Plant-Wide Waste Management. 1. Synthesis and Multi-Objective Design

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Abstract

Combinatorial process synthesis is a novel paradigm for flowsheet synthesis. Its two-staged synthesis algorithm generates all feasible operational alternatives followed by rigorous optimization of structurally superior flowsheets. In the conventional practice, process synthesis aims at minimizing total annualized cost. However, designs with maximum economic performance may cause unbalanced environmental impact. It should not surprise that subsequent cleanup and waste treatment efforts often compound actual process overhead unaccounted for in the traditional design philosophy. Therefore, environmental considerations should be accommodated alongside economic performance. In this first paper of a triple series, we will introduce the concept of combinatorial process synthesis for developing plant-wide recovery and treatment policies for batch manufacturing sites. The flowsheet generation step combined with multi-objective optimization will render operating policies with optimal trade-off among the conflicting objectives cost and environmental impact. The discussion includes case studies illustrating the systematic and fully automatic waste management procedure.

Keywords: Process synthesis, pollution prevention, recovery and treatment selection

1. Introduction:

The drug approval process distinguishes batch process development for pharmaceuticals from continuous commodity businesses. After the approval of the original recipe by the Food and Drug Administration (FDA) in the early stages of the drug development, the operating parameters of a batch
recipe must not be changed during its entire lifetime. Any adaptation to the authorized recipe perhaps in favor of a more benign raw material or the deployment of more selective solvents requires new approval for the entire manufacturing route.

Another distinction concerns drug manufacturing in multi-purpose plants in campaigns of several weeks to months. The complex organic reaction mechanisms require multi-stage reaction networks. Stringent purity requirements call for multiple solvents in abundant quantities. Often, kinetic data about these complex reaction mechanisms are lacking; the stoichiometry of side-reaction may be uncertain. Difficult separation steps like crystallization are carried out without knowing all species properties. Although valuable solvents are recovered, they are seldom recycled into the original batch recipe due to the uncertainty and high purity standards.

Due to the formal approval proceedings and the special manufacturing practices, reintegration of pollution prevention efforts with the original operating scheme are less customary as this is the case in dedicated continuous plants. In effect, a large number of different types and levels of effluents are leaving pharmaceutical production campaigns and need material recovery and/or adequate treatment, see Fig. 1.1 In the industrial practice, treatment allocation and solvent recovery decisions are frequently taken in an ad-hoc fashion using company-specific selection criteria. It is customary to remove hazardous solid wastes via incineration, while waste-water is mostly directed to a biological treatment facility. For solvent recovery, batch and semi-batch conventional distillation, entrainer-based distillation, physical absorption and extraction is available.2 Destructive treatment options include wet-air oxidation, per-oxidation and catalytic incineration.3 When stepping up solvent recovery via physical separations, or introducing novel recovery or destructive methods such as supercritical extraction and
oxidation, a myriad of different scenarios for reducing raw material utilization needs to be considered. Discovering viable reactive and separation tasks for a single effluent stream is already a formidable synthesis problem. Addressing the recovery and treatment selection for an entire manufacturing facility with hundreds of ever changing effluents becomes an overwhelming challenge.

Currently there is no systematic methodology for managing the total accumulation of unavoidable by-products and effluents from different campaigns on a plant-wide level. It would be desirable to conceive an automatic computer procedure to answer two key questions:

- What are feasible recovery and treatment options?
- Which policy can optimally handle all recovery and treatment tasks for the entire manufacturing site?

1.1. Prior work:

Open-ended design problems such as flowsheet synthesis remain a challenging research topic. Broadly, two approaches can be distinguished: (i) reasoning-based and (ii) mathematical programming. Reasoning-based methods exploit physical property information and process knowledge to construct structurally feasible flowsheets, e.g. AIDES. A hierarchical decomposition principle guided subsequent developments, e.g. BALTAZAR, PIP. Barnicki and Fair developed a comprehensive rule base for the separation of liquid and gaseous mixtures. Gani and coworkers devised a process synthesis methodology driven by thermodynamic insights.

Fewer methods have focused on batch processes, e.g. PROVAL. BatchDesign-Kit (BDK) offers interactive development of batch recipes with ecological considerations. The EASY environment