Parameter Estimation of a Rigorous Rate Base Model for Distillation in Packed Columns

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Abstract: This papers presents the formulation, analysis and parameter estimation of a steady state Rate Base Model (RBM) for a pilot-scale distillation column. A packed column is considered, using non-equilibrium stages to represent the packing segments and accounting for the special structure such that sparsity can be exploited in the non-linear parameter estimation problem. Model parameters are tuned to fit the model with experimental data from multiple experiments. A sensitivity analysis with respect to parameters to estimate is performed in order to properly select the parameters that can be estimated from the available temperature measurements. The tuned model is validated with experimental data.

Keywords: Distillation, parameter estimation, nonlinear optimization.

1. INTRODUCTION

Distillation is the most common unit operation in chemical industry and it often contributes to more than 50% of the total energy consumption in a plant. The best way to reduce the operating costs and energy consumption of existing units is to improve the process efficiency by an appropriate control of its variables (applied heat, temperatures, concentrations, flows, etc). However, to reach the control and optimization stages, models which describe accurately the behavior of the plant are desired. Developing models which include most of the physical properties involved in this kind of process is a challenge, since a more accurate representation in the model requires more complexity in the formulation and more efficient techniques to solve the model equations. Although distillation is performed in several industrial applications using tray-based columns, packed columns are in general more efficient since the vapor and liquid are continuously in contact through the packing surface enhancing the mass and energy transfer. On the other hand, pressure drops are smaller allowing for operation under vacuum.

Packed columns can be modeled using concepts from tray based columns such as stage efficiency and height equivalent to theoretical plate (HETP). However, these concepts do not account for departure from equilibrium properly. General approaches to model packed distillation consider the packing either as a continuous media, leading to partial differential equations (Karacan et al., 1998), or divides the packing in segments and model them as a mass and energy transfer unit (Khrishnamurthy and Taylor, 1985), (Taylor and Krishna, 1993). The latter approach is considered in the current study.

2. PILOT PLANT DESCRIPTION

The experimental setup involves a computer controlled packed distillation column (see Figure 1). The column has an internal diameter of 7 cm containing three sections of 960 mm each with Sulzer CY packing (Sulzer, Winterthur). Each section is subdivided into six smaller packing segments of 160 mm length, leading to 18 packing segments. For this particular packing material the column could be modeled using an equivalent representation of approx. 34 theoretical trays[1] if a tray based approach is used. The feed stream containing a mixture of methanol and isopropanol can be introduced into the column between the packed sections S_1 and S_2 or S_2 and S_3. The temperature of the feed can be adjusted by an electric heater of maximum 250 W. At the bottom of the column a reboiler is present containing two electric heaters of maximum 3000 W each. In the reboiler, a part of the liquid is vaporized while the rest is extracted as bottom stream. At the column top a total condenser allows to condense the entire overhead vapor stream, which is then collected in a reflux drum whose level is maintained constant. A part of the condensed liquid is fed back to the column as reflux, while the remainder leaves the column as the distillate stream. In this setup the following four variables can be manipulated: the reboiler duty Q_R (W), the feed rate F (g/min), the duty of the feed heater Q_F (W) and the reflux flow rate L_N (g/min). The distillate flow D (g/min) is adjusted to maintain a constant drum level. Measurements are available for the reflux flow rate L_N, the distillate flow rate D, the feed flow rate F and twelve temperatures,

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[1] This equivalence can be obtained using height equivalent to theoretical plate per meter (HETP/m) data from Sulzer Chemtech.
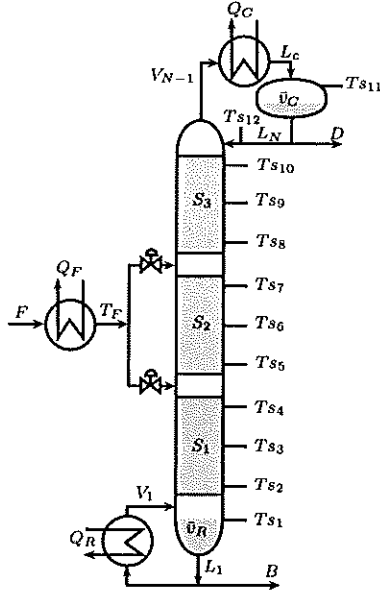
Fig. 1. General layout of the distillation setup with the distribution of the temperature sensors.

i.e., the reflux temperature $T_{s_{12}}$, the temperature at the top of the condenser $T_{s_{11}}$, the temperatures in the center and extremes of each packing section (T_{s_2} to $T_{s_{10}}$), the temperature of the feed point T_F, and the temperature in the reboiler T_{s_1}. A Labview (National Instruments, Austin) program is developed to control the actuators and to register the variables. There is no online measurement of the concentrations in the distillate and bottom streams but it is possible to measure them offline by sampling the output streams.

3. RATE BASE MODEL FOR PACKED COLUMNS

The classical approach for modeling stagewise columns employs models where the stages are considered in thermo-dynamic equilibrium. However, this equilibrium-stage approach is not completely valid since, in general, vapor and liquid leaving a stage are not at the same temperature. To cope with this problem the concept of stage efficiency was introduced, nevertheless the stage efficiency method is still deficient when multicomponent process are analyzed or the efficiency is relatively low (Seader and Henley, 2006). To this end, mass-transfer considerations are used to better model the behavior of the interaction between vapor and liquid phases along the column. In this approach each stage is assumed in mechanical but not thermal equilibrium and it is composed of two bulk phases, liquid and vapor, which are in contact at the stage interface. Figure 2 shows a non-equilibrium stage as considered by the RBM. Mass and energy transfer are performed between the bulk phases through the interface due to temperature and composition gradients.

The following assumptions are made to simplify the model.

- A binary mixture is considered, i.e, $i = 1, 2$.
- Bulk phases are assumed to be perfectly mixed.
- Vapor-liquid equilibrium is only assumed at the vapor-liquid interphase.
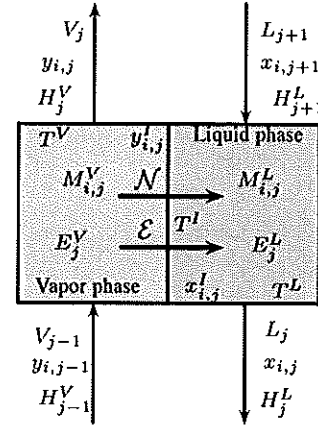- The reboiler and condenser are assumed to be in thermodynamical equilibrium.

Fig. 2. Non-equilibrium stage in the rate base model.

- The liquid volumes of reboiler and reflux drum, $\bar{v}_R$ and $\bar{v}_C$, are perfectly controlled.
- Each stage is in mechanical equilibrium.
- The condenser is at atmospheric pressure.
- The system is analyzed in steady state.

The following set of equations describe mass-transfer operations for the distillation system.

3.1 Reboiler

The reboiler is considered as an equilibrium stage and is modeled using mass, energy balances and holdups. The steady state model is summarized as follows:

$$0 = L_2 x_{i,2}^I - B x_{i,1}^I - V_1 y_{i,1}^I, \quad i = 1, 2 \tag{1}$$

$$0 = L_2 H_2^L - B H_1^L - V_1 H_1^V + Q_R - Q_1^L, \tag{2}$$

$$0 = M_{1,1}^L + M_{2,1}^L - M_{t_1}^L, \tag{3}$$

$$0 = M_{t_1}^L H_1^L - E_1^L, \tag{4}$$

$$0 = v_{t_1}^L M_{t_1}^L - \bar{v}_R, \tag{5}$$

$$0 = y_{i,1}^I - K_{i,1} x_{i,1}^I, \quad i = 1, 2, \tag{6}$$

$$0 = y_{1,1}^I + y_{2,1}^I - x_{1,1}^I - x_{2,1}^I, \tag{7}$$

$$0 = P_2 + \Delta P_2 - P_1. \tag{8}$$

3.2 Non-equilibrium stages

The stages modeling the structured packing segments are not considered in equilibrium. Consequently, balances are formulated for each bulk phase and mass and energy flow through the interface between the two bulk phases .

The following set of equations are defined for the non-equilibrium stages, i.e., $j = 2, \ldots, N - 1$.

Mass and energy balance.

$$0 = L_{j+1} x_{i,j+1} - L_j x_{i,j} + F_j^L x_{i,j}^F + \mathcal{N}_{i,j}, \quad i = 1, 2, \tag{9}$$

$$0 = V_{j-1} y_{i,j-1} - V_j y_{i,j} + F_j^V y_{i,j}^F - \mathcal{N}_{i,j}, \quad i = 1, 2, \tag{10}$$

$$0 = L_{j+1} H_{j+1}^L - L_j H_j^L + F_j^L H_{F,j}^L - Q_j^L + \mathcal{E}_j^L, \tag{11}$$

$$0 = V_{j-1} H_{j-1}^V - V_j H_j^V + F_j^V H_{F,j}^V - Q_j^V - \mathcal{E}_j^V. \tag{12}$$

Mass and energy holdups. Holdups are calculated from the geometry of the packing section as:

$$0 = M_{1,j}^L + M_{2,j}^L - M_{t,j}^L,\tag{13}$$

$$0 = M_{t,j}^L - \frac{\pi}{4}d^2 l h_{t_j}^L c_{t_j}^L,\tag{14}$$

$$0 = E_j^L - \frac{\pi}{4}d^2 l h_{t_j}^L c_{t_j}^L H_j^L,\tag{15}$$

$$0 = M_{1,j}^V + M_{2,j}^V - M_{t,j}^V,\tag{16}$$

$$0 = M_{t,j}^V - \frac{\pi}{4}d^2 l(\epsilon - h_{t_j}^L)c_{t_j}^V,\tag{17}$$

$$0 = E_j^V - \frac{\pi}{4}d^2 l(\epsilon - h_{t_j}^L)c_{t_j}^V H_j^V.\tag{18}$$

Mass and Energy Transfer Rates. Mass and energy transfer are assumed at the interface. The algebraic equations for mass transfer are implicit in the transfer rates $\mathcal{N}_{i,j}$ and are calculated according to Taylor and Krishna (1993):

$$0 = \mathcal{N}_{1,j} - a^I c_t^L k_j^L(x_{1,j}^I - x_{1,j}) - x_j(\mathcal{N}_{1,j} + \mathcal{N}_{2,j}),\tag{19}$$

$$0 = \mathcal{N}_{1,j} - a^I c_t^V k_j^V(y_{1,j} - y_{1,j}^I) - y_j(\mathcal{N}_{1,j} + \mathcal{N}_{2,j}).\tag{20}$$

The energy fluxes $\mathcal{E}_j$ are calculated from conductive and convective fluxes as:

$$0 = h_j^V a_j^I(T_j^V - T_j^I) + \sum_{i=1}^{2}\mathcal{N}_{i,j}\bar{H}_{i,j}^V,\tag{21}$$

$$0 = h_j^L a_j^I(T_j^I - T_j^L) + \sum_{i=1}^{2}\mathcal{N}_{i,j}\bar{H}_{i,j}^L,\tag{22}$$

$$0 = \mathcal{E}_j^V - \mathcal{E}_j^L.\tag{23}$$

Interface Equilibrium

$$0 = y_{i,j}^I - K_{i,j}x_{i,j}^I, \quad i = 1,2\tag{24}$$

$$0 = x_{1,j}^I + x_{2,j}^I - 1,\tag{25}$$

$$0 = y_{1,j}^I + y_{2,j}^I - 1.\tag{26}$$

Pressure Pressure at each stage is obtained from:

$$0 = P_{j+1} + \Delta P_{j+1} - P_j,\tag{27}$$

where the pressure drop ΔP_j is calculated from the geometry of the packing.

3.3 Condenser

To model the top stage, a total condenser ($L_c = V_{N-1}$) plus reflux drum is considered. It is important to mention that the real setup provides a subcooled condensate. Hence, a rigorous model requires the condenser to be modeled as a non-equilibrium stage. However, a non-equilibrium stage for the condenser requires the calculation of molar holdups for liquid and vapor phases, as long as mass transfer rates, making the model more complex. Here, the condenser is assumed in equilibrium, for simplicity, and the subcooled liquid is achieved by modeling the heat loss in the reflux drum. This loss accounts for the extra heat removed in the condenser and it has the final effect of providing a subcooled liquid in the reflux. The following set of equations defines the stage behavior.

Equilibrium total condenser.

$$0 = V_{N-1}H_{N-1}^V - L_cH_c^L + Q_c,\tag{28}$$

$$0 = y_{i,N}^I - K_{i,N}x_{i,N}^I, \quad i = 1,2,\tag{29}$$

$$0 = x_{1,N}^I + x_{2,N}^I - 1,\tag{30}$$

$$0 = y_{1,N}^I + y_{2,N}^I - 1,\tag{31}$$

$$0 = y_{1,N}^I - y_{1,N-1}.\tag{32}$$

Reflux drum

$$0 = L_c x_{i,N}^I - (L_N + D)x_{i,N}, \quad i = 1,2.,\tag{33}$$

$$0 = L_c H_c^L - (L_N + D)H_N^L,\tag{34}$$

$$0 = M_{1,N}^L + M_{2,N}^L - M_{t,N}^L,\tag{35}$$

$$0 = M_{t,N}^L H_N^L - E_N^L,\tag{36}$$

$$0 = v_{t_N}^L M_{t,N}^L - \bar{v}_C.\tag{37}$$

3.4 Model formulation

The presented model equations can be organized in such a form that structure in the formulation is preserved, i.e., the model equations are ordered by stage, i.e., reboiler, non-equilibrium stages and condenser. This formulation leads to a nonlinear algebraic system of the form

$$F(x,p) = 0,\tag{38}$$

such that $x \in \mathbb{R}^{20N-17}$ and $F(x,p) \in \mathbb{R}^{20N-17}$, where $N - 2$ is the number of packing segments. The sparse and banded jacobian, $\partial F(x,p)/\partial x$, obtained by this formulation can be exploited when solving (38) with derivative-based methods.

4. PHYSICAL PROPERTIES OF COMPONENTS

To complete the presented equations, mass and energy transfer coefficients have to be calculated as well as specific liquid holdups and pressure drops for the packing segments. Those features depend on physical properties of the mixture, e.g., viscosity, diffusion and density. Table 1 shows the references used to determine the physical properties.

Table 1. References for physical properties.

Property	Source
Activity coefficients	Wilson (1964)
Diffusion coefficients	Fuller et al. (1966), Reid et al. (1977)
Density	Daubert and Danner. (1989)
Heat capacities	Sandler (1999)
Heat of vaporization	Daubert and Danner. (1989)
Heat of mixing	Christensen (1982)
Heat Transfer Coeff.	Seader and Henley (2006)
Enthalpy	Seader and Henley (2006)
Mass Transfer Coeff.	Billet and Schultes (1999)
Viscosity	Reid et al. (1977)
Pressure drop	Billet and Schultes (1999)
Thermal conductivities	Daubert and Danner. (1989)
Specific liquid holdup	Billet and Schultes (1993)
Packing parameters	Kister (1992)

Although packing dependent coefficients for pressure drops, liquid holdup and mass transfer for some structured packing internals are listed in Billet and Schultes (1999), a proper tuning of those parameters is required since a different kind of packing is used in the studied pilot plant.

Liquid holdup. Billet and Schultes (1993) performed an extensive study with 56 different kinds of packings to predict liquid holdup in two phase countercurrent columns using a model of the form:

$$h_t = C_h^{\frac{2}{3}} f(\eta^L, \rho^L, u^L, a). \qquad (39)$$

The dimensionless holdup parameter C_h is packing depending its estimation is analyzed the current study.

Pressure drop. Likewise, pressure drops are calculated as function of the dry pressure drop ΔP_0 and the liquid holdup, following the model proposed in Billet and Schultes (1999):

$$\Delta P = \Delta P_0 f(\epsilon, h_t, a, u^L), \qquad (40)$$

$$\Delta P_0 = C_p f(a, u^V, \rho^V, \epsilon, \eta^V). \qquad (41)$$

The value of the parameter C_p is packing depending and is not described for Sulzer-CY packing. However, Billet and Schultes (1999) provide a range of values for it.

Mass transfer coefficients. The mass transfer rates are calculated as in Khrishnamurthy and Taylor (1985) using the transfer coefficients k^L and k^V from Billet and Schultes (1999):

$$k^L = C_L f(u^L, D^L, h_t), \qquad (42)$$

$$k^V = C_V f(h_t, D^V, u^V, \eta^V, \rho^V). \qquad (43)$$

The tuning of C_L and C_V is studied in the sensitivity analysis in Section 5.

Heat losses. To account for heat losses, the relation:

$$Q_j^L = \phi_L(T_j^L - T_{\text{amb}}) \qquad (44)$$

$$Q_j^V = \phi_V(T_j^V - T_{\text{amb}}) \qquad (45)$$

is proposed. Here, the vapor and liquid heat losses coefficients ϕ_L and ϕ_V, respectively, are scalar parameters. Independent heat losses parameters ϕ_R and ϕ_C are considered for the reboiler and condenser, due to the different geometry of those stages compared to the rest of the column.

5. THE PARAMETER ESTIMATION PROBLEM

The following section describes the experiments performed along with the formulation of the optimization problem for the parameter estimation.

5.1 Experimental data

A set of experiments is performed on the distillation setup by changing the reboiler duty Q_R, and the inflow F. Data is recorded when the system reaches steady state. Table 2 shows the values of some variables on each of the experiments. Flows are in g/min, applied heat in kW and temperature in K.
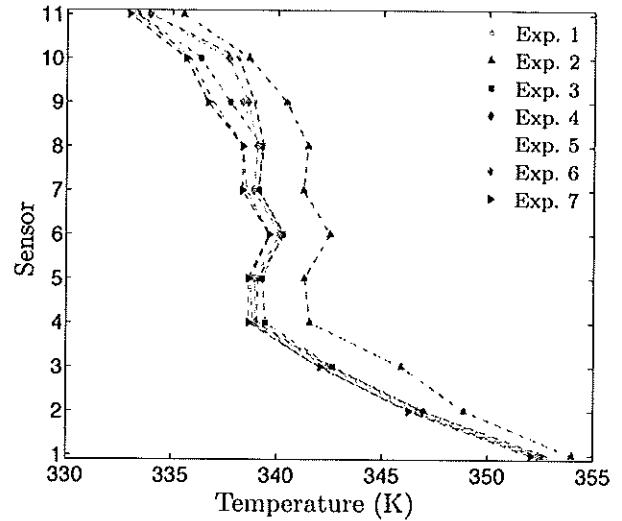

Fig. 3. Experimental data coming from the 11 sensors located along the column as illustrated in Figure 1. Temperature of the reflux, around 315 K, has not been included in the plot but is used in the estimation.

5.2 Sensitivity Analysis

To perform the estimation process, it is useful to know if the available measurements are informative enough to identify the set of proposed parameters. This requirement can be translated to check how sensitive are the states to fit with respect to model parameters, i.e., to calculate $\partial x/\partial p$. Analytical expressions for sensitivities are hard to obtain due to the complexity of the nonlinear equations describing the model. Hence, a numerical method based on finite differences is used. The model sensitivities $\partial x/\partial p$ are:

$$\left. \frac{\partial x}{\partial p} \right|_{\substack{x=x_0 \\ p=p_0}} = \left(\frac{\partial F(x,p)}{\partial x} \right)^{-1} \left. \frac{\partial F(x,p)}{\partial p} \right|_{\substack{x=x_0 \\ p=p_0}} \qquad (46)$$

Since only temperature measurements are available, the parameters which have the highest sensitivity with respect to the vapor and liquid temperature provided by the model are selected[2]. It is important to mention that this approach requires an initialization point for the parameters p_0 and the states x_0. In the current study, initialization is based on knowledge of the process and reported studies on separation using structured packing. Figure 4 gives an estimation of the sensitivity of vapor and liquid temperatures with respect to model parameters along with sensitivities

[2] Changes in those parameters have the highest effect on the trajectories to fit.

Table 2. Steady state experiments used for identification and validation.

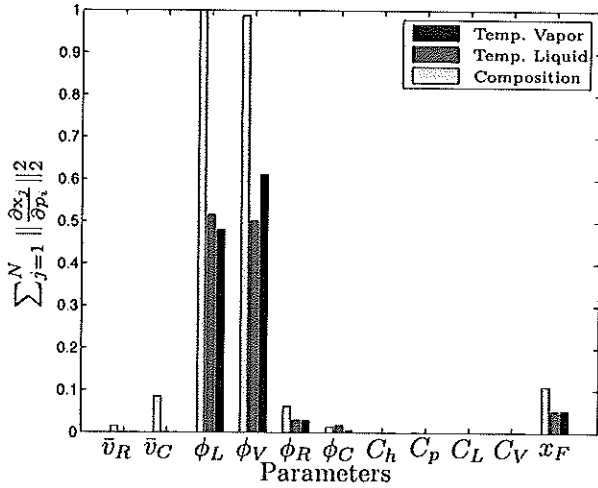| Exp	Q_R	L_N	F	T_F	T_{amb}	D	B
1	4.0	60.0	150	313.15	292.90	70	80
2	4.5	86.0	110	313.15	292.95	70	40
3	4.5	80.0	150	318.15	292.45	70	80
4	4.0	59.0	150	313.15	295.20	70	80
5	4.5	76.5	150	313.15	298.85	70	80
6	4.0	65.0	150	313.15	294.95	70	80
7	4.5	77.2	150	313.15	287.45	70	80

Fig. 4. Norm on the sensitivity of some model states with respect to the model parameters. Sensitivities are calculated around the pair (x_0, p_0) such that $F(x_0, p_0) = 0$.

for the liquid composition at top and bottom[3]. Table 3 shows the initial guess for the parameter vector p_0.

Since only parameters $\phi_L, \phi_V, \phi_R, \phi_C$ and x_F have a considerable influence on the temperature, these parameters are selected to be tuned. Hence, the number of parameters is reduced from eleven to five. However, the experiments are performed under different conditions allowing for to different input concentration, x_F. Consequently, a different concentration is estimated for each one of the experiments. This increases the number of parameters again to $N_p = 4 + M$ where M is the number of experiments used for identification. It is important to mention that the neglected parameters are discarded here due to a lack of proper measurements that allow their estimation.

5.3 Problem formulation

The parameter estimation problem can be formulated only in terms of the parameter vector, p, and solved using Gauss-Newton method (Nocedal and Wright, 2006). However, (38) has to be solved at each Newton-iteration. Consequently, the model equations are introduced as an

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[3] These compositions can be measured offline and integrated to the parameter estimation problem.

Table 3. Initial parameter vector p_0

Parameter	Initial value	Bounds	Optimum*	Units
$\bar{v}_R$	5	[3 6]	-	1
$\bar{v}_C$	2	[1 3]	-	1
ϕ_L	1	[0 10]	0.0	W/K
ϕ_V	0.5	[0 10]	2.1	W/K
ϕ_R	8	[0 100]	0.0	W/K
ϕ_C	5	[0 100]	8.5	W/K
C_h	0.8	[0.5 1.1]	-	
C_p	0.5	[0.19 0.5]	-	
C_L	0.5	[0.5 1.5]	-	
C_V	0.7	[0.15 0.7]	-	
x_F	0.67	[0.4 0.7]	0.4948	mol/mol

* Only identifiable parameters are optimized.

equality constraints, and the problem is optimized in parameters and states x at the same time. This is a more efficient approach that preserves sparsity in the optimization, at the cost of increasing the number of optimization variables. Hence, the optimization problem is cast as:

$$\min_{x,p} \quad \|\bar{y} - Cx\|^2_{Q_x} \tag{47}$$

$$\text{s.t.} \quad F(x, p) = 0 \tag{48}$$

$$x_{min} \leq x \leq x_{max} \tag{49}$$

$$p_{min} \leq p \leq p_{max} \tag{50}$$

where the vector $\bar{y}$ represents the measurement data, C is a positive-semidefinite diagonal matrix with zero entries in the diagonal corresponding to the states that are not measured and Q_x a weight matrix. Here it is assumed that the measurements correspond to the liquid phase temperatures. Note that this formulation accounts only for one experiment. In order to use multiple experiments, the optimization vector, the residual vector and the constraints are increased such that:

$$\tilde{y}^T = [\bar{y}_1^T, \ldots, \bar{y}_M^T], \tag{51}$$

$$w^T = [x_1^T, \ldots, x_M^T, p], \tag{52}$$

$$F(w)^T = [F(x_1, p)^T, \ldots, F(x_M, p)^T] \tag{53}$$

and the problem is formulated as

$$\min_w \quad \|\tilde{y} - \tilde{C}w\|^2_{Q_w} \tag{54}$$

$$\text{s.t.} \quad F(w) = 0 \tag{55}$$

$$w_{min} \leq w \leq w_{max} \tag{56}$$

with appropriate matrices Q_w, $\tilde{C}$, and bounds.

Five experiments are used for the estimation task, leading to $N_p = 9$ an a total size of the optimization problem of $M(20N - 17) + N_p$. Due to the structure of the setup, a $N = 20$ is selected, yielding an optimization vector $w \in \mathbb{R}^{1924}$. Figure 5 (top) illustrates the fitting results for the identification set containing data from the first five experiments presented in Figure 3.

6. RESULTS AND DISCUSSION

The optimized values are summarized in Table 3. The input concentration value, x_F, that gives the smallest error for the validation test among the five obtained from the identification is selected. It is noticed that the liquid temperature described by the model adjusts better the measurements. A possible reason for this is the fact that sensors can be cooled by liquid falling over the column internal walls. Note that most of the losses are centered in the reflux drum due to the subcooling in the condenser. In this particular setup, extra heat is removed from the top stage in order to condensate all the vapor and avoid the light component escaping from the column. The liquid is subcooled when falling along the spiral condenser, this liquids falls into the reflux drum decreasing its temperature. The presented model assumes that the liquid coming out from the condenser is at equilibrium (it cannot reach temperatures that the modified Rault's
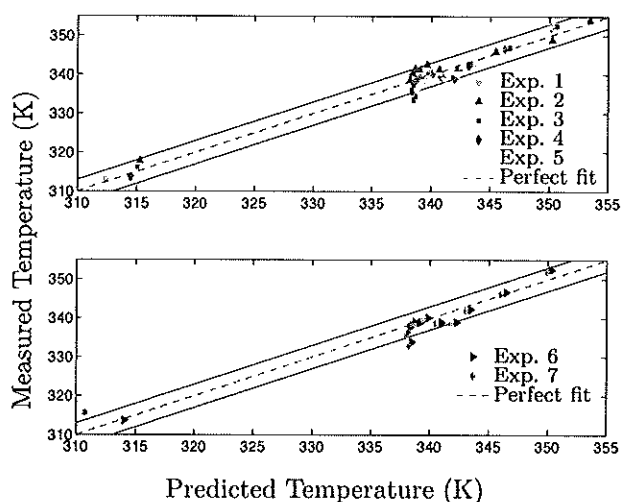
Fig. 5. Fitting results for five steady state experiments (top), and validation test with two new experiments (bottom). Note that almost all the predicted temperatures lie in a ±3K error band.

law does not predict). Consequently, the heat that is removed by the sub-cooling of the liquid falling in the real condenser is compensated by the reflux drum losses in the model. A better representation of what is happening in the condenser can be achieved by using a non-equilibrium stage. This implies increasing the complexity of the model, since holdups for the non-equilibrium condenser have to be estimated from its geometry.

Nevertheless, the model with these parameters is able to correctly predict the vapor temperatures for a new set of experiments. Figure 5 (bottom) illustrates the vapor temperature predictions for the validation set. Note that the prediction errors still lie in a band of ±3K for almost all the measurement points. Consequently, The rigorous model presented is not only able to predict the temperature profiles but can also provide information about internal flows, energy and mass transfer inside the packing allowing for a better understanding of the separation.

NOTATION

a : Specific interface area, m^{-1}
a^I: Net interfacial area, m^2
B : Bottom Flow, mol/s
c_t : Molar density, mol/m^3
C : Condenser
d : Column internal diameter in m
D : Distillate flow, mol/s
D^p : Phase (p) diffusion coefficient, m^2/s
E : Energy holdup, kJ
ϵ : Packing void fraction %
F : Feed flow, mol/s
f : A general nonlinear function
h : Heat transfer coefficient, kJ/mol
h_t : specific liquid holdup, dimensionless
H : Molar enthalpy, kJ/mol
$\bar{H}$: Partial molar enthalpy, kJ/mol
I : Interface
k : Mass transfer coefficient, m/s
K_i : Equilibrium constant for component i
l : Packing segment length, m
L, V : Liquid and vapor flow, mol/s

M_i : Component molar holdup, mol
M_t : Total molar holdup, mol
$\mathcal{N}$: Mass transfer flux, mol/s
η : Mixture viscosity, Pa.s
P_j : Pressure at stage j, Pa
ρ : Phase mass density, kg/m^3
Q : Heat added or removed, kW
R : Reboiler
T : Temperature , K
x_i : Liquid composition for component i, mol/mol
y_i : Vapor composition for component i, mol/mol
v_t^p: Molar volume of phase p, m^3/mol

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