



# Model predictive control of reactive distillation for benzene hydrogenation



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## ABSTRACT

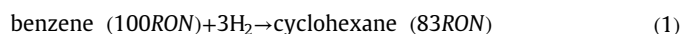
Benzene hydrogenation via reactive distillation is a process that has been widely adopted in the process industry. However, studies in the open literature on control of this process are rare and seem to indicate that conventional decentralized PI control results in sluggish responses when the reactive distillation column is subjected to disturbances in the feed concentration. In order to overcome this performance limitation, this work investigates model predictive control (MPC) strategies of a reactive distillation column model, which has been implemented in gPROMS. Several MPCs based upon different sets of manipulated and controlled variables are investigated where the remaining variables remain under regular feedback control. Further, MPC controllers with output disturbance correction and, separately, with input disturbance correction have been investigated. The results show that the settling time of the column can be reduced and the closed loop dynamics significantly improved for the system under MPC control compared to a decentralized PI control structure.

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## 1. Introduction

Benzene is carcinogenic and has been classified by the Environmental Protection Agency (EPA) as a Mobil Source Air Toxic (MSAT) due to its presence in gasoline (Environmental Protection Agency, 2000). The EPA regulates automobile emissions of benzene by limiting the amount of benzene in gasoline to 0.62 vol% (Environmental Protection Agency, 2007). The gasoline pool in a refinery consists of a blend of streams from several different sources which also have different benzene concentrations. While the reformat stream is one of the most important sources for blending, as it enhances the octane number of the pool, it is also the main contributor of benzene (Environmental Protection Agency, 2006). As such, removal strategies for benzene from reformat streams are essential for gasoline production. A variety of different approaches exist, ranging from removing compounds that form benzene in the reformat feed, to removal of benzene via solvent extraction or hydrotreating (Palmer, Kao, Tong & Shipman, 2008). The latter approach will be investigated in this work and it involves hydrogenation of benzene in the presence of a catalyst.

However, this reaction is not selective and toluene, which is a desirable component of the reformat stream and present in significant amounts, is also reduced. As toluene has a high octane rating (RON), it is desirable to maintain it in the final product; see Eqs. (1) and (2) for detail of the reactions.



The issue of selectivity can be overcome by using a reactive distillation (RD) column as reactive distillation can make use of the different volatilities of the components. Fig. 1 shows a schematic of a reactive distillation column used for benzene hydrogenation.

Reactive distillation can enable selective reactions as separation and reaction are simultaneously occurring in the same vessel, e.g., the catalyst zone can be located in a part of the column where one or more of the components of the undesirable side-reaction are not present in significant concentrations. In addition to enhancing the selectivity of the reactions, using reactive distillation can result in savings in capital expenditure and also energy utilization for some processes (Harmsen, 2007).

While reactive distillation for benzene hydrogenation can have benefits over a conventional process, combining separation and reaction in a single vessel can lead to operational challenges as

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**Notation**

$a$	geometric surface area of packing per unit volume, $\text{m}^2 \text{m}^{-3}$
$A$	cross section area of column
$C_A$	concentration, $\text{mol m}^{-3}$
$d_p$	packing particle diameter, m
$d_s$	column diameter, m
$D$	distillate flow rate, $\text{mol s}^{-1}$
$E_a$	reaction activation energy, $\text{J mol}^{-1}$
$F$	feed flow rate, $\text{mol s}^{-1}$
$h_i$	total liquid holdup based on empty column, $\text{m}^3 \text{m}^{-3}$
$H_{l,j}$	molar enthalpy of liquid stream on stage $j$ , $\text{J mol}^{-1}$
$H_{v,j}$	molar enthalpy of vapor stream on stage $j$ , $\text{J mol}^{-1}$
$HETP$	height equivalent to a theoretical stage, m
$k$	reaction rate constant, $\text{mol s}^{-1} \text{kg}^{-1}$
$K$	wall factor
$K_A$	reaction adsorption coefficient, $\text{m}^3 \text{mol}^{-1}$
$K_H$	reaction adsorption coefficient, $\text{m}^3 \text{mol}^{-1}$
$L$	liquid flow rate, $\text{mol s}^{-1}$
$m$	number of manipulated variables
$M$	mass holdup, kg
$M_{l,j}$	liquid molar holdup on stage $j$ , mol
$M_{v,j}$	vapor molar holdup on stage $j$ , mol
$N$	number of stages
$P$	pressure, Pa
$\Delta P_{0,j}$	dry column pressure drop across stage $j$ , Pa
$\Delta P_j$	irrigated column pressure drop across stage $j$ , Pa
$Q$	external heat energy input, J
$Q$	process noise covariance matrix
$r$	number of controlled variables
$R$	reflux ratio
$R$	measurement noise covariance matrix
$R_{\text{gas}}$	gas constant, $\text{J mol}^{-1} \text{K}^{-1}$
$Re_v$	vapor Reynolds number

$rxn$	reaction rate, $\text{mol s}^{-1} \text{kg}^{-1}$
$s$	Laplace variable
$T_0$	reaction reference temperature, K
$T_{\text{cond}_{in}}$	temperature of cooling water entering the condenser, K
$T_{\text{cond}_{out}}$	temperature of cooling water leaving the condenser, K
$T_j$	temperature on stage $j$ , K
$u$	specific liquid load, $\text{m s}^{-1}$
$V$	vapor flow rate, $\text{mol s}^{-1}$
$v$	measurement noise
$w$	process noise
$x$	liquid mole fraction
$y$	vapor mole fraction
$y^*$	equilibrium vapor mole fraction
$z$	feed mole fraction

**Greek letters**

$\epsilon$	packing void fraction
$\phi_{l,i}$	liquid fugacity coefficient of component $i$ on stage $j$
$\phi_{v,i}$	vapor fugacity coefficient of component $i$ on stage $j$
$\rho_{\text{cat}}$	catalyst density, $\text{kg m}^{-3}$
$\eta$	Murphree efficiency
$\lambda$	relative gain
$\Lambda$	relative gain array
$\tau$	transfer function time constant, s
$\tau_c$	controller design parameter, s
$\theta$	transfer function time delay, s
$\psi$	resistance coefficient

**Subscripts**

$i$	component index
$j$	stage index

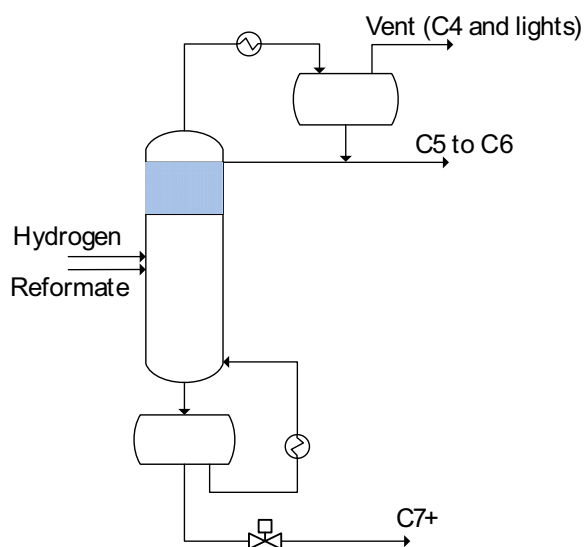


Fig. 1. Schematic of a reactive distillation column.

(Environmental Protection Agency, 2006). This makes it challenging to develop a control system for the process as the control system needs to effectively maintain all the controlled variables at their set points and at the same time rapidly reject disturbance effects.

It is essential for any control system to be tested in an industrial setting or, in a first step, in detailed simulations. In this regard, this work makes use of a rigorous first principles-based dynamic model of the benzene hydrogenation reactive distillation column. This model has been implemented in gPROMS as part of a recent study and consists of over 2400 differential and 5000 algebraic equations (Mahindrakar & Hahn, 2014). This prior study developed a decentralized control scheme in conjunction with a feedforward controller for this process. While the investigated control configuration worked reasonably well, it had the drawback that the feedforward controller was only beneficial if the delay associated with the feed composition measurement was small, which in turn requires a composition analyzer which can be expensive to purchase and maintain (Luyben, 2006). In order to address these drawbacks, this work investigates several MPC control structures in order to improve the closed loop dynamics of the RD column for disturbance rejection without requiring continuous and near instantaneous measurements of the feed concentrations.

The outline of this paper is as follows. Section 2 presents preliminary information about the dynamic model of the reactive distillation column and model predictive control relevant to this work. The details of the model predictive control scheme are provided in

there are fewer controlled and manipulated variables than if separate reaction and separation processes would be used. This can be especially challenging for benzene hydrogenation because this process is known to be subjected to significant feed concentration fluctuations. For example, the reformate stream benzene concentration can vary between 3 vol% and 11 vol% on a regular basis

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