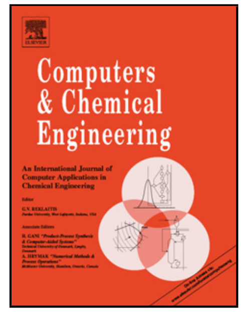
Accepted Manuscript



Title: Closed-loop Reactor Network Synthesis with Guaranteed Robustness

Author: Xiao Zhao Wolfgang Marquardt

PII: S0098-1354(17)30256-9
DOI: http://dx.doi.org/doi:10.1016/j.compchemeng.2017.06.010
Reference: CACE 5841

To appear in: *Computers and Chemical Engineering*

Received date: 27-9-2016
Revised date: 4-6-2017
Accepted date: 6-6-2017

Please cite this article as: Xiao Zhao, Wolfgang Marquardt, Closed-loop Reactor Network Synthesis with Guaranteed Robustness, <*![CDATA[Computers and Chemical Engineering]]*> (2017), http://dx.doi.org/10.1016/j.compchemeng.2017.06.010

Closed-loop Reactor Network Synthesis with Guaranteed Robustness☆

Xiao Zhao[a], Wolfgang Marquardt[a,1]

[a] Aachener Verfahrenstechnik, Process Systems Engineering, RWTH Aachen University, Templergraben 56, D-52056 Aachen, Germany.

Abstract

This paper presents a systematic methodology to design closed-loop reactor networks with guaranteed robustness. The methodology is based on the superstructure approach for reactor network synthesis and extends our previous work [1] to simultaneously design the process and the control system structure. The spectral abscissa of the Jacobian matrix of the closed-loop reactor network is chosen to measure the response speed of the designed process. A mixed-integer nonlinear program (MINLP) with complementarity constraints and a robust eigenvalue constraint is formulated and solved sequentially by a two-step solution strategy. Structural alternatives of the process and the control system as well as parametric uncertainties are considered in an integrated framework. A case study involving continuous stirred-tank (CSTR) and plug flow (PFR) reactors is presented to illustrate the novel approach and compared with an established two-step design approach.

Keywords: reactor network synthesis, decentralized control structure selection, superstructure approach, integration of process and control system design, normal vector approach, robust optimization

1. Introduction

The analysis and control of interconnected systems is one of the challenges of modern engineering science [2]. A closed-loop reactor network is an instance of an interconnected system, in which reactors are connected by material flows and control loops. Reactor network design requires decisions on the operating point, the process flowsheet and control structure, and also on equipment design parameters. When process uncertainty (e.g., unknown quality in the feed flow) and model uncertainty (e.g., uncertain reaction kinetic constants) have to be considered additionally, the task of designing reactor networks becomes very challenging. This paper will present a superstructure-based methodology to address the design of closed-loop reactor networks with robust dynamic properties.

For open-loop reactor network synthesis problems, there exist three types of methods: the superstructure approach [3], the attainable region method [3] and the state-space framework [4, 5, 6, 7]. The superstructure approach starts by postulating a network of idealized reactors and performing a structural optimization on this enlarged network or "superstructure" by using optimization techniques [3]. The attainable region is defined as the set of all possible points in concentration space that are attainable through reaction and mixing from a given feed point. Consequently, this region quantifies the performance of a reacting system [5]. The state space framework decomposes the overall process network into two parts: the distribution network (DN) where all possible mixing, splitting, recycling and bypassing of process streams occur; and the process operator (OP) where the action of process unit operations is quantified [7]. Within the state space framework, reactor network synthesis problem is formulated as an infinite dimensional convex (linear) optimization problem [5] and the optimal value of this infinite linear optimization is approximated through solutions of a sequence of finite linear programs [7].

[1] Corresponding author. Email: Wolfgang.Marquardt@avt.rwth-aachen.de; present address: Forschungszentrum Juelich GmbH, 52425 Juelich, Germany