Nonsmooth methods for process integration

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Process integration is a promising method to improve sustainability and reduce waste in chemical processes by recovering excess resources such as heat, water, or other materials. However, calculating the maximum amount of resource that can be reused is challenging because resource sinks can only take in resource if it is of high enough quality. As a result, most current integration methods are either limited and heuristic or use large superstructure formulations that must assess all possible matches between the resource sources and sinks.

Therefore, this thesis presents new computational methods for maximizing resource recovery that use nonsmooth functions to compactly describe the resource that is available at different qualities. This work can be divided into three main contributions that improve process integration for systems with different resources and assumptions:

1) A generalized approach to process integration that uses a system of two nonsmooth equations to describe optimal reuse for a wide variety of resources, including multiple resources simultaneously,
2) An extension of this general approach to more complex mass and water systems with multiple contaminants that can limit their reuse,
3) A nonsmooth optimization formulation that applies our integration approach to design variable-temperature cogeneration systems that convert process waste heat into electricity.

By utilizing nonsmooth equations, each of these contributions exhibits improved scaling compared to other integration methods and have numbers of equations or constraints that remain the same regardless of the size and complexity of the system. In addition, unlike other methods, our approaches have the flexibility to either determine resource requirements or the process variables that achieve a given target.

This thesis describes the formulation and implementation of each of these nonsmooth approaches and applies them to a wide of range of example applications. These applications include carbon-constrained energy planning, hydrogen conservation networks, water recovery from petroleum refining with multiple contaminants, and designing improved cogeneration systems for sulfuric acid and cement production processes. The results from these examples show the flexibility and scalability of our approaches and the breadth of improvements they can provide. Together, our contributions increase the applicability of computationally efficient process integration methods to improve the sustainability of a wide range of chemical processes.