

# RESEARCH ARTICLE

## **OPTIMIZATION OF WOOD CARBONIZATION: NUMERICAL MODELING**

## Houénagnon Nestor Agbossaga Badoussi<sup>1</sup>, Comlan Jean-Louis Fannou<sup>1</sup>, David Gildas Farid Adamon<sup>2</sup> Macaire Agbomahena<sup>3</sup> and Codjo Roland Houéssouvo<sup>4</sup>

- 1. Laboratory of Engineering Sciences and Mathematics of the National University of Sciences, Technologies, Engineering and Mathematics of Abomey (INSTI/UNSTIM), Cotonou-Benin.
- 2. Department of Energy, National Higher Institute of Industrial Technology of the National University of Sciences, Technologies, Engineering and Mathematics of Abomey (INSTI/UNSTIM), Cotonou-Benin.
- 3. Department of Mechanical Energy, Abomey-Calavi Polytechnic School of the University of Abomey-Calavi (EPAC/UAC), Cotonou-Benin.
- 4. Laboratory of Electronics, Telecommunications and applied Computer Science /LETIA/Polytechnic School of Abomey Calavi/ EPAC

### Manuscript Info

### Abstract

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In the face of the progressive depletion of fossil fuel resources, the increasing global energy demand, and the growing awareness of international leaders regarding the challenges of climate change, the search for alternatives, such as renewable energy sources, has become a priority in the 21st century. In this context, wood energy, particularly charcoal, holds significant interest and is the subject of numerous scientific studies aimed at optimizing its production process, known as carbonization or slow pyrolysis.Our objective is to optimize this wood carbonization process through numerical modeling. To conduct this study, bibliographic research was carried out on several online databases, such as Google Scholar, Science Direct, Scopus, Web of Science, as well as other databases specialized in environmental sciences, to collect data related to the chosen model. The collected data was then analyzed using MATLAB software to perform numerical simulations, utilizing the fourth-order Runge-Kutta method. The results obtained are consistent with the data available in the literature. The kinetic optimization approach, achieved by adjusting the implemented data to the rate constant to favor carbonization over gasification, led to key actions, detailed below. Furthermore, the optimization through numerical simulation of mass balance equations applied to the model allowed us to validate our data and define an optimal temperature range for carbonization, between 590 and 610 K, with a mass yield evaluated at 66%.

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#### Introduction:-

Research on the modeling of the wood carbonization process for optimizing yield and charcoal quality, the main product, has been the subject of numerous publications for several years. The work of Bamford et al. (1946) [1] was the very first study conducted in this field. Several other studies followed, attempting to provide more precision to

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## Corresponding Author:-H.N. Agbossaga Badoussi

Address:-Laboratory of Engineering Sciences and Mathematics of the National University of Sciences, Technologies, Engineering and Mathematics of Abomey (INSTI/UNSTIM), Cotonou-Benin.

the concept (Diblasi, 2009 [2], Chan et al. 2010 [3], A. Mahmoudi et al., 2014 [4]...). Thus, several kinetic models have been developed through various approaches. However, the issue of process modeling remains relevant to this day. Indeed, a glance at this literature reveals a divergence in the ideas developed by different authors. Finding a point of convergence between these ideas towards a comprehensive optimization approach that takes into account all aspects of the process would represent a significant advancement in the science of carbonization. This study aims to contribute innovatively to this issue through a theoretical and experimental approach. It brings together several approaches around a kinetic model leading to the numerical optimization of the process. By presenting the results of an in-depth bibliographic study concerning the different models developed to date for the thermochemical description of wood pyrolysis, we chose to adopt the model with three parallel and competitive primary reactions, followed by two secondary reactions, to achieve our objectives.

## Materials and Methods:-

## Materials:-

The materials used for the development of this study are of two types: numerical modeling and experimental validation, both enriched by mathematical data and formulas derived from the literature. Regarding mathematical modeling, the material used is based on the MATLAB mathematical data processing software, implemented on a laptop for numerical simulations. For experimental validation, a chainsaw is used for harvesting and shaping the wood, followed by a precision balance to weigh the wood before exposure for drying and at the beginning of carbonization.

## Methods:-

In the of the present study on numerical modeling, bibliographic research was conducted using various sources of information such as scientific journals, online databases, specialized books, and websites of research institutions and organizations. These investigations on kinetic models led to the selection of a two-step model. The first step consists of three competitive parallel primary reactions where wood decomposes into charcoal, gas, and tar, and the second step consists of two secondary reactions of tar cracking into gas and charcoal. The experimental and theoretical data collected were used in a MATLAB code for model simulation.

## **Results and Discussion:-**

## **Results:-**

## Choice of the pyrolysis model

Allowed us to gain insight into the various works carried out and the criteria for selecting a model. The first type of model presented by Ganhou (2020) [5] is a model developed by Shafizadeh and al. (1977) [6]. Park and al. (2009) [7] combined this model with another to derive a theoretical and empirical model. Thurner and Mann [8], as well as Font and al. [9], studied the same model under different operating conditions. Therefore, it is a fairly flexible model capable of adapting to various operating conditions. It is illustrated by the kinetic scheme below.



Figure n°1: Kinetic diagram of the model.

The reactions with rate constants  $\mathbf{k}_{char1}$ ,  $\mathbf{k}_{tar}$ , and  $\mathbf{k}_{gas1}$  are the primary competitive reactions, while the reactions with rate constants  $\mathbf{k}_{char2}$  and  $\mathbf{k}_{gas2}$  are the secondary reactions in the mechanism, corresponding respectively to the cracking of tar into gas and its repolymerization into charcoal. This repolymerization of tar was made possible by trapping it in the carbonization chamber. The parameters used for this model by Park and al. are presented in Table 1 below.

Reactions	Charcoal	Tar	Gas	Tar <sub>2</sub>	Gas <sub>2</sub>
$A_i(s^{-1})$	3,27	1,08	4,38	1,08	4,28
	$*10^{6}[10]$	$*10^{10}[10]$	$*10^{9}[10]$	$* 10^{5}[11]$	* 10 <sup>6</sup> [12]
$E_i(J.mol^{-1})$	111,700 [10]	148,000 [10]	152,700 [10]	108,000 [11]]	108,000 [12]
$\Delta h_i k J. k g^{-1}$	64 [15	64 [15]	64 [15]	-42 [3]	-42 [3]

For this same model, the parameters of Thurner and Mann are presented below:

#### Table n° 2:-Parameters of Thurner and Mann [14].

Reactions	$A(s^{-1})$	E(J/mol)
Reaction with constant kgaz1	14345	88600
Reaction with constant k <sub>goudr</sub>	41250000	112700
Reaction with constant k <sub>char1</sub>	737666.666	106500

The same model will be used by Font et al. for the pyrolysis of almond shells, but with newly recalculated kinetic parameters. The kinetic parameters they calculated are summarized in the table below.

#### Table n° 3:-Kinetic Parameters of Font et al. [9].

Réaction	$A(s^{-1})$	E(J/mol)
Reaction with constant kgaz	253500	139000
Reaction with constant k <sub>goudr</sub>	97516,66	119000
Reaction with constant k <sub>char1</sub>	49,68	73000

The process is thus modeled by the simplified diagram below, highlighting the inputs and outputs along with the various physicochemical phenomena that occur.

Mass, balance Equations	Chosen Model: Model with three parallel primary reactions followed by two secondary
	reactions
Mass balance for Wood:	$\frac{\partial \rho_w}{\partial t} = S_w = -(k_{tar} + k_{gas} + k_{char})\rho_w  (1)$
Mass balance for Charcoal:	$\frac{\partial \rho_{char}}{\partial t} = S_{char} = +k_{char}\rho_w + k_{char2}\rho_{tar} $ (2)
Mass Balance for Gases:	$\frac{\partial(\epsilon\rho_{gaz})}{\partial t} + \frac{1}{r^2} \left( r^2 V \rho_{gaz} \right) = S_{gaz} = k_{gaz} \rho_a - k_{gaz} \rho_{gou} $ (3)
Mass balance for Tars:	$\frac{\partial(\epsilon\rho_{tar})}{\partial t} + \frac{1}{r^2}(r^2 V \rho_{tar}) = S_{tar} = k_{tar}\rho_w - (k_{char2} + k_{gas2})\rho_{tar} $ (4)

## Table n°4: Model Equations [7]

#### Numerical Optimization of Carbonization Kinetic Optimization Approach The Rate Constant

"The rate constant is a key kinetic parameter when it comes to controlling and optimizing a chemical reaction. Mastery of this parameter is a major issue regarding the rate of formation and disappearance of a chemical species in a process, which is crucial for its optimization. We studied the evolution of the rate constants for the reactions involved in the model under investigation through a comparative approach using data from different authors on the same model. The analysis of these curves allowed us to make adjustments to optimize the carbonization among the various reactions. The curve in the figure below represents the variations in the rate constants based on the data from Park and al



Figure n° 2:- Simplified diagram of the process showing the inputs and outputs.

The mass balance equations of the model for the different chemical species present in the reaction medium are presented in the table below



Figure 3:-Variations of the rate constants of the model reactions using the data from Park et al.



Figure 4:-Variation of the rate constants using the data from Thurner and Mann.

This figure shows the variations in the rate constants of the five reactions in the model (three primary and two secondary). It is obtained by utilizing the data from various authors presented by Park et al. [7]. For temperatures

between 450 and 600K, the rate constants of the different reactions are virtually zero. Above 600K, there is a sharp increase in this parameter for all five reactions, with the highest being the rate constant related to the wood decomposition into tar, and the lowest growth is seen in the repolymerization of tar into charcoal. Thus, wood decomposition into tar is more favored than decomposition into charcoal, followed by tar cracking into gas, while wood decomposition into gas ranks fourth. Finally, the repolymerization of tar into charcoal is the least favored according to these data. For the data used by Thurner and Mann [8], only the three primary reactions of wood decomposition into gas, tar, and charcoal are considered. The curve in the figure below shows the variations in the rate constants for the data from Thurner and Mann [8].

Similar to the previous figure, the rate constants for the three reactions studied show the same trend. They are virtually zero for temperatures between 450 and 600K and increase starting from 600K. Unlike the curves from the data presented by Park et al. [7], for the curves from the data of Thurner and Mann [8], it is the wood decomposition into charcoal that predominates, while wood decomposition into tar is the least favored. This indicates that in the competition between the three reactions studied, decomposition into charcoal dominates. For our data, the curve in the figure below shows the evolution of the rate constants for the five reactions in the model. The following figure presents the curves derived from our data.



Figure n°5:- Variations of the reaction rate kinetic constants from our data.

Here, the situation is also similar to what was observed with the data from Park et al., with the difference that wood decomposition into charcoal is the most favored of the three primary reactions, while decomposition into gas is the least favored, and decomposition into tar falls in between these two reactions. For the secondary reactions, we observe low values for the rate constants of the two repolymerization reactions of tar formed in the primary stage into gas2 and char2. However, it is important to note that the repolymerization of tar into gas2 is the most favored among these secondary reactions.

#### Kinetic approach to process optimization for carbonization.

This approach initiated in this study consisted of the theoretical optimization of the carbonization process through data adjustment to favor carbonization among the various reactions involved in the thermal decomposition of wood. Indeed, the bibliographic research conducted as part of this study informs us that the rate constant developed in

various studies follows the Arrhenius law (P. Rousset and al. [15], T. Madjid [16], Vikram andal. [17], Sadhukhan and al. [18], Sinha and al. [19], Wang and al. [20]... to name a few). This constant, following the Arrhenius law, is given by the equation :

$$k_i = A_i * \exp\left[\frac{E_i}{R*T}\right] (5)$$

Where Ai is the frequency factor expressed in  $s^{-1}$ , Ei is the activation energy of reaction iexpressed in J/mol, T is the temperature in Kelvin, and R is the ideal gas constant. As indicated by the curves derived from our data (Figure 5), the rate constant related to primary carbonization (the transformation of wood into charcoal) is significantly dominant in terms of comparative growth of the rate constants of the various reactions. This situation theoretically indicates that the yield of charcoal is higher than that of gas and tar. It is therefore possible to optimize carbonization based on the model of Park et al. by adjusting the data. This optimization relies on prior measurements regarding the raw material and the reaction environment, aimed at effectively directing the process under specific conditions. These conditions, once developed, constitute our kinetic approach for optimizing the carbonization process. They are based on the following actions:

i) The use of specific catalysts to promote charcoal formation by increasing the frequency factor of the reactions.

ii) Adjusting temperatures, favoring lower temperatures to promote reactions leading to charcoal formation at the expense of those responsible for the decomposition into gas and tars.

iii) Pre-treatment of wood by prior drying, allowing its moisture content to be reduced before carbonization, thus steering the reaction towards charcoal production rather than gas and tar generation.

iv) Adjusting reaction parameters, aiming to favor the decomposition of wood into charcoal over competing reactions.

v) Controlling the heating rate, opting for gradual heating, to allow for more controlled carbonization and thus favor the formation of charcoal over that of gases and tars.

These measures offer an integrated approach to improving charcoal production under optimal conditions.

# Optimization through numerical simulations of the model Simulation results

The model equations are solved numerically in MATLAB over a temperature range from 600K to 700K by implementing data from the literature and data related to the present study. The fourth-order Runge-Kutta method is used for this purpose.

The figures below represent the variations in the densities (volumetric masses) of the species (wood, tar, gas, and charcoal) during carbonization as a function of time, using data from different authors.

According to the different curves in the figure above, we observe a decreasing trend in the wood density, while for the other species produced by the process, the trend is increasing. This observation is quite normal since the wood (reactant) in the process decomposes under the effect of heat. This thermal decomposition of the wood produces gas, tar, and charcoal, which are the reaction products. Particularly for tar, the trend remains increasing up to 1300 seconds (s), where the peak is reached, and the trend then becomes decreasing until the end of the simulation. We deduce that the secondary cracking and repolymerization reaction of tar consumes more tar than is formed in the primary reaction after the observed peak. The curves in Figures 7 and 8 show the variations of the species at temperatures of 650K and 700K, using data from the same authors.



Figure n° 6:- Variation of species densities (wood, gas, tar, and charcoal) over time at a carbonization temperature of 600 K using the data from Park and al.



Figure n° 7:- Variation of species densities (wood, gas, tar, and charcoal) over time at a carbonization temperature 650 K using the data from Park and al.

For the work of Thurner and Mann, the kinetic scheme studied is the same, but with different formulations of the model equations. A simulation of the equations studied by Park et al. for their model with these data shows an increase in the mass fraction of charcoal formed with carbonization temperature, while for tar and gas, the opposite trend is observed, which contradicts the results available in the literature. We conclude that the data related to the primary reactions are not adaptable to the equations developed by Park et al.

The various observations made in light of these results led us to adjust the data to optimize carbonization at the expense of other reactions competing with it. The table below presents the readjusted data.



Figure n° 8:- Variation of species densities (wood, gas, tar, and charcoal) over time at a carbonization temperature of 700 K using the data from Park and al.



Figure n°9:- Variation of species densities (wood, gas, tar, and charcoal) over time at a carbonization temperature of 600 K using the data from Thurner and Mann.

A comparison of the variations in the mass densities of the products reveals that the mass fraction of gas formed increases with the carbonization temperature, while for charcoal, it increases up to a carbonization temperature of 640K and then decreases for the remaining carbonization temperatures. These results are consistent with those available in the literature according to several authors. The data from Thurner and Mann [8] are also used. In their study on the chosen model, these authors provided theoretical data to predict the evolution of the process, but with different equations. The figures below show the variations in the densities of the species during the process for the respective carbonization temperatures of 600K, 650K, and 700K.



Figure n°10:- Variation of species densities (wood, gas, tar, and charcoal) over time at a carbonization temperature of 650 K using the data from Thurner and Mann.



Figure n°11:- Variation of species densities (wood gas, tar, and charcoal) over time at a carbonization temperature of 700 K using the data from Thurner and Mann.

For the work of Thurner and Mann, the kinetic scheme studied is the same, but with different formulations of the model equations. A simulation of the equations studied by Park et al. for their model with these data shows an increase in the mass fraction of charcoal formed with carbonization temperature, while for tar and gas, the opposite trend is observed, which contradicts the results available in the literature. We conclude that the data related to the primary reactions are not adaptable to the equations developed by Park et al.

The various observations made in light of these results led us to adjust the data to optimize carbonization at the expense of other reactions competing with it. The table below presents the readjusted data.

-	Char1	Char2	Gas1	Gas2	Tar
Frequency	$4,416.10^{6}$	$1,00.10^5$	4,38.10 <sup>8</sup>	$4;28.10^{5}$	3,415.10 <sup>9</sup>
factors A $(s^{-1})$					
Activation	111700	108000	152700	108000	148000
energies E					
(J/mole)					

The figures 12, 13, and 14 below show the variations in the densities of the species for carbonization temperatures of 600 K, 650 K, and 700 K, respectively.



Figure 12:- Variation of species densities (wood, gas, tar, and charcoal) over time at a carbonization temperature of 600 K using our data.



Figure 13:- Variation of species densities (wood, gas, tar, and charcoal) over time at a carbonization temperature of 650 K using our data.



Figure 14:- Variation of species densities (wood, gas, tar, and charcoal) over time at a carbonization temperature of 700K using our data.

For the adjusted data, we observe an increase in the density of charcoal for temperatures ranging from 580K to 600K, followed by a decrease in charcoal density for the remaining carbonization temperatures. On the other hand,

the density of the gas formed increases with the carbonization temperature. These observations are in line with the results from the literature according to Ganhoun al al. [5] and Faradji (2011) [21].

For a detailed analysis, simulations are conducted on the distribution of charcoal, gas, and tar using data from each author and the adjusted data from this study. The curve in Figure 14 below shows the variations in the yields of gas, charcoal, and tar using the data from Park and al



Figure 15:- Variation of yields in coal, gas, and tar as a function of temperature with the data from Park and al.

According to the curve, the yield of charcoal based on the data from Park et al. is approximately constant, hovering around 20%. On the other hand, the yield of gas increases with temperature, rising from 40% to 80%. Conversely, the yield of tar shows a decreasing trend with carbonization temperature, starting at 40% and almost reaching zero by 700K.

As for the adjustment of Thurner and Mann's data to the model, the variations in yields as a function of the reaction temperature are shown in Figure 16 below.



Figure 16:- Variation of yields in coal, gas, and tar as a function of temperature based on the adjustments of data from Thurner and Mann.

The data from Thurner and Mann are used in a study on hydrogen production based on the present model. Paradoxically, we observe that the yield of charcoal increases with the carbonization temperature, rising from 54% to around 74%, while the yields of gas and tar show a decreasing trend. Although this situation favors optimal charcoal production, it warrants review through an experimental approach to validate it or not. The curve in Figure 17 below shows the variations in yields of charcoal, gas, and tar using our data.



Figure 17:- Variation of yields in coal, gas, and tar as a function of temperature with our data.

The variations observed in the figure show two trends for the yield of charcoal. From 550K to 600K, the yield increases with the carbonization temperature and then decreases for carbonization temperatures above 600K. Such a situation is in agreement with the results available in the literature on carbonization. Indeed, according to Ganhou et al. [5] and Spencer et al. [22], lower carbonization temperatures are quite favorable for optimal charcoal production. Thus, our data implemented in the model of Park et al. are numerically validated. As a result, the optimal temperature for charcoal production is between 590K and 610K.

## Summary of the Numerical Simulation Results

The results presented above can be summarized in four key points:

- Variability of species densities during the wood carbonization process: During simulations over the chosen temperature range, the density of wood decreases significantly, while the densities of gas and tar initially increase. The density of tar reaches a peak at 1300 seconds before decreasing, indicating that secondary reactions consume more tar than they produce after this peak.
- Yield evolution with temperature: The mass fraction of gas formed increases with the carbonization temperature, while that of charcoal increases up to 600K and then decreases. These results suggest that charcoal production is optimal at temperatures ranging from 590K to 610K.
- Validation of adjusted data: The adjustment of kinetic parameters related to reaction rate constants shows an increase in charcoal yield from 580K to 600K, followed by a decrease at higher temperatures. The gas yield, on the other hand, increases with temperature, consistent with the results in the literature.
- **Optimal temperature for charcoal production**: The simulations indicate that the optimal temperature to maximize charcoal production is between 590K and 610K, confirming that lower temperatures favor carbonization into charcoal rather than gas or tar

## **Discussion of Results:-**

### **Choice of Pyrolysis Model**

The choice of the pyrolysis model based on the work of Shafizadeh et al. (1977), later presented by Ganhou (2020) and other authors, demonstrates the importance and flexibility of the approach adopted to model the complex reactions involved in wood pyrolysis. The model with three primary parallel reactions and two secondary reactions allowed for a better understanding of the reaction interactions between the different chemical species generated during the process. This choice is justified by the model's ability to adapt to various operational conditions, as illustrated by the comparative studies conducted by Chan et al. (2009), Thurner and Mann, and Font et al.

The analysis of kinetic parameters reveals significant variations between studies. The reaction rate constants and activation energies show that wood decomposition into gas is favored at high temperatures, while charcoal formation appears to be optimized at lower temperatures (around 600K). The differences between studies (e.g., between the results of Park et al. and Thurner and Mann) highlight the importance of selecting experimental data and the analysis method for modeling purposes.

The adjustment of kinetic parameters in this study, following the Arrhenius law, is relevant for optimizing charcoal production. By considering catalysts, temperatures, and pretreatments, our optimization approach steers the process towards charcoal formation, while reducing the production of gas and tars. This multidimensional approach underscores the complexity of pyrolysis and the need for a deep understanding of the reaction mechanisms.

## **Carbonization Optimization**

Optimization through the adjustment of reaction parameters showed promising results. The use of specific catalysts and temperature control theoretically enabled an increase in charcoal yield, particularly by favoring wood decomposition at optimal temperatures. Our results suggest that the carbonization temperature of 600K is indeed a tipping point, where charcoal yield is maximized, which is consistent with previous observations in the literature. The numerical simulations show a reduction in wood density in line with an increase in the densities of pyrolysis products, highlighting the efficiency of the carbonization process. The curves illustrating the variation of species densities with different data highlight the competition between charcoal formation and other products, indicating the dominance of the wood decomposition reaction into charcoal at appropriate temperatures.

## **Comparison with Literature Data**

The of yields in charcoal, gas, and tar with the data from Park et al. and Thurner and Mann shows interesting divergences. Our approach allowed us to identify trends that confirm some existing theories while proposing adjustments that could be experimentally validated. For example, the constant charcoal yield of 20% in the data from Park et al. contrasts with the optimized results of this study, which show an increase in yield with appropriate adjustment of pyrolysis conditions.

The results this study have practical implications for semi-industrial and industrial carbonization process optimization. By adjusting kinetic parameters and controlling operational conditions, it is possible to significantly increase charcoal yield while reducing undesirable by-products. This could lead to improved efficiency in carbonization technologies and a reduction in associated environmental impacts. In the future, experimental studies should be conducted to validate the numerical approaches and the adjusted parameters. A more in-depth exploration of the effects of different catalysts and pretreatment techniques could also offer new perspectives for optimizing wood carbonization.

Over the past few decades, several authors have invested in both theoretical and experimental studies to better describe the complex mechanisms occurring during the thermal degradation of biomass. Beyond the single-reaction model, which dominated the discussions for several years and became a reference for most of these authors, several other models have been developed.

Based on the reaction rate constants, we optimized the carbonization process with concrete actions aimed at achieving optimal carbonization. The simulation of the mass balance equations was performed in MATLAB using the 4th-order Runge-Kutta method. The results obtained are in line with information available in the literature. Beyond the optimization techniques developed based on the reaction rate constants, another major outcome of this study concerns the optimal carbonization temperature, estimated between 590K and 610K, highlighting the importance of numerical modeling and optimization of reaction parameters in wood carbonization. This is our first step toward finding sustainable solutions for the production of wood energy. The results are promising and pave the way for future studies on the experimental validation of this work, particularly through the optimization of wood carbonization technologies.

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