STUDY OF THE INFLUENCE OF WOOD PROPERTIES ON THE CHARCOAL PRODUCTION: APPLYING THE RANDOM FOREST ALGORITHM

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1 Received on 30.06.2020 accepted for publication on 15.10.2020.
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ABSTRACT – The understanding of the relationship between the properties of wood and charcoal makes it possible to improve the production of charcoal. Therefore, the random forest algorithm was used in this study to analyze the influence of eucalyptus wood properties on the quality of charcoal as well as the accuracy of the predicted values concerning the results estimated by support vector regression and multiple linear regression. Six properties of wood and six properties of charcoal obtained from the hybrid Eucalyptus grandis x Eucalyptus urophylla and from twelve clones of Corymbia torelliana x Corymbia critriodora at the age of seven were measured. In the analysis, the measure of mean decrease in node impurity (residual sum of squares) calculated with the random forest and the copula correlation was used to evaluate the relationship between properties of wood and charcoal. The random forest was compared to the support vector regression and multiple linear regression through the coefficient of determination, linear correlation between observed and predicted values, mean absolute error and root mean squared error. The accuracy of the random forest was greater than that obtained with the support vector regression and multiple linear regression, mainly in terms of the coefficient of determination and the linear correlation between observed and predicted values. The yield and quality of the charcoal produced from clones were mainly influenced by the holocellulose content, heartwood/sapwood ratio, and basic wood density. The apparent relative density of charcoal was the variable in which the random forest algorithm reached the best level of explanation of the variability as a function of the properties of wood, while the minor error was observed for the fixed carbon content.

Keywords: Supervised learning, Corymbia, Random forest.

ESTUDO DA INFLUÊNCIA DAS PROPRIEDADES DA MADEIRA SOBRE A PRODUÇÃO DE CARVÃO VEGETAL: APLICANDO O ALGORITMO RANDOM FOREST

RESUMO – O entendimento das relações entre as propriedades da madeira e do carvão vegetal possibilita a melhoria da produção de carvão. Sendo assim, neste estudo utilizou-se o algoritmo random forest para análise da influência de propriedades da madeira de eucalipto sobre a qualidade do carvão vegetal, bem como avaliou-se a acurácia dos valores preditos em relação às estimativas do support vector regression e da regressão linear múltipla. Foram mensuradas seis propriedades da madeira e seis do carvão do híbrido Eucalyptus grandis x Eucalyptus urophylla e de doze clones de Corymbia torelliana x Corymbia critriodora com sete anos de idade. Nas análises, foi utilizado a medida de redução média da impureza do nó (soma de quadrados residual) do random forest e a correlação de cúpulas para avaliar a relação entre propriedades da madeira e do carvão. O random forest foi comparado ao support vector regression e à regressão linear múltipla por meio do coeficiente de determinação, correlação linear entre valores observados e preditos, erro médio absoluto e raiz quadrada do erro quadrático médio. A acurácia do random forest foi maior que a do support vector regression e da
regressão linear múltipla, principalmente em termos de coeficiente de determinação e correlação linear entre valores observados e preditos. O rendimento e qualidade do carvão vegetal dos clones foram influenciados, principalmente, pelo teor de holocelulose, relação cerne/alburno e densidade básica da madeira. A densidade relativa aparente do carvão foi uma variável em que o random forest atingiu o melhor nível de explicação da variabilidade em função das propriedades da madeira, enquanto para o teor de carbono fixo o algoritmo forneceu previsões com menor erro.

Palavras-Chave: aprendizagem supervisionada, Corymbia, Random forest.

1.INTRODUCTION

The heterogeneity of the charcoal quality is one of the main problems faced by the steel industries while controlling the reduction of iron ore process. The charcoal properties are influenced by the carbonization process and by inherent characteristics of the source material, such as species or genotype, chemical characteristics of the wood and age of the trees (Protásio et al. 2012; Soares et al. 2015).

Among the wood properties that influence the quality of charcoal, Oliveira et al. (2010) highlight the basic density, calorific value, chemical constitution and moisture content as the most important characteristics for the selection of genotypes that are suitable for the charcoal production. Soares et al. (2014) emphasize that the knowledge about the relationship between the properties of wood and those of charcoal still needs to be deepened. Furthermore, a better understanding of the chemical reactions that occur in wood during the carbonization process is required.

The relationship between the characteristics of wood and charcoal has been studied by estimating the linear correlation coefficient (Santos et al. 2011; Medeiros Neto et al. 2014; Soares et al. 2014), by simple linear regression (Brito and Barrichelo 1980; Brand et al. 2013; Santos et al. 2016) and by canonical correlation analysis (Protásio et al. 2012; Castro et al. 2013).

There is a more complex method of data analysis that associates statistical principles with computer programming and machine learning. This method allows the implementation of algorithms able to recognize patterns, learn and execute analysis in an automated way (Dantas 2017). Some methods that are already widely used, such as regression analysis and multivariate techniques, can be included in this context (Biamonte et al. 2017). The great contribution of machine learning is related to the systematic increment of programming, which allows the production of advanced and robust algorithms, like the random forest (RF).

The RF algorithm is based on decision/regression trees, which, according to Breiman (2001), provides a numerical estimate that is the average of all $k$ trees when used for regression. In some cases, the RF proved to be more accurate than other algorithms, such as neural networks and support vector machine (Caruana et al. 2008). The performance of RF has been demonstrated in researches executed in the most diverse areas of knowledge, such as applications in remote sensing (Girolamo Neto et al. 2015), studies of soil physics (Carvalho Júnior et al. 2016), health area (Lento 2017), in the field of electromechanical energy (Lopes 2017) and many others.

In this study, the random forest algorithm was used to analyze the influence of some wood properties on the charcoal quality from Eucalyptus and Corymbia clones, as well as the accuracy of the predicted values concerning the results estimated by support vector regression (SVR) and multiple linear regression (MLR).

2.MATERIALS AND METHODS

The study was performed using data acquired in an experimental field area located in the city of Dionísio, Minas Gerais. This region has a humid subtropical climate, with the average annual temperature between 20 and 23 ºC and the average annual rainfall usually between 1100 and 1400 mm (Motta et al. 1996).

The planting of 13 eucalyptus genotypes, specifically one hybrid of Eucalyptus grandis x Eucalyptus urophylla and twelve of Corymbia torelliana x Corymbia citriodora, was carried out in 2008 in a land of Red-Yellow Latosol, with a plant spacing of 3.0 x 2.5 m. The plantings were seven years old when the trees were felled to collect the samples. These samples were obtained for the analysis of wood properties (heartwood/sapwood
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ratio, basic wood density, higher calorific value, total lignin content, holocellulose content and extractive content) and charcoal properties (higher calorific value, gravimetric yield in carbonization, friability, apparent relative density, content of volatile materials and fixed carbon content).

2.1 Anatomical and physical properties of wood

The heartwood/sapwood ratio was measured according to Castro et al. (2013). Basic density was measured according to the standard ABNT NBR 11941 (2003) and the higher calorific value was determined according to the ABNT NBR 8633 (1984).

2.2 Analysis of the chemical composition of wood

The total extractive content was determined according to the TAPPI 204 cm-97 standard (TAPPI 1997) and the total lignin content was quantified according to Gomide and Demuner (1986) and Goldshimid (1971). The holocellulose content was calculated by deducting the percentages of total lignin and extractives from 100%.

2.3 Gravimetric yield and charcoal properties

The gravimetric yield of carbonization was determined by the relationship between the charcoal mass and the dry wood mass. Apparent relative density of the charcoal was determined by using the hydrostatic method, according to Vital (1984). Friability was obtained according to the methodology proposed by Oliveira et al. (1982). The contents of volatile materials and ashes were measured according to the NBR 8112 (ABNT 1986). Fixed carbon content was calculated by deducting the contents of volatile materials and ashes from 100% and the higher calorific value was measured according to the NBR 8633 (ABNT 1984).

2.4 Parameterized algorithms

All analysis were performed using the statistical packages of the software R. The RF regression trees were built through the randomForest function, which is part of the package with the same name (R Core Team 2018). For the three basic parameters of the function (Breiman 2002) – number of trees, variables randomly selected by node and number of terminal nodes – there were 500 trees, four variables per node and five terminal nodes established, respectively. In the SVR training, the radial basis function kernel (RBF kernel) was used by means of the train function of the caret package (R Core Team 2018). The train function was also applied to adjust the MLR.

The wood properties were classified according to the importance of its influence on the charcoal features using the measure of mean decrease in node impurity (MDNI) of the trees in the RF algorithm, calculated by the residual sum of squares. Furthermore, the level of dependence between the properties of wood and charcoal was measured by the Spearman's rank correlation coefficient (Spearman's ρ) calculated with an elliptical copula, using the pobs function (R Core Team 2018) in order to convert data to an uniform distribution. This coefficient is equivalent to the Pearson's correlation coefficient (Pearson's r), with the additional feature of also measuring non-linear correlations (Ding and Li 2013). The training of trees was only repeated in function of the most important variables, aiming the measurement of the influence of these predictor values on the yield and quality of charcoal through the coefficient of determination ($R^2$).

To evaluate the effectiveness of RF in relation to SVR and MLR, data was randomly divided into 75% for training and 25% for validation. The methodologies were compared based on the performance outcomes on the data of validation, following the criteria used in the papers of Hallak and Pereira Filho (2011), Aitkenhead and Coull (2016), Carvalho Junior et al. (2016) and Malone et al. (2016), in which the coefficient of determination ($R^2$), the Pearson's correlation coefficient between observed and predicted values ($r_YY$), the mean absolute error (MAE) and the root mean squared error (RMSE) were calculated. To calculate the accuracy criteria, the postResample function of the caret package was used (R Core Team 2018).

3.RESULTS

3.1 Wood properties vs yield and quality of charcoal

According to the MDNI measurements, it was noticed that the holocellulose content of wood was the variable that mostly influenced the yield of carbonization, volatile materials content and friability of charcoal. Heartwood/sapwood ratio was the most important variable for the fixed carbon content of
Inferring about the apparent relative density and higher calorific value of the charcoal, basic density of wood was the property of greatest influence. The measure of the influence of wood variables on charcoal is shown by the MDNI graph, in whom, the more to the right is the point referring to the variable, the more explanatory the variable is in the algorithm (Fig. 1).

Table 1 shows that, with the exception of friability as a function of holocellulose, and apparent relative density of charcoal as a function of basic wood density, all the other relationships were inversely proportional. By analyzing the coefficients of determination (Table 1), it is possible to ensure that most of the variability of the charcoal properties is explained by the most important wood variables in terms of RF modeling.

Figure 1 – Influence of wood properties on carbonization yield, volatile material content, fixed carbon content, friability, apparent relative density and higher calorific value (H.C.V.) of charcoal produced from eucalyptus clones. RMIN: mean decrease in node impurity in the random forest (RF) algorithm.

Figura 1 – Influência das propriedades da madeira sobre o rendimento da carbonização, teor de materiais voláteis, teor de carbono fixo, friabilidade, densidade relativa aparente e poder calorífico superior (H.C.V.) do carvão vegetal produzido a partir de clones de Eucalyptus. RMIN: redução média na impureza do nó no algoritmo random forest.
3.2 Performance of the models

The performance of the RF algorithm regarding the measures of the coefficient of determination ($R^2$), linear correlation between observed and predicted values ($r\hat{y}$), mean absolute error (MAE) and root mean squared error (RMSE), was superior to the other algorithms tested for all the charcoal variables (Tables 2 and 3). It is important to point out that the results of performance that are presented in this paper refer to the data intended for validation, which, in this study, includes only 12 observations, therefore featuring a small sample. The values of $R^2$ and $r\hat{y}$ regarding to the RF algorithm were relatively high, with most of them presenting values above or close to 90% when including all the independent variables, and always remaining above 60% in the estimates containing only the most influential independent variable (Tables 2 and 3). In both estimation cases, the $r$ values for the RF were significant, which did not occur in the same magnitude for the SVR and MLR (Table 3).

The best results in terms of $R^2$ and $r\hat{y}$ were obtained while estimating the apparent relative density of charcoal. On the other hand, considering the measures of MAE and RMSE (Table 4), it is noticed that the accuracy was higher while estimating fixed carbon. The results of EMA and REQM also suggest that the differences in RF accuracy for SVR and MLR are narrow, mainly in the prediction of fixed carbon and the yield of carbonization. The different interpretations that can be extracted from $R^2$, $r\hat{y}$, MAE and RMSE may imply an unsureness about the more appropriate measure for the comparison of the evaluated methods. In this case, it is important to emphasize that the MAE and RMSE measured the difference between the observed and predicted values directly. Consequently, these error measures become more reliable to compare and evaluate the different prediction methods.

4. DISCUSSION

Unlike the dependence considered high ($R^2 = 61.65\%$) that was observed for the relationship between the carbonization yield and wood holocellulose content, Santos (2008) obtained a low linear correlation ($r = -0.15$) between these two variables. It is consistent to what was observed in the work of Soares et al. (2014), in which the carbonization yield granted a greater dependence on the higher calorific value of the wood. In practice, the carbonization yield is usually higher when wood has a bigger lignin content, since this macromolecule is

### Table 1 – Spearman’s rank correlation coefficient ($\rho$) and coefficient of determination ($R^2$) of the random forest algorithm (RF) implemented only with the most influential properties for the yield and quality of charcoal produced with eucalyptus clones.

| Dependent variable       | Predictor          | $\rho$(%) | $R^2$(%) |
|--------------------------|--------------------|-----------|----------|
| Yield of carbonization   | Holocellulose      | -55.19    | 61.65    |
| Volatile material content| Holocellulose      | -37.90    | 62.84    |
| Fixed carbon content     | Heartwood/Sapwood  | -12.92    | 61.74    |
| Friability               | Holocellulose      | 41.59     | 77.48    |
| Apparent relative density| Basic density      | 84.84     | 85.23    |
| Higher calorific value   | Basic density      | -33.07    | 80.45    |

1Referring to charcoal; 2Referring to wood; 3About validation data.

### Table 2 – Coefficient of determination ($R^2$) for the random forest (RF), support vector regression (SVR) and multiple linear regression (MLR) considering six wood predictor variables (1st estimate) and only the most important variable (2nd estimate), using validation data.

| Dependent variable       | RF       | SVR      | MLR       |
|--------------------------|----------|----------|-----------|
| Yield of carbonization   | 87.10    | 49.50    | 55.94     |
| Volatile material content| 88.26    | 33.88    | 20.00     |
| Fixed carbon content     | 89.12    | 0.36     | 0.09      |
| Friability               | 89.62    | 42.76    | 30.66     |
| Apparent relative density| 93.70    | 64.95    | 68.56     |
| Higher calorific value   | 90.30    | 34.17    | 4.64      |

1Referring to charcoal; 2Referring to wood; 3About validation data. 

### Table 2 – Coeficiente de determinação ($R^2$) para o random forest (RF), support vector regression (SVR) e regressão linear múltipla (MLR) considerando as seis variáveis preditoras da madeira (1ª estimativa) e apenas a variável mais importante (2ª estimativa), utilizando os dados para validação.

| Dependent variable       | RF       | SVR      | MLR       |
|--------------------------|----------|----------|-----------|
| Yield of carbonization   | 87.10    | 49.50    | 55.94     |
| Volatile material content| 88.26    | 33.88    | 20.00     |
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more stable to the thermal degradation than the other
existent chemical compounds (Trugilho et al. 2001;
Pereira et al. 2013).

The relationship between holocellulose and
volatile material content in terms of linear correlation
was almost null in the study made by Soares et al.
(2014), in a way that the main influence reported by the
authors on the volatile materials of charcoal was the
carbon-hydrogen ratio of wood. According to Oliveira
et al. (2010), the volatile content also depends on the
carbonization temperature and heating rate.

Brito and Barrichelo (1977) noticed that more
lignified eucalyptus wood leads to a charcoal with a
higher fixed carbon content, which, according to the
authors, is a direct consequence of the composition
of lignin, as this polymer contains approximately
65% of elemental carbon. Even though the results
indicate an inverse relationship between fixed carbon
and heartwood/sapwood ratio, wood that has a greater
heartwood/sapwood ratio can increase the fixed
carbon content in the charcoal, since heartwood tends
to have a lignin content that is greater than – or even
equal – to that observed on sapwood (Klitzke et al.
2008; Costa et al. 2017; Fonte et al. 2017). It is also
important to emphasize that the production process is
the most important factor that interferes with the fixed
carbon content of charcoal (Róz et al. 2015).

| Table 3 – Coefficient of linear correlation between observed and predicted values ($r_{xy}$) for the random forest (RF), support vector regression (SVR) and multiple linear regression (MLR) considering six wood predictor variables (1st estimate) and only the most important variable (2nd estimate), for validation data. |
| Dependent variable | RF | SVR | MLR | RF | SVR | MLR |
|---------------------|-----|-----|-----|-----|-----|-----|
| Yield of carbonization | 93.65* | 70.35* | 74.80* | 78.52* | 54.67* | 0.24* |
| Volatile material content | 93.94* | 62.54* | 43.58* | 79.27* | 52.46* | -4.65* |
| Fixed carbon content | 94.40* | 5.99* | 3.01* | 78.57* | 47.87* | -36.31* |
| Friability | 94.67* | 65.39* | 55.37* | 88.02* | 30.94* | 20.18* |
| Apparent relative density | 96.80* | 80.59* | 82.80* | 92.32* | 83.99* | 77.41* |
| Higher calorific value | 95.03* | 58.46* | 21.53* | 89.69* | 40.83* | 49.00* |

*Significant according to the t test at 5% of significance; ns: not significant.

| Table 4 – Mean absolute error (MAE) and root mean squared error (RMSE) for the random forest (RF), support vector regression (SVR) and multiple linear regression (MLR) using six wood predictor variables (1st estimate) and only the most important variable (2nd estimate), considering validation data. |
| Dependent variable | RF | SVR | MLR | RF | SVR | MLR |
|---------------------|-----|-----|-----|-----|-----|-----|
| Yield of carbonization | 0.88* | 1.14 | 1.26 | 1.27 | 1.63 | 1.45 |
| Volatile material content | 1.73 | 2.21 | 3.21 | 2.37 | 2.90 | 3.65 |
| Fixed carbon content | 0.63 | 1.18 | 1.19 | 0.81 | 1.09 | 1.26 |
| Friability | 6.84 | 10.80 | 12.36 | 7.43 | 11.83 | 13.22 |
| Apparent relative density | 3.02 | 7.50 | 6.96 | 4.59 | 6.53 | 8.3 |
| Higher calorific value | 1.19 | 2.14 | 2.35 | 1.41 | 2.31 | 2.32 |

*As a percentage of the average.

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Previous studies that evaluated the friability of charcoal produced from different species, correlate the highest fines generation mainly to the diameter of the logs, the carbonization time and the wood moisture (Coutinho and Ferraz 1988; Silva 1988; Pinheiro 2013). Coutinho and Ferraz (1988) state that the generation of fines is caused by the formation of internal stresses during the moisture loss process. These stresses are directly influenced by the heartwood area and by the variation of density between the pith and the bark of the wood.

The variation of the apparent density of the charcoal as a function of basic density of the wood is well known, as demonstrated by Brito and Barrichelo (1980) in a simple linear equation with R² of 97% for this relationship. The higher is the density of the wood, the greater is the density and mechanical resistance of the charcoal. These characteristics, with the addition of the granulometry, are the most important ones for the operation of the blast furnace in the steel industry (Brito 1993; Pereira 2012).

Although the higher calorific value of the charcoal as a function of the basic density of wood presented a high R² value, there is no research that demonstrates any direct relationship between these two variables. According to Couto (2014), a higher calorific value of charcoal is dependent on the elemental chemical composition of the material. An increase in the higher calorific value can be obtained by raising the carbonization temperature, which also results in a rise of the fixed carbon content caused by the elimination of volatile materials (Figueiredo et al. 2018).

Unlike what was observed in this present study, Montaño (2016) obtained better results in the prediction of the volume of Pinus taeda, and in the projection of the biomass content and the height of Acacia mearnsii, when using the SVR compared to the RF. In the study of Carvalho Junior et al. (2016), better results were obtained with the use of MLR than with RF, in order to estimate the density of the soil in function of the physicochemical properties of the samples. Rodriguez-Lado et al. (2015), on the other hand, obtained better results by applying RF to estimate soil density as a function of organic matter and texture than by applying artificial neural networks and MLR to it.

This divergence of outcomes and lack of unanimity on which technique or algorithm is more efficient considering the most diverse areas of knowledge, highlights the importance of testing different methodologies and parameter settings, so that it turns possible to define a set of procedures that is effectively more appropriate for each research field.

5. CONCLUSIONS

Using the random forest algorithm, the yield and quality of the charcoal produced from clones of eucalyptus were mainly influenced by the holocellulose content, heartwood/sapwood ratio and basic wood density.

The apparent relative density of the charcoal was the variable that the random forest algorithm reached the best level of explanation of the variability as a function of the properties of the wood, in addition to being the variable with the greatest reduction in the error of the predictions, when compared to the other two tested techniques. The fixed carbon content observed the minor error provided by the algorithm predictions.

The accuracy of the random forest algorithm was greater than that obtained with the support vector regression and multiple linear regression. Therefore, the estimation of the yield and quality properties of charcoal as a function of wood properties through machine learning using the random forest is possible to be executed. Notwithstanding, considering the error measures, the use of support vector regression and multiple linear regression also leads to accurate predictions for most of the dependent variables.

6. AUTHOR CONTRIBUTIONS

Kaléo D. Pereira: data analyze and text written, Antônio P. S. Carneiro: research supervision and text review, Gerson R. Santos: conception and data analyze, Angélica C. O. Carneiro: technical review, Hélio G. Leite: technical review and Felipe P. Borges: text review and translation.

7. ACKNOWLEDGMENTS

To the company ArcelorMittal BioFlorestas and the Laboratory of Wood Panels and Energy – LAPEM of the Federal University of Viçosa - UFV for providing the wood samples and carrying out the laboratory analyzes, respectively. To the Coordination
for the Improvement of Higher Education Personnel - CAPES for granting a postgraduate scholarship - Financing Code 001.

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