MATHEMATICAL MODELLING OF OVERALL HEAT TRANSFER COEFFICIENTS IN CONCENTRATION OF LEMON JUICE USING RECONCILED DATA

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***Abstract*— Citrus production is one of the main agro-industrial activities in Tucuman, Argentina, with a value in 2017 estimated at US$1,178 million. Production of lemon juice concentrate requires the use of evaporation systems. Those systems are critical for water and energy consumption in process industries. Precise knowledge of process variables is therefore extremely important for evaluation of the efficiency, economic parameters, etc. of the whole plant. In this work, data reconciliation and gross error detection were performed for a lemon juice concentration system. Data were collected from an industrial plant located in Tucuman, Argentina. From reconciled data, the overall heat transfer coefficients (OHTC) for all evaporators were calculated. In addition, a mathematical model was developed to predict the overall heat transfer coefficients. The parameters of the model were fitted to experimental and reconciled data. The OHTC models could be used to estimate the behavior of the plant under different scenarios.**

***Keywords*— mathematical modelling, overall heat transfer coefficient, data reconciliation, lemon juice processing.**

I. INTRODUCTION

In Argentina, primary production of lemon consists of the culture, harvest and hand picking of the fruit from May to September, with high labor requirements.

The secondary production or industrialization involves two sections,

- Packing: Tasks involved in this section are classification, washing, quality control and, preparation (waxing, labeling and wrapping) of the fresh fruit. The lemons that do not accomplish the desired standards are sent to the industrial section.
- Industrial section: Lemons are used in the elaboration of products such as essential oil, concentrated juice, dehydrated peel and freeze pulp. These products are widely used in human or animal food industries, as well as in pharmaceutical, cosmetics and perfume industries.

In Argentina, the lemon fruit and lemon-derived products are commercialized in the domestic as well as international markets. In 2017, Argentina´s lemon fruit production reached 1,676,000 tons, which represents 19.0% of worldwide production. Argentina is one of the main exporters of fresh lemon fruit (224,000 tons in 2017). It is also one of the largest exporters of lemon products with a market share of 56.15% in the period 2016/2017. In 2017, the value of citrus industry reached the amount of US$1,178 million (Federcitrus, 2018).

Industrial plants commonly employ heating processes in order to achieve product-specific properties. In the specific case of lemon juice production, evaporation lines are used to obtain the concentration of the juice that meets the market specifications. Since evaporation is a critical point for efficient water and energy management, precise knowledge of process variable values becomes extremely important.

Process variable measurements are usually performed for quality control, yield and efficiency evaluation, and operation optimization of the plant. Due to technological advances in the last decades, data acquisition and data storage are done automatically, allowing manipulation of large amounts of data collected at high frequency. Furthermore, computational tools for management and data verification have also been developed. Nevertheless, although the instrument accuracy and precision have improved, occurrence of various types of errors is inevitable during measurement, processing and transmission of the data.

In order to detect and eliminate gross errors in measured data, several techniques can be used. Different strategies that use data reconciliation have been proposed to achieve this objective (Madron, 1985; Tjoa and Biegler, 1991, Madron and Veverka, 1992; Romagnoli and Sanchez, 2000; Arora and Biegler, 2001; Yuan *et al*., 2015; and Xie *et al*., 2019). Data reconciliation has been widely used in different processes (Weiss *et al*., 1996; Colombo *et al*., 1999; Lid and Skogestad, 2008; Srinivasan *et al*., 2015, Maciel *et al*., 2017). In this work, data reconciliation and gross error detection were performed for the lemon juice concentration process in an industrial plant located in Tucumán, Argentina. A mathematical model for the overall heat transfer coefficients (OHTC) of the evaporators was also developed. Parameters of the heat transfer phenomena in the evaporator system were estimated from experimental and reconciled plant data. The mathematical model of the OHTC could be used for

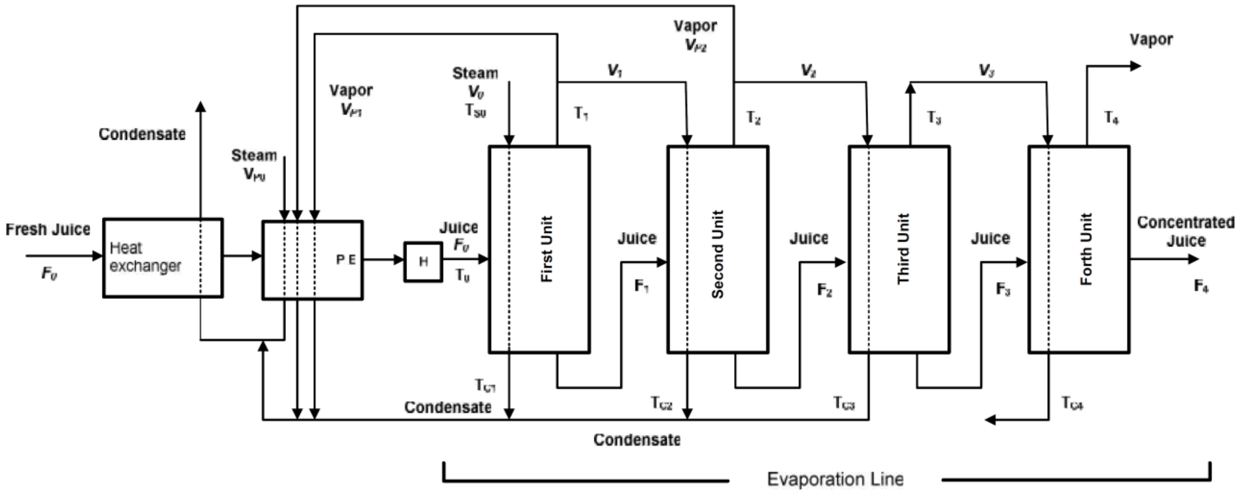

Figure 1: Lemon juice concentration process.

several purposes, e.g. to predict the behavior of the plant or to calculate the energy efficiency under different circumstances.

II. LEMON JUICE CONCENTRATION PROCESS

A scheme of the lemon juice concentration process is shown in Fig. 1. The fresh juice is previously heated and then pasteurized. Condensates from the pasteurization equipment (PE) and from the first and second units of the evaporation system are used to heat up the fresh juice. Pasteurization is performed using steam produced in a boiler as well as vapor generated at the first and second units. In order to increase the residence time, the juice is fed to a compact tubing device, denoted as H in Fig.1, before entering the evaporator.

The evaporation system consists of 4 different stainless-steel plate evaporators working in series as shown in Fig.1. In the first unit, the juice is concentrated using steam generated at the boiler. The vapor produced in the first unit is used to heat the following unit, and so on for units 2 and 3. Unit 4 is heated with vapor coming from unit 3. The vapor produced in unit 4 is condensed as it is not useful for heating. The juice leaving the fourth unit is the product that is then frozen before being shipping to clients. The flow of juice was measured with floatbased or electromagnetic flowmeters. All concentration values were obtained with a refractometer. Most of the studied variables are actually measured at the plant on a regular basis but some of them were acquired exclusively for this work.

III. METHODOLGY

The aim of this work was to obtain a mathematical model that can predict the OHT Coefficients of the evaporation system. The following procedure was followed.

i) Data reconciliation of the lemon juice evaporation process was performed which allowed OHTC (Ur) calculation for all 4 evaporation units.
ii) Mathematical models for the OHTC (U) for all four units were developed. The mathematical models depend on the following physical properties of the lemon juice: viscosity, thermal conductivity and specific heat.
iii) Expressions of the physical properties of the juice were obtained from bibliography. The parameters of the expressions were determined by the method of least squares to obtain an optimum fit to experimental data.
iv) The parameters of the model were adjusted with an optimization program (NLP) that minimizes the errors between the OHTC calculated by data reconciliation (Ur) and the ones predicted by the model (U).

Through data reconciliation, a set of statistically adjusted process variables was obtained. Let´s consider a mathematical model represented by a set of nonlinear equations f

$$f(x,y) = 0 \tag{1}$$

where x and y represent vectors of measured and unmeasured variables, respectively. The following model represents the variable measurements

$$\hat{x} = x + e. \tag{2}$$

where $\hat{x}$ represents the measured value, x the real value of the variable, and e the measurement error. It is assumed that e are random quantities with zero mean value and with a known positively definite covariance matrix F. In most cases F is a diagonal matrix with squares of the standard deviation on the diagonal ($F_{ii} = \sigma_i^2$). The reconciliation is carried out as follows. Statistically adjusted values $\tilde{x}$ are searched. For $\tilde{x} = \hat{x} + v$, where v is the vector of adjustments.

The adjusted values must satisfy exactly the equations of the mathematical model and, at the same time, they have to be minimal in some way. The quadratic function of adjustments is then minimized (so-called generalized least squares method) (Veverka and Madron, 1997).

$$\Phi_{min} = v^T F^{-1} v. \tag{3}$$

The presence of gross errors in the system can occur due to nonrandom events such as malfunctioning or inexact calibration of instruments, leaks in the tubing, nonsteady state of the system, wear or corrosion of sensors, and solid deposits. The presence of gross errors invalidates all data reconciliation results. The measurement credibility method was used to detect the presence of gross errors (Madron, 1985). The "Status" parameter can be used to indicate the presence of gross errors. The definition of the "Status" parameter is given in Eq. 4.

$$Status = \frac{\Phi_{min}}{\Phi_{crit}}. \tag{4}$$

Assuming Normal distribution of the errors, a χ^2 test can be performed and Φ_{crit} is thus obtained for a given significance level.

When data reconciliation is performed for the system, the $Status$ parameter is calculated and if its value is less than 1, no gross error is present in the system.

IV. OVERALL HEAT-TRANSFER COEFFICIENT ESTIMATION

A. Determination of Ur from Reconciled Plant Data

A mathematical model consisting of mass and energy balances, and heat transfer expressions was used to perform data reconciliation of the evaporation system.

The following methodology was adopted for data reconciliation.

- System configuration survey
- Data acquisition at the industrial plant in steady state
- Formulation of the mathematical model (f) of the plant based on conservation of mass and energy, and heat transfer equations
- Use of data reconciliation for gross error detection and as a tool for monitoring of key variables

The following assumptions have been considered in deriving the mathematical model (f).

a) Negligible boiling point increase.
b) No solute loss in the system.
c) No solute is removed with the evaporating water.
d) Constant conditions at the evaporation units during operation.

Eleven assays were performed during the steady state operation of the plant. Reconciled data for one of the assays are shown in Table 1. The heat transferred per unit of time (Q) in each unit was not measured but calculated (observable variable). Q was calculated using the heat transfer equation with logarithmic mean temperature difference as driving force. In all data reconciliation assays the confidence level was 95%. No gross errors were detected in any of the 11 assays performed. In Table 1 the value of the "Status" parameter for the correspondent test is also informed. The "Status" values for the 11 assays oscillate between 0.01128 and 0.55367.

B. Mathematical Model for the OHTC

OHTC for all evaporation units were estimated using Eq. 5 where the conduction resistance to heat transfer of the metal interface was consider negligible

$$\frac{1}{U_i} = \frac{1}{hv_i} + \frac{1}{hl_i} \tag{5}$$

Both convective heat-transfer coefficients were calculated by the Colburn expression (Bird, 2001) given by Eq. 6. Colburn expression is suitable for the evaporation system considered in this work (Coulson, 1985).

Table 1: Measured and reconciled values of the lemon juice evaporation system.

Status			0.27596		
Variable	**Units**	**Type**	**MV**	**RV**	**SD**
F_0	Mass flow(kg/s)	MC	6.314	6.303	0.029
	X (%)	MC	8.48	8.49	0.08
F_1	Mass flow(kg/s)	NO	-	4.89	0.03
	X (%)	NO	-	10.9	0.1
F_2	Mass flow(kg/s)	NO	-	3.55	0.02
	X (%)	NO	-	15.1	0.2
F_3	Mass flow(kg/s)	NO	-	2.294	0.017
	X (%)	NO	-	23.3	0.2
F_4	Mass flow(kg/s)	NO	-	1.01	0.02
	X (%)	NO	52.8	52.8	0.5
V_0	Mass flow(kg/s)	NO	-	1.51	0.01
V_1		NO	-	1.29	0.01
V_2		NO	-	1.20	0.09
V_3		NO	-	1.25	0.01
V_{P0}		MC	0.0625	0.0625	0.0007
V_{P1}		MC	0.118	0.118	0.002
V_{P2}		MC	0.149	0.149	0.002
Q_1	(J/s)	NO	-	953000	6650
Q_2		NO	-	822000	6125
Q_3		NO	-	764000	5600
Q_4		NO	-	811000	5425
T_{C1}	(K)	MC	371.85	371.65	1.98
T_{C2}		MC	363.15 3	63.03	1.99
T_{C3}		MC	356.35	356.31	1.99
T_{C4}		MC	343.95	343.93	1.99
T_0		MC	355.45	355.99	1.71
T_1		MC	364.75	364.64	1.98
T_2		MC	357.95	357.87	1.99
T_3		MC	345.65	345.60	1.99
T_4		MC	333.75	333.72	1.99
T_{S0}		MC	373.15	373.16	1.99

MV (measured value); RV (reconciled value); SD (standard deviation); MC (measured variable, adjustable); NO (unmeasured variable, observable).

$$N_{Nu} = c \cdot N_{Pr}^m \cdot N_{Re}^q \cdot \left(\frac{\mu}{\mu_w}\right)^s \tag{6}$$

where c, m, q, s: dimensionless parameters which depend on the flow regime and the geometry of the heat exchanger.

The flow inside a plate heat exchanger is turbulent when the Reynold number reaches the critical value between 10 and 400 (Marriott, 1971). That condition was verified for all exchangers during the assays done for this work. Therefore, the ratio $\frac{\mu}{\mu_w}$ is considered equal to 1 because the fluid and exchange wall temperatures are considered identical due to turbulent flow of the juice. Hence, Eq. 6 can be rewritten as the following expression.

$$N_{Nu} = c \cdot N_{Pr}^m \cdot N_{Re}^q \tag{7}$$

By substituting the expressions of the dimensionless Nusselt, Prandtl, and Reynolds numbers in Eq.7, the convective heat-transfer coefficients of the vapor and of the juice can be expressed by Eqs. 8 and 10, respectively. The corresponding dimension less parameters are noted as cl, ml and ql for the juice, and cv, mv, and qv for water vapor

$$hl_i = zl_i \cdot Cpl_i^{ml_i} \cdot kl_i^{1-ml_i} \cdot \mu l_i^{ml_i - ql_i} \cdot (F_{i-1})^{ql_i} \tag{8}$$

where,

$$zl_i = cl_i \cdot De_i^{ql_i - 1} \cdot S_i^{-ql_i} \cdot ncl_i^{-ql_i} \tag{9}$$

and,

$$hv_i = zv_i Cpv_i^{mv_i} \cdot kv_i^{1-mv_i} \cdot \mu v_i^{mv_i - qv_i} \cdot (V_{i-1})^{qv_i} \tag{10}$$

where,

$$zv_i = cv_i \cdot De_i^{qv_i - 1} \cdot S_i^{-qv_i} \cdot ncv_i^{-qv_i} \tag{11}$$

The physical properties of water vapor can be considered constant for all range of temperatures of the lemon juice evaporation system. The equivalent diameter as well as the transverse section of flow are parameters that depend on the equipment design. If all parameters are included in a single variable yv_i, Eq. 10 can be rewritten as follows

$$hv_i = yv_i \cdot (V_{i-1})^{qv_i} \tag{12}$$

where yv_i is given by Eq.13 and it is a constant for a given evaporator and for all its range of working temperature.

$$yv_i = cv_i \cdot De_i^{qv_i - 1} \cdot S_i^{-qv_i} \cdot ncv_i^{-qv_i} \cdot Cpv_i^{mv_i} \cdot kv_i^{1-mv_i} \cdot \mu v_i^{mv_i - qv_i} \tag{13}$$

The mathematical expression of U is obtained by substituting Eqs. 12 and 8 in Eq. 5.

$$U_i = \frac{1}{\frac{1}{yv_i \cdot (V_{i-1})^{qv_i}} + \frac{1}{zl_i Cpl_i^{ml_i} \cdot kl_i^{1-ml_i} \cdot \mu l_i^{ml_i - ql_i} \cdot (F_{i-1})^{ql_i}}} \tag{14}$$

The expression of U given by Eq. 14 depends on the physical properties of the lemon juice, the flow regime and the geometry of the evaporator unit.

C. Determination of physical properties of the lemon juice

In order to determine the physical properties of the lemon juice, experimental data from bibliography were used. The specific heat of the lemon juice was calculated using Eq. 15. The parameters of Eq. 15 were fitted by regression using experimental values (Minim *et al*., 2009).

$$Cpl_i = \frac{X_i}{100}\left(-0.85051 + 0.01057\tau_i - 9.363 \cdot 10^{-5}\tau_i^2\right) + \left(1 - \frac{X_i}{100}\right)\left(4.021 + 5.768 \cdot 10^{-4}\tau_i - 8.307 \cdot 10^{-8}\tau_i^2\right) \tag{15}$$

Equation 15 can be used to determined Cpl of lemon juice for a concentration from 8 to 61.9 ºBrix and juice temperature between 273.15 to 373.75 K.

Two different expressions were used to calculate the viscosity of lemon juice. Equation 16 was used for juice concentrations between 8.2 and 22 ºBrix.

$$\mu l1_i = 0.00074 e^{\left(\frac{2123.075}{T_i} + 0.03623 X_i\right)} \tag{16}$$

Equation 17 was used for juice concentrations between 22 and 52ºBrix.

$$\mu l2_i = 0.000142 e^{\left(\frac{2560.079}{T_i} + 0.04811 X_i\right)} \tag{17}$$

Parameters of Eqs. 16 and 17 were adjusted by regression using experimental values of the viscosity (Alvarado, 1993). In both cases, the expressions can be used to predict lemon juice viscosity in the range of temperature between 303.15 and 393.15 K.

Equation 18 was used to predict the values of thermal conductivity of the juice at different concentrations and temperatures.

$$kl_i = 0.29908 + 9.7 \cdot \tau_i - 0.00246 \cdot X_i - 1.74 \cdot 10^{-5} \cdot X_i^2 \tag{18}$$

Parameters of Eq.18 were also fitted from experimental values of thermal conductivity of lemon juice (Minim *et al*., 2009). The model of thermal conductivity must be used in the concentration range between 10 and 61.9 ºBrix, and in the temperature range between 273.45 and 363.75 K.

D. Determination of the parameters of the OHTC mathematical models

In order to adjust the values of the parameters ml, ql, zl, yv, and qv of the mathematical model of the OHTC for the evaporators of the system (Eq.14), a nonlinear optimization model (NLP) was developed.

The objective is to minimize the errors between the experimental values Ur obtained by performing data reconciliation and the values U predicted by the mathematical model as shown in Eq. 19.

The optimization model has the following objective function and constraints.

$$\min e = \sum_{j=1}^{n} \left(U_{i,j} - Ur_{i,j}\right)^2 \tag{19}$$

s.t.

Eq. 5: OHTC

Eqs. 9, and 11: convective heat transfer coefficient for the lemon juice

Eqs. 12 and 13: convective heat transfer coefficient for the vapor

Bounds:

$$0.35 \le ml_i \le 0.45$$
$$0.65 \le ql_i \le 0.85$$

Bounds for ml and ql parameters were obtained from bibliography (Marriott, 1971).

The resulting model is nonlinear (NLP) with 95 continuous variables and 90 constrains. The mathematical model was implemented in the GAMS language (Brooke *et al*., 1992) and solved with CONOPT solver.

V. RESULTS AND DISCUSSION FOR THE CASE STUDY

In this work, plant data were collected and processed in order to verify that no gross errors were detected. Most of those plant data are routinely measured and automatically recorded.

Measured variables allowed calculating the OHTC for all the evaporators in the plant. In Table 2, the mean values of the OHTC and standard deviation for the 11 data reconciliation assays are shown.

Reconciled values of the variables obtained from the 11 assays were used to solve the optimization problem developed above. The results of the optimization model are shown in Table 3. Those variable values can only be used for the actual plant configuration and within the limits of validity of the equations that predict the physical properties of the juice. The *t* Test allowed to confirm that

Table 2: Mean value of the OHTC from data reconciliation assays

	Mean values J/(s m^2 K)	Standard deviation
$\overline{U_{r1}}$	1308.7	65.5
$\overline{U_{r2}}$	3193.6	145.9
$\overline{U_{r3}}$	3080.6	155.8
$\overline{U_{r4}}$	3858.9	596.6

Table 3: Results of the optimization model.

	Evaporation Unit			
	1	2	3	4
ml_i	0.45	0.35	0.45	0.35
ql_i	0.85	0.65	0.85	0.85
zl_i	1.81	229.26	28.57	1521.38
yv_i	16389.41	10828.92	12614.48	10872.60
qv_i	0.65	0.74	0.85	0.85
U (J/(s m2 K))	1456±29	3402±63	3318±52	3757±187

the predicted OHTCs have no significant difference with the OHTCs calculated using reconciled plant data.

The overall heat transfer coefficient estimations could be used by plant personnel for different purposes, e.g. process behavior prediction by simulation under different scenarios, optimization of the industrial plant operation, estimation of the amount of energy needed for the evaporation system at different operating conditions.

VI. CONCLUSIONS

In this work, data reconciliation and gross error detection were performed for a lemon processing plant. This allowed obtaining more precise values of the process variables of the juice concentration system. Mathematical models for the OHTC for the evaporation units were developed from heat transfer principles. Those models depend on physical properties of the lemon juice. The expressions for the various physical properties of the lemon juice were obtained from the experimental data.

A nonlinear optimization program (NLP) was developed to determine the values of the parameters of the OHTC in the mathematical models of the evaporation units of the lemon juice concentration system. The results of 11 data reconciliation assays at an industrial plant located in Northern Argentina were used to determine the parameter values of the model.

The adjustment of the parameters for the determination of OHTC will allow predicting the behavior of the juice concentration system at different operating conditions.

NOTATION

Cpl	Specific heat of lemon juice (kJ / kg K)
Cpv	Specific heat of water vapor (kJ / kg K)
D_e	Equivalent diameter of plate evaporator (m)
F	Lemon juice mass flow (kg/s)
hl	convective heat-transfer coefficient of the lemon juice (J/s m^2 K)
hv	convective heat-transfer coefficient of water vapor (J/s m^2 K)
kl	Thermal conductivity of lemon juice (W/m K)
kv	Thermal conductivity of water vapor (W/m K)
ncl	Number of channels for juice flow
ncv	Number of channels for water vapor flow
N_{Nu}	Nusselt number
N_{Pr}	Prandtl number
N_{Re}	Reynolds number
Q	Transferred heat per unit of time (J/s)
S	Cross-section of the evaporator (m^2)
T	Temperature of juice, steam or vapor (K)
T_{Ci}	Temperature of the condensate leaving the evaporator (K)
U	Predicted OHTC (J/s m^2 K)
Ur	Reconciled OHTC (J/s m^2 K)
$\overline{U_r}$	Mean value of reconciled OHTC (J/s m^2 K)
V	Steam/vapor mass flow (kg/s)
V_{P0}	Steam fed to the pasteurization equipment (kg/s)
V_{P1}	Vapor from 1st evaporator fed to the pasteurization equipment (kg/s)
V_{P2}	Vapor from 2nd evaporator fed to the pasteurization equipment (kg/s)
X	Lemon juice concentration ºBrix (%)

GREEK LETERS

μ	viscosity of the fluid (mPa s)
μ_w	viscosity of the fluid at exchange wall temperature (mPa s)
μl	Viscosity of lemon juice (mPa s)
μv	Viscosity of water vapor (mPa s)

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i	Number of unit at the evaporation system
j	Number of data reconciliation assay

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