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MODELLING THE INTERNAL TEMPERATURE OF AN AUTOCLAVE USING PARAMETER ESTIMATION

Francisco Carlos de Amorim Terceiro [1], *Roberto Vieira da Fonseca Lopes* [2], *Hélio Koiti Kuga* [3]

[1]INPE, São José dos Campos-SP, Brazil, amorim@dem.inpe.br
[2]INPE, São José dos Campos-SP, Brazil, roberto.lopes@dss.inpe.br
[3]INPE, São José dos Campos-SP, Brazil, hkk@dem.inpe.br

Abstract: The purpose of this work is to obtain a model that describes temperature behavior of an autoclave used in pharmaceutical industries for sterilization. After formulating a model described by differential equations, an amount of data is processed in a nonlinear least squares estimator to find the model parameters.

Keywords: Modeling, Nonlinear Estimation, Gradient Method.

1. INTRODUCTION

Sterilization process through saturated water vapor (steam) is widely used in pharmaceutical and food industries. The sterilization process purpose is to eliminate microorganisms of any nature, [1]. The goal of this work is to propose a model capable of forecasting an autoclave temperature behavior. An autoclave simulator also will be developed. Some experiments were realized in order to gather necessary data amount to identify the model parameters. Once there are uncertainties in the model and data obtained by the sensors, a parameter estimation procedure will be used to process this data and find the model parameters.

2. SYSTEM DESCRIPTION

The focused system is a vertical cylindrical autoclave, with 1.60 m high and 1 m diameter. An autoclave is a pressurized device that enables the heating of aqueous solutions up to temperatures above the boiling point of water. The device has a top cover for product entrance and exit. A temperature sensor is installed at 1.17 m height inside the vessel. A control system maintain the inner pressure at 2 kgf/cm^2. The saturated steam supply is a boiler installed solely for this purpose. The steam distribution causes the water motion inside the autoclave. This motion is intended to homogenize the autoclave inner temperature.

2.1. Sterilization Cycle

The operational procedure for product sterilization cycle starts by putting the non-sterile products inside the autoclave, closing its top cover and immersing the product in water. Thus, the pressure control system is activated followed by the temperature control system. The temperature control system should maintain the temperature at 102 ± 2 °C for one hour, after that period this control is turned off. Thus, the water inside the autoclave is drained, the pressure control system is turned off and a pressure valve is opened to make the autoclave inner pressure equalize with the ambient pressure. Then the top cover is opened and the now sterilized products removed from the autoclave.

2.2. Temperature Control System

The temperature control system is discrete. Its control action is the bang-bang type, opening and closing the steam valve completely. The controller compares the measured temperature with a reference. When the measured temperature value is lower than the reference the controller opens the steam valve, when it is above the reference the controller closes the steam valve. The controller has two reference values, one for heating period and other for sterilization period. The heating period is the time period when the autoclave temperature did not reach 102 °C for the first time. The sterilization period is time period between the first time that temperature reaches 102 °C and time instant when the temperature control system is turned off. The reference for heating period is 100 °C and for sterilization period is 102 °C. The purpose of this difference is to prevent overheat when the first temperature peak is reached, see Fig. 1. The value informed as control in Fig. 1 is just for illustration, finding this value is one of the tasks of this work.

3. MODEL

The system model aims to predict the autoclave inner temperature behavior, mainly the time period when the system reaches the first temperature peak. This is the period when more commonly product losses by overheating occur.

Modeling should pursue simplicity and accuracy, but in general they are conflicting characteristics. The first attempts led to complex models that treated the problem with distributed heat capacitance ruled by partial differential equations. But those models were unsuited to use with regular control theory. Searching for a simpler model, it was decided to use a model ruled by ordinary differential equations, leading to model with lumped heat capacitance and assuming that heat is transferred by conduction.

Suppose that the system is quickly submitted to a temperature change at the time $\theta = 0$. Suppose also that the temper-

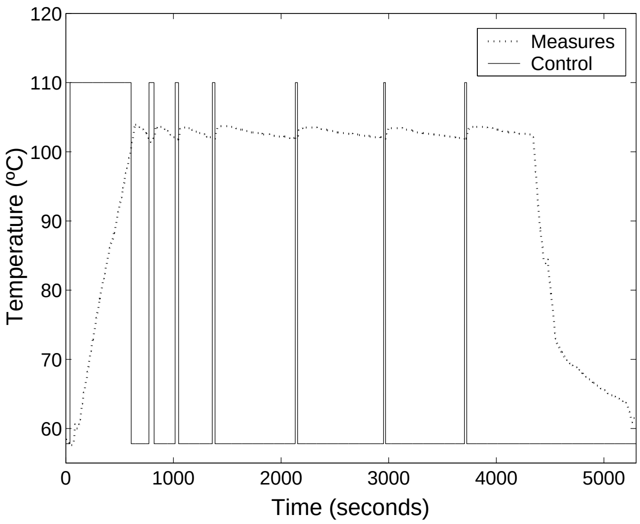

Figure 1 – Sterilization Cycle

ature, $T(\theta)$, is measured with respect to ambient temperature, T_0. Assuming that at beginning the system temperature is equalized with the ambient temperature, thus $T(0)+T_0 = T_0$ which implies that $T(0) = 0$. So the initial system condition is null. From the balance energy equation the Eq. 1 is derived, [2].

$$RC\frac{dT(\theta)}{d\theta} + T(\theta) = T_\infty \tag{1}$$

$T(\theta)$ $\rightarrow$ System inner temperature, with respect to ambient temperature.
T_∞ $\rightarrow$ Temperature imposed to system, with respect to ambient temperature.
θ $\rightarrow$ Time.
R $\rightarrow$ Thermal resistance.
C $\rightarrow$ Thermal capacitance.

Once that Eq. 1 has null initial conditions it can be written in transfer function form, as seen in Eq. 2.

$$T(s) = \frac{T_\infty}{(RC\,s+1)} \cdot \frac{1}{s} \tag{2}$$

Observing the system working it was noticed that it does not answer immediately when submitted to an input. In order to make the model more faithful with reality, a delay was added to the model. This delay is known as transport delay. The model with transport delay is shown in Eq. 3.

$$T(s) = \frac{T_\infty}{(RC\,s+1)} \cdot \frac{e^{-s\tau}}{s} \tag{3}$$

Where τ is the delay quantity measured in seconds. But the term $e^{-s\tau}$ is hard to treat with inverse Laplace transform. However an approximation for this term can be used in order to make this term easily treated, that is, Padé approximation to the exponential function, indeed a first order Padé approximation.

$$T(s) = \frac{T_\infty}{(RC\,s+1)} \cdot \frac{1}{s} \cdot \frac{2-\tau s}{2+\tau s} \tag{4}$$

Expanding the Eq. 4 in partial fractions one has Eq. 5.

$$T(s) = T_\infty \left[\frac{1}{s} - \left(\frac{2RC\,+\tau}{2RC\,-\tau}\right)\left(\frac{1}{s+\frac{1}{RC}}\right) + \left(\frac{2\tau}{2RC\,-\tau}\right)\left(\frac{1}{s+\frac{2}{\tau}}\right)\right] \tag{5}$$

Using the inverse Laplace transform in Eq. 5 results in the algebraic and deterministic model, Eq. 6 that will be used in the parameters estimation procedure.

$$T(\theta) = T_\infty \left\{1 - \left(\frac{1}{2RC\,-\tau}\right) \left[(2RC\,+\tau)\,e^{-\left(\frac{\theta}{RC}\right)} - 2\tau e^{-\left(\frac{2\theta}{\tau}\right)}\right]\right\} \tag{6}$$

4. PARAMETERS ESTIMATION

Observing the system working it is clear that it does not work as smooth as the model response seen in Eq. 6. The reason for that is because the model has many simplifications. The pressure control system, the ambient temperature, they act continuously as a temperature disturbance and they were not included in the model. Another source of uncertainties comes from measures made by the sensors, [3]. All those uncertainties are assumed to be in the stochastic vector variable called **v**, shown in the stochastic model of measurements in Eq. 7, [4].

$$\mathbf{z} = \mathbf{h}(\mathbf{x}) + \mathbf{v} \tag{7}$$

Where
$\mathbf{z}$ $\rightarrow$ Observation vector, order (n,1), n is quantity of measurements used for estimation.
$\mathbf{h}(\mathbf{x})$ $\rightarrow$ Model answer vector, order (n,1). composed of a non-linear function of the parameters vector.
$\mathbf{x}$ $\rightarrow$ Parameters vector, order (m,1), where m is the quantity of parameters that will be estimated. In this case $\mathbf{x} = [T_\infty\ RC\ \tau]$.
$\mathbf{v}$ $\rightarrow$ Observation error vector, order (n,1). This is a vector stochastic variable, where all vector elements have probability density function assumed to be $N(0, W)$.

4.1. Estimator

To estimate the model parameters from the observation vector will be required a nonlinear estimator. A maximum likelihood estimator was chosen, in order to find a best estimate for the vector **x**, also called $\hat{\mathbf{x}}$. First it is needed to define on which terms $\hat{\mathbf{x}}$ is best, so we can define the functional $J(\mathbf{x})$ seen in Eq. 8. Finding a $\hat{\mathbf{x}}$ that minimizes this functional, is the same as finding a $\hat{\mathbf{x}}$ that minimizes the quadratic error of the measurements with respect to the model.

$$J(\mathbf{x}) = \left(\tfrac{1}{2}\right)[\mathbf{z}-\mathbf{h}(\mathbf{x})]^T\,\mathbf{W}^{-1}\,[\mathbf{z}-\mathbf{h}(\mathbf{x})] \tag{8}$$

4.2. Finding a Minimum

Once that functional $J(\mathbf{x})$ has a quadratic form, is assumed that it has only one extremum and this extremum is a minimum. So if there is a value of **x** that makes $\mathbf{J}^{(1)}(\mathbf{x}) = 0$ this value, $\hat{\mathbf{x}}$, minimizes $J(\mathbf{x})$. $\mathbf{J}^{(1)}(\mathbf{x})$ is called the gradient vector. For the problem treated in this paper the gradient vector is shown in Eq. 9.

$$\mathbf{J}^{(1)}(\mathbf{x}) = \frac{\partial J(\mathbf{x})}{\partial \mathbf{x}} = \left[\frac{\partial J(\mathbf{x})}{\partial T_\infty} \quad \frac{\partial J(\mathbf{x})}{\partial RC} \quad \frac{\partial J(\mathbf{x})}{\partial \tau} \right] \tag{9}$$

The iterative method for finding a minimum, fundamentally solves the difference equation in Eq. 10. Once the method uses the gradient vector for guiding the solution to a minimum the method is called Gradient Method.

$$\mathbf{x}_{i+1} = \mathbf{x}_i - \mathbf{P}(i) \left[\mathbf{J}^{(1)}(\mathbf{x}) \right]^T \tag{10}$$

where $\mathbf{P}(i)$ is a weight matrix that weighs at every iteration the step of the vector **x** to the $\hat{\mathbf{x}}$. The stop criteria is when $\mathbf{x}_{i+1} - \mathbf{x}_i$ is less then a ϵ or the number of iterations are greater than k. The values for ϵ and k can be chosen empirically. When the method stops it is assumed convergence, that is, $\hat{\mathbf{x}} = \mathbf{x}_{i+1}$.

Therefore one has:

$$\left[\mathbf{J}^{(1)}(\mathbf{x}) \right]^T = - \left[\mathbf{H}^{(1)}(\mathbf{x}) \right]^T \mathbf{W}^{-1} \left[\mathbf{z} - \mathbf{h}(\mathbf{x}) \right] \tag{11}$$

$$\left[\mathbf{H}^{(1)}(\mathbf{x}) \right]^T = \frac{\partial \mathbf{h}(\mathbf{x})}{\partial \mathbf{x}} = \begin{bmatrix} \dfrac{\partial h_1(\mathbf{x})}{\partial T_\infty} & \cdots & \dfrac{\partial h_n(\mathbf{x})}{\partial T_\infty} \\ \dfrac{\partial h_1(\mathbf{x})}{\partial RC} & \cdots & \dfrac{\partial h_n(\mathbf{x})}{\partial RC} \\ \dfrac{\partial h_1(\mathbf{x})}{\partial \tau} & \cdots & \dfrac{\partial h_n(\mathbf{x})}{\partial \tau} \end{bmatrix} \tag{12}$$

where $\mathbf{H}^{(1)}(\mathbf{x})$ is known as Jacobian Matrix of $\mathbf{h}(\mathbf{x})$ related to **x**, and n is the order of the observation vector **x**. Using the Eq. 11 in Eq. 10 results the Eq. 13.

$$\mathbf{x}_{i+1} = \mathbf{x}_i + \mathbf{P}(i) \left[\mathbf{H}^{(1)}(\mathbf{x}_i) \right]^T \mathbf{W}^{-1} \left[\mathbf{z} - \mathbf{h}(\mathbf{x}_i) \right] \tag{13}$$

The sequence of weight matrices $\mathbf{P}(i)$, also known as covariance matrices is shown in Eq. 14, [4].

$$\mathbf{P}(i) = \left[\left[\mathbf{H}^{(1)}(\mathbf{x}_i) \right]^T \mathbf{W}^{-1} \mathbf{H}^{(1)}(\mathbf{x}_i) \right]^{-1} \tag{14}$$

5. RESULTS

In order to make the estimation of the value of **x**, many sterilization cycles were logged, but a few were selected to be used in the estimation. For every cycle the data used came from the time period between the instant when the steam valve is opened for the first time and the instant when the steam valve is closed for the first time. The valve closes when the inner temperature reaches 100 °C for the first time. The reason for using only this data window is because the model was obtained for a step response. Thus the first period when the steam valve is opened behaves as a step input.

The gradient method described in the last section was implemented in MATLAB® environment. The algorithm results in the following estimative:

$$\begin{aligned} T_\infty &= 128.9508 \pm 5.7356\,^\circ C, & \sigma_{T_\infty} &= 5.7356\,^\circ C \\ RC &= 1309.9218 \pm 71.1249\, s, & \sigma_{RC} &= 71.1249\, s \\ \tau &= 51.0636 \pm 1.1597\, s, & \sigma_\tau &= 1.1597\, s \end{aligned}$$

Such estimates were used in a simulator implemented in SIMULINK® environment. The measured result compared with the simulated, Fig 2, lead to a mean square error of approximately 0.7354 °C.

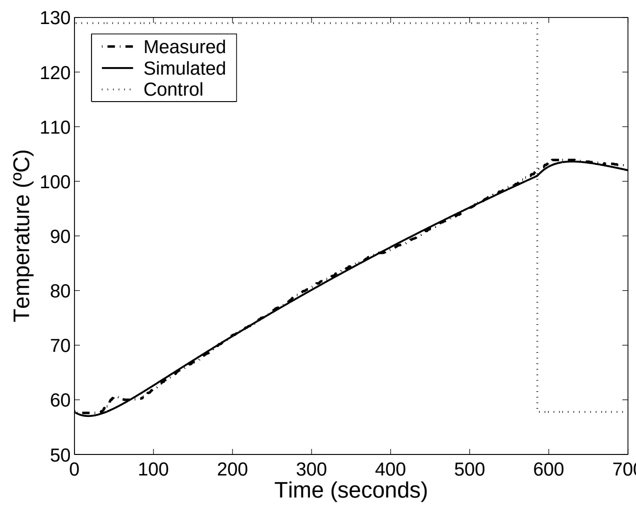

Figure 2 – Simulated Result compared with Measures

The most critical period is when the system reaches the first temperature peak. This period will be analyzed more carefully. The Fig. 3 shows a comparison of results, during the first temperature peak, comparing the measured result, the simulated result and the simulated result using the $T_\infty \pm \sigma_{T_\infty}$ instead of T_∞ as a parameter. The Fig. 4 also shows a comparison but now the parameter changed is the RC. Same for Fig. 5 that alters the parameter τ.

6. CONCLUSION

The temperature model proposed in this work, despite its simplicity, achieved the expectations. The model has shown really satisfactory performance in forecasting the autoclave inner temperature. The estimator and the method used for finding the best estimate also accomplished the task. One should remark that during the estimation trials it was observed that a previous knowledge of the parameters are necessary to initialize the algorithm, because the iterative method convergence showed to be very sensible to initial values set to initialize the procedure.

The results presented herein were considered worthwhile to the laboratory that made the autoclaves available for real-

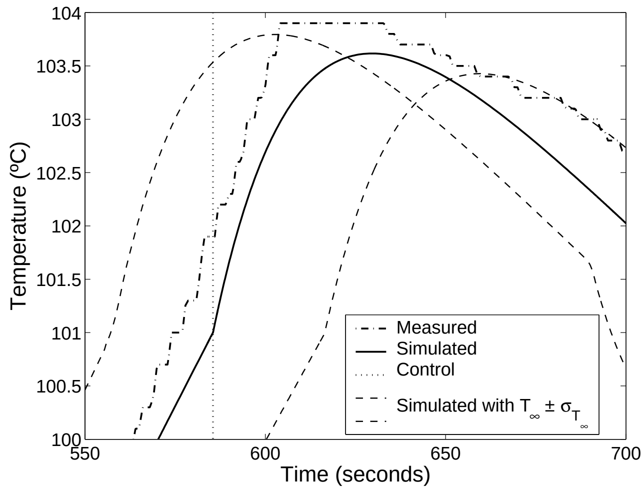

Figure 3 – Simulation realized varying the parameter T_∞

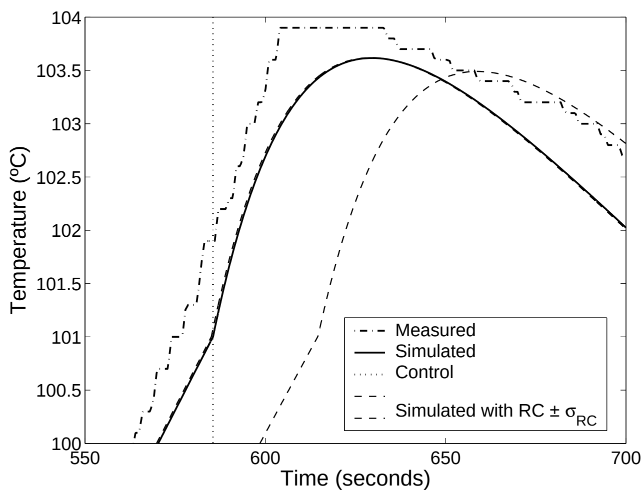

Figure 4 – Simulation realized varying the parameter RC

ization of this work. With the system simulator developed it was chosen a better reference value for the heating period, reducing the temperature peak and the product loss caused by overheating. It was also possible to find a reference value, that even reducing losses, did not increase the time for sterilization cycle. This certainly would represent a production hindrance.

Future works could come with a better solution to the temperature control system, once now it is possible to simulate the system behavior. An improvement in this control would represent a cost reduction with respect to steam generation and valves fading. Other enhancements to the system model could be achieved if more sensors are installed, for instance, two sensors, one at the maximum temperature location and other at the minimum. On doing that it would be feasible to build a simulator capable of forecasting more characteristics of this system.

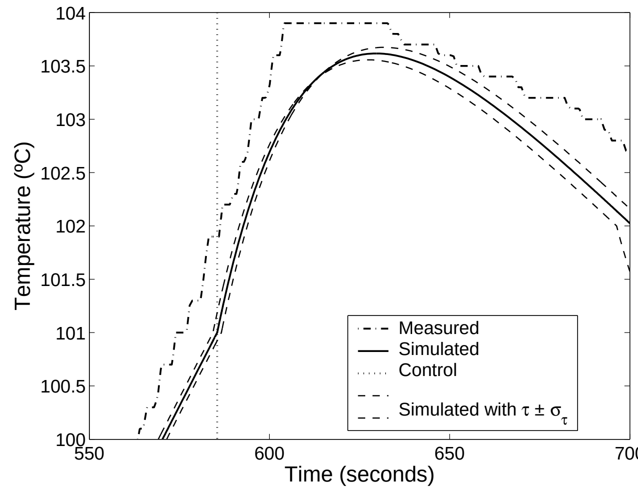

Figure 5 – Simulation realized varying the parameter τ

7. ACKNOWLEDGMENT

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