Plant-Wide Waste Management. 2. Decision Making under Uncertainty

Aninda Chakraborty* and Andreas A. Linninger*

Laboratory for Product and Process Design, Department of Chemical Engineering, University of Illinois at Chicago, Chicago, Illinois 60607

The synthesis and optimization of plant-wide waste management policies under uncertainty is the subject of this paper. The combinatorial synthesis methodology (Chakraborty, A.; Linninger, A. A. Ind. Eng. Chem. Res. 2002, 41 (18), 4591–4604) was adapted to incorporate variations in the expected waste loads. In its first stage, automatic generation of recovery and treatment flowsheet produces a superstructure that embeds all plant-wide waste management policies. In the subsequent optimization phase, plant-wide policies with a desired degree of operational flexibility against uncertainty are developed. The proposed problem formulation leads to linear mathematical models for quantifying the probability of uncertain parameter variations affecting expected operating cost, emissions, and plant capacities. The paper discusses different flexibility measures, their purpose for process design under uncertainty, and mathematical models for their application to the synthesis of robust plant-wide waste management policies. The case studies demonstrate the application of the methodology to industrial design problems at batch manufacturing sites. The linear problem formulation together with the sampling technique suggested in the paper provide a practicable solution approach to open-ended flowsheet synthesis problems under uncertainty previously deemed intangible.

1. Background and Overview

In part 1 of this series,1 we introduced the combinatorial process synthesis methodology for the generation and design of optimal recovery and treatment policies for entire manufacturing sites using a two-stage procedure. In the first step, a linear planning algorithm synthesized a tree of all feasible recovery and treatment options. As input, the reason-based search required (i) state information on the effluent streams, W, (ii) a set of models for available recovery and treatment options, T, and (iii) a database of environmental emission regulations, R. Unrealistic or impractical reaction or separation steps were eliminated immediately according to unsuitable physical property ranges of the chemicals involved or insufficient regulatory compliance. The resulting network of all feasible treatment options for all effluent streams was termed superstructure.

Phase two of the methodology produced plant-specific operating policies embedded in the superstructure by optimizing a desired performance function through the adjustments of (i) structural decisions for the best combination of operational tasks and/or (ii) optimal operating conditions for each unit operation. We also demonstrated how to arrive at operating procedures with optimal trade-off among economic and ecological targets, while satisfying site-specific emission, logistic, and plant capacity constraints. The approach of part 1 of the series relied on the availability of perfect state information. Clearly, this is a very strong assumption. A more realistic picture in closer agreement with the industrial practice considers variability and uncertainty in the operating conditions.2,3 We investigate in this paper how to plan optimal design policies for an entire manufacturing site in the presence of uncertainty in the effluent streams. We will develop optimal policies considering the variability in the flow rates of the processing streams. It will be our objective to quantify the cost associated with uncertain operating conditions. Moreover, we study the effect of process uncertainties on structural decisions such as the choice of treatment options.

Outline. In this paper we will derive a novel mathematical framework for quantifying the impact of certain types of uncertainty on waste management policies at batch manufacturing sites. Section 2 develops the mathematical background of the design methodology. It will introduce a probabilistic representation of the uncertain parameters and adjustments to the combinatorial synthesis paradigm for the design under uncertainty in the process streams. Different flexibility measures and their suitability to treatment selection will be discussed. Section 3 will demonstrate the flexibility index for the robust design of a distillative solvent recovery task. Section 4 will derive a detailed mathematical framework for plant-wide effluent management under uncertainty using a stochastic approach. Section 5 will suggest implementation issues aimed at reducing the computational effort via specialized sampling techniques. In section 6, we will demonstrate industrial applications for optimal waste treatment under uncertainty. We will also give detailed results and a discussion of a larger case study with the purpose of finding Pareto optimal plant-wide treatment policies.

2. Methodology

First, we develop a mathematical problem representation that incorporates uncertainty into the combinatorial process synthesis approach. Figure 1 gives an overview of the combinatorial process synthesis methodology composed of superstructure generation and superstructure optimization. Because its two phases were discussed in part 1 of this series, we will only present the modifications for the design under uncer-
Our proposed framework for the optimal design of recovery and treatment options in the presence of uncertainty is composed of three components: (i) waste scenarios; (ii) superstructure synthesis for uncertain systems; (iii) optimization of operating policies under uncertainty. Waste scenarios quantify uncertainty in each effluent stream by relating the extent of variations with their probability. Using the waste scenarios as input, we synthesize a network of feasible recovery and treatment options in the superstructure generation phase. Subsequently, the mathematical program for finding plant-wide optimal design policies embedded in the superstructure in the presence of uncertainty will be discussed. In the optimization part, we will also propose different metrics to measure the sensitivity of particular design policies to process uncertainty.

2.1. Waste Scenarios. The first phase of the combinatorial process synthesis methodology synthesizes a network of feasible reaction and separation steps using a set of waste states \( W = \{ w_1, w_2, \ldots \} \) covering amount, temperature, pressure, and composition. For the design under uncertainty, we shall now introduce a probabilistic model termed a waste scenario \( \omega \) as a set of random variables representing expected state variations in each of the effluent streams.

Impact of Uncertainty. Pressure and temperature variations of the processing streams are of minor importance for the design because they do not affect the selection of feasible recovery and treatment options. Typically, they are dissipated as routine disturbances by the process control equipment. More significant are variations in the amount and composition of effluent streams. Excessive compositional changes may render a treatment infeasible. Hence, large composition variations may invalidate the available treatment flowsheet embedded in the superstructure. In this paper, however, we shall assume that composition variations do not affect the structural validity of the superstructure. Methods to overcome this limiting conjecture are discussed elsewhere.

Quantification of Uncertainty. Variations in extensive process variables, i.e., mass, molar flow rate, etc., are modeled by means of a normal probability distribution function (PDF) given by a mean value \( w_k \) and a standard deviation \( \sigma_k \) as given in eq 1. Thus, possible outcomes for a waste scenario and their likelihood can be computed as a convolution of constituent waste load variations. A waste scenario, \( W^\omega \), is a random event associated with a particular state realization for each effluent stream. The probability of a scenario, \( P(W^\omega) \), is given by the joint PDF of independent random variables corresponding to each waste stream. When the waste loads vary independently of one another, the scenario probability \( P(W^\omega) \) simplifies to the product of the individual probabilities of each outcome, \( w_k \) (eq 2).

\[
P(w_k) = \frac{1}{\sqrt{2\pi}\sigma_k} \exp\left\{ -\frac{1}{2}\left( \frac{w_k - w_k^*}{\sigma_k} \right)^2 \right\} \quad (1)
\]

\[
P(W^\omega) = \prod_{k,j} P(w_k) \quad (2)
\]

In case the process streams exhibit strong correlations, as is often the case in real manufacturing sites, principal component analysis (PCA) can effectively eliminate dependencies among the waste load variations.

2.2. Superstructure Synthesis for Uncertain Systems. In complete analogy to the deterministic case, we propose to generate the network of possible treatment steps by means of the reasoning mechanism described in part 1 of this series. For the uncertain case, we propose the application of the superstructure generation mechanism using the waste scenarios as inputs. With the mean flow rate \( w_k^* \) of waste streams at nominal conditions, the three-step reasoning cycle entails (i) diagnosis, (ii) preselection, and (iii) step execution. In diagnosis, the physical and chemical properties of each effluent stream are checked against health safety and environmental regulations, \( R \). In preselection, the algorithms proceeds to identify any treatment tasks capable of eliminating at least one rule violation. This phase involves a data-driven search of the treatment database for feasible and effective recovery and chemical treatment tasks, i.e., separations and chemical reactions. Annual operating cost and residuals resulting from its implementation are computed for all feasible and effective operational tasks in the execution.
step. The residuals leaving the separator or reactor are examined in another diagnosis, preselection, and execution cycle until all residuals are compliant. The resulting superstructure is an acyclic tree of treatment options connecting the original effluents with final emissions via a sequence of reaction and separation steps. In addition, its nodes store important information such as the state of all residual streams, total energy requirements, and total estimated treatment cost attained at the nominal values. The resulting superstructure embeds all of the structurally different policies for handling all process effluents.

**Dynamic Linearization.** Clearly, the actual flow rate of each uncertain process stream during plant operation may differ from its nominal value. A tedious approach to assessing the impact of possible realizations of the waste scenarios would require reevaluation of all mass and energy balances of the superstructure network. Even for a modest number of process streams, time and space complexity of such an attempt would render this method impractical. It would be more effective to devise a mechanism for extracting information about waste load variations from the superstructure data available at the nominal values. Dynamic linearization suggests computing cost or residual state for each waste scenario by linear extrapolation of the results obtained for the nominal load. The true value of desired properties in a particular realization can thus be approximated by a linear expansion around its nominal conditions. The magnitude of the linear perturbation is a product of the local gradient of the property evaluated at the mean, and the distance of the sample from the mean. The property gradient can be computed by a finite difference formula. This step requires one additional evaluation of the model equations for all recovery and treatment tasks embedded in the superstructure, i.e., step execution for cost and residual calculations. The gradients of nonlinear transfer functions change according to the levels of waste loads; see Figure 2. In effect, dynamic linearization captures the overall nonlinear trend of cost and state properties observed for different levels of waste loads. An example for the linearized cost function is given in eq. 3. It shows a dynamically linearized treatment cost

\[
\frac{\partial c_{k,i}}{\partial w_k} \Delta w_k = c_{k,i} + \rho_{k,i} \Delta w_k
\]

of operation, i, as a function of the uncertain process effluent, \(w_k\). Linearity of scenario properties greatly simplifies the solvability of the mathematical program in the subsequent superstructure optimization phase.

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**2.3. Decision Making under Uncertainty.** The second stage in combinatorial process synthesis methodology termed superstructure optimization (Figure 1, bottom) aimed at identifying plant-wide optimal treatment policies. In part 1 the open decision variables in that design problem were discrete, i.e., selection of treatment paths, and continuous, i.e., level of operating parameters such as reflux ratios, reaction temperatures, pressures. However, the deterministic model assumed accurate information of all material states. In this paper, we shall consider plant-wide design with flexibility against process uncertainty. Before attempting to formulate the mathematical framework for design under uncertainty, we need to discuss robustness metrics.

The flexibility index of a particular process flowsheet measures the maximum tolerable deviations from the nominal values of uncertain design variables or parameters without violating any design constraint. The design is guaranteed to work within the uncertain parameters range prescribed by the flexibility index. The concept of the flexibility index and its computation via mathematical programming techniques has been studied intensively by Grossmann and co-workers.8–12 They developed several solution strategies converting the original max–min–max problem13 into a succession of mixed-integer programs (direct search) or a single M1-NLP (active constraint method). Proofs of correctness and convergence of their algorithms were given for problems with quasi-convex constraints in the uncertain parameters. Uncertain parameter variations within a continuous bounded interval have entered the definitions of similar metrics such as the resilience index for processing plants14 or the flexibility measure for decisions in production planning.15

Kubic and Stein16,17 performed failure analysis of different designs with both stochastic and fuzzy uncertainties. For failure analysis involving random uncertainties, they recommend a probabilistic measure of uncertainty defined as the stochastic reliability. For uncertain events that can be categorized into discrete outcome sets, the concept of fuzzy reliability was introduced. The fuzzy reliability is the possibility that a design will be feasible.

Stochastic flexibility introduces the notion of expected values into a design optimization. Different metrics maximize expected cost, which can be interpreted as a mean value of the performance function.18–20 Alternatively, models focus on reducing the variance of an optimal design solution. The concept of robust design by Taguchi measures the “signal-to-noise” ratio.21 Robust decision making involves choosing designs with good “average” performance and minimum variance.22 A trade-off between the expected performance and its variance can be obtained by different multiobjective formulations. The resulting Pareto-optimal solutions are also termed stochastically dominant.23,24

In the subsequent chapter, we shall select suitable flexibility measures for plant-wide optimal waste management and discuss their purpose for design under uncertainty.

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3. Decision Making for Flexible Designs: Deterministic Approach

Classical process design determines optimal design decisions by maximizing a performance function subject to conservation principles, state equations, and design