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Development and application of linear process model in estimation and control of reactive distillation

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Abstract

This paper presents a comprehensive formulation of a linearized state space process model for a generic two-reactant-two-product reactive distillation system. The development of the model requires the knowledge of the desired steady state design data, including liquid holdups and composition profiles. The application of the developed linear process model in composition estimation and control of the system is demonstrated. The effect of controller tuning on the performance of the estimator-based control system is explored. It is shown that effective controller tuning is necessary for a robust performance of a closed-loop reactive distillation system that relies on a state estimator. A robust linear state estimator can be developed and implemented in a feedback control system of a reactive distillation when the process can be approximated by a linear model.

Keywords: Reactive distillation; Linear state space model; State estimation and control

1. Introduction

The growing application of reactive distillation processes has necessitated a better understanding of its process dynamics and control. The classical problem of implementing a feedback control on a system is the means to provide the controllers the required feedback states. In practice, the use of online analyzer to measure the concentration in a reactive distillation column is unsatisfactory because of its economic implications. Besides, the large time delay between taking the sample and the output of the analyzer makes it difficult to be used in a feedback control system. Therefore, the use of a state estimator to provide the state estimates, when needed in the control system of a reactive distillation system, is an attractive alternative.

Recent publications on reactive distillation control emphasize the need to have the knowledge of internal composition profiles in order to design an effective control for reactive distillation (Al-Arfaj & Luyben, 2000, 2002a, 2002b, 2004; Bisowarno, Tian, & Tade, 2003; Wang, Wong, & Lee, 2003). Unless an excess of one of the reactants is incorporated in the process design, some detection of the inventory of one of the reactants in the column is required so that a feedback trim can balance the reaction stoichiometry (Al-Arfaj & Luyben, 2000).

Reactive distillation columns are generally being modeled by a set of highly nonlinear first order differential equations (Baur, Taylor, & Krishna, 2001; Kumar & Daoutidis, 1999; Roat, Downs, Vogel, & Doss, 1986; Taylor & Krishna, 2000). However, many model-based controllers use linear models because the linear models are easier to analyze and require less computational recourses than nonlinear models. Besides, most of the nonlinear systems often have the same general phase-plane behavior as the model linearized about the steady state condition when the system is close to that particular condition. Therefore, it is important to derive a suitable linearized dynamic model that when used in the model-based control applications could yield an effective and robust control system.

Few papers have emerged on the development of a linear model for a typical distillation column. Marquardt and Amrhein (1994) developed a linear distillation model for multivariable controller design of binary distillation columns. Their modeling idea draws on the wave propagation phenomena characterizing distillation column dynamics. The process nonlinearities were nicely averaged by using a 5th order linear model. Luyben (1987) derived a simple but effective method to determine suitable linear transfer functions for highly nonlinear distillation columns. He presented an effective design procedure that uses

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Nomenclature

A	reactant component
A	matrix of state variables for the linearized process model
B	reactant component
B	matrix of inputs for the linearized process model
C	product component
C	matrix of outputs for the linearized process model
d	disturbance variables' vector
E	matrix of the disturbance variables for the linearized process model
F_A	fresh feed flowrate of reactant A (kmol/s)
F_B	fresh feed flowrate of reactant B (kmol/s)
G	matrix of measurement noise
ΔH_v	heat of vaporization (cal/mol)
K	gain matrix
K_B	specific reaction rate of the reverse reaction (kmol s^{-1} $kmol^{-1}$)
K_c	Controller gain
K_F	specific reaction rate of the forward reaction (kmol s^{-1} $kmol^{-1}$)
KF	Kalman filter
L	liquid flowrate (kmol/s)
M_i	liquid holdup on stage i (kmol)
nf_1	first tray of reactive section (entrance of feed F_A)
nf_2	last tray of reactive section (entrance of feed F_B)
N	total number of stages including reboiler and reflux drum
P	column pressure
$R_{i,j}$	rate of production of component j on tray i (kmol/s)
T_i	temperature in stage i including reboiler (K)
U	input variables' vector
v	measurement noise
V_i	vapor flowrate on tray i (kmol/s)
V_S	vapor flowrate from the reboiler (kmol/s)
w	plant noise
$x_{bot,D}$	composition of D in the bottoms
$x_{dis,C}$	composition of C in the distillate
$x_{i,j}$	liquid mole fraction of component j on tray i
X	state vector of the variables
$\hat{X}$	state estimate vector
$X_{nf_1,A}$	composition of A in tray nf_1
$X_{nf_2,B}$	composition of B in tray nf_2
X_0	initial conditions of the plant model
X_0 err	initial condition error vector
Y	output vector
$\hat{Y}$	observation vector
Z	measured output vector
Z_a	composition of fresh feed F_A
Z_b	composition of fresh feed F_B

Greek letters

α_j	relative volatility of component j with respect to heavy component
δ_m	standard deviation of the measurement noise
δ_p	standard deviation of the plant noise
θ	lumped model parameters
λ	heat of reaction (cal/mol)

Astrom's method (relay feedback) to get critical gains and frequencies for each diagonal element of the plant transfer matrix. He concluded by emphasizing the effectiveness of the method in handling highly nonlinear column efficiently.

This study deals with the formulation of a linearized state space model, and demonstrates its applicability in an estimator-based control system of a generic reactive distillation. A linear state estimator is developed from a linear process model and implemented in a feedback control system of a reactive distillation. The function of the state estimators is to provide the required states for feedback. The robustness and reliability of a linear estimator at different operating conditions are examined by comparing the performance of an estimator based-control system to that of a system that assumes a perfect composition measurement. Section 2 presents a detailed nonlinear process model for a generic reactive distillation under study. Because the performance of a state estimator largely depends on the accuracy of the process model in which it is based on, Section 3 is devoted to developing a reliable linear process model for the system. The linearization of this nonlinear reactive distillation model is challenging because of the presence of reaction and separation in a single column. Complexity in its dynamics arises from the interaction of the reaction kinetics and distillation concept of vapor–liquid equilibrium in the system. The development of a linear state estimator is presented in Section 4. The performance of a dual-end composition control structure when all of the compositions are estimated by the linear estimator, and when the linearized process model is used to describe the reactive distillation process is investigated in Section 5.

2. Nonlinear process model

Various types of models, involving different levels of complexity, can be used to simulate the dynamics of reactive distillation column. In this work, we considered the simple and generic reactive distillation system studied by Al-Arfaj and Luyben (2000) as shown in Fig. 1. The system model captures the main features of the unit dynamics with simple vapor–liquid equilibrium, kinetics and physical properties. The reversible liquid-phase elementary reaction occurring in the reactive zone is

$$A + B \Leftrightarrow C + D \tag{1}$$

The assumptions considered are the following: constant liquid holdups; equimolar overflow except in the reaction zone where vapor boilup changes due to heat of reaction, which vaporizes some liquid on each tray; constant relative volatilities; fixed heat of reaction and vaporization; saturated liquid feed and reflux