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Integration of process design and controller design for chemical processes using model-based methodology

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ABSTRACT

In this paper, a novel systematic model-based methodology for performing integrated process design and controller design (*IPDC*) for chemical processes is presented. The methodology uses a decomposition method to solve the *IPDC* typically formulated as a mathematical programming (optimization with constraints) problem. Accordingly the optimization problem is decomposed into four sub-problems: (i) pre-analysis, (ii) design analysis, (iii) controller design analysis, and (iv) final selection and verification, which are relatively easier to solve. The methodology makes use of thermodynamic-process insights and the reverse design approach to arrive at the final process design–controller design decisions. The developed methodology is illustrated through the design of: (a) a single reactor, (b) a single separator, and (c) a reactor–separator-recycle system and shown to provide effective solutions that satisfy design, control and cost criteria. The advantage of the proposed methodology is that it is systematic, makes use of thermodynamic-process knowledge and provides valuable insights to the solution of *IPDC* problems in chemical engineering practice.

1. Introduction

Traditionally, process design and controller design are two separate problems that are dealt with sequentially. The process is designed first to achieve the design objectives, and then, the operability and control aspects are analyzed and resolved to obtain the controller design. This traditional-sequential approach is often inadequate since many process control challenges arise because of poor design of the process and may lead to overdesign of the process, dynamic constraint violations, and may not guarantee robust performance (Malcom, Polam, Zhang, Ogunnaike, & Linninger, 2007). Another drawback has to do with how process design decisions influence the controllability of the process. To assure that design decisions give the optimum economic and the best control performance, controller design issues need to be considered simultaneously with the process design issues. The research area of combining process design and controller design considerations is referred here as integrated process design and controller design (*IPDC*). One way to achieve *IPDC* is to identify variables together with their target values that have roles in process design (where the optimal values of a set of design variables are obtained to match specification on a set of process variables) and controller design (where the same set of design variables serve as the actuators or manipulated variables and the same set of process variables become the controlled variables). Also, the optimal design values become the set points for the controlled and manipulated variables. Using model analysis, controllability issues are incorporated to pair the identified actuators with the corresponding controlled variables. The integrated design problem is therefore reduced to identifying the dual purpose design-actuator variables, the process-controlled variables, their sensitivities, their target-set-point values, and their pairing.

The importance of an integrated process-controller design approach, considering operability together with the economic issues, has been widely recognized (Allgor & Barton, 1999; Bansal, Perkins, Pistikopoulos, Ross, & Van Schijndel, 2000; Bansal, Sakizlis, Ross, Perkins, & Pistikopoulos, 2003; Kookos & Perkins, 2001; Luyben, 2004; Meeuse & Grievink, 2004; Patel, Uygun, & Huang, 2008; Ricardez Sandoval, Budman, & Douglas, 2008; Schweiger & Floudas, 1997). The objective has been to obtain a profitable and operable process, and control structure in a systematic manner. The *IPDC* has advantage over the traditional-sequential method because the controllability issues are resolved together with the optimal process design issues. Meeuse and Grievink (2004) used the Thermodynamic Controllability Assessment (*TCA*) technique to incorporate controllability issues into the design problem. The *IPDC* problem, however, involved multi-criteria optimization and needed trade-off between conflicting design and control objectives. For example, the process design issues point to design of smaller

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Nomenclature

B	bottom flowrate
C^0_{EO}, $C_{EO,F}$	feed concentration of ethylene oxide
C^0_W	feed concentration of water
C_{DEG}	concentration of diethylene glycol
C_{EG}	concentration of ethylene glycol
C_{EO}	concentration of ethylene oxide
C_{TEG}	concentration of triethylene glycol
C_W	concentration of water
C_p, C_{pc}	heat capacity for component and coolant
D	distillate flowrate
Da	Damköhler number
$\mathbf{d}$	set of disturbance variables
FD_i	driving force
F_c	coolant flowrate
F_j	feed flowrate on the jth stage
$F_{EO,F}$	ethylene oxide feed flowrate
$F_{W,F}$	water feed flowrate
f_W	dimensionless water feed flowrate
ΔH_R	heat of reaction
H_j	reactor enthalpy of stream j
H^c_j	jacket enthalpy of stream j
h^l_j	specific heat content of liquid emanating from stage j
h^v_j	specific heat content of vapor emanating from stage j
J	objective function
k_i	reaction kinetic of reaction i
$K_{i,j}$	equilibrium constant of component i on the jth stage
L_j	liquid flowrate on the jth stage
$M_{i,j}$	holdup of component i on the jth stage
M_j	holdup on the jth stage
m_{EO}	dimensionless ethylene oxide mixer flowrate
N	number of stage
N_F	feed stage
P^{opt}	optimal pressure
P^*_i	partial pressure of component i
P	pressure
$P_{1,j}$	design objective term
$P_{2,j}$	control objective term
$P_{3,j}$	economic objective term
Q_c	condenser duty
Q_r	reboiler duty
Q_R	heat transfer between the jacket and the reactor
r_i	reaction rate of component i
R_i	net reaction rate of reaction i
RB, $RB_{\min}$	real reboil ratio, minimum reboil ratio
RR, $RR_{\min}$	real reflux ratio, minimum reflux ratio
S	reactor effluent flowrate
t	time
T_j	temperature of stream j
T_{co}, T_c	coolant temperature (input and output)
T^m_i, T^b_i	melting and boiling point of component i
U_i	holdup internal energy on the jth stage
$\mathbf{u}$	set of design/manipulated variables
$\mathbf{v}$	set of chemical system variables
V	reactor volume
V_j	vapor flowrate on the jth stage
V_R	real reactor volume
w_j	weight factor assigned to each objective term
$\mathbf{x}$	set of process/controlled variables
$x_{i,j}$	liquid mole fraction for component i on the jth stage
Y	binary decision variables
$y_{i,j}$	vapor mole fraction for component i on the jth stage
$z_{i,j}$	feed composition for component i on the jth stage

Greek symbols

$\alpha_{i,jk}$	relative volatility of component i
$\alpha_{Y,S}$	recovery of ethylene oxide at stream Y w.r.t. stream S
$\beta_{Y,S}$	recovery of water at stream Y w.r.t. stream S
$\chi_{Y,S}$	recovery of ethylene glycol at stream Y w.r.t. stream S
$\delta_{Y,S}$	recovery of diethylene glycol at stream Y w.r.t. stream S
$\varepsilon_{Y,S}$	recovery of triethylene glycol at stream Y w.r.t. stream S
$\boldsymbol{\theta}$	set of constitutive variables
ξ_i	dimensionless extent of reaction of component i
ρ, ρ_c	density for component and coolant
τ_R	reaction residence time

process units in order to minimize the capital and operating costs, while, process control issues point to larger process units in order to smooth out disturbances (Luyben, 2004).

A number of methodologies have been proposed for solving *IPDC* problems (Sakizlis, Perkins, & Pistikopoulos, 2004; Seferlis & Georgiadis, 2004). In these methodologies, a mixed-integer nonlinear optimization problem (*MINLP*) is formulated and solved with standard *MINLP* solvers. The continuous variables are associated with design variables (flowrates, heat duties) and process variables (temperatures, pressures, compositions), while binary (decision) variables deal with flowsheet structure and controller structure. When an *MINLP* problem represents an *IPDC*, the process model considers only steady-state conditions, while a *MIDO* (mixed-integer dynamic optimization) problem represents an *IPDC* where steady state as well as dynamic behaviour is considered.

A number of algorithms have been developed to solve the *MIDO* problem. From an optimization point of view, the solution approaches for *MIDO* problems can be divided into simultaneous and sequential methods, where the original *MIDO* problem is reformulated into a mixed-integer nonlinear program (*MINLP*) problem (Sakizlis et al., 2004). The former method, also called complete discretization approach, transforms the original *MIDO* problem into a finite dimensional nonlinear program (*NLP*) by discretization of the state and control variables. Avraam, Shah, and Pantelides (1999), Flores-Tlacuahuac and Biegler (2007) and Mohideen, Perkins, and Pistikopoulos (1996) applied this complete discretization approach and solved the resulting *MINLP* problem using outer approximation (*OA*) and generalized Benders decomposition (*GBD*) frameworks. However, this method typically generates a very large number of variables and equations, yielding large *NLPs* that may be difficult to solve reliably (Exler, Antelo, Egea, Alonso, & Banga, 2008; Patel et al., 2008), depending on the complexity of the process models.

As regards the sequential method, also called control vector parameterization approach, only control variables are discretized. The *MIDO* algorithm is decomposed into a sequence of primal problems (nonconvex *DO*s) and relaxed master problems (Bansal et al., 2003; Mohideen, Perkins, & Pistikopoulos, 1997; Schweiger & Floudas, 1997; Sharif, Shah, & Pantelides, 1998). Because of nonconvexity of the constraints in *DO* problems, such solution methods are possibly excluding large portions of the feasible region within which an optimal solution may occur, leading to the suboptimal solutions (Chachuat, Singer, & Barton, 2005).