

# A comparison of the performance of profile position and composition estimators for quality control in binary distillation

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## Abstract

In this study a number of control strategies have been developed for control of the overhead composition of a binary distillation column. The nonlinear wave model as presented in the literature, has been substantially modified in order to express it in variables that can easily be measured and make it more robust to feed flow and feed composition changes. The new model consists essentially of the equation for wave propagation and a static mass and energy balance across the top section of the column. Taylor series developments are used to relate the temperature on the measurement tray to the temperature and concentration on the tray where the inflection point of the concentration profile is located. The model has been incorporated in control of the overhead quality of a toluene/*o*-xylene benchmark column. In addition, a number of partial least squares (PLS) estimators have been developed: a nonlinear estimator for inferring the overhead composition from temperature measurements and a linear and nonlinear estimator for inferring the inflection point of the concentration profile in the column. These estimators are also used in a cascade control strategy and compared with use of the wave propagation model. Finally a control strategy consisting of a simple temperature controller and a composition controller were implemented on the simulated column. The study shows that the inferential control using PLS estimators performs equally well than control using the nonlinear wave model. In all cases the advantage of using inferential controllers is substantial compared with using single tray temperature control or composition control.

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*Keywords:* Binary distillation; Partial least squares; Wave propagation model

## 1. Introduction

Systems with distributed parameters, such as distillation columns, exhibit dynamic characteristics that resemble traveling waves (Luyben, 1972; Marquardt, 1986; Hwang, 1991, 1995).

Luyben (1972) pioneered a temperature profile position controller by measuring the temperature on five trays and calculating ‘between which trays a temperature in the middle of break lies’. This control strategy exhibited an increased sensitivity to feed changes. Marquardt (1986) analyzed the behavior of binary distillation columns by showing that a relationship exists between the product composition and the inflec-

tion point of the temperature profile. The idea behind the use of a profile for composition control is the fact that the shape of the profile does not necessarily have to be the same in order to guarantee a constant top (and/or bottom) composition, it only requires conformity of the profile.

Betlem (2000) has also shown experimentally that in batch columns the inflection point under constant top quality control remains constant despite the fact that the bottom composition changes continually and consequently, the dominant first order time constant remains the same.

Hwang (1991, 1995) gave a comprehensive discussion on how the shift in sharp concentration profiles in a distillation column can be explained by nonlinear wave theory.

The nonlinear wave model can be a very helpful tool for the implementation of dual composition control since it provides a fast method to infer the response of

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**Nomenclature**

$A$	constant in Antoine equation
$B$	constant in Antoine equation
$D$	molar distillate flow
$dy/dx$	derivative of vapor–liquid equilibrium relationship
$F$	molar feed flow rate
$H$	molar enthalpy
$K$	ratio between partial component pressure and system pressure
$L$	molar liquid flow rate
$M$	molar holdup
$N$	total number of trays
$p$	Pressure
$q$	vapor fraction of the feed
$Q$	heat released in the condensor
$r$	ratio between molar vapor and liquid holdup
$S$	dimensionless spatial coordinate
$t$	time or score
$T$	temperature
$u$	wave propagation velocity
$V$	molar vapor flow
$x$	mole fraction light component
$y$	vapor fraction light component
$z$	feed fraction light component
$\Delta$	difference between two sides of shock wave
<i>Subscripts</i>	
LD	liquid distillate
LS	liquid on representative tray
m	measurement
S	spatial coordinate of representative tray
VS	vapor flow on representative tray

product compositions to feed composition and feed flow changes. It is, therefore, not surprising that various control applications have been reported in the literature (Gilles & Retzbach, 1980, 1983; Balasubramhanya & Doyle, 1997, 2000; Han & Park, 1993; Shin, Seo, Han & Park, 2000). The latter two authors implement the nonlinear wave model in a dual composition Generic Model Control framework. In all cases the authors report that the control strategy based on the nonlinear wave model outperforms all other tested control strategies.

Another interesting approach to control the top and/or bottom composition in distillation columns is the use of a Partial Least Squares estimator for composition control (Mejdell & Skogestad, 1991; Kano, Miyazaki, Hasebe & Hashimoto, 2000).

Mejdell proposed three estimators for the composition, (i) an estimator using 12 weighted column temperatures, (ii) an estimator using logarithmic transformation of the composition and no weighting on the temperatures and (iii) an estimator using logarithmic transformations on temperatures and composition. Kano et al. carried out a comprehensive study

of dynamic Partial Least Squares (PLS) for composition estimation and concluded that the estimation of column top and bottom quality should be based on reflux flow rate, reboiler heat duty, pressure and multiple tray temperatures. The cascade control system studied consisted of inner temperature control loops and outer inferential composition control loops. No feedback on actual composition was, however, included in the control strategy.

In this study the nonlinear wave model will be revisited, the model is formulated such that it is dependent on easily measurable variables. The problem of maintaining a constant inflection point of the concentration profile is reduced to proper estimation of the vapor and liquid flow and of the concentration and temperature on the tray, where the inflection point of the concentration profile is located. It will be shown that several, relatively simple models can be developed to accomplish estimation of concentration and temperature. In addition, it will be shown that using the nonlinear wave model in a cascade composition control structure provides the advantage of fast response of the controlled variable.

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