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A Modeling Framework for Conventional and Heat Integrated Distillation Columns

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Abstract: In this paper, a generic, modular model framework for describing fluid separation by distillation is presented. At present, the framework is able to describe a conventional distillation column and a heat-integrated distillation column, but due to a modular structure the database can be further extended by additional configurations. The framework provides the basis for fair comparison of both steady state and dynamic performance of the different column configurations for a given binary or multicomponent separation.

Keywords: Fluid separations, Distillation columns, Diabatic distillation, Dynamic modeling

1. INTRODUCTION

Multi-stage distillation is the most widely used industrial technique for continuously separating liquid mixtures. At the same time Conventional Distillation Columns (CDiC, Figure 1a) are energy intensive and operate at Second-Law efficiencies as low as 5-20 % (de Koeijer and Kjelstrup, 2000). Despite the fact that distillation is considered a mature technology, alternative configurations are under consideration, primarily due to increased attention paid to environmental issues and resource management. Alternative column configurations which reduce the amount of external energy utility are the Heat-Pump Assisted Distillation Columns for example the Mechanical Vapor Recompression Columns (MVR, Figure 1b). These configurations do not fundamentally change the fact the energy is degraded through the column, which causes low Second-Law efficiencies. Diabatic distillation has been proposed as a means to increase the Second-Law efficiency and hence the reversibility of the process. In this type of operation, the heat required to perform the separation is added and/or removed throughout the column. An example is the heat-integrated distillation column (HIDiC, Figure 1c). Internal heat transfer in the HIDiC is realized by operating the rectifying section at higher pressure than the stripping section by employing vapor recompression, thereby enabling heat transfer between the sections. This heat transfer facilitates gradual boil-up throughout the stripping and condensation throughout the rectifying section leading to an improved Second-Law efficiency (Nakaiwa et al., 1998b). The HIDiC uses significantly less utility in form of steam and cooling water compared to the CDiC. Instead, electrical energy needs to be supplied to the compressor. Even though electricity is several times more expensive than supplying energy through steam, this operation may significantly reduce the operation cost of the separation (Olujic et al., 2003). As a result of the promising features of the HIDiC, extensive efforts have been made to develop this technology during the past 15 years, both theoretically (Jana, 2010; Nakaiwa et al., 2003; Gadalla et al., 2007) and experimentally (Naito et al., 2000; Bruinsma et al., 2012). However, despite demonstrations of large energy savings of the HIDiC compared to the CDiC, it has not yet been accepted by industry. This could be due to lack of mature methods for designing and analyzing these more complex configurations, although such methods are beginning to appear (Gadalla et al., 2007; Wakabayashi and Hasebe, 2013; Suphanit, 2010; Ho et al., 2010). Furthermore operation becomes more complex as a result of the higher degree of process integration (Nakaiwa et al., 1998a; Zhu and Liu, 2005a).

One fundamental problem in the literature analyzing the operability and potential benefits of novel distillation solutions, is the use of simplistic models and different means of analysis of energy efficiencies. This can lead to bias towards one given configuration. Current studies report very different figures for potential energy savings which clearly constitutes a problem in relations to achieving industrial acceptance. Among others, Harwardt and Marquardt (2012); Shenvi et al. (2011) have addressed this issue by proposing systematic evaluations of the HIDiC. Furthermore, published case studies of industrial relevance are limited to a quite narrow range of separations. Most attention has been directed to ideal, binary systems of close boiling mixtures of hydrocarbons such as separations of equimolar mixtures of benzene/toluene (Bisgaard et al., 2013; Zhu and Liu, 2005b) or propane/propene (Ho et al., 2009). There is a need for research and comparative studies which can help to provide analysis of the pros and cons of novel and intensified distillation processes compared to conventional columns for a broader range of separations. These studies must address both static as well as dynamic analysis.

This paper presents a generic and modular modeling framework which provides solutions for a range of dis-

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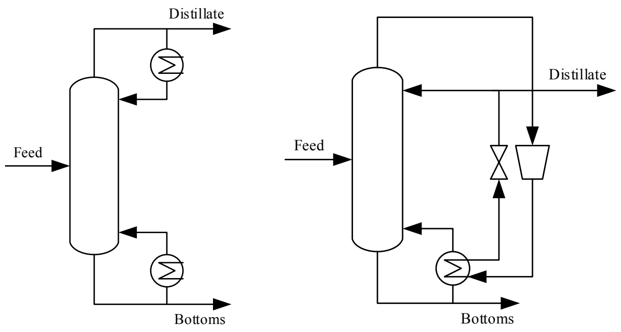
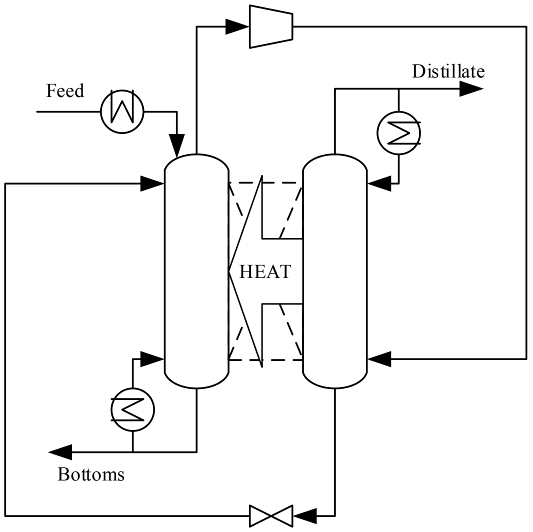


(a) CDiC (b) MVR



(c) General HIDiC

Fig. 1. Schematic representations of three column configurations: The conventional distillation column, (a), the mechanical vapor recompression column, (b), and the general heat-integrated distillation column (c) respectively.

tillation configurations including the CDiC and HIDiC configurations for separation of multicomponent mixtures. The framework provides the basis for fair comparison of steady state and dynamic performance of different column configurations for a given separation task, since the same level of detail is used for each of the modules featured in the individual column configurations. This modeling framework represents a significant improvement of the fundamental modeling of the HIDiCs often reported in literature and hence forms a better basis for quantitative performance evaluations.

The paper is organized with the detailed modeling of the columns in section 2. This is systematically divided into subsections, where section 2.5 contains the configuration specific equations and section 2.6 illustrates the required calculation sequence. A simulation study is provided in section 3 to briefly illustrate the validity of the model before finalizing remarks are listed in section 4.

2. DYNAMIC MODELING

It is the purpose of this section to provide the model equations for the framework. The following major assumptions are applied in the framework:

(i) A staged column model is used
(ii) Ideal mixing and equilibrium on each stage
(iii) Ideal vapor phases
(iv) Incompressible liquid (hence $\Delta U = \Delta H$)
(v) Negligible vapor mass and energy holdup compared to liquid holdup

Note that dynamic pressure variations are accounted for in the model as well as sensible heat effects. These are commonly neglected elsewhere for e.g. control studies.

2.1 First-principles Balances

This section provides mass and energy balances for four modules (column, total condenser, partial reboiler and compressor) which comprise the building blocks of the relevant distillation column configurations. The nomenclature is illustrated in Figure 2.

Column A schematic representation of a column module is given in Figure 2a. Let $j = 1, ..., N_C$ denote the N_C components and let $i = \{1, ..., N_S\}$ denote the stage number for a column with N_S stages counted from top. Then conservation of mass of all components on all stages is expressed in moles:

$$\frac{d}{dt}M_{1,j} = L_{top}x_{top,j} + V_2 y_{2,j} + F_1 z_{1,j} - L_1 x_{i,j} - V_1 y_{1,j} \tag{1}$$

$$\frac{d}{dt}M_{i,j} = L_{i-1}x_{i-1,j} + V_{i+1}y_{i+1,j} + F_i z_{i,j} - L_i x_{i,j} - V_i y_{i,j}, \qquad i = 2, ..., N_S - 1 \tag{2}$$

$$\frac{d}{dt}M_{N_S,j} = L_{N_S-1}x_{N_S-1,j} + V_{btm}y_{btm,j} + F_{N_s}z_{N_S,j} - L_{N_S}x_{N_S,j} - V_{N_S}y_{N_S,j} \tag{3}$$

Conservation of energy is expressed:

$$\frac{d}{dt}(M_{1,j}h_1^L) = L_{top}h_{top}^L + V_2 h_2^V + F_1 h_{F,1} + Q_1 - L_1 h_i^L - V_1 h_1^V \tag{4}$$

$$\frac{d}{dt}(M_{i,j}h_i^L) = L_{i-1}h_{i-1}^L + V_{i+1}h_{i+1}^V + F_i h_{F,i} + Q_i - L_i h_i^L - V_i h_i^V, \qquad i = 2, ..., N_S - 1 \tag{5}$$

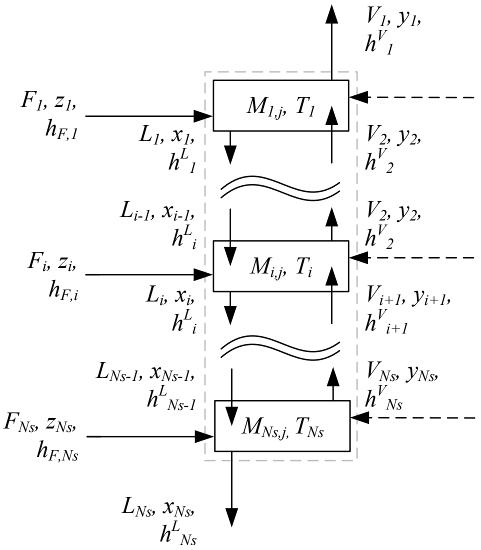
$$\frac{d}{dt}(M_{N_S,j}h_{N_S}^L) = L_{N_S-1}h_{N_S-1}^L + V_{btm}h_{btm}^V + F_{N_S}h_{F,N_S} + Q_{N_S} - L_{N_S}h_{N_S}^L - V_{N_S}h_{N_S}^V \tag{6}$$

Total Condenser A schematic representation of a total condenser module is given in Figure 2c. Conservation of mass for all components:

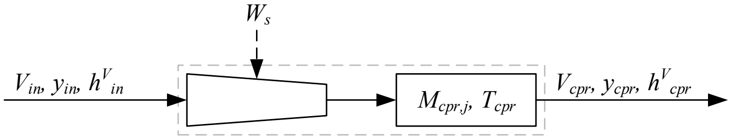
$$\frac{d}{dt}M_{cnd,j} = V_1 y_{1,j} - (L_{cnd} + D)x_{cnd,j} \tag{7}$$

Conservation of energy:

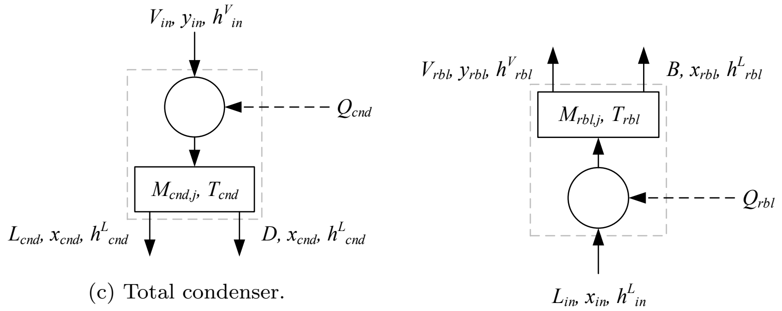
$$\frac{d}{dt}(M_{cnd,j}h_{cnd}^L) = V_1 h_1^V - (L_{cnd} + D)h_{cnd,j}^L + Q_{cnd} \tag{8}$$



(a) General stage model of a column section.



(b) Compressor.



(c) Total condenser.

(d) Partial reboiler

Fig. 2. Schematic representation of the modular units. Abbreviations: Bottom (btm), condenser (cnd), reboiler (rbl), and compressor (cpr). Lines represent mass flows and dashed lines represent energy flows.

Partial Reboiler A schematic representation of a partial reboiler module is given in Figure 2d. Conservation of mass for all components:

$$\frac{d}{dt}M_{rbl,j} = L_1 x_{1,j} - B x_{rbl,j} - V_{rbl} y_{rbl,j} \tag{9}$$

Conservation of energy:

$$\frac{d}{dt}(M_{rbl,j} h^L_{rbl}) = L_1 h^L_1 - B h^L_{rbl} - V_{rbl} h^V_{rbl} + Q_{rbl} \tag{10}$$

Compressor A schematic representation of a compressor module is given in Figure 2b. The total molar holdup is assumed to be constant, leading to the mass balance:

$$\frac{d}{dt}M_{cpr,j} = (y_{in,j} - y_{cpr,j})V_{cpr} \tag{11}$$

Conservation of energy:

$$\frac{d}{dt}h^V_{cpr} = \frac{1}{M_{T,cpr}}\left[(h^V_{in} - h^V_{cpr})V_{cpr} + W_S\right] \tag{12}$$

The pressure of the compressor exit is assumed to be given by following simplified expression for an isentropic balance:

$$P_{cpr} = P_{in}\left[\eta\left(\frac{T_{cpr}}{T_{in}} - 1\right) + 1\right]^{\dfrac{\kappa}{\kappa - 1}} \tag{13}$$

Here η is the efficiency of compression, and κ is the isentropic expansion factor which is treated as temperature independent to maintain consistency from the deviation of Eq. (13).

2.2 Thermodynamics

Vapor-Liquid Equilibrium Assuming an ideal vapor phase and a negligible contribution from Poynting correction, Modified Raoult's law states:

$$y_{i,j} = x_{i,j}\gamma_{i,j}P^{sat}_{i,j}/P_i \tag{14}$$

The vapor pressure of a liquid is calculated by the DIPPR 101 (AIChE, DIPPR) correlation. Finally the pressure can be calculated by a bubble pressure calculation, derived from Dalton's law combined with Eq. (14):

$$P_i = \sum_{j=1}^{N_C} x_{i,j}\gamma_{i,j}P^{sat}_{i,j} \tag{15}$$

Various liquid activity coefficient models are available in literature and they are typically on the form $\gamma_j = f(T, x)$. For example the Wilson model is suitable for describing a wide variety of polar mixtures and has the advantage in this application of its incapability of predicting false liquid-liquid phase splits.

Enthalpy The reference state has been chosen as pure components in ideal gas state at 298.15 K. The constant pressure heat capacity from DIPPR 107 (AIChE, DIPPR) correlation. The vapor enthalpy thus becomes:

$$h^V_{i,j} = h^{\circ}_{ref,j} + \int_{T=T^{\circ}}^{T_i} C^V_{P,i,j}\,dT \tag{16}$$

$$h^V_i = \sum_{j=1}^{N_C} y_{i,j}h^V_{i,j} \tag{17}$$

The heat of vaporization, $\Delta_{vap}H_{i,j}$, of component j is given by the DIPPR 106 (AIChE, DIPPR) correlation. The liquid enthalpy is obtained from following expression:

$$h^L_{i,j} = h^V_{i,j} - \Delta_{vap}H_{i,j} \tag{18}$$

$$h^L_i = \sum_{j=1}^{N_C} x_{i,j}h^L_{i,j} \tag{19}$$

2.3 Tray Hydraulics

It is the scope to express the liquid and vapor flow rates as functions of intensive variables. In a trayed column, liquid is entering a tray from the downcomer and leaving from the weir outlet. Furthermore vapor enters a tray in the bottom and passes through the liquid while it partly condenses until it enters the vapor phase of the tray. From the vapor phase a flow, caused by a pressure gradient, leaves the tray.

Liquid flow can be described by the Francis weir formula in which the amount of liquid over a weir is proportional to the volumetric, liquid flow rate leaving the weir to the power of 2/3 (Wittgens and Skogestad, 2000), hence:

$$L_i = \begin{cases} C_i^L \dfrac{\rho_i^L}{MW_i^L} h_{oW,i}^{1.5}, & h_{oW,i} > 0 \\ 0, & h_{oW,i} \leq 0 \end{cases} \tag{20}$$

$$h_{oW,i} = h_{cl,i} - h_W \tag{21}$$

$$h_{cl,i} = \frac{M_{T,i} MW_i^L}{\rho_i^L A_t} \tag{22}$$

Where C_i^L is a constant depending on the liquid loading of the individual trays. A_t is the active area of a tray, h_W is the weir height, $h_{cl,i}$ is the clear liquid height (any froth is ignored), and $h_{oW,i}$ is the liquid heigh above the weir. Both A_t and h_W are dimensional parameters of the column.

The vapor flow through perforated plates can be described as suggested by Kolodzie Jr. and van Winkle (1957). In this work, the volumetric flow rate is simplified to be proportional to the square root of the pressure gradient in terms of liquid height, thus:

$$V_i = C_i^V \frac{(\rho_i^V)^{0.5}}{MW_i^V} (\Delta P_i - \Delta P_{s,i-1})^{0.5} \tag{23}$$

$$\Delta P_i = P_i - P_{i-1} \tag{24}$$

$$\Delta P_{s,i-1} = \rho_{i-1}^L g h_{cl,i-1} \tag{25}$$

Where C_i^V is a constant depending on the vapor loading of the individual trays. g is the gravitational constant and $\Delta P_{s,i}$ is the static pressure drop caused by the liquid height, h_{cl}.

2.4 Miscellaneous Equations

The following definitions are used for respectively the liquid mole fraction and the total stage holdup:

$$x_{i,j} = M_{i,j}/M_{T,i} \tag{26}$$

$$M_{T,i} = \sum_{j=1}^{N_C} M_{i,j} \tag{27}$$

Molecular weights of the liquid and vapor phases can be calculated as follows from those of the pure components:

$$MW_i^L = \sum_{j=1}^{N_C} x_{i,j} MW_j, \quad MW_i^V = \sum_{j=1}^{N_C} y_{i,j} MW_j \tag{28}$$

Liquid mixture liquid density:

$$\rho_i^L = MW_i \left(\sum_{j=1}^{N_C} \frac{x_{i,j} MW_{i,j}}{\rho_{i,j}^L} \right)^{-1} \tag{29}$$

Where the pure liquid densities are calculated from the DIPPR 105 (AIChE, DIPPR) correlation. Vapor density:

$$\rho_i^V = \frac{MW_i^V P_i}{RT_i} \tag{30}$$

2.5 Configuration Specific Equations

Since the feed flow rates, composition and enthalpy must be specified for each stage, mixing relations must be applied in order to combine streams when needed. Furthermore, additional configuration specific relations must be specified. These relations are listed in this section.

Conventional Distillation Column The conventional distillation column (as illustrated in Figure 1a), operates adiabatically:

$$Q_i = 0, \qquad i = 1, ..., N_S \tag{31}$$

The operation degrees of freedom are the reflux flow rate L_{cnd}, the distillate flow rate, D, the condenser duty, Q_{cnd}, the reboiler duty, Q_{rbl}, and the bottoms flow rate, B.

Ideal Heat-Integrated Distillation Column Diabatic operation with heat transfer on multiple stages:

$$\begin{aligned} Q_k &= UA_k(T_k - T_p) && k \in \{1, ..., N_F - 1\} \\ Q_p &= -Q_k && p \in \{N_F, ..., N_S\} \\ Q_i &= 0 && i \in \{1, ..., N_S\} \backslash \{k, p\} \end{aligned} \tag{32}$$

Here UA_k parameter at stage k resembling the product of the overall heat transfer coefficient and heat transfer area. Only an ideal HIDiC is considered in this paper, meaning a HIDiC without external reflux or boilup. The operation degrees of freedom are the distillate flow rate, D, the bottoms flow rate, B, the compressor duty, W_S, and the feed preheat duty, Q_F.

The driving pressure in Eq. (23) for the vapor flow between the column sections is given by:

$$\Delta P_{N_F} = P_{cpr} - P_{N_F - 1} \tag{33}$$

Here N_F denote the top stage in the stripping section, i.e. the feed stage for a single feed configuration.

2.6 Model Discussion

The calculation sequence of the model equations is based on the framework provided by Gani et al. (1986). In this framework, the model equations are decomposed into subsets which can be solved sequentially and individually from one another. The framework is summarized in Figure 1. Assuming pressure independent enthalpies as in Eq. (16–19), the energy balances in the current form of Eqs. (4–5, 8, 10, 12) can be rewritten is terms of temperature derivatives by applying the chain rule. With respect to assumption (v), the mass balances are formulated in terms of liquid holdup instead of total stage holdup, which is reasonable for columns operating at pressures below 10 atm (Choe and Luyben, 1987). The presented model contains a C_i^L (Eq. 20) and a C_i^V (Eq. 23) for each L_i and V_i, respectively, together with a weir height h_W, a tray area A_t, and UA which is the product of the available heat transfer area at a stage and the overall heat coefficient. This high number of parameters can represent a weakness of the model since these have an impact on the dynamic behavior of the considered distillation column. Alternative to the Francis weir formula, linearized tray hydraulics can be applied as proposed by e.g. Wittgens and Skogestad (2000). The combination of a modular structure with the partitioning of the model equations in subsets, enables a flexible model with respect to configurations types and

Table 1. Model framework for implementation with calculation sequenced from top. *Requires pure and activity coefficient model parameters. † Requires distillation column dimensional parameters. ‡Requires control loop tuning parameters (optional).

Subset	Calculation
Subset 1: Thermo-dynamic*	a) Obtain states M and T b) Calculate $x = f(M)$ c) Calculate $P = f(T, x)$ d) Calculate $y = f(T, P, x)$
Subset 2: Properties*	a) Calculate $\rho^L = f(T, x)$ and $\rho^V = f(T, P)$ b) Calculate $h^L = f(T, x)$ and $h^V = f(T, y)$ c) Calculate $MW^L = f(x)$ and $MW^V = f(y)$
Subset 3: Hydraulics†	a) Calculate $L = f(M, \rho^L, MW^L)$ b) Calculate $V = f(M, \rho^L, MW^L, \rho^V, MW^V, \Delta P)$
Subset 4: Couplings†‡	a) Calculate $Q = f(T)$ etc. b) Control loops (optional)
Subset 5: Mass and energy balances	For required modules from Fig. 2, calculate $dM/dt = f(L, x, V, y, F, z)$ and $dT/dt = f(L, h^L, V, h^V, F, h_F, Q)$

ultimately a generalized foundation for comparisons. An analogous, modular framework for a HIDiC in which a floating, top stage pressure model was presented by Ho et al. (2009). In this floating pressure model, mass balances were constructed separately for the liquid and the vapor phase at the top stage. Given the top stage pressure, the propagation of pressure changes between the stages in the rectifying section was then approximated by a first order lag for each stage.

3. SIMULATION STUDY

This section provides a demonstration of the model on a separation of a binary mixture of a saturated equimolar, liquid mixture of benzene/toluene at the feed stage pressure. The purpose of this demonstration is to provide numerical and graphical examples of one of the configurations which is made possible to model with the framework. For this purpose, an ideal HIDiC with 20 stages (10 stages in stripping and 10 in rectifying section) and without external boil up and reflux will be considered. The feed is partly vaporized before its fed to the column, and heat exchange is carried out on every tray with the trays being paired according to the sequences 1-11, 2-12, ..., 10-20. Additional heat exchange is performed on the stream leaving the compressor due to slightly superheated vapor.

The model consisting of the equations summarized in this paper is implemented in the MATLAB® R2012b environment in the sequence illustrated in Table 1. The model parameters are obtained by solving the mass and energy balances subjected to the constraints listed in Table 2. Specifications of the stationary operation point are listed in Table 3. It can be seen that a compression ratio of 4.26 is required to perform the separation in the HIDiC.

Table 2. Constraints for distillation column design.

Variable	Value	Unit	Range
$y_{i,1}$	0.95	-	-
$x_{N_S,1}$	0.05	-	
P_{11}	0.101325	MPa	$i = 11$
ΔP_i	1000	Pa	$i = 2, ..., N_S$
$M_{T,i}/F$	0.5	min	$i = 1, ..., N_S - 1$
UA_i	3000	$\mathrm{W \cdot K^{-1}}$	$i = 1, ..., N_S$
$A_{t,i}$	1.34	$\mathrm{m^2}$	$i = 1, ..., N_S$
h_W	5	cm	-

Table 3. Selected variables at stationary operation point.

Desciption	Variable	Value	Unit
Feed flow	F	100	$\mathrm{kmol \cdot h^{-1}}$
Distillate flow	D	50	$\mathrm{kmol \cdot h^{-1}}$
Bottoms flow	B	50	$\mathrm{kmol \cdot h^{-1}}$
Feed composition	z	0.5000	-
Compressor duty	W_s	435.4	kW
Feed duty	Q_F	126.6	kW
Compressor heat exchanger duty	Q_{cpr}	-19.41	kW
Pressure between sections	$P_{N_F-1} - P_{N_F}$	0.326	MPa

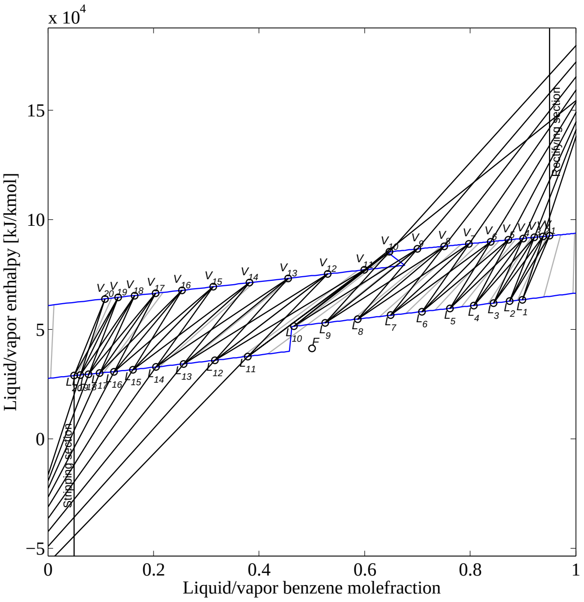
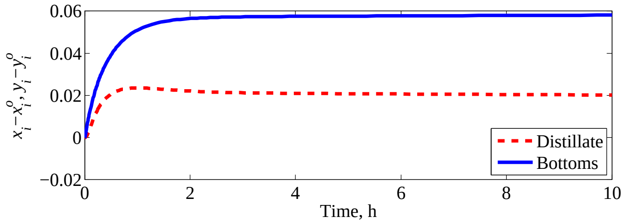


Fig. 3. Enthalpy-composition (Hxy) diagram.

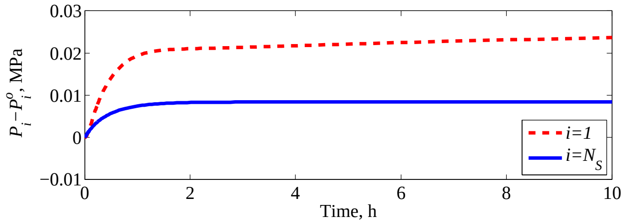
Diabatic operation makes energy balances significant and therefore enthalpy-composition (Hxy) diagrams can beneficially be used to illustrate the operating point for binary mixtures as an alternative to the xy-diagram (Ho et al., 2010). The Hxy-diagram is given in Fig. 3. Dynamic, open-loop responses to a +10% step change in feed flow rate are given in Fig. 4.

4. SUMMARY AND PERSPECTIVES

A model framework has been presented, being capable of describing both adiabatic and diabatic distillation columns. The model framework enables studies to gain



(a) Distillate (y_1) and bottoms purities (x_{N_S}) in deviation variables.



(b) Top and bottom stage pressures in deviation variables.

Fig. 4. Dynamic open-loop responses to +10% step change in feed flow rate.

insights into e.g. static properties and the dynamic behaviors. These insights can cover utility consumption accounts, energy efficiencies, operation expenses, as well as dynamics and control. In addition, the framework offers a flexibility of extending current configuration libraries due to the modular structure. Preliminary studies suggest that sensible heat effects are significant for the stream between the column sections when it comes to separation performance.

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