Semi-mechanistic Modeling of an Osmotic Dehydration Process.

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Abstract: This article presents a semi-mechanistic model (a hybrid of the classic and fuzzy models) of an osmotic dehydration process of pineapple. The fuzzy model (Takagi-Sugeno) represents a kinetic parameter of the physical process and it is developed through fuzzy classification of data (Gustafson-Kessel algorithm). The fuzzy model is then incorporated in the mass conservation equation (classic model) aiming at the numerical prediction of the process. Experiments and validations are presented.

Key Words: Physics Model, Osmotic Dehydration

1 Introduction

In complex systems, such as the processes that are carried out on an industrial level, physical modeling can be approached through two methodologies. The first is the classical modeling methodology and it focuses the study of the process on the fundamental principles of physics such as the mass, energy and moment conservation theorems. Mathematically, this kind of model is represented through difference equations, which are defined using state variables, constants and parameters.

The second methodology is fuzzy modeling, where the identification of the parameters is done by using soft-computing techniques (which include fuzzy models, neural networks and adaptive network-based fuzzy inference system or ANFIS). ANFIS has had a growing use in representing physical, chemical and biochemical processes, where partially known expressions exist, such as kinetic parameters, which involve the handling of highly empiric models that are valid only for certain conditions or circumstances in the process. As an application of the semi-mechanistic model, the osmotic dehydration of pineapple process has been modeled combining these two methods.

The article is organized as follows. Section 2 describes the studied process and the experimental conditions of the process, the experiment and the dehydration plant. Section 3 presents the classical model. Section 4 reviews the fundamental concepts of fuzzy classification, identification and modeling techniques. Section 5 poses the semi-mechanistic model. Section 6 compares the results of the semi-mechanistic and classic models. Section 7 concludes the article, explaining the importance of the obtained results.

2 Process Description

Osmotic dehydration is defined as a process where two phenomena are combined (dehydration and osmosis) and occur through a semi-permeable membrane: the cell wall [1],[2].

Pineapple is a completely heterogeneous, highly watery and porous food, that when submerged in solutions with high concentration of soluble solids (sugar), provokes two simultaneous upstream main flows (Figure 1) [3],[4]:

1. Transfer of soluble solids (sugar) from the solution to the food.
2. Flow of water from the food to the solution.
The mass transfer mechanisms at atmospheric pressure and room temperature are mainly diffusion (Fick’s laws of diffusion) and are originated by the concentration differences between the food and the osmotic solution [2], [5].

The sugar concentrations found in the osmotic solution and the food (mechanically extracted juice of the pineapple sample) are obtained for each sample time, $\Delta T$. These measurements are registered by refractometers and reported in refraction indexes or Degrees Brix. Sugar concentration changes have been analyzed in terms of mass balances for sugar gain $X^S$ and loss $Y^S$. The plant worked in Fed-Batch regime (Figure 2). A secondary tank (tank 2) has been used, with a high concentration in sugar $[Y^S]_{cte} = 0.65$ Degrees Brix and initial volume of $[V]_1 = 40$ liters, to feed the main tank (tank 1, the reactor where the fruit dehydration process takes place), aiming at maintaining its sugar concentration above an initial and reference value $[Y^S]_{ref} = 0.6$ Degrees Brix.

This article is limited to Fed-Batch regime experiments because it generates better results in the dehydration. The used raw material was pineapple (ananas comosus in the cayena lisa variety) in a geometric shape (eighths of slice of 1 cm of thickness without any previous treatment).

The attributes of the osmotic solution for each tank were:

- Tank 2: Constant. $[Y^S]_{cte} = 0.65$ Degrees Brix. This is obtained by mixing approximately 61.5 kg of sugar with 40 kg of water.
- Tank 1: Reference. $[Y^S]_{ref} = 0.6$ Degrees Brix. This is obtained by mixing approximately 83.3 kg of sugar with 50 kg of water.

The plant was operating for a Fed-Batch regime experiment with ascending linear entry flow. $[U_1] = \text{From 0 to 2.09 L/min in 180 minutes.}$

### 3 Classic Model

The dynamic process is discrete, with a sampling time of $\Delta T$, which is practically the time that the fruit spends submerged in the solution. For this time, the available information is the flow entering tank 1, $[U]_k$, and the sugar concentrations are being measured simultaneously in the food, $[X^S]_k$, and in the solution, $[Y^S]_k$, (Figure 2).

Based on multiple investigations developed around the kinematics of the dehydration process, [3], [5], [6], [8], the classic model, in terms of mass balance carried away in a fixed time interval, is formulated in difference equations and represented as follows:

- Variation of sugar concentration for the solution:

$$[Y^S]_{k+1} = [Y^S]_k - B[C]_k[X^S]_k \Delta T + ([Y^S]_{cte} - [Y^S]_k)\frac{[U]_k \Delta T}{[V]_k}$$

(1)

- Variation of sugar concentration for the food:

$$[X^S]_{k+1} = [C]_k[X^S]_k \Delta T + \frac{[U]_k[X^S]_k \Delta T}{[V]_k}$$

(2)

Where:

- $[V]_k$ is the variation of tank 1 volume:

$$[V]_{k+1} = [V]_k + [U]_k \Delta T$$

(3)

- $[C]_k$ is the specific rate of sugar concentration in food:
\[ [C]_k = \mu \frac{[Y^S]_k}{K_{Y^S} + [Y^S]_k} \]  

- \( B \) is a dimensionless proportion factor between the concentration variation of the food and that of the solution:

\[ B = \frac{[Y^S]_f - [Y^S]_o}{[X^S]_f - [X^S]_o} \]  

- \( \mu \) is the maximum change rate in sugar growth for the food. It is represented by:

\[ \mu = \frac{ln\left(\frac{[X^S]_f}{[X^S]_o}\right)}{t_f - t_0} \]  

- \( K_{Y^S} = 0.65 \) (gr. of sugar / gr. of osmotic solution in tank 1) is the saturation constant for sugar concentration in tank 1.

The calculation of the kinetic parameter \([C]_k\) and the kinetic constants \(\mu\) and \(B\) is empirically done with the data and the equations 5 and 6 respectively. The results of the calculations for the experiment are: \(\mu = 0.0008\) and \(B = 0.51\). Figure 3 presents the experimental data and the weighing of \([C]_k\).

![Figure 3: Experimental data and calculation of \([C]_k\) for the classic model](image)

4 Fuzzy Logic Principles

Within the fuzzy scope, models are defined through membership functions and rules, which are found using the system’s input and output data with classification algorithms. The Takagi-Sugeno Model (T-S) is a fuzzy model made of \(R_i\) rules, like follows [8], [9], [10], [11], [12], [13]: \(R_i: if \ x_1, \ldots, x_k\) then

\[ Y_i = a_i^T x + b_i; \quad i = 1, 2, \ldots, k \]  

Where \( x \) is the input vector, \( A_i \) is the fuzzy set (multidimensional), \( Y_i \) is the output of the \( i \)-th rule, \( a_i \) is a parametric vector and \( b_i \) is the scalar displacement, namely, the antecedent is calculated through fuzzy rules, while the consequent is a linear combination of the variables of the antecedent. Therefore, the inputs \( x \), that are \( A_i \), are represented as a combination of monodimensional propositions defined by each component of the input vector \( x \).

The Gustafson-Kessel Algorithm (G-K), based on C-means was used for classification. The classification techniques seek to find subsets with certain degree of similitude within a set of data, whether it is on a quantitative level or qualitatively. The data are observations of a process (physical, chemical, etc.). Each observation consists of \( n \) measured variables, expressed in an \( n \)-dimensional column \( z_k = [z_{1k}, \ldots, z_{nk}]^T, z_k \in \mathbb{R}^n \). A set of \( N \) observations is denoted by \( \{Z_k \mid k = 1, 2, \ldots, N\} \) and it is repre-
represented as a $n \times N$ matrix:

$$Z = \begin{bmatrix}
    z_{11} & z_{12} & \cdots & z_{1N} \\
    z_{21} & z_{22} & \cdots & z_{2N} \\
    \vdots & \vdots & \ddots & \vdots \\
    z_{n1} & z_{n2} & \cdots & z_{nN}
\end{bmatrix} \quad (8)$$

Before reviewing the classification techniques, it is convenient to define a \textit{cluster} as a group of objects that are more similar among them than other members of other groups [8]. The concept of "similarity" can be understood as a mathematical likeness, measured in metric spaces and defined through a distance norm. The distance can be measured between the same data vectors or as a distance from one data vector to some prototypical object (centers) of the cluster [9].

One of the first proposed classification techniques that uses objective function optimization is C-means by Bezdek in 1981. The similarity measurement of this technique is capable of detecting a cluster in a circular shape. Gustafson and Kessel extended the C-means algorithm by using an adaptative distance norm for differently shaped cluster location effects in the set of data. Each cluster has its own induced norm matrix, $A_i$, which originates the norm of the internal product \cite{10,11}.

The clusters obtained by data classification are a local linear approximation of the regression hypersurface. The whole of the global model can be represented by a T-S model. Then each cluster is converted into a T-S rule, defined by parameters of the consequent and the membership functions of the antecedent, that are obtained from the fuzzy partition matrix \cite{8,9}.

5 Physical model: a hybrid of the classic and fuzzy models

A block representation of the semi-mechanistic model, using a white-box (classic model) and black-box (Takagi-Sugeno fuzzy model) is presented in figure 4. The white box is directly associated to the balance and flow equations 1, 2, 3, defined in section 3. The black box is originated by previously defining an unknown dependency between $[C]^k$ with $[X^S]^k$ and $[Y^S]^k$, which is represented in the form:

$$[C]^k = f([X^S]^k, [Y^S]^k) \quad (9)$$

This dependence in modeling terms could be represented as a fuzzy model (black-box) with 2 inputs: $[X^S]^k$ and $[Y^S]^k$ and an output: $[C]^k$. The purpose of this methodology is precisely to define the unknown dependency $f(\cdot)$ from a Takagi-Sugeno fuzzy model. The previously defined fuzzy model is used as a numeric predictor of $[C]^k$ and the obtained prediction is explicitly replaced in equations 1 and 2 of the classic (white-box) model. To determine the T-S model, the Gustafson-Kessel algorithm was used and the experimental data which was organized in a data matrix $Z$ like follows:

$$Z = \begin{bmatrix}
    [Y^S]^1 & [X^S]^1 & [C]^1 \\
    \vdots & \vdots & \vdots \\
    [Y^S]^n & [X^S]^n & [C]^n
\end{bmatrix} \quad (10)$$

In the validation of the T-S model, the data of section 3 was used. Meanwhile, the identification was done with different experimental data than those used in the validation, but taken under the same experimental conditions, which allowed the \textit{a-posteriori} estimation of $[C]^k$. The previously exposed methodology allows making comparisons between the classic and the semi-mechanistic models from the two interpretations available to define $[C]^k$ for each case. In the following graphs, the obtained T-S model for predicting $[C]^k$ is shown. In the model estimation process, three clusters were used, which allowed the definition of the three rules and six membership functions (figures 6, 7). These results have been obtained using the Babuska fuzzy modeling and identification toolbox \cite{13}.

The validation of the models was done through
Figure 5: Validation of the T-S model that defines $[C]_k$ for the semi-mechanistic model. Purple line: output forecast by T-S model. Blue line: experimental $[C]_k$ output. $E_{RMSD} = 0.00021$.

Figure 6: Membership functions $[X^S]$ of the T-S model for the $[C]_k$ forecast in the semi-mechanistic model, obtained by G-K algorithm

The obtained rules from the T-S model for the $[C]_k$ forecast in the semi-mechanistic model were:

1. If $[X^S]$ is $A_{11}$ and $[Y^S]$ is $A_{12}$ then
   $[C] = 3.50 \times 10^{-3}[X^S] - 3.18 \times 10^{-3}[Y^S] + 1.82 \times 10^{-3}$

2. If $[X^S]$ is $A_{21}$ and $[Y^S]$ is $A_{22}$ then
   $[C] = 7.70 \times 10^{-4}[X^S] - 1.46 \times 10^{-4}[Y^S] + 3.78 \times 10^{-4}$

3. If $[X^S]$ is $A_{31}$ and $[Y^S]$ is $A_{32}$ then

The validation of the T-S model that forecast $[C]_k$, based on equation 11 and the data used in figure 6 is $E_{RMSD} = 0.00021$. Based on the validation process of the previously exposed T-S models, it can be stated that they make a very efficient estimation.

6 Results

Through the methodologies used to determine $[C]_k$, developed in sections 3 and 5, their respective structures were used to generate a prediction of the sugar concentration variations in food $[X^S]_{k+1}$ and the osmotic solution $[Y^S]_{k+1}$. For this, an .m file was developed in Matlab®, which loads the input data for the model, compiles the predictions and calculates the root-mean-squared deviation between the prediction and the experimental data. For the model validation, the RMSD equation has been re-interpreted, which is defined by equation 11, where $N$ is the number of used data, $y_j$ is the experimental data and $\hat{y}_j$ is the estimated output of the classic and semi-mechanistic models in each of the state variables $[X^S]$ and $[Y^S]$. As a comparison, figure 8 shows the prediction for the classic and semi-mechanistic models plus the experimental data in experiment 1. Table 1 presents the validation of the experiment, based on equation 11 and the information available in figure 8.

After the validation process of these previously explained models, it can be concluded that they have an acceptable performance in predicting the behavior of the analyzed osmotic dehydration process.
Figure 8: Comparison of model predictions and experimental data for experiment 1. Blue: experimental data. Red: Classic model. Green: Semi-mechanistic model.

Table 1: Validation of classic and semi-mechanistic models for the experiment

<table>
<thead>
<tr>
<th>E1 (eq. 24)</th>
<th>Classic model</th>
<th>Semi-mech. model</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E1 - [X^S]$</td>
<td>0.006248</td>
<td>0.003073</td>
</tr>
<tr>
<td>$E1 - [Y^S]$</td>
<td>0.006446</td>
<td>0.003165</td>
</tr>
</tbody>
</table>

7 Conclusions

- The G-K classification and the fuzzy modeling and identification techniques given by R. Babuska’s fuzzy modeling and identification toolbox are important tools that can be used as a complement of the numerical techniques of classical modeling to generate semi-mechanistic models.

- The recurring structure of the classic and semi-mechanistic models allows them to be used as numeric predictors of the process by defining the initial conditions of the process, the flow entry $[U]^k$ and the kinetic parameter $[C]^k$.

- The structures of the semi-mechanistic and classic models respectively, based on the approximation of $[C]^k$ through a model T-S technique and the calculation of $[C]^k$ through empirical methods in kinetics, may be used in the controller design field by using PID and non-linear control techniques.

- The obtained models open work perspectives around the interesting but not so trivial techniques of parametric optimization and identification.

- Agroindustrial and Food Production Engineering is another promising field where the automation and control theory techniques can deepen in favor of obtaining high-quality food products for commercial and industrial ends.

References:


