

Hybrid Modelling Development for a Continuous Industrial Kraft Pulping Digester

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Abstract

The kraft pulping process (introduced in 1979), is a complicate process which involve mass transfer of cooking chemical into wood structure and complex heterogeneous chemical reactions between wood components and the cooking chemicals. In this work a hybrid model is developed for a kraft digester, which is a fundamental stage in pulp production coupluy a deterministic model with artificial neural network. The deterministic model is built-up for a kraft Pulping Process of *Eucalyptus* by combining intrinsic kinetic equations Lignin, Cellulose, Hemicellulose, Extractives and diffusion mass transfer equations, will provide the data to verify the performance of the artificial neural network modelling. The aim of this work is to develop a mathematical model which at some time is able to represent the main phenomena taking place in the process and suitable to be used in control and optimization applications. The performance of hybrid model is compared to a validated deterministic model, so that different operation conditions may be used to verify the prediction capabilities of the proposed model. The hybrid modelly approach proposed in this work has as main advantage compared to the existing models the fact that it allows to obtain a final kappa numbers with smaller number of process variables. Regarding the deterministic model is important to mention its adaptation in order to consider the delignification reactions as simultaneously reactions with three different types of lignin, with the most reactive lignin reacting more quickly. This approach presents a new point of view for the theory of three phases of the reaction, interpreting its results as if the reaction of each lignin was responsible for a specific phase of the reaction

Keywords: kraft pulping, hybrid model, kinetic equation, mathematical model, artificial neural network

1. Introduction

Wood is a complex structure of fibres glued together by lignin. In order to make pulp, it is necessary to separate them, which can be done mechanically, chemically or by a combination of the two processes. The digestion process can be either batch or continuous. The continuous digester is a tubular reactor in which wood chips react with an aqueous solution of sodium hydroxide and sodium sulfide (Kraft Pulps), referred to

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as white liquor, to remove the lignin from the cellulose fibres. The product of the digesting process is cellulose fibres, or pulp, which is used to make paper products (Al-Awami et al.,1999).

The continuous digester is a large pressurized vessel, divided into three basic zones: an impregnation zone, one or more cooking zones, and a wash zone. The white liquor penetrates and diffuses into the wood chips as they flow through the impregnation zone. The first zone is responsible for the impregnation of the wood with liquor. It is very important that the wood receives liquor entirely and uniformly, so that at the end of the cooking the pulp is uniform and the amount of rejects is minimum. A heating zone follows the impregnation zone, leading the process to the suitable temperature for the lignin reaction which predominates over the carbohydrates reactions. The white liquor and wood chips are then heated to reaction temperature and the lignin is removed through one or more cook zones (Assumpção et al., 1988). The chips stay in the cooking zone for a period, and then proceed to the washing and discharge zones. The free liquor is in either cocurrent or countercurrent flow with respect to the wood chips in the cooking zones, where the majority of the delignification reactions occur. The wash zone is the end of the digester where a countercurrent flow of free liquor washes the degradation products from the pulp (Al-Awami et al., 1999). A simplified scheme is shown in Figure 1.

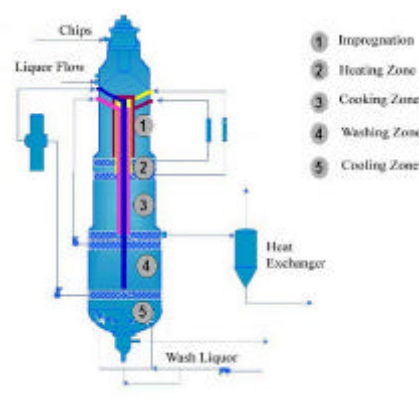


Figure 1. Continuous Digester

The proposed model considers three types of lignins with one reacting faster and another one suffering a slow reaction, and a third one is inert. The reactions of the major carbohydrates components (two types of cellulose and two types of hemicellulose) are considered as following the same general equation. Unlike most models in literature, this one considers the fast and simple consumption of alkaline in extractive reactions (also wood components), usually disregarded due to very high dissolving rates.

2. Model of Kraft Cooking

A kraft cook model should take into consideration the kinetics of the removal of wood components and the transport of cooking chemicals, dissolved wood components and heat between cooking liquor and the wood chips.

2.1 Kraft Cook Kinetics

The first attempt to model the kinetics was made by Vroom (1957), and an Arrhenius type expression for the reaction rate temperature dependence to derive the “H factor” was used. The H factor, which combines the cooking temperature and cooking time into variable, is at the heart of many control schemes used for kraft pulping (Saltin, 1992). Most of models use the same general form, although some simplifications and modifications are usually applied (Aguar and Maciel Filho, 1997):

$$-dW/dt = \left(k_1 [OH^-]^a + k_2 [OH^-]^b [HS^-]^c \right) (W - W_\infty) \quad (1)$$

where: W is the wood component concentration; k1,k2 are the Arrhenius constants; W_∞ is the wood component after infinite time; a,b,c are the kinetic orders; [OH⁻] and [HS⁻] are the OH- and HS⁻ concentrations, respectively, and t is time.

In this work, the model for a continuous digester considers the diffusion into the wood pores initiated during the impregnation of the chips. Another characteristic of the model is its adaptation in order to consider the delignification reactions as simultaneously reactions with three different types of lignin, with the most reactive lignin reacting more quickly. This approach presents a new point of view for the theory of three phases of the reaction, interpreting its results as if the reaction of each lignin was responsible for a specific phase of the reaction (initial delignification, bulk and residual). Regarding the solution of the model it is based on “Line Method”, which consist on usage of Orthogonal Collocation for discretization of the partial differential equations. The temporal integration of the ordinary differential equations is solved by integrator LSODE (Vasco de Toledo, 1999).

2.2 Equations

The proposed model considers three types of lignins to know, one reacting faster, another one suffering a slow reaction, and a third one is inert. The reactions with the major carbohydrates components (two types of cellulose and two types of hemicellulose) are considered as following the same general equation. Taking into account the reactions for lignin, hemicellulose, cellulose and extractives, the deterministic model equations can be written as follows:

$$\frac{dL_i}{dt} = k_{L_i} \exp\left(\frac{E_{L_i}}{RT}\right) [OH]^a [HS]^b L_i \quad (2)$$

$$\frac{dH_i}{dt} = k_{H_i} \exp\left(\frac{E_{H_i}}{RT}\right) [OH]^a H_i \quad (3)$$

$$\frac{dC_i}{dt} = k_{C_i} \exp\left(\frac{E_{C_i}}{RT}\right) [OH]^a C_i \quad (4)$$

$$\frac{dE}{dt} = -0.6E \quad (5)$$

$$D = 60 \times 10^{-4} \sqrt{T} \exp\left(\frac{-223 \times 10^3}{RT}\right) \times (124 \times 10^{-2} - 1.12 \times 10^{-4}) \times [L + H + C + E] \quad (6)$$

$$\frac{\partial HS}{\partial t} = \frac{1}{X^2} \frac{\partial}{\partial x} \left(D \frac{\partial HS}{\partial x} \right) \quad (7)$$

where: L is the lignin; H is the hemicellulose; C is the cellulose; E is the extractives; D is the Diffusion Coefficient, R is the gas constant, T is temperature, t is the time; x is the dimensionless distance from the center of the chip; X is the half the chip thickness; OH is the alkali concentration and HS is the sulfide ion concentration in the liquid. This deterministic model will be used to develop this hybrid model for a pulping digester.

3. Hybrid Model

This work proposes a hybrid model, based on the known part of a first principle model, combined to a neural network to account for the phenomena that is not comprised in the deterministic equations, in order to overcome limitations of both methods. Hybrid models may be developed in many different combinations. Knowledge of the process may be used to impose constraints (as inequalities) to the neural model. The network can also be used as default, but the deterministic model should be used when the variables are out of training range. Also, the mathematical model may be used in situations when data is not available. A common approach is having the first principles model as the basis, with the neural net calculating unknown parameters. Still, the network can be used to learn the deviation between the mathematical model output and the aimed output. In fact, this may be easier than learning the complex relationships between input variables and process results.

Other possible approach is using the deterministic model as reinforcement for the function relationship between inputs and outputs. The choice of how to combine both parts depends on the precedence of data or first principle system knowledge, and it is particular to each case. The approach considered in this work uses the mathematical model as reinforcement for the relationship between inputs and outputs. The hybrid net was trained according to backpropagation algorithm, where sets of mill inputs and correspondent results were iteratively fed to the net and net parameters adjusted until the input-output relationship was learned. The mathematical model receives information from process variables and generates the kappa number according to the kinetic equations. The result is then fed into the net along with other process variables, and the net yields a final kappa number. The scheme is described in Figure 2.

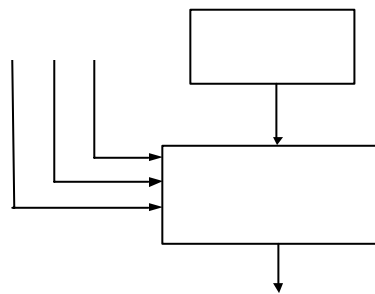


Figure 2. Hybrid model scheme

The algorithm used in this work is the Generalized Delta Rule (GDR) algorithm, a gradient descent method that minimizes the sum of squares of the residual (Savkovic-Stevanovic, 1994).

4. Discussion of Results

Many adjustments in network configuration and analysis of the input variables set must be done in order to obtain the best network configuration for the modeled process. Industrial data were carefully collected, observing retention time in the reactor for different production rates, to be used as input for the first principles model as well as for hybrid net training. The hybrid model was trained, the net configuration was optimized, and the results reproduced industrial data properly. The net was initially set to be trained with one hidden layer and all 22 available variables. However, it did not converge to the predetermined minimum error. Changes in net configuration were done gradually until best results were obtained. The parameters to be optimized in a neural network are: number of layers and neurons in each layer, momentum term, offset, learning rate, error tolerance, transfer function and random initial weights algorithm.

The predicted variable in the model is the Kappa number, due to its importance to the next sections of the process and its significance for mill personnel. Regression and graphical analysis of the data are carried out in order to eliminate the variables that do not affect Kappa number significantly. As a result, only 9 variables were used to feed the input neurons in the network. The inputs variables are: white liquor flow, wood density, total alkali charge, temperature (top, CD1, CD2), effective alkali (top, CD1, CD2), white liquor flow (top, CD1, CD2) H factor (top, CD1, CD2) and sulfidity. Figure 3 illustrates the improvement obtained for kappa number prediction with previous data analysis.

At this stage it was found that the number of industrial profiles was not the desired number of training sets for a neural network but it reflects the potential of the proposed model even with relatively few data. In any case, it is expected that when more data is gathered, network prediction will improve considerably.

A new set for training was derived from industrial data in order to improve the net efficiency. Correlation curves between kappa number and each variable were determined and a better behaved training set composed of new values attained from correlation curves were used to train the network. Real data from the mill was used to test and validate the model. Figure 4 presents prediction results, considered satisfactory, specially for a network trained with a reduced number of training sets.

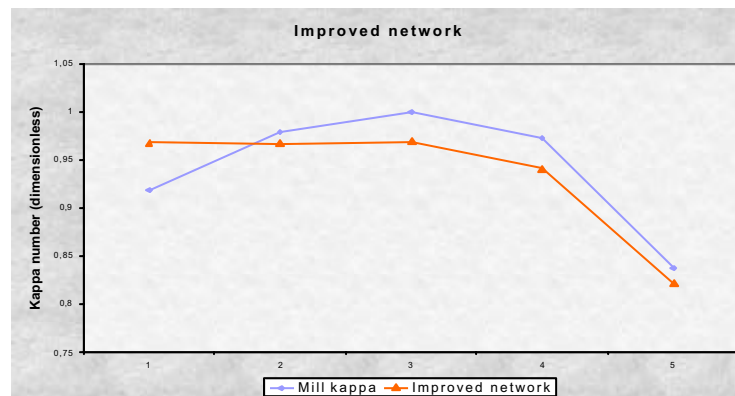


Figure 3. Kappa prediction

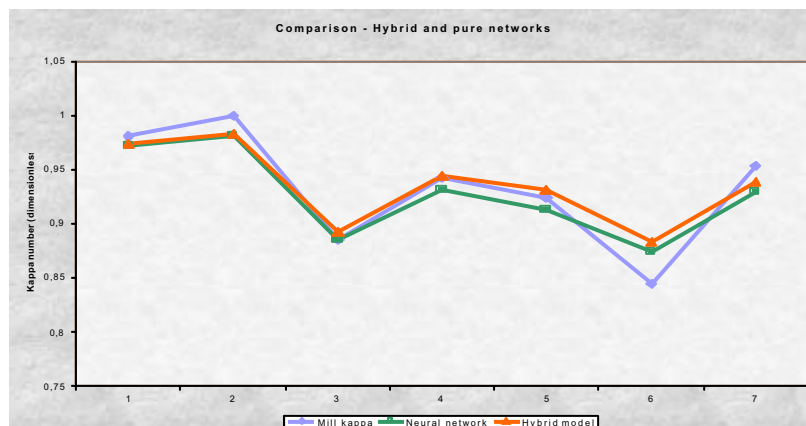


Figure 4. Comparison between hybrid model and neural model predictions

5. Conclusion Remarks

Both, neural network and hybrid network models produced similar results, showing to be adequate tools to model an industrial cooking process, even with a reduced number of training sets. The mathematical model developed in this work is valid over a significant range of operation it has shown to be used in control and on-line optimisation. The simple approach used to combine first principles knowledge and neural network features produced improved results when compared to the pure net. However, it should be seen as the starting point for a more complex model, where process knowledge and pattern learning capacity can be better combined in order to improve prediction capability and to provide a more complete approach of the process (when all variables and relevant phenomena influencing results are accounted for). The expected benefit is that simulation program assists in decision making on process policies according to the desired product characteristics, and enables mill personnel to correct the process before undesired pulp grades are produced. Furthermore the program can be used to design specific pulp characteristics that are requested by customers, and can be achieved by specific parameters controlled in the process. It can also be a useful tool for training operators and engineers.

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