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M.Sc. Xiao Zhao,
Xinjiang

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Reactor network synthesis with guaranteed robust performance

Berichte aus der
Aachener Verfahrenstechnik - Prozesstechnik

RWTH Aachen University

Reactor Network Synthesis With Guaranteed Robust Performance

Synthese von Reaktornetzwerken mit robust garantierten Eigenschaften

Von der Fakultät für Maschinenwesen der Rheinisch-Westfälischen Technischen Hochschule Aachen vorgelegte Dissertation zur Erlangung des akademischen Grades eines Doktors der Ingenieurwissenschaften

vorgelegt von

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In this work a systematic model-based approach for reactor network synthesis problem with guaranteed robust dynamic performance will be presented. The work is based on the superstructure approach and aims to find an optimal process flowsheet with determined connection patterns of reactors, reactor types, design parameters and operating conditions. In comparison to the classical design methods, certain specified dynamic properties are guaranteed simultaneously under parametric uncertainty. Structural alternatives in the flowsheet, i.e., how reactors are interconnected, as well as in the control system, i.e., how controlled and manipulated variables are paired, are subject to design degrees of freedom. It is allowed that idle reactors and controllers can appear in the reactor network superstructure, so that a fixed number of non-idle reactors and controllers does not have to be assumed as a priori. The optimal reactor network design in either open- or closed-loop is determined by solving a single optimization problem.

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Aachen, in May 2017

Contents

Notation

We summarize the symbols for reactor network modeling and the derived problem formulations in Chapter 3 and 4. The symbols for the introduction part of nonlinear systems in Chapter 2 and the symbols for reviewing different numerical optimization methods shown in Chapter 5 are not presented here. The meaning of these symbols is always introduced together with the corresponding texts.

Symbols for the reaction example

A	propylene
B	allyl chloride
C	chlorine
c_A, c_B, c_C	concentration of component A, B or C
R	gas constant
a_1, a_2, a_3	reaction constants
H_1, H_2, H_3	heat of reaction per mol
c_p	heat capacity
T	temperature
V	reactor volume
L	reactor length
r_1, r_2, r_3	reaction rates
R_A, R_B, R_C	reaction rates for component A, B, C
$\dot{n}_A^0, \dot{n}_B^0, \dot{n}_C^0$	mole flowrates of inlets
$\dot{Q}^0$	energy flowrate of inlets
Q_h	energy duty of heat exchanger
$c_A^{sys}, c_B^{sys}, c_C^{sys}$	concentration in system's inlet
E^{sys}	energy density in system's inlet
N_d	number of discretized points of each PFR

Symbols for open-loop reactor network design

i	index of subsystems
j	index of outlet ports
k	index of inlet ports
N	total number of reactors
(i, j)	index of the j-th outlet port of subsystem i
(i, k)	index of the k-th inlet port of subsystem i
$l(i, j)$	index of an inlet port, which is connected to (i, j)
$h(i, k)$	index of an outlet port, which is connected to (i, k)

$(i,j) \triangleright (i',k')$	pipe connection from (i,j) to (i',k')
$\bar{l}(i,j)$	index of a subsystem, one of its inlets is connected to (i,j)
$\bar{h}(i,k)$	index of a subsystem, one of its outlets is connected to (i,k)
N_c	number of necessary chemical components to model reactions
x_i	states (concentrations, temperature) of reactor i
$u_{i,k}$	component flowrates and energy flowrate through inlet port (i,k)
$q_{i,j}$	volumetric flowrate through the (i,j)-th outlet port
p_i	design parameters of reactor i
$f_i(\cdot)$	function for mass and energy balances of reactor i
$y_{i,j}$	component flowrates and energy flowrate through outlet port (i,j)
$g_{i,j}(\cdot)$	function for reactor's outlets
y_{sys}	component flowrates and energy flowrate in system's outlet
p_{sys}	molar concentration and energy density in the system's feed
$\mathcal{I}$	index set of all reactors
$\mathcal{I}_{id}$	index set of idle reactors
$\mathcal{I}_{nid}$	index set of non-idle reactors
J_{tot}	Jacobian matrix of the open-loop reactor network
J_{id}	Jacobian matrix of idle reactors
J_{nid}	Jacobian matrix of non-idle reactors
$\bar{J}$	a constructed matrix
c	predefined constant for the upper bound of eigenvalue constraints
$\alpha(\cdot)$	spectral abscissa function
D_o	definition domain of function $\alpha_{J_{nid}}(\cdot)$
P^*	steady state of the 2-reactor network example
φ	objective function in optimization
π_τ	vector of uncertain variables
$\bar{\pi}_\tau$	nominal values of uncertain variables
$\Delta\bar{\pi}_\tau$	uncertain range of uncertain variables
z_i	integer for the existence of reactor i
z	a vector of z_i, $i = 1, ..., N$
M	sufficiently large positive constant in big-M method
I	identity matrix
ψ_o	degrees of freedom of the open-loop model
ϵ	a small positive number

Symbols for simultaneous reactor network design and control

u	candidate MV of reactor network
y	candidate CV of reactor network
e	state variables of PI controllers
$\bar{u}$	offset values of u
$\bar{y}$	reference signals of y
$\bar{q}$	offset values of q
u_i	candidate MV of reactor i (elements of p_i)
d_i	equipment design parameters of reactor i (elements of p_i)

u_{p1}	candidate MV, which belong to idle reactors
u_{p2}	candidate MV, which do not belong to idle reactors
n_c	dimension of y, i.e. total number of candidate CV
n_m	dimension of u, i.e. total number of candidate MV
(i,r)	index of the r-th candidate measurement of reactor i
	index of the (i,r)-th candidate PI controller
n_c^i	dimension of all candidate CV of reactor i
$e_{i,r}$	state variable of (i,r)-th PI controller
π	variables in ψ_o, which are not in u
v	location index for candidate MV
	location index for rows of control gain matrix K
w	location index for candidate CV
	location index for columns of control gain matrix K
$[u]_v$	v-th element in vector u
$[y]_m$	m-th element in vector y
Θ_i	index set for candidate MV of reactor i
$y_{i,r}$	r-th candidate CV of reactor i
$\phi_{i,r}(\cdot)$	function for candidate CV
$\varrho(\cdot,\cdot)$	function for transforming the subscripts of $[y]_m$ and $y_{(i,r)}$
K	proportional control gain matrix
$[K]_{v,w}$	(v,w)-th element in matrix K
K_v	vector of variables in matrix K
K^+, K^-, $\hat{K}$	auxiliary matrices for control structure selection
T	integral control gain matrix
$t_{i,r}$	integral control gain for state $e_{i,r}$
T_v	vector of variables in matrix T
ψ_c	degrees of freedom of the closed-loop model
$\mathcal{U}$	index set of all candidate MV
$\mathcal{U}_{id}$	index set of candidate MV, which are not subject to control
$\mathcal{U}_{nid}$	index set of candidate MV, which are subject to control
$\mathcal{C}$	index set of all PI controllers
$\mathcal{C}_{id}$	index set of idle PI controllers
$\mathcal{C}_{nid}$	index set of non-idle PI controllers
$z_{i,r}$	integer for the existence of the (i,r)-th PI controller
z_r	a vector of z_i (existence of reactors)
z_c	a vector of $z_{i,r}$ (existence of controllers)
x_{id}	states of idle reactors
x_{nid}	states of non-idle reactors
e_{id}	states of idle controllers
e_{nid}	states of non-idle controllers
J_{tot}	Jacobian matrix of the closed-loop reactor network model
J_{id}, J'_{id}, J_{nid}, J'_{nid}	Submatrices in J_{tot}
$F_{id}(\cdot)$	state functions of all idle reactors and controllers
$F_{nid}(\cdot)$	state functions of all non-idle reactors and controllers
$\bar{J}$	a constructed matrix

Mathematical notations

$\mathbb{R}$	real line
$\mathbb{R}^n$	real n-dimensional space
$\mathbb{R}^n_+$	non-negative orthant of $\mathbb{R}^n$
$\mathbb{C}$	complex plane
$\mathcal{C}^k$	space of k-th order continuously differentiable functions
$\frac{\partial f}{\partial x}$	partial derivatives of function $f(x)$ to x
$\overline{B}$	topological closure of a set B

Acronyms

NLP	nonlinear optimization
MINLP	mixed-integer nonlinear optimization
MILP	mixed-integer linear optimization
MIDO	mixed-integer dynamic optimization
GDP	generalized disjunctive programming
MPCC	mathematical programs with complementarity constraints
MPEC	mathematical programs with equilibrium constraints
SIP	semi-infinite programming
GSIP	generalized semi-infinite programming
EVO	eigenvalue optimization
SDP	semi-definite programming
NSO	non-smooth optimization
DOF	degrees of freedom
SA	spectral abscissa
NVA	normal vector approach
CV	controlled variable
MV	manipulated variable
B&B	branch and bound (with respect to binary variables)
sB&B	spatial branch and bound
GBD	generalized bender's decomposition
VI	variational inequalities
MFCQ	Mangasarian Fromovitz constraint qualification
LICQ	linear independence constraint qualification
KKT	Karush Kuhn Tucker
SQP	sequential quadratic programming
NCP	nonlinear complementary problem
FB	Fischer-Burmeister
BL	bi-level
EPF	elementary process functions
AR	attainable region
PI	proportional-integral
RGA	relative gain array
SV	singular values

NI	Niederlinski index
SSV	structured singular value
MIMO	multi-input multi-output
ODE	ordinary differential equations
DAE	differential algebraic equations

Abstract

Typical continuous process flowsheets include reaction section, separation section and recycles. The reaction section is often the most important part of a chemical process, which may contain several interconnected reactors. The superstructure approach is a widely used model-based process design method for reactor network synthesis. It starts from a reactor network superstructure and uses mathematical models and optimization tools to select the best process design. The superstructure approach results in an optimal process flowsheet with determined connection patterns of reactors, reactor types, design parameters and operating conditions of each reactor.

In this work, a systematic model-based approach for reactor network synthesis problems with guaranteed robust dynamic performance will be presented. The work is based on the superstructure approach, but in comparison to the classical methods, not only economic optimality with respect to a static objective function, but also certain specified dynamic properties, i.e. dynamic stability and response speed, are guaranteed simultaneously under parametric uncertainty. Structural alternatives in the flowsheet, i.e., how reactors are interconnected, as well as in the control system, i.e., how controlled and manipulated variables are paired, are subject to design degrees of freedom. Moreover, it is allowed that idle reactors and controllers can appear in the reactor network superstructure, so that a fixed number of non-idle reactors and controllers does not have to be assumed as a priori. The optimal reactor network design in either open- or closed-loop is determined by solving a single optimization problem.

The proposed approach allows an integrated treatment of parametric uncertainties, which may either result from model uncertainties, such as reaction kinetic constants or heat transfer coefficients, or from process uncertainties, including slow disturbances in load or the quality of raw materials. A robust eigenvalue constraint to guarantee the robust performance of the designed reactor network is formulated. Efficient formulations of interconnecting reactors and novel complementarity-based constraints for control structure selection are proposed. The method results in a semi-infinite mixed-integer nonlinear optimization problem with complementarity constraints, disjunctions and a robust eigenvalue constraint. A hybrid two-step solution method is proposed to solve the synthesis problem, which integrates candidate solution algorithms of related optimization problems. The proposed solution method is applied to a case study of allyl chloride production with up to ten plug flow and continuous stirred tank reactors.

Kurzfassung

Übliche kontinuierliche Prozesse enthalten einen Reaktionsteil, eine Trennsequenz und Rückführungen. Der Reaktionsteil stellt meist den wichtigsten Teil eines chemischen Prozesses dar, der aus vielen untereinander verknüpften Reaktoren bestehen kann. Der Überstrukturansatz beschreibt eine oft genutzte, modellgestützte Methode zur Erstellung von Reaktornetzwerken mit strukturellen Freiheitsgraden. Ausgehend von einer Überstruktur des Reaktornetzwerkes werden mathematische Modelle und Optimierungswerkzeuge genutzt, um den besten Prozessentwurf zu finden. Der Überstrukturansatz resultiert in einem optimalen Prozessfließbild mit festgelegten Verknüpfungen der Reaktoren eines bestimmten Reaktortyps sowie mit den zugehörigen Designparametern und Betriebsbedingungen für jeden Reaktor.

In dieser Arbeit wird ein systematischer, modellgestützter Ansatz für den Entwurf von Reaktornetzwerken mit garantiert robusten dynamischen Eigenschaften präsentiert. Die Arbeit basiert auf dem Überstrukturansatz. Im Vergleich zu konventionellen Methoden wird jedoch nicht nur die ökonomische Optimalität in Bezug auf eine statische Zielfunktion, sondern auch bestimmte spezifische dynamische Eigenschaften, insbesondere die dynamische Stabilität und die Geschwindigkeit des Responses, gleichzeitig unter parametrischer Unsicherheit garantiert. Strukturelle Fließbildalternativen, insbesondere die Verknüpfung von Reaktoren untereinander und Alternativen in Bezug auf die Regelungsstruktur, d.h. insbesondere die Kopplung von geregelten und manipulierten Variablen, zählen zu den Freiheitsgraden des Entwurfsprozesses. Des Weiteren werden unbenutzte Reaktoren und Regler im Netzwerk zugelassen, sodass a-priori keine feste Anzahl von benutzten Reaktoren und Reglern vorgegeben werden muss. Der optimale Entwurf des Reaktornetzwerks im offenen oder geschlossenen Regelkreis wird durch die Lösung eines einzelnen Optimierungsproblems ermittelt.

Der vorgeschlagene Ansatz erlaubt eine integrierte Behandlung von parametrischen Unsicherheiten, die entweder aus Modellunsicherheiten resultieren, wie z.B. Konstanten in der Reaktionskinetik oder Wärmeübergangskoeffizienten, oder aus Prozessunsicherheiten, die auch langsame Veränderungen des Zuflusses oder der Qualität der Edukte einschlieen. Es wird eine robuste Zwangsbedingung für die Eigenwerte formuliert, um ein robustes Verhalten des entworfenen Reaktornetzwerkes zu garantieren. Effiziente Formulierungen zur Verknüpfung von Reaktoren und neue Zwangsbedingungen zur Auswahl der Regelungsstruktur, die auf Komplementarität basieren, werden vorgeschlagen. Die Methode resultiert in einem semi-infiniten gemischt-ganzzahligen nichtlinearen Optimierungsproblem mit Komplementaritätsbdingungen, Disjunktionen, und einer robusten Eigenwert-Nebenbedingung. Es wird eine hybride zweistufige Lösungsmethode vorgeschlagen, welche die Lösungsalgorithmen des verwandten Optimierungsproblems integriert. Die vorgeschlagene Lösungsmethode wird auf eine Fallstudie der Allylchlorid-Produktion mit bis zu zehn Rohrreaktoren bzw. Rührkesselreaktoren angewandt.