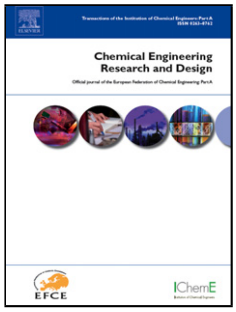

Title: A Superstructure Optimization Approach for Process Synthesis under Complex Reaction Networks

Authors: Gautham Madenoor Ramapriya, Wangyun Won, Christos T. Maravelias

PII: S0263-8762(18)30354-X
DOI: https://doi.org/10.1016/j.cherd.2018.07.015
Reference: CHERD 3269

To appear in:

Received date: 26-3-2018
Revised date: 9-7-2018
Accepted date: 10-7-2018

Please cite this article as: Ramapriya, Gautham Madenoor, Won, Wangyun, Maravelias, Christos T., A Superstructure Optimization Approach for Process Synthesis under Complex Reaction Networks.Chemical Engineering Research and Design https://doi.org/10.1016/j.cherd.2018.07.015

A Superstructure Optimization Approach for Process Synthesis under Complex Reaction Networks

Gautham Madenoor Ramapriya[1,2], Wangyun Won[1], Christos T. Maravelias[1,2,*]

[1] Department of Chemical and Biological Engineering University of Wisconsin-Madison, Madison, WI 53706

[2] DOE Great Lakes Bioenergy Research Center Univ. of Wisconsin-Madison, Madison, WI 53726

Highlights

- Optimization methods for synthesis of systems subject to complex reaction network.
- Extent-based reactor model for multiple simultaneous reactions.
- Model detects limiting reactant of each reaction based on variable inlet component flows.
- New stream-conditioning modeling approach to determine the associated work/duty.
- Methods enable the synthesis of systems with hundreds of reactions.

ABSTRACT

In this work, we present mixed integer linear programming methods for the synthesis of processes that involve complex reaction networks. Specifically, we consider the modeling of reactors and interconnecting streams in systems where the composition of the reactor inlet streams can vary substantially, thereby making the determination of the limiting component as well as the calculation of the stream heating/cooling and power requirements challenging. First, towards the modeling of reactors we develop an extent-based method which detects the limiting reactant of each reaction occurring in parallel with others, based on the inlet flows of the reactants. Second, we develop a computationally tractable method for the calculation of the work and heating/cooling duty needed to condition any stream of a process based on simple calculations that can be performed offline. Finally, we present how the two aforementioned components can be integrated in an optimization model generated based on a process superstructure. We demonstrate the application of the developed methods for the synthesis of a biorefinery.