

Rigorous Dynamic Model of  
Distillation Columns

Young-Soon Choe  
KAIST, Chemical Process Lab.

ABSTRACT

For distillation columns, dynamic models which consider variable pressure and vapor holdup were studied.

A most rigorous model which used the vapor hydraulic equation was studied with implicit methods.

Vapor holdup must be considered in high pressure columns in order to predict dynamic responses accurately.

The effect of pressure changes on the tray was only important for the vacuum column, particularly when heat input disturbances occurred.

The rigorous vapor hydraulic model was shown to be useful, despite the fact that it is extremely stiff, provided an implicit integration algorithm (LSODES) is employed.

INTRODUCTION

Most dynamic models of distillation columns incorporate many simplifying assumptions. Two assumptions commonly applied are: (1) Negligible vapor holdup (2) Constant tray pressures.

These are reasonable when the column is operated under moderate pressure. For example, Fuentes and Luyben (ref.1) compared three different dynamic models which calculate vapor flow

rates from algebraic forms of the energy balance equation for Methanol - Water system. The elimination of the energy differential equation by using the approximated algebraic form made the system less stiff, therefore they could use the simple Euler integrator for the dynamic simulation.

But for high pressure columns, the vapor phase holds significant amounts of material. For the  $C_2$ -splitter, whose steady state design parameters are given in Table 1, the ratio of vapor to liquid holdup is about 0.5 at an operating pressure of 30 atmospheres. So vapor holdup will not be negligible for high pressure columns.

In moderate to high pressure columns, the relative changes in pressure are typically very small. However, in vacuum or low pressure columns, the effect of variable pressure will not be small. Condenser pressure may be considered as constant by controlling it, but the change in vapor rates gives a significant change in tray pressure drops. This produces changes in process variables, particularly in tray temperatures. Therefore, we can not assume constant tray pressures in dynamic simulation for low pressure columns.

A rigorous vapor hydraulic model was developed to apply any kind of dist-

illation columns comprehensively, particularly for vacuum columns. It uses the vapor hydraulic equation to calculate vapor rates instead of the algebraic form of the energy equation.

This paper explores these dynamic models applied to three different real chemical systems. Openloop responses to four disturbances were studied: feed flow rate, feed composition, reflux rate, and reboiler heat input. The systems studied were:

- (1) Methanol - Water system for an atmospheric column
- (2) Toluene - m-Xylene system for a vacuum column
- (3) Ethylene - Ethane (C<sub>2</sub>-splitter) system for high pressure columns.

Methanol - Water system was studied to confirm the negligible effect of vapor holdup and variable pressure to this moderate pressure column.

Accurate dynamic models are important for control studies. If the model does not predict the real dynamic behavior, it is hard to develop the best control strategy. The rigorous model developed here will be useful for control studies of columns operating under high pressure and vacuum conditions.

#### VAPOR HOLDUP

The differential equations for each tray arising from total mass and component balances for a binary system are:

$$\frac{d}{dt}(m_n + M_n) = L_{n+1} + V_{n-1} - L_n - V_n \quad (1)$$

$$\frac{d}{dt}(m_n x_n + M_n y_n) = L_{n+1} x_{n+1} + V_{n-1} y_{n-1} - L_n x_n - V_n y_n \quad (2)$$

where  $m_n$  = moles of liquid holdup  
 $M_n$  = moles of vapor holdup

The algebraic form of the energy equation can be used and variable tray pressure is not important for the high

pressure column.

At each point in time, the numerical integration of equations (1) and (2) will give us values of all trays of the quantities  $(m_n + M_n)$  and  $(m_n x_n + M_n y_n)$ . The variables  $m_n$ ,  $M_n$ ,  $x_n$ ,  $y_n$  can be calculated by an iterative solution. (ref. 2) Figure 1 gives the openloop responses of the C<sub>2</sub>-splitter to step change in heat input. If vapor holdup is neglected, the process time constant is incorrectly predicted to be 60 minutes. But in fact it is more than 50% great (90 minutes when vapor holdup is included).

#### VARIABLE PRESSURE

Figure 2 shows the importance of variable pressure for low pressure column. Model 3 in the figure is a model in Fuentes and Luyben's work. (ref.1) By including variable tray pressure we will get accurate steady state values.

To handle variable pressure for a vacuum column, the use of a rigorous 'vapor hydraulic model' was proposed.

Instead of making simplifying assumptions about the energy equation to reduce it to an algebraic form, the dynamic energy equation can be numerically integrated. This makes the system of differential equations extremely stiff and can lead to excessive computation times if explicit integration algorithms are used. (see Table 2) A practical way to handle this problem will be discussed later.

This model is a very natural and appealing one, and it permits us to handle variable pressure and incorporate vapor holdup if we wish.

In case of negligible vapor holdup, three differential equations describing each tray of a binary column are:

$$\frac{d}{dt}(m_n) = L_{n+1} + V_{n-1} - L_n - V_n \quad (3)$$

$$\frac{d}{dt}(m_n x_n + M_n y_n) = L_{n+1} x_{n+1} + V_{n-1} y_{n-1} - L_n x_n - V_n y_n \quad (4)$$

$$\frac{d}{dt}(m_n h_n + M_n H_n) = L_{n+1} h_{n+1} + V_{n-1} H_{n-1} - L_n h_n - V_n H_n \quad (5)$$

The model for binary systems is illustrated, but its use in multicomponent is straight forward. We simply add one additional component balance for each additional component. There is no change in the energy balance equation.

The known initial values from the steady state design are  $m_n$ ,  $x_n$  and  $h_n$  on each tray. Temperature and pressure are calculated from the thermodynamic relationships. Liquid rates are calculated from the Francis weir formula. (ref. 3)

Vapor rates are determined from pressure drops using a vapor hydraulic equation. (ref.3)

$$V_n = f(\Delta P_n) \quad (6)$$

This equation includes the standard relationship between dry hole pressure drop and vapor velocity.

Energy responses much faster than liquid holdup or liquid composition to a disturbance. Adding a fast changing differential equation to the system causes stiffness problem. To solve the stiffness problem of this model, several 'stiff system integrators' were tested as suggested by Schiesser. (ref.4)

Among them LSODES(ref.5) did an excellent job. (see Table 2) The LSODES algorithm is much more complex than the simple Euler, but the software is readily available, well documented and reasonably easy to use.

## CONCLUSIONS

Vapor holdup should be included in dynamic models of high pressure columns. For columns where pressure changes are significant (vacuum column), a rigorous vapor hydraulic model is recommended, using the implicit stiff-system integrator LSODES.

Table 1. Steady state design specifications

System	M-W	T-X	E-E
Feed flowrate, g-mole/min	27240	18000	5000
composition	0.5	0.67	0.5
temperature, °C	70	95	-7
pressure, mm-Hg	760	90	22800
Distillate flowrate, g-mole/min	13620	5934	2500
composition	0.999	0.999	0.95
Bottoms flowrate, g-mole/min	13620	12066	2500
composition	0.001	0.001	0.05
Reflux drum pressure, mm-Hg	760	90	22800
Reflux ratio	1.023	1.206	7.32
Temperatures, °C			
Base	100	110	-1.4
Reflux drum	64.5	60	-11.5
$\Delta P_{n,ave}$ , mm-Hg	6.46	8.0	2.175
$\Delta P_{total}$ , mm-Hg	200.24	203	104.4
$\alpha_{ave}$	4.47	2.52	1.29
NT	32	29	47
NF	6	14	25
$Q_B$ , $10^6$ Kcal/hr	14.225	15.082	4.65

Table 2. Comparison of Computation Times

cpu seconds on Cyber 850/minute of process time

Algorithm	M-W	T-X	E-E
Explicit Euler	150	130	89400
DGEAR	10	-	-
LSODES	0.5	0.4	0.4

Notes:

M-W; Methanol - Water system

T-X; Toluene - m-Xylene system

E-E; Ethylene - Ethane system

$\alpha_{ave}$ ; average relative volatility through the column

NT; total tray number

NF; feed tray location

$Q_B$ ; reboiler heat input

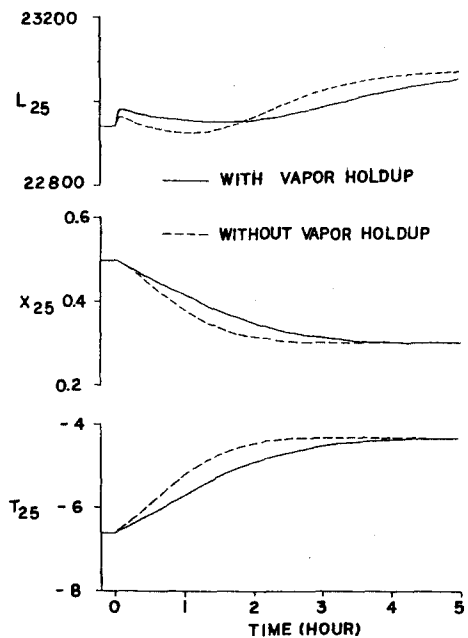


Figure 1. Responses to Heat Input( $Q_B$ ) Change for E-E on the top tray

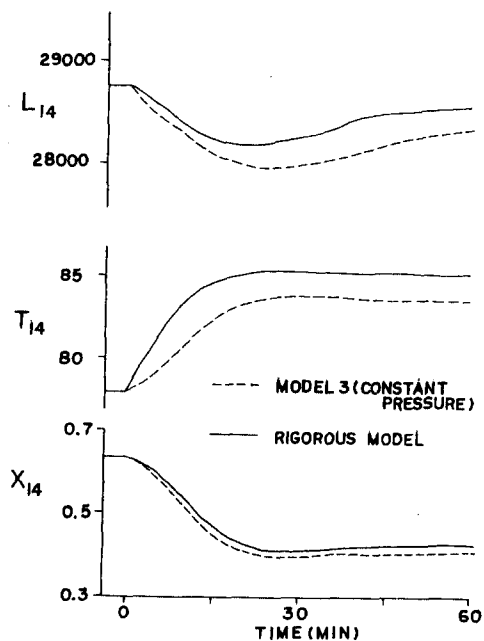


Figure 2. Responses to Heat Input( $Q_B$ ) change for T-X on the feed tray

#### NOMENCLATURE

$h_n$	liquid enthalpy
$H_n$	vapor enthalpy
$L_n$	liquid flow rate
$V_n$	vapor flow rate
$m_n$	liquid holdup
$M_n$	vapor holdup
$x_n$	liquid mole composition
$y_n$	vapor mole composition
$n$	$n^{\text{th}}$ tray
$P_n$	tray pressure
$T_n$	tray temperature

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