Combinatorial Process Synthesis

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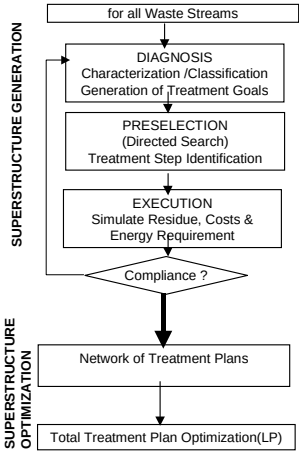
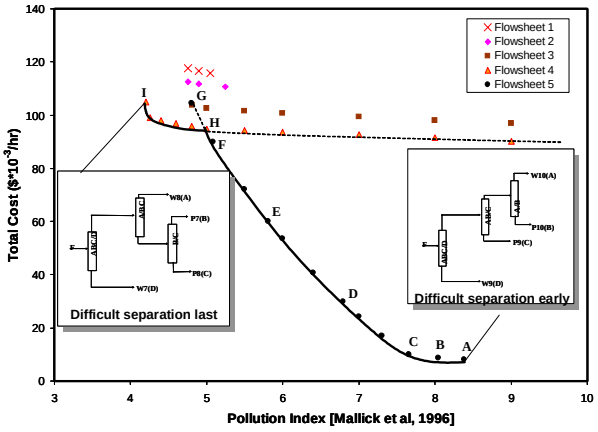
In pharmaceutical and specialty chemical manufacturing, complex multi-stage chemical reactions and stringent product purity requirements often leads to high waste to product ratios. Seasonal variations and fluctuations in product demands contribute to the large degree of uncertainty associated with the operating conditions and process streams. In such a dynamic environment, selection of recovery and treatment options for an entire manufacturing facility becomes an overwhelming task. In order to address this problem, I have developed a novel methodology, *Combinatorial Process Synthesis*. This methodology consists of two phases (see Figure 1): *(i) Superstructure synthesis*, a linear planning algorithm which generates a network of feasible solvent recovery and waste treatment options for all unavoidable by-product streams at a manufacturing site. Permutations of all possible treatment alternatives within the superstructure constitute plant-wide *treatment policies*. Each policy is composed of an ordered sequence of reaction or separation tasks transforming wastes into compliant residuals. *(ii) Superstructure optimization*, a large-scale mathematical program that finds the best plant-wide policies embedded in the superstructure. My research addressed three major problems:

- Design of plant-wide waste management policies with best trade off between process economics and environmental impact (c.f. Figure 2)
- Multi-objective design of plant-wide operations while considering uncertainty in the process streams (Figure 3).
- A predictive closed loop control algorithm for optimal plant operation and investment decisions for the entire manufacturing site over a planning horizon of 5 to 10 years (Figure 4).

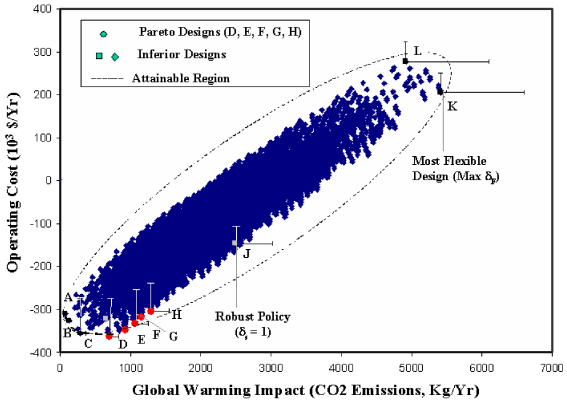
Significance. Previously there was no systematic methodology for managing entire manufacturing sites. A significant challenge not considered in any research so far was the impact of regulatory changes onto the manufacturing practice. This novel computer-aided approach solves open-ended industrial decision-making problems previously deemed intangible. The success of this methodology has been proven with application to industrial size problems from Eastman Chemical Company, TN and Abbott Laboratories, IL.



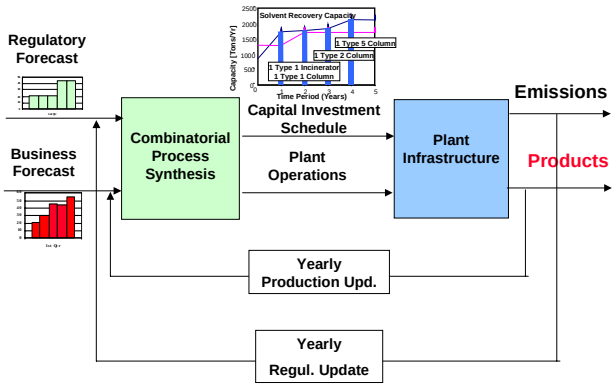
(1) Combinatorial Process Synthesis - Overview:



(2) Trade-off Curves: Cost v.s. Environmental Impact



(3) Trade-offs under Uncertainty



(4) Schematic of Long-Term Planning