A novel approach to white liquor control in a continuous digester using the Box-Jenkins methodology to predict chip bulk density

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ABSTRACT: Alkali charge is one of the most relevant variables in the continuous kraft cooking process. The white liquor mass flow rate can be determined by analyzing the chip bulk density fed to the process. At the mills, the total time for this analysis usually is greater than the residence time in the digester. This can lead to an increasing error in the mass of white liquor added relative to the specified alkali charge. This paper proposes a new approach using the Box-Jenkins methodology to develop a dynamic model for predicting chip bulk density. Industrial data were gathered on 1948 observations over a period of 12 months from a Kamyr continuous digester at a bleached eucalyptus kraft pulp mill in Brazil. Autoregressive integrated moving average (ARIMA) models were evaluated according to different statistical decision criteria, leading to the choice of ARIMA (2,0,2) as the best forecasting model, which was validated against a new dataset gathered during 2 months of operations. A combination of predictors has shown more accurate results compared to those obtained by laboratory analysis, allowing a reduction of around 25% of the chip bulk density error to the alkali addition amount.

Application: The results of this study may help mills to review the alkali addition methodology to reduce the chip bulk density error in white liquor flow rate.

Complex processes with significant time delays are difficult to optimize and control. This is because of the large number of variables that affect the quality of the final product and the significant time between input and output process operations. A typical example of such equipment in the pulp industries is the continuous digester. The cooking plant is one of the major unit operations in the pulp mill, and its proper control is very important to the pulp quality. Continuous digester is a complex reactor in which the delignification of wood chips takes place through chemical and physical processes. Strong interactions between many process variables in this equipment, and frequent disturbances, are observed. Steady-state operation is, therefore, difficult to maintain for a long time.

At the cooking plant, the first problem that hampers good monitoring is to control variables that are not directly or instantaneously measurable. These variables are obtained from process stream samples periodically collected and then measured in the laboratory. The second problem is the long time taken for analysis. The result is that adjustments based to the process, based on the control variables, are done belatedly. White liquor addition control is an issue affected by both of these challenging problems. Besides the physical and chemical properties of the wood, the most relevant variables in a continuous kraft cooking process are temperature, residence time, and white liquor charge, which is consumed in chemical reactions with lignin, carbohydrates, organic acids, and resins or is adsorbed by cellulose fibers [1].

For a continuous digester, process variables are measured at different frequencies. Chip density for instance, does not have the same frequency of the white liquor flow rate, alkali concentrations, etc. Numerous chip properties vary during daily operations. Chip density is just one of them, and its value is important to determine the white liquor flow rate.

A common procedure in pulp mills is to measure chip bulk density according to TAPPI Useful Method UM-23 (2010) "Bulk density of woodchips," which usually takes 4 h, including sampling, analysis, and results display to operators. This 4 h period is commonly higher than the digester residence time. This means that when the analysis result is available to operators, the fed chips analyzed were already cooked and out of the digester. The white liquor quantity is a dependent function of chip density, which in turn demands a long time to be analyzed. Consequently, results needed to make changes during a previous shift are not available until the next. Delays cannot be eliminated by the control system, but an alternative control might minimize its effects.

Different models for kappa number prediction in kraft pulping are described in the literature. Kumar and Gustafson [2], for example, concluded that about half of the variability observed in kappa for the digester and the oxygen reactor can be explained by inadequate control of process variables. Rubini and Yamamoto [3] evaluated mathematical models capable of predicting the outlet kappa number from an industrial delignification reactor, using kinetic models. Yang and Liu [4] proposed a new kinetic step mechanism for the heterogeneous delignification reaction during the kraft pulping process. The derived kinetic model showed that the mechanism can be used to predict the pulping pattern under a variety of conditions with a good accuracy. Galicia and colleagues [5] performed experiments in simulation disturbances and industrial cases in a partial least squares model of delignification predictions. Despite abundant reports regarding the kraft pulping kinetics model, few works deal with mathematical modeling or investigations concerning chip properties prediction applications [6,7].

Over the years, the ability to accurately predict different types of events has improved, providing better tools to make better decisions. The uses of formal forecasting methods are the means by which this development is taking place [8].

The objective of this study was to identify a chip bulk density prediction model, using the Box-Jenkins methodology to overcome time delay analysis limitations, to be used in white liquor addition control. The main advantages of this methodology are its ability to handle modeling errors and that it is auto-adjustable for the next step, using information from the previous one, based on eventual deviations in the predicted values. A better accuracy in the chip bulk density is important, considering the tendency of mills to end the cook at a higher kappa number to preserve yield [9,10]. Running at high kappa values increases the risk of plugging at the screen plant. In this context, a better accuracy for chip bulk density values will directly affect the amount of white liquor additions, the cooking alkaline concentrations, and temperatures, allowing an economy of the added alkali, and especially a reduction on kappa number variations.

PROCESS DESCRIPTION

In the process we studied, eucalyptus pre-steamed wood chips and white liquor are fed into a continuous digester. At the top of the digester, the chips are heated to reach the cooking temperature using direct steam and the delignification reaction begins. During the cooking process, the alkali in the white liquor is consumed by reactions with lignin, carbohydrate dissolution, and reactions with various organic acids (from the wood or produced by pulping hydrolysis). Most of the alkali consumed is used in neutralizing the acids formed by carbohydrates degradation. The alkali consumption starts as soon as it contacts the chips and increases with temperature. The amount of alkali consumed in the digester depends on the wood properties (chemical and physical), chip impregnation, cooking temperature, desired kappa number, and residence time. Alkali consumption affects yield and pulp quality. Celluloses and hemicelluloses are unstable in alkaline solutions. In the delignification process, undesirable reactions of hydrolytic glucosidic linkages break, causing separation of groups or side chains and the breaking of the main carbohydrates chains. Such degradation reactions result in the formation of soluble low molecular weight compounds, and consequently, a yield decrease.

The kappa number represents the residual lignin content in the pulp. An increase in chip bulk density results in a lower delignification degree because the digester control is based on the chips volumetric feed rate (on chip meter speed). As a result, the chemicals-to-wood mass ratio decreases, causing a higher kappa number at blow. High kappa number may cause shives quality problems, disturbances at the screen plant, high organic load to effluent treatment, and high chemicals consumption. On the other hand, the higher the effective alkali addition, the greater the yield loss, and lower the pulp viscosity. The kappa number is strongly affected by the alkali content [11]. The white liquor flow rate to the continuous digester is calculated according to Eq. (1):

$$WL = 60\,(AC)\,(RPM)\,(V)\,\varrho\,/\,(EA) \tag{1}$$

where:

WL	= white liquor flow, m^3/h
AC	= alkali charge, %
RPM	= chip meter speed
V	= chip meter volume, m^3
EA	= white liquor alkali concentration, g/L
ϱ	= chip bulk density, kg/m^3

The alkali charge (AC) is set by operators, and the other variables in Eq. (1) are fixed values (V), or measured on line (RPM, *EA*), except for chip bulk density (ϱ), which has discrete values depending on the frequency of laboratory analysis.

The total time of sample collection, chip bulk density procedure analysis, and data processing usually takes around 4 h, which means that the density value used at Eq. (1) has an undesirable time delay.

TIME SERIES METHOD OF BOX-JENKINS

A time series is a set of observations generated sequentially in time. Depending on the dataset, it may be continuous or discrete. The use at time, *t*, of available observations from a time series to forecast its value at some future time, *t+1*, can provide a basis for control and optimization of industrial processes. Much of statistical methodology is concerned with models based on the independence assumption of the observations. In many applications, dependence between the observations is regarded as a nuisance. However, a great set of data in engineering and industries occurs in the form of time series where observations are dependent and where the nature of this dependence itself is of great interest. The body of techniques available for analysis of such a series of dependent observations is called time series analysis (a set of observations generated sequentially in time), which may be classified as linear or nonlinear. Linear models are the most popular because of their simplicity and ease of use. Examples of widely used linear methodologies are the autoregressive integrated moving average (ARIMA) models. These have been studied extensively by George Box and Gwilym Jenkins, and their names have frequently been used synonymously with general ARIMA processes applied to time series analysis, forecasting, and control [12].

Most time series analysis consists of elements that are serially dependent, in the sense that a statistical model with one or more parameters may be estimated to describe the relationship of consecutive observations and to forecast future values of the series from a specific time [13].

In time series analysis, an ARIMA model is a generalization of an autoregressive moving average (ARMA) model. These models are fitted to time series data, either to better understand the data or to predict future points in the series. They are applied in some cases where data show evidence of non-stationarity, where an initial differencing step (corresponding to the "integrated" part of the model) can be applied to remove the non-stationarity. The model is generally referred to as an ARIMA (p,d,q) model, where the parameters p, d, and q are non-negative integers that refer to the order of the autoregressive, integrated, and moving average parts of the model, respectively. When the series is stationary, the model is called ARMA (p,d).

The autoregressive model specifies that the output variable depends linearly on its own previous values. The moving average specifies a dependence relationship among the successive error terms, which in this time terminology should not be confused with the use of the same phrase in other statistical methods. The term "moving average" is used only in reference to a series of terms involving errors at different periods. The methodology proposed by Box and Jenkins to adjust ARIMA models uses an iterative three-stage modeling approach [12]:

- *Model identification and model selection*: Making sure that the series is stationary, identifying seasonality in the dependent series (seasonally differencing it if necessary), and using plots of the autocorrelation and partial autocorrelation functions of the dependent time series to decide which (if any) autoregressive or moving average component should be used in the model.
- *Parameter estimation*: Using computation algorithms to determine the coefficients that best fit the selected ARMA model. These parameters may be estimated by least squares or maximum likelihood [14] methods.
- *Model checking*: Testing whether the estimated model conforms to the theoretical specifications. In particular, the residuals should be independent of each other and constant in mean and variance over time. The normal distribution is also required to perform statistical inferences. If the estimation is inadequate, it is necessary to return to the first step and attempt to build a better model.

In addition to these three steps, it is important to validate the obtained model over a new dataset to confirm the model fitting.

Autoregressive (AR) models may be effectively coupled with moving average (MA) models to form ARMA models, a very general and useful class of stationary time series models expressed by Eq. (2):

$$Y_t = \delta + \phi_1 Y_{t-1} + \phi_2 Y_{t-2} + \cdots + \phi_p Y_{t-p} + \varepsilon_t - \theta_1 \varepsilon_{t-1} - \theta_2 \varepsilon_{t-2} - \cdots - \theta_q \varepsilon_{t-q} \quad (2)$$

where:

Y_t = value of the output variable Y at the time t

δ = $\mu\,(1-\sum_{i=1}^{p}\phi_i)$, with μ denoting the process mean

$\phi_1, \ldots, \phi_p$ = the parameters of the AR model

$\theta_1, \ldots, \theta_q$ = the parameters of the MA model

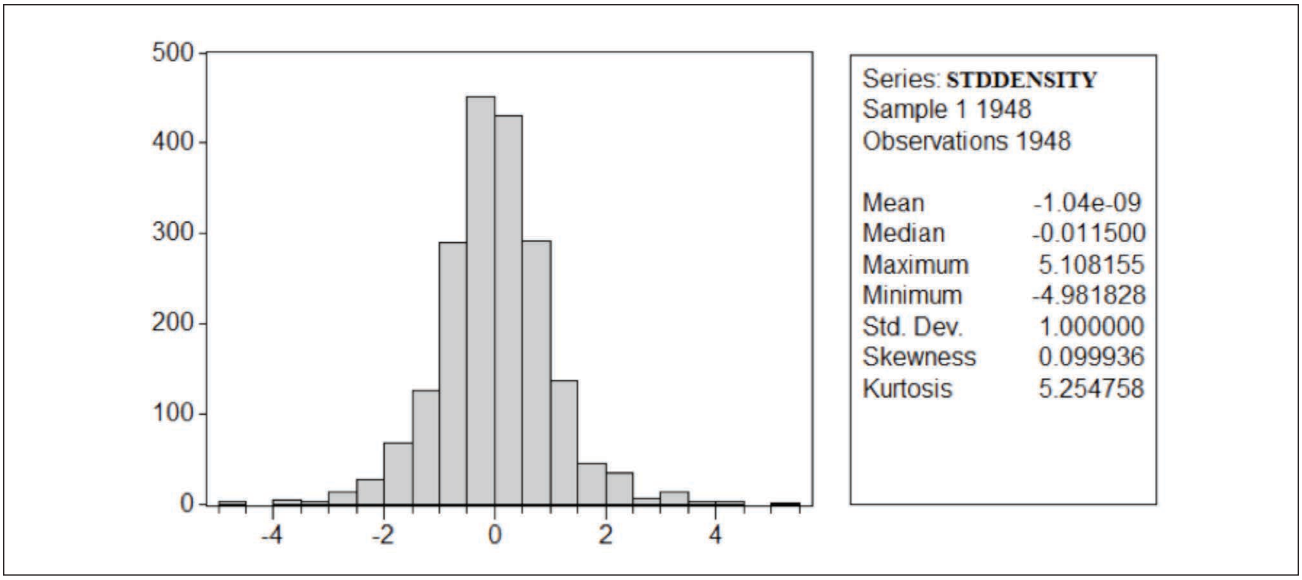
ε_t = the random error component at time t. The errors are independent with zero means and same variance (white noise series).

To adjust an ARMA model, the input series needs to be stationary. It should have a constant mean, variance, and autocorrelation through time. To determine the stationarity, it is necessary to examine the plot of the data and autocorrelogram. Not only does the model have to be stationary, it also has to be invertible. The invertibility is independent of the stationarity condition and is also applicable to the nonstationary linear models. The requirement of invertibility is needed if there is an interest in the association of the occurrence of the present events with past happenings in a sensible manner. There is a "duality" between the moving average process and the autoregressive process. The moving average equation can be rewritten (inverted) into an autoregressive form (of infinite order). However, this can only be done if the moving average parameters follow certain conditions; that is, if the model is invertible. Otherwise, the series will not be invertible and the model is not identifiable [12].

In other words, each observation is a function of a random error component and a linear combination of prior observations and prior random shocks. In recent years, the use of time series models for conducting forecasts in datasets has proved to be an important and reliable tool in such different areas as water resources and environmental systems [15], energy engineering [16] , pulp and paper [17], and several other applications [18,19].

DATA ACQUISITION

Statistical modeling techniques were used to evaluate eucalyptus chip bulk density data generated at a market pulp mill in Minas Gerais state, Brazil. The mill produces bleached eucalyptus kraft pulp, and the fiber line has a single vessel vapor-phase Kamyr extended modified continuous cooking (EMCC) digester with a capacity of 500,000 a.d. metric tons/year.



1. Histogram and descriptive statistic of the standardized chip bulk density (STDDENSITY).

Chip samples were collected in 4 h periods. A total of 2306 observations were divided into two data sets. The first was used to build the parameters of the model during 12 months operation and the second comprising a total of 358 observations in a period of 2 months, which was used to validate the model. The data set had their chip bulk density analyzed according to TAPPI UM-23, which is used to determine the weight on a moisture-free basis per unit volume of wet wood chips.

DATA ANALYSIS

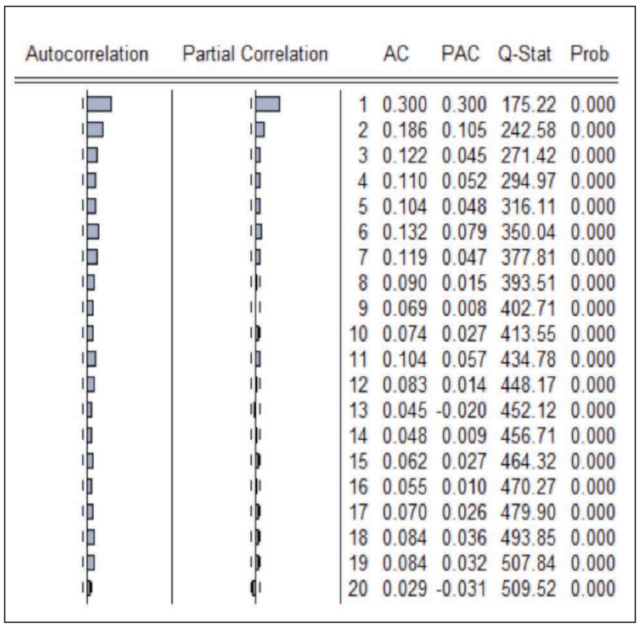
Assumptions of normality, linearity, and homogeneity of variance were evaluated at building model data set.

Models were evaluated according to different statistical decision criteria, such as mean absolute deviation (MAD), mean absolute percent error (MAPE), rooted mean square error (RMSE), Akaike information criterion (AIC), Schwarzs Bayesian criterion (SBC), Durbin Watson (DW), and Theil inequality coefficient (TIC). Lower means were considered better in the evaluation of all these criteria, except for Durbin Watson, for which the closest possible of number two was best. These and related scalar measures to choose between alternative models in a class are discussed in various texts on statistics [8,13,18].

We used EViews 5 (HIS Global; Irvine, CA, USA) software to estimate the parameters for the Box-Jenkins models and statistical analysis.

Figure 1 presents the histogram and descriptive statistics of the standardized values of the chip bulk density. Data were auto-scaled to unit variance (i.e., each data point was divided by the standard deviation) and mean centered. Assumption of normality is providing by large sample size and visual evidence of the graphic.

By examining the autocorrelation function (AC) and partial correlation (PAC) of the chip density data in **Fig. 2**, it is possible to observe significant autocorrelations (at significance level of 5%) in the first 2 lags.

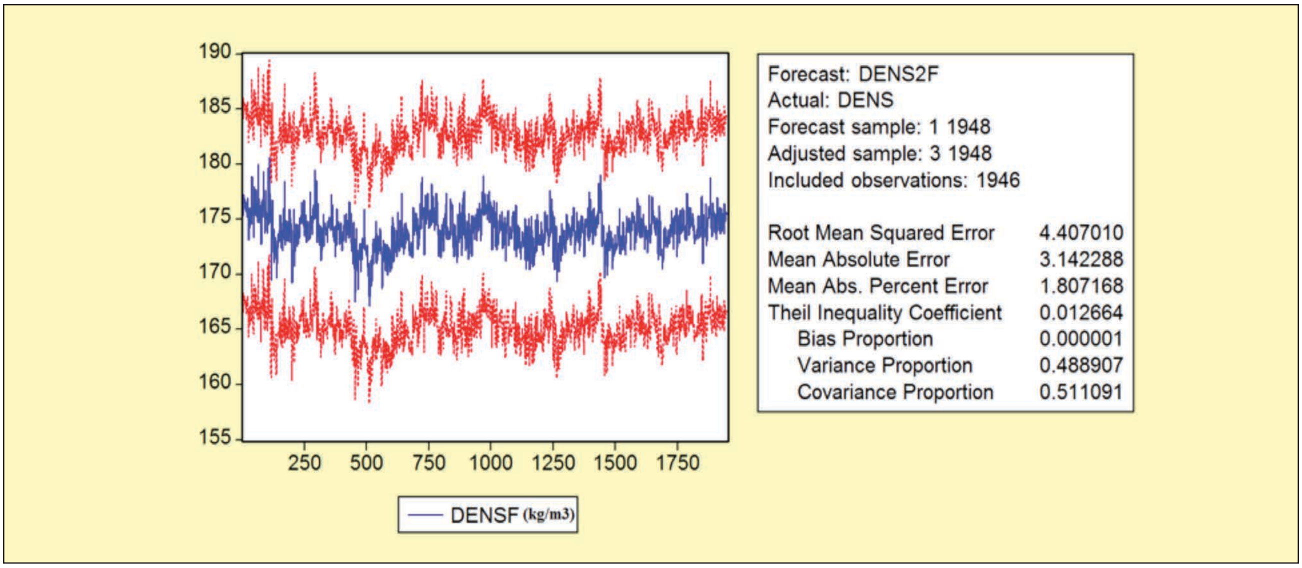


2. Autocorrelation (AC) and partial correlation (PAC) function.

The ARMA (1,1), ARMA (1,2), ARMA (2,1), and ARMA (2,2) models were evaluated. Considering accuracy and parsimony properties, the ARMA (2,2) ARMA (1,2) and ARMA (2,1) models (in this order) showed good results according to the statistical decision criteria (MAD, MAPE, RMSE, AIC, SBC, DW, and TIC), as indicated in **Table I**. According to these statistical decision criteria (**Fig. 3** and **Table II**), the best forecasting model was the ARMA (2,2).

The estimated parameters of model ARMA (2,2) are also presented in Table II using the 1,948 forecast sample.

Figure 4 shows actual and theoretical autocorrelation



3. ARMA (2,2) parameters.

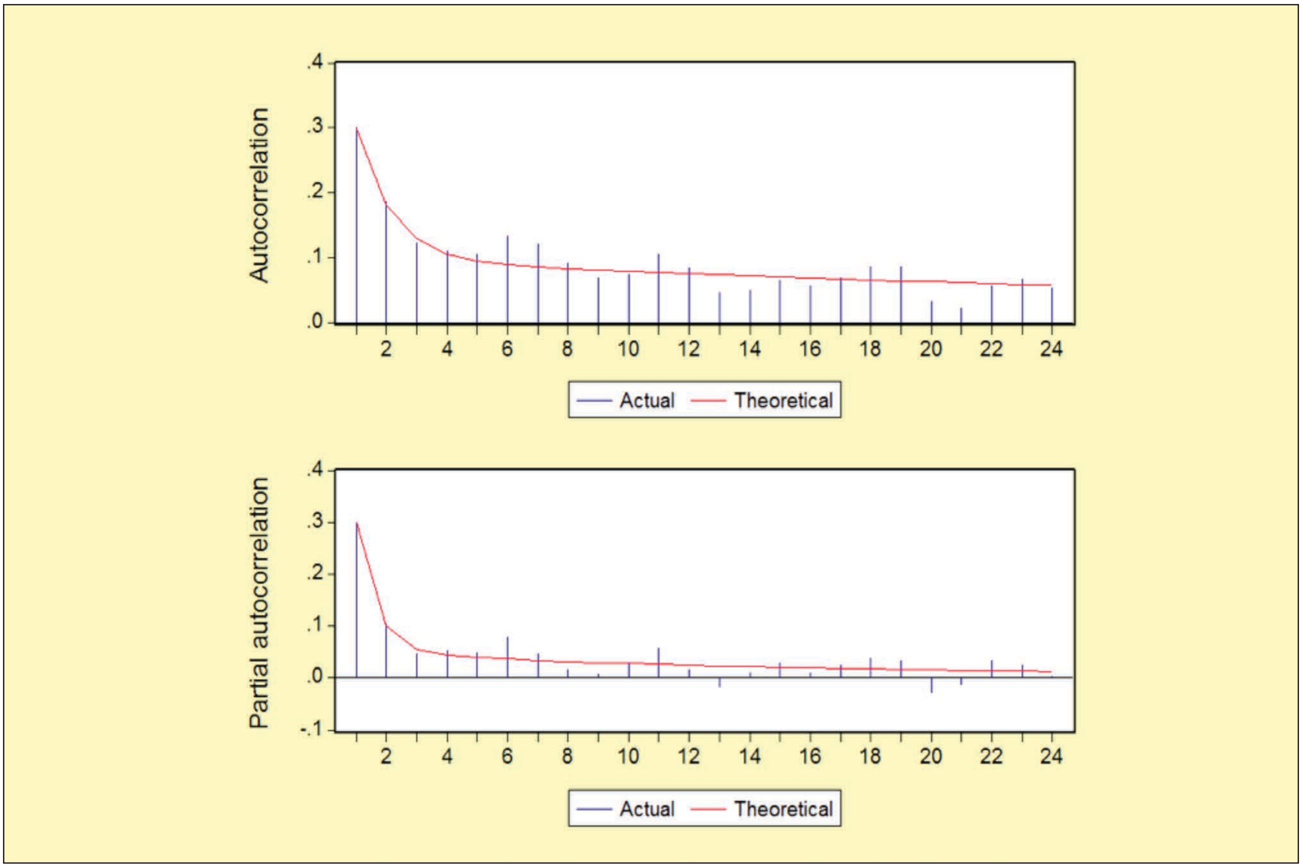
Model	AR (1)	MA (1)	ARMA (1,1)	ARMA (2,1)	ARMA (1,2)	ARMA (2,2)
AIC	5.8360	5.8550	5.8190	5.8100	5.8110	5.8090
SBC	5.8410	5.8610	5.8280	5.8210	5.8230	5.8124
DW	2.0630	1.9250	1.9440	2.0110	1.9860	2.0010
RMSE	4.4720	4.5150	4.4340	4.4100	4.4140	4.4070
MAD	3.2090	3.2780	3.1610	3.1550	3.1640	3.1420
MAPE	1.8460	1.8860	1.8170	1.8150	1.8190	1.8070
TIC	0.0128	0.0128	0.0127	0.0127	0.0127	0.0127

Abbreviations: AR = autoregrassive; MA = moving average; ARMA = autoregressive moving average; AIC = Akaike information criterion; SBC = Schwarzs Bayesian criterion; DW = Durbin Watson; RMSE = rooted mean square error; MAD = mean absolute deviation; MAPE = mean absolute percent error; TIC = Theil inequality coefficient.

I. Results of the statistical forecasting criteria of tested models.

Variable	Coefficient	Std. Error	t-Statistic	Prob.
C	173.9198	0.344822	504.3753	0.0000
AR (1)	1.404277	0.099330	14.13751	0.0000
AR (2)	- 0.417042	0.095448	- 4.36933	0.0000
MA (1)	- 1.157647	0.104792	- 11.04707	0.0000
MA (2)	0.201239	0.093597	2.15005	0.0317
R-squared	0.116660	Mean dependent var	173.9539	
Adjusted R-squared	0.114840	S.D. dependent var	4.690204	
S.E. of regression	4.412683	Akaike info criterion	5.809409	
Sum squared resid	37794.71	Schwarz criterion	5.823729	
Log likelihood	-5647.555	F-statistic	64.08541	
Durbin-Watson stat	2.001810	Prob (F-satistic)	0.000000	
Inverted AR Roots	0.98	0.43		
Inverted MA Roots	0.94	0.21		

II. ARMA (2,2) forecasting parameters.



4. Autocorrelation and partial correlation of model ARMA (2,2).

Lag	AC	PAC	Q-Stat	Prob
1	-0.001	-0.001	0.0037	
2	0.006	0.006	0.0793	
3	-0.013	-0.013	0.4253	
4	0.000	0.000	0.4258	
5	-0.002	-0.001	0.4312	0.511
6	0.041	0.041	3.7375	0.154
7	0.029	0.029	5.3828	0.146
8	0.001	0.000	5.3833	0.250
9	-0.019	-0.018	6.1010	0.297
10	-0.010	-0.009	6.2902	0.391
11	0.035	0.035	8.6480	0.279
12	0.011	0.009	8.8919	0.351
13	-0.032	-0.035	10.860	0.285
14	-0.020	-0.020	11.620	0.311
15	0.001	0.003	11.620	0.393
16	-0.014	-0.013	12.028	0.443
17	0.003	0.000	12.047	0.524
18	0.021	0.018	12.943	0.531
19	0.032	0.033	14.910	0.458
20	-0.035	-0.031	17.342	0.364

5. Residuals of autocorrelation and partial correlation.

and partial correlation, indicating a good adjustment between actual and theoretical line.

The study of residuals (or errors of fit) is very important for deciding on the appropriateness of a given forecasting model. If the errors are essentially random, then the model may be a good one. **Figure 5** shows residuals autocorrelation and partial correlation, demonstrating a white noise model.

MODEL VALIDATION

Applying coefficients indicated in Fig. 3 at Eq. (2), Eq. (3) (ARMA 2,2) was obtained to validate the second dataset:

$$Y_t = -2.220086 + 1.404277\, Y_{t-1} - 0.417042\, Y_{t-2} - 1.157647 e_{t-1} + 0.201239\, e_{t-2} \tag{3}$$

where:

Y_t = chip bulk density at time t

e_t = chip bulk density error at time t (observed – estimated)

This second data set was obtained from 2 months of regular operation of the cooking plant and the model (3) has presented a MAPE of 1.64%. As expressed in **Table III**, using the laboratory analysis to calculate the white liquor amount, a MAPE of 2.17% is achieved because of the undesirable time delay between sample collection and analysis result. The combination of predictors have presented more accurate results when compared with those obtained by simple laboratory analysis, resulting in a reduction of approximately 25% of the density error, allowing a better accuracy of

Model	ARMA (1,1)	ARMA (2,1)	ARMA (1,2)	ARMA (2,2)	Laboratory
MAD	3.3082	3.2580	2.8589	2.8437	3.7795
RMSE	4.9455	4.9457	4.2561	4.2377	5.5800
MAPE	1.8968	1.8681	1.6370	1.6291	2.1691
MAPE reduction (%)	12.5536	13.8769	24.5289	24.8930	0
Abbreviations: ARMA = autoregressive moving average; MAD = mean absolute deviation; RMSE = rooted mean square error; MAPE = mean absolute percent error.					

III. Results of the statistical forecasting criteria of validation model.

cooking chemicals concerning the chip bulk density variations.

The ARMA (2,2) model was applied in an electronic spreadsheet for digester operators inserting the current density value, receiving the predicted value as an answer to use at white liquor addition flow rate calculus.

CONCLUSIONS

This paper proposed new inferential models for predicting eucalyptus chip bulk density based on the Box and Jenkins methodology for time series analysis, applied in the white liquor addition amount control. From the results, analysis of the residuals and different statistical forecasting indexes indicate good model fitting of autoregressive and moving average models of order 1 and 2. The error in calculated values of chip density using the prediction model was reduced in 25%, when compared with the ones obtained in the laboratory. This technique is a useful tool for pulp mills because it can be applied to the cooking process optimization and control, and may be easily included in any electronic spreadsheet and updated from time to time as more data become available.

The model has proven to be effective in industrial operation and the parameters have been updated every 3 months. **TJ**

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ABOUT THE AUTHORS

Wood is one of the highest costs for a pulp mill. It is also an item of great variability, considering the different forest soil and climate conditions. We were looking for alternatives to reduce the effects of that variability in the pulping process and to reduce alkali costs as well. Considering the large digester residence time and the time required for the chip density analysis, the statistical evaluation of the chip density data showed us that it was possible to reduce the chip bulk effects on white liquor amount.

Investigations of the raw material to reduce cooking process variability are rare, considering forest and chip wood yard limitations. Our work had a different focus, studying statistical modeling in the woodchip data to improve the control of white liquor to the continuous digester.

Statistical analysis of industrial data requires critical evaluation. One of the main difficulties was the time series evaluation through the four seasons of the year. In the various statistical forecasting methods, it is important to check which best applies to existing data series. To resolve this issue, we performed different trials and tests in different models.

There are numerous possible applications of statistical forecasting techniques. When we studied time series, we did not imagine that we could apply this technique in a continuous pulping process. The good fitting of the data to the model, despite large variations in forests, was really interesting.

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The information from this study may help mills improve control of the white liquor addition to their continuous digester, reducing the error of chip bulk density.

The next step is to evaluate other practical applications of time series analysis in additional stages of the kraft pulping process.

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