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SEMI-EMPIRICAL MODEL FOR ESTIMATING MOLAR FRACTION OF SYNGAS PRODUCED BY THERMAL CRACKING OF WOOD TAR

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ABSTRACT

To optimize the efficiency of the wood gasification, tar which limits the use of syngas in thermal engines must be reduced. The quantity, quality and composition of syngas produced after thermal cracking of tar were analysed, and mathematical equations formulated based on Newton's bivariate polynomial interpolation were used to estimate the molar fraction of the gases. The conceptual analysis of the problem was based on experimental data on temperature and residence time, and the semi-empirical model was simulated using Matlab to predict the composition of the syngas and the tar content in the gas mixture. The thermal cracking of tar increased the amount of syngas produced; in particular, the molar fraction of carbon monoxide and hydrogen. The gasification energy efficiency also improved with temperature and residence time, as the quantity of tar was reduced during cracking. The model was validated by comparing experimental and numerical data.

Key words: Syngas, Gasification, Pyrolysis, Residence time, Thermal cracking of tar, Semi-empirical model

1. INTRODUCTION

Gasification is a thermo-chemical process involving pyrolysis and reduction reactions of the tar to produce syngas, chars and tars. The reduction reactions are Boudouard reaction (redox reaction of a mixture of CO and CO_2 in chemical equilibrium at a given temperature) and Water gas reaction (CO and water vapour to form CO_2 and hydrogen).

Several experimental, analytical and numerical studies have been conducted to examine the processes of gasification in order to determine the molar composition of the syngas [1]. The synthesis gas contains heavy hydrocarbons, and the tars make the gas unsuitable for running thermal engines, and therefore requires complete or partial removal [2 - 6]. The recommended concentration of tar are 10 - 50 mg/m^3 for engines and 8mg/m^3 for gas turbines [4]. The tar removal can be achieved by catalytic reforming in the gasifier using dolomites which decompose tar into gases [6, 7]. A model of three endothermic parallel reactions producing tar, gas and intermediate solid, and subsequent exothermic decomposition of the intermediate solid to char and decomposition of tar to char and gas has been developed [8].

The operating temperatures that reduce the residual tar content in the fuel gas in downdraft gasifiers range from 700 - 1000 °C, and results in decreased quantity of tar [9]. Tar removal by two-steps of decomposition and adsorption from the pyrolysis gas show reduction of the gravimetric tar mass by 78 % in the case of thermal cracking, and in the range of 77 – 92 % for steam and air forming [10]. Other techniques of purifying synthesis gas include washing with water to remove NH_3, wet electrostatic filtering and catalytic cracking, but the processes are either complex or very expensive for implementation. Simulation of the effect of input power and tar cracking on pyrolysis of wood for both microwave-induced and conventional heating has been studied [11].

To investigate the effect of residence time and temperature on the performance of gasification and tar thermal cracking for purifying the synthetic gasses, a semi-empirical model based on Newton polynomial method is presented in this paper. The model algorithm to estimate the amount of tar and syngas produced after the thermal cracking using bivariate or two variable functions of Newton form was developed. A Matlab code was implemented to simulate optimal conditions for production of the syngas, and model was validated using published experimental data for oak wood [5].

2. Experimental Data

Experimental data on molar fraction of syngas for residence time from 0.2 s to 4.3 s over temperature range of 500 to 900 °C in step of 100 °C during gasification of oak wood obtained by Fagbemi *et. al.* [1, 5], were used as input to develop the model. Tables 1 and 2 show data obtained from the experiments during pyrolysis with thermal cracking of the tar. (For completeness. (**Data for 600, 700 and 800 °C**)?

Table 1. Molar composition of pyrolysis gases for different residence times at 500 ˚C

% Pyrolysis Gas produced	Residence time (s)				
	0.4	**1.5**	**2.3**	**3.2**	**4.3**
CO	39.7	40.2	38.0	36.8	39.2
CO_2	36.6	41	37	31.5	31.0
H_2	7.6	4.5	6.4	7.2	10.6
CH_4	12.8	12	13	12.7	14.6

Table 2. Molar composition of pyrolysis gases for different residence times at 900 ˚C

% Pyrolysis Gas produced	Residence time (s)			
	0.2	**0.9**	**1.5**	**2.0**
CO	56.1	53	54	55
CO_2	6.5	4.7	4.1	3.5
H_2	25.3	28	30.1	32
CH_4	12.1	12	11.8	9.5

2. Kinetics of Thermal Cracking of Tar

The number of moles of syngas mixture (n_{gas}) and the mass fraction of the gas mixture (P_{gas}) produced by pyrolysis were calculated as [**reference**]

$$n_{gas} = \frac{P_{gas} M_{dw}}{100 \sum P_i M_i} \tag{1}$$

where M_{dw} is mass of dry wood, $\sum P_i M_i$ is average molar mass, P_i is molar fraction of gas i derived from the pyrolysis and M_i is molecular mass of gas i. **What is n_i ?**

$$n_i = P_i \times \frac{n_{gas}}{100} \tag{2}$$

The amounts of char, steam and residual tar were determined as molar fraction of char (n_{char}), molar fraction of steam (n_{H_2O}) and mass fraction of tar (m_{tar}) generated during pyrolysis were calculated by

$$n_{char} = \frac{M_{pc} M_{dw}}{12 \, x \, 100} \tag{3}$$

$$n_{H_2O} = \frac{M_{H_2O} M_{dw}}{18 \, x \, 100} \tag{4}$$

$$n_{tar} = \frac{M_{tar} M_{dw}}{100} \tag{5}$$

where M_{pc}, M_{H2O} and M_{tar} are respectively mass of pyrolysis char, mass of steam, and mass of tar. (**eqn. (6), is molecular mass of tar 1 ?**)

The residual mass of tar produced after cracking (production rate), P_{tar}, was calculated at cracking temperature T and residence time t by first-order kinetics for known tar production rate P_g as [**reference**],

$$P_{tar} = P_g e^{-Ct} \tag{6}$$

where t_s is residence time and C is kinetic constant defined by Arrhenius equation,

$$C = Ae^{-E/_{RT}} \tag{8}$$

activation energy E = 5.58×10^3 cal/mol, and A = 4.34 s^{-1} [1].

If P_g is amount of syngas produced by gasification, the amount of syngas produced from thermal cracking is [**reference**],

$$P_{gc} = (P_g - P_{tar}) \tag{9}$$

while the total amount of gas obtained from the pyrolysis (including thermal cracking of tar) is

$$P_{gr} = (P_{gazpyro} + P_{gc}) \tag{10}$$

where P_{gc} is amount of gas produced by thermal cracking and $P_{gazpyro}$ is amount of gas from the pyrolysis (without tar cracking).

The molar composition of gas and water vapor produced by the gasifier n_t is the sum of molar compositions of each gas species in **each zone** (**specify zones**), where $n_{CO}, n_{CO_2}, n_{H_2}, n_{CH_4}$ and n_{H_2O} respectively represent the amounts of CO, H_2, CO_2, CH_4, and steam at the end of pyrolysis,

$$n_t = n_{CO} + n_{CO_2} + n_{H_2} + n_{CH_4} + n_{H_2O} \tag{11}$$

so that end of the gasification,

$$n_{CO}^f = n_{CO} + \frac{n_{char}^1 (R_2)}{R_1} \tag{12}$$

$$n_{H_2}^f = n_{H_2} + \frac{n_{char}^1 \times R}{R_1} \tag{13}$$

$$n_{CO_2}^f = n_{CO_2} + q - \frac{n_{char}^1}{R_1} \tag{14}$$

$$n_{H_2O}^f = n_{H_2O} - \frac{n_{char}^1 \times R}{R_1} \tag{15}$$

$$n_{CH_4}^f = n_{CH_4} \tag{16}$$

$$n_{char}^1 = n_{Char} - q \tag{17}$$

where R_2 and R_1 are kinetic constant of Boudouard and Water gas reaction, defined as

$$R = \frac{R_2}{R_1} = 0.786\alpha\left(1 + P_{CO_2}\right) \frac{P_{H_2O}}{P_{CO_2}} e^{\left[\frac{-2000}{1.987T}\right]} \tag{18}$$

$\alpha = 8$ for $T < 800$ °C, $\alpha = 3$ for $T > 800$ °C.

The partial pressures of steam (H_2O) and CO_2 are calculated from the molar composition of the gases up to end of combustion, as

$$P_{H_2O} = \frac{n_{H_2O}}{n_t} \tag{19}$$

$$P_{CO_2} = \frac{n_{CO_2}}{n_t} \tag{20}$$

where $n_t = n_{CO} + n_{CO_2} + n_{H_2} + n_{CH_4} + n_{H_2O}$.

3. Modeling molar fractions of gases

3.1. Formulation of Newton bivariate polynomial interpolation

If a dependent variable z = f(x,y) is a two-variable function with tabular arranged data for interpolation, the two fit procedures for interpolation approximation are the successive univariate polynomial approximation and discrete multivariate polynomial approximation [12, 13]. Algorithms are required for computation of Newton form of polynomial function z =

f(x,y), and computation of the coefficients of the Newton form polynomial at reduced complexity to O(n^2).

For successive univariate approximation, a set of univariate approximation functions is fitted at each value of one of the independent variable, x_i, such that $z_i(y) = f(x_i,y)$. Interpolation is then performed on each of the univariate approximation functions to yield values of the desired operation at the specified value of the other independent variable, e.g. $z_i(y^*) = z_i(x_i, y^*)$. The final process of interpolation is performed on that univariate approximation function of any functional form.

Using successive univariate quadratic polynomial interpolation,
$z(x_i, y) = a + by + cy^2$
can be fitted at each x_i to interpolate for the value of y at y_i. The coefficients or constants a, b, c are solved by Gaussian elimination. Error in results is $z_i(x_i,y_i) = f(x_i,y_i)$ – data value fit.

Discrete multivariate polynomial approximation of bivariate function, z = f(x, y) and set of tabular data, can be fitted by multivariate polynomial of the general form,
$z = a + bx + cy + dxy + ex^2 + fy^2 + gx^2y + hxy^2 + jx^3 + ky^3 + lx^3y + mxy^3 + nx^4 + py^4 + rx^4y + sxy^4$. The number of data points must equal to the number of coefficients of the polynomial. Linear bivariate polynomial in x and y is obtained by including the first 4 terms, while quadratic bivariate polynomial in x and y is obtained by including the first 8 terms. The number of terms in the approximating polynomial increases rapidly as the degree of approximation increases, leading to ill-conditioned system of linear equations for determining the coefficients.

The interpolating polynomial with the form, $p(x,y) = \sum_{i=0}^{n}\sum_{j=0}^{n-1} a_i\, x^{i,j}$ has total n = degree [p(xy)] and defined uniquely in the following set of $n = \binom{m+2}{n}$ interpolations.

Recursive algorithm for computation of the Newton interpolation of a given two variable function, permits determination of multivariate interpolating function which interpolates a given data set over a set of multivariate basis functions.

3.2. Algorithms and Solution analysis

To find a value of unknown function f at point (x, y), values of f at four points $Q_{11}(x_1, y_1)$, $Q_{12}(x_1,y_2)$, $Q_{21}(x_2,y_1)$ and $Q_{22}(x_2,y_2)$ were assumed to be known. The key is to perform bilinear interpolation, which is an extension of linear interpolation for interpolation function of two variables, e.g. perform (x,y) in a rectilinear two dimensional grid in one direction, and then followed in the other direction. Although each step is linear in the sampled value and in the position, the interpolation as a whole is not linear, but rather quadratic in the sample location [13]. The steps for the bilinear interpolation algorithm are:

Step 1: Perform linear interpolation in x-direction to yield:

$$f(x,y_1) \approx \frac{x_2-x}{x_2-x_1}f(Q_{11}) + \frac{x-x_2}{x_2-x_1}f(Q_{21}) \quad (21)$$

$$f(x,y_2) \approx \frac{x_2-x}{x_2-x_1}f(Q_{12}) + \frac{x-x_2}{x_2-x_1}f(Q_{22}) \quad (22)$$

Step 2: Proceed by interpolating in the y-direction to obtain the desired estimate:

$$f(x,y) \approx \frac{y_2-y}{y_2-y_1}f(x,y_1) + \frac{y-y_1}{y_2-y_1}f(x,y_2)$$

$$\approx \frac{y_2-y}{y_2-y_1}\left(\frac{x_2-x}{x_2-x_1}f(Q_{11}) + \frac{x-x_1}{x_2-x_1}f(Q_{21})\right) +$$

$$\frac{y-y_1}{y_2-y_1}\left(\frac{x_2-x}{x_2-x_1}f(Q_{12}) + \frac{x-x_2}{x_2-x_1}f(Q_{22})\right)$$

$$= \frac{1}{(x_2-x_1)(y_2-y_1)}\big(f(Q_{11})(x_2-x)(y_2-y)$$
$$+f(Q_{21})(x-x_1)(y_2\,y)f(Q_{12})(x_2-x)(y-y_1)$$
$$+f(Q_{22})(x-x_1)(y-y_1)\big)$$

$$= \frac{1}{(x_2-x_1)(y_2-y_1)}\begin{bmatrix} x_2-x & x-x_1 \end{bmatrix}$$
$$\begin{bmatrix} f(Q_{11}) & f(Q_{12}) \\ f(Q_{21}) & f(Q_{22}) \end{bmatrix}\begin{bmatrix} y_2-y \\ y-y_1 \end{bmatrix} \quad (23)$$

The same result is obtained if the interpolation is done first along the y-direction and then along the x-direction.

By alternative algorithm, the solution to the interpolation problem is of the form,
$f(x,y) \approx a_0 + a_1x + a_2y + a_3xy$
where the coefficients are found by solving the linear system,

$$\begin{bmatrix} 1 & x_1 & y_1 & x_1y_1 \\ 1 & x_1 & y_2 & x_1y_2 \\ 1 & x_2 & y_1 & x_2y_1 \\ 1 & x_2 & y_2 & x_2y_2 \end{bmatrix}\begin{bmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} f(Q_{11}) \\ f(Q_{12}) \\ f(Q_{21}) \\ f(Q_{22}) \end{bmatrix} \quad (24)$$

If a solution is preferred in terms of f(Q) then,

$$f(x,y) \approx b_{11}f(Q_{11}) + b_{12}f(Q_{12}) + b_{21}f(Q_{21}) + b_{22}f(Q_{22}) \quad (25)$$

where the coefficients are found by solving

$$\begin{bmatrix} b_{11} \\ b_{12} \\ b_{21} \\ b_{22} \end{bmatrix} = \left(\begin{bmatrix} 1 & x_1 & y_1 & x_1y_1 \\ 1 & x_1 & y_2 & x_1y_2 \\ 1 & x_2 & y_1 & x_2y_1 \\ 1 & x_2 & y_2 & x_2y_2 \end{bmatrix}^{-1}\right)^{T}\begin{bmatrix} 1 \\ x \\ y \\ xy \end{bmatrix} \quad (25)$$

Table 3. Constants of the Syngas functions

Constants for CO function	$A_0 = 4657.819$	$A_1 = -27.663$	$A_2 = 6.093 \times 10^{-2}$	$A_3 = -5.857 \times 10^{-5}$	$A_4 = 2.079 \times 10^{-8}$
	$B_0 = -7407.943$	$B_1 = 44.293$	$B_2 = -9.745 \times 10^{-2}$	$B_3 = 9.368 \times 10^{-5}$	$B_4 = -3.328 \times 10^{-8}$
	$C_0 = 3280.374$	$C_1 = -19.716$	$C_2 = 4.365 \times 10^{-2}$	$C_3 = -4.232 \times 10^{-5}$	$C_4 = 482.025 \times 10^{-8}$
	$D_0 = -482.025$	$D_1 = 2.932$	$D_2 = -6.586 \times 10^{-3}$	$D_3 = 6.495 \times 10^{-6}$	$D_4 = -2.376 \times 10^{-9}$
Constants for H_2 function	$A_0 = -1398.635$	$A_1 = 8.483$	$A_2 = -1.884 \times 10^{-2}$	$A_3 = 1.831 \times 10^{-5}$	$A_4 = -6.546 \times 10^{-9}$
	$B_0 = 5707.424$	$B_1 = -34.272$	$B_2 = 7.554 \times 10^{-2}$	$B_3 = -7.261 \times 10^{-5}$	$B_4 = 2.574 \times 10^{-8}$
	$C_0 = -3512.859$	$C_1 = 21.098$	$C_2 = -4.653 \times 10^{-2}$	$C_3 = 4.476 \times 10^{-5}$	$C_4 = -1.588 \times 10^{-8}$
	$D_0 = 529.614$	$D_1 = -3.182$	$D_2 = 7.024 \times 10^{-3}$	$D_3 = -6.763 \times 10^{-6}$	$D_4 = 2.402 \times 10^{-9}$
Constants for CH_4 function	$A_0 = 844.62$	$A_1 = -5.358$	$A_2 = 1.268 \times 10^{-2}$	$A_3 = -1.303 \times 10^{-5}$	$A_4 = 4.898 \times 10^{-9}$
	$B_0 = -6145.736$	$B_1 = 37.078$	$B_2 = -8.275 \times 10^{-2}$	$B_3 = 8.098 \times 10^{-5}$	$B_4 = -2.931 \times 10^{-8}$
	$C_0 = 4643.694$	$C_1 = -28.116$	$C_2 = 6.295 \times 10^{-2}$	$C_3 = -6.178 \times 10^{-5}$	$C_4 = 2.242 \times 10^{-8}$
	$D_0 = -901.697$	$D_1 = 5.489$	$D_2 = -1.236 \times 10^{-2}$	$D_3 = 1.22 \times 10^{-5}$	$D_4 = -4.453 \times 10^{-9}$
Constants for CO_2 function	$A_0 = 2357.79$	$A_1 = -13.755$	$A_2 = 3.016 \times 10^{-2}$	$A_3 = -2.912 \times 10^{-5}$	$A_4 = 1.041 \times 10^{-8}$
	$B_0 = -3558.844$	$B_1 = 22.161$	$B_2 = -5.028 \times 10^{-2}$	$B_3 = 4.952 \times 10^{-5}$	$B_4 = -1.792 \times 10^{-8}$
	$C_0 = 2580.398$	$C_1 = -15.906$	$C_2 = 3.584 \times 10^{-2}$	$C_3 = -3.510 \times 10^{-5}$	$C_4 = 1.265 \times 10^{-8}$
	$D_0 = -488.254$	$D_1 = 2.981$	$D_2 = -6.669 \times 10^{-3}$	D_3 6.499×10^{-6}	$D_4 = -2.334 \times 10^{-9}$

3.3. Estimating Molar fractions of the gases

Estimation of the molar fractions of pyrolysis gases from the thermal cracking tar was formulated from a function of two variables, temperature (T, °C) and the residence time (t, s), of the wood in the gasification reactor, such that n = f(T, t). Knowing the four points consisting of t as abscissa and T as ordinate, the molar fractions for temperatures 500, 600, 700 and 800 °C (Tables 1 and 2) were set up as a quadratic function to express the molar fraction of gas as a function of the variables T and t.

For T=500 °C,

$$\%gas = f(t) = a_0 + b_0 t + c_0 t^2 + d_0 t^3 \quad (26)$$

where t is residence time and a_0, b_0, c_0, $d_0 \neq 0,0,0,0$, are constants. Similarly, for T = 600 °C, 700°C, 800 °C and 900 °C respectively,

$$\%gas = f(t) = a_1 + b_1 t_s + c_1 t^2 + d_1 t^3$$
$$\%gas = f(t) = a_2 + b_2 t_s + c_2 t^2 + d_2 t^3$$
$$\%gas = f(t) = a_3 + b_3 t_s + c_3 t^2 + d_3 t^3$$
$$\%gas = f(t) = a_4 + b_4 t_s + c_4 t^2 + d_4 t^3$$

and in general form;

$$\%gas = a + b t_s + c t^2 + d t^3 \quad (27)$$

The constants a, b, c, d in eqn, (27) of the function are expressed as an equation of degree 4 in terms of temperature T,

$$a = A_0 + A_1 \times T + A_2 \times T^2 + A_3 \times T^3 + A_4 \times T^4$$
$$b = B_0 + B_1 \times T + B_2 \times T^2 + B_3 \times T^3 + B_4 \times T^4$$
$$c = C_0 + C_1 \times T + C_2 \times T^2 + C_3 \times T^3 + C_4 \times T^4$$
$$d = D_0 + D_1 \times T + D_2 \times T^2 + D_3 \times T^3 + D_4 \times T^4$$

and upon substitution of the constants into general eqn. (22), gave expression for the molar fraction of the syngas by Newton's method as,

$$\%gas = (A_0 + A_1 T + A_2 T^2 + A_3 T^3 + A_4 T^4) + (B_0 + B_1 T + B_2 T^2 + B_3 T^3 + B_4 T^4)t + (C_0 + C_1 T + C_2 T^2 + C_3 T^3 + C_4 T^4)t^2 + (D_0 + d_1 T + D_2 T^2 + D_3 T^3 + D_4 T^4)t^3 \quad (28)$$

Equation (28) was used as the function for estimating the molar fraction of the various gases of pyrolysis resulting from thermal cracking of wood tar for different residence times and temperatures.

Following the analysis of Newton bivariate polynomial interpolation in Section 3.1, and applying the algorithms set up in Section 3.2, a Newton Method Matlab Code shown in Appendix I was developed to calculate the coefficients in eqn. (28), and hence, evaluate the molar fraction of CO, H_2, CH_4, and CO_2 produced after tar thermal cracking of wood chips. The calculated coefficients of eqn. (31) are given in Table 3.

4. Model Results and Validation

The Matlab code was implemented to simulate the gasification, pyrolysis and thermal cracking of chips of wood at temperatures of 500 °C, 700 °C and 900 °C and residence times of 0,4 s, 1.1 s and 2 s to determine the numerical values of the molar fraction of the syngas produced.

These numerical values were compared with the experimental data to examine the residual errors associated with the modeling of the fuel gases as shown in Table 4. The numerical values are in agreement with the experimental data, testifying to the accuracy of the model and precision of the results.

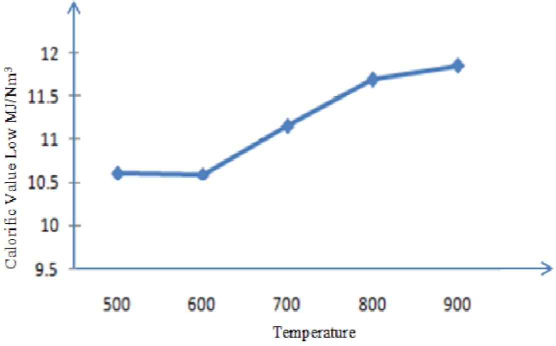
Table 4. Residual error analysis of model data and experimental data

Test Conditions	**Pyrolysis gas**	**Numerical Values (%)**	**Experimental values(%)**	**Residuals (%)**
T=500°C t_s = 0.4s	CO	3.9699e+001	39.7	0.001
	H_2	7.599e+000	7.6	0.001
	CH_4	1.280e+001	12.8	0.0
	CO_2	3.6599e+001	36.6	0.099
Test Conditions	**Pyrolysis gas**	**Numerical Values (%)**	**Experimental values (%)**	**Residuals (%)**
T=700°C t_s = 1.1s	CO	4.4999e+001	45	0.001
	H_2	1.6699e+001	16.7	0.001
	CH_4	1.6399e+001	16.4	0.001
	CO_2	1.6100e+001	16.1	0.0
Test Conditions	**Pyrolysis gas**	**Numerical Values (5)**	**Experimental values (5)**	**Residuals (%)**
T=900°C t_s = 2.0 s	CO	5.4999e+001	55	0.001
	H_2	3.1999e+001	32	0.001
	CH_4	9.499e+000	9.5	0.001
	CO_2	3.499e+000	3.5	0.001

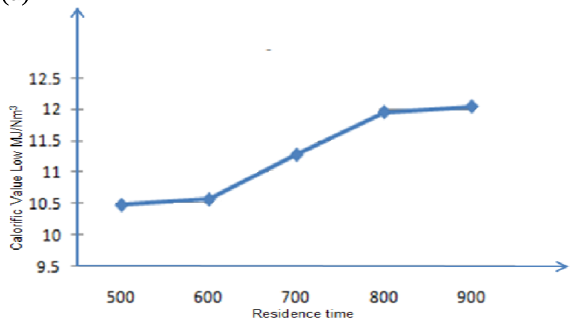
5. Numerical Experimentation

5.1. Calorific value of syngas

The semi-empirical model was applied to examine the influence of thermal cracking of the tar on calorific value and quantity of syngas produced at different temperatures and residence times. One mole of wood chips of 10 % water content (**dry or wet basis?**) was gasified with a mole of oxygen for residence times of 0.3 s, 1.1 s, and temperatures of 500, 600, 700, 800 and 900°C. At the end of gasification, the calorific value of syngas were predicted as shown in Fig. 1 (a, b). (**How were the data obtained for the graphs; simulations required**)



(a)



(b)

Fig. 1. Calorific value at different temperature for residence time (a). 3 s, (b). 1.1 s

(**The plot must be in black lines, not blue**?)

5.2. Quantity of syngas

For the syngas produced after the numerical experimentation for t = 0.35, 1.4 and 3.8 s at T = 600 °C, and t = 0.3, 1.1 and 3.1 at T = 800 °C, the evolution of the molar composition and quantity of the syngas are illustrated in Figs 2, 3, and 4.

From the graphs, the quantity of gas produced at end of gasification appreciably increased according to the residence time whatever the temperature of the reaction, which is opposite to the results for molar fractions. The molar fractions of CO_2 and CH4 show reduction and slow growth at the low temperatures, compared to values at high temperatures; while the molar fractions of H_2 and CO respectively showed slow increase and reduction at all temperatures of reaction.

6. DISCUSSION

The increase in quantity of syngas increased with increase in temperature and residence time as observed by Hellgren and *al.* [14]. There was a reduction in the amount of carbon dioxide, an increase in molar fraction of hydrogen and a high production of carbon monoxide dependence on high temperatures, as confirmed by Houben et *al.* [15] and Morf et *al.* [3]. In addition, the significant increase of the calorific value of gas of gasification was dependent on temperature and residence time.

7. CONCLUSIONS

A semi-empirical model was developed to determine the molar composition of syngas produced by gasification, pyrolysis and thermal cracking of the wood over different regimes of temperatures and residence times.

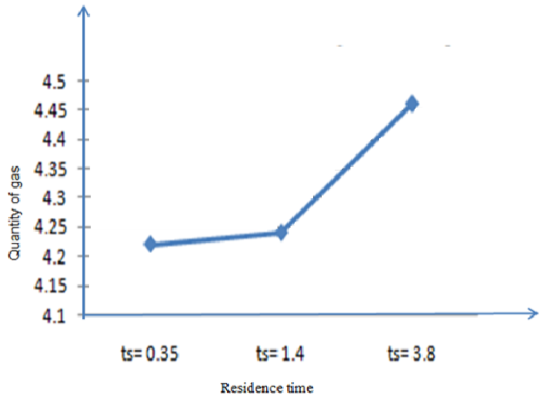


Fig 2. Evolution of quantity of gas produced at T = 600 °C for different residence times

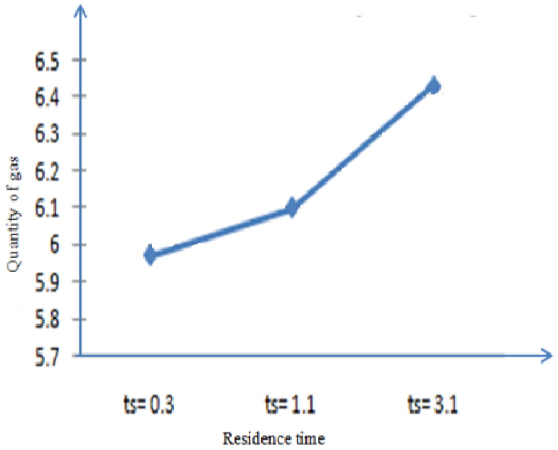


Fig 4. Evolution of quantity of gas produced at T=800°C for different residence times.

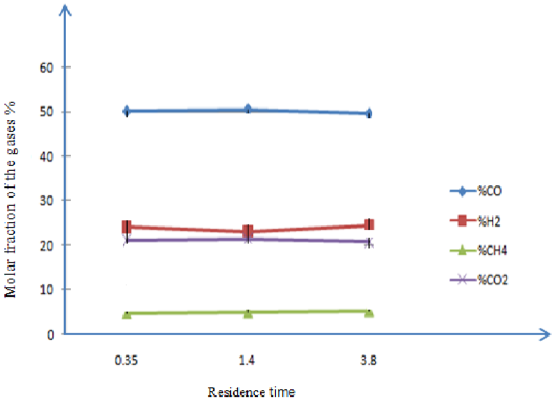


Fig 5. Evolution of the molar fractions of gases as function residence time at T=600°C

The model was based on fitting Newton’s polynomial functions to experimental data to predict the molar fractions of the gasses produced. Thermal cracking of the tar of pyrolysis improved qualitatively and quantitatively the syngas output of the process of gasification.

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Appendix I: Newton Method Code

```
n=-4;
while n<=0
n = input('Enter the number of points: ');
if (n<=0)
     disp('you must enter only a positive number');
end
end
     de=0;
     while (n>de || n<de)
x = input('Entrer in the ascending order the abscissa of the points in form X=[ x1 x2 x3   xn]:');
dim=size(x);
de=dim(2);
if (n>de || n<de)
    disp('you must enter numbers on abscissa corresponding to the number of points');
end
   end
de=0;
while (n>de || n<de)
y = input('Enter in ascending order of ordinate of the points in the form Y=[ y1 y2   yn]:');
dim=size(y);
de=dim(2);
if (n>de || n<de)
    disp('you must enter numbers on ordinate corresponding to the number of points');
end
  end
tab=diffdiv(x,y);
disp('Here is the table of differences divided:');
disp(tab);
s=size(x);
d=s(1,2);
disp('here are the coefficients of the polynomial:');
for i=1:d
    coef(i)=tab(1,i);
    disp(coef(i));
end
disp('Here are the abscissa to be used in the establishment of the function:');
for j=1:(n-1)
    c(j)=x(j);
    disp(c(j));
end
i=1;
for t=500:0.0001:600
   f(i)=evaluation1(n,coef,c,t);
   i=i+1;
end
S=500:0.0001:600;
```

```
plot(S,f);
  r=1;
while r<2
t = input('Entrer the abscissa of point to have the ordinate:');
U=evaluation1(n,coef,c,t);
disp(U);
r=input('Type 1 to change the abscissa: ');
end
function table=diffdiv(x,y)
s=size(x);
d=s(1,2);
table=zeros(d,d);
for i=1:d table(i,1)=y (i) ;
end
for k=2:d
for i=1:d-k+1
table(i,k)=((table(i+1,k-1)-table(i,k-1))./(x(i+k-1)-x(i)));
%disp(table(i,k));
end
end

for j=1:i
    for l=1:k
    table(j,l);
end
end
end
function val=evaluation1(n,a,c,t)
%Evaluation of a polynomial function at point t
somme=0;
for i=1:n
produit=1;
for j=1:i-1
produit=produit*(t-c(j));
%disp('abscissa');
%disp(c(j)); end
somme=somme+a(i)*produit;
%disp('coeficient');
%disp(a(i));
end
val=somme;
end
```