

DIFFERENTIAL EVOLUTION METHOD APPLIED TO KINETIC PARAMETERS ESTIMATION OF BAGASSE PYROLYSIS

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Abstract. In the present paper, the Independent Parallel Reaction Model (IPR Model) is applied to describe the slow dynamic pyrolysis of sugar cane bagasse, which is studied by thermogravimetric analysis of three ranges of particles diameter. The kinetic parameters and mass fraction of each principal pseudo-component of biomass (hemicellulose, cellulose and lignin) are estimated using the Differential Evolution Algorithm. Good fits to weight loss curve were obtained at different heating rates. The mass fractions and Arrhenius parameters estimated are compared with the experimental values reported by literature with good agreement.

1 INTRODUCTION

The pyrolysis process have been widely studied and considered as a good alternative to renewable energy generation, since it can generate products with high calorific power from reusable materials. This process consists in producing gases, liquid fuels (volatiles) and char by the thermal decomposition, in absence of an oxidant agent, like O₂ (Di Blasi, 1998).

Many materials types have been extensively used for power generation from pyrolysis, that includes biodegradable products (Kopinke et al., 1996; Soares et al., 2006), municipal waste (Islam et al., 2004; Garcia et al., 1995), animal substances (Ayllón et al., 2006; Purevsuren et al., 2004; Wiggers et al., 2009), residues from agriculture (Shinogi and Kanri, 2003; Uzun et al., 2006), as well as forestry (Paradela et al., 2009) and related industries (Chen et al., 2001; Moltó et al., 2009; Huang and Tang, 2009; Lee, 2007; Yang and Jiang, 2009).

The processing of sugar cane, much used in the production of sugar and alcohol, creates large quantities of fibrous residue called bagasse. Due to his abundance in the central region of Brazil, sugarcane bagasse was selected as material to carry out the pyrolysis in this work. Like most of biomass waste, the bagasse is basically composed by hemicellulose, cellulose and lignin (González et al, 2003). Some kinetic models are based in individual decomposition of these pseudo-components, like the three independent parallel reaction model.

The knowledge of kinetic and transport phenomena that characterize the reactor is essential to design and optimization of pyrolysis process (Hu et al., 2007), in order to achieve industrial application. Thermogravimetric analysis (TG) is a simple and straightforward manner to obtain mass loss data in kinetic control regime, in order to estimate the parameters which describe the pyrolysis kinetic. The thermogravimetric technique also shows that characteristics of pyrolysis process are dependent of kind of biomass and the specific proportions of the components present in it (Li et al., 2008).

Some kinetic models are available in literature, like single reaction model (González et al, 2003, Varhegyi et al., 1989; Radmanesh et al., 2006; Conesa et al., 2004; Senneca, 2007; Brink and Massoudi, 1978; Roberts and Clough, 1956), consecutive reaction model (Gronli et al., 1999; Mui et al., 2008; González et al., 2003; Rao et al., 1998; Williams and Besler, 1993), pseudo-components reaction model, also called independent parallel reaction model (Gómez, 2006; Vamvuka et al., 2003; Manyà and Araùzo, 2008; Várhegyi, et al., 2002; Órfão et al., 1999; Manyà et al., 2003; Gómez, et al., 2004; Müller-Hagedorn and Bockhorn, 2007). Due to the high variability in composition from one biomass species to another, exists an inherent difficulty to fit DTG curves (Gómez, 2006). The Independent Parallel Reaction Kinetic Model is a practical mathematic way to describe the DTG curve. Here, the pseudo-components are degraded individually in the same temperature range, guaranteeing a possible simultaneous decomposition. So, the rate of weight loss is calculated considering the individual reaction rates and their respective mass fraction. Hu et al. (2007) applied this model to estimate the mass fraction of each subcomponent and the reaction orders. The results of devolatilization of biomass reported in literature show that this model provides consistent parameters values (Hu et al., 2007, Gómez, 2006; Vamvuka et al., 2003; Manyà and Araùzo, 2008; Várhegyi, et al., 2002; Órfão et al., 1999; Manyà et al., 2003; Gómez et al., 2004; Müller-Hagedorn and Bockhorn, 2007), and presents a very low fitting error.

In the parameter estimation context, optimization methods based on the natural phenomena and structural approaches have been developed to overcome the problems associated with the classical optimization methods (Deb, 2001, Storn et al., 2005). Differential Evolution Algorithm (DE), developed by Storn and Price (1995) is one of the most of promising methods. This approach has been empirically demonstrated to be an efficient and robust optimization method that outperforms some traditional Genetic Algorithm (Babu and Sastry,

1999). DE has been applied with success (Storn et al., 2005; Maciejewski et al., 2007; Souza et al., 2007; Lobato et al., 2010).

In this work, a three independent parallel reaction model is used to estimate the kinetic parameters of sugarcane pyrolysis from thermogravimetric experiments. The estimation is carried out applying the Differential Evolution Algorithm. The activation energy, pre-exponential factor of Arrhenius equation and the mass fraction of each subcomponent of biomass are calculated and compared with literature data, showing good agreement.

2 MATERIAL AND METHODS

2.1 Preparation and Characterization of Bagasse

The bagasse was initially dried at 353 K for 24 h. After grinding, the bagasse was sieved to obtain three sets of particles: S_1 ($d_p < 0.35$ mm), S_2 ($0.35 \leq d_p < 1.18$ mm) and S_3 ($1.18 \leq d_p < 2$ mm). The Table 1 shows the chemical composition, in % (wt/wt), from classical elemental analysis, values of density, ash content and moisture for each set of particle.

The elemental analysis was performed on the equipment Ea1108 Fisons Instruments. The moisture content was estimated gravimetrically before and after the drying in an oven at 398 K for 24 h. The density was measured by gas pycnometer method, using N_2 . The surface area of sample was estimated in equipment Asap 2020 (Micrometrics), while the ash content was calculated from tests in muffle.

The moisture content of bagasse showed no clear relationship with the particle diameter, as demonstrated in. As expected, the set of smaller particle diameter have a greater surface area and consequently, higher ash content. García-Pérez et al. (2002) studied the vacuum pyrolysis of sugarcane bagasse and found the same relationship between particle size and ash content. The density value of particles increases with the decreasing of particle size. The highest density of smaller particles is explained by lower contain of micro-pores.

Set of particles	d_p [mm]	Elementary Analysis			Ash (%)	Moisture (%)	Density [$g\ cm^{-3}$]	Surface Area [$m^2\ g^{-1}$]
		N(%)	C(%)	H(%)				
S_1	<0.35	0.44	45.78	5.72	8.34	8.02	1.335	0.6446
S_2	0.35 – 1.18	0.45	45.99	5.78	2.93	7.21	1.243	0.4685
S_3	1.18 - 2	0.38	47.32	5.91	1.43	8.97	1.141	0.2399

Table 1 – Sugar cane bagasse proprieties.

2.2 Thermogravimetry tests

The experiments have been performed with a thermogravimetric analyzer TGA 50 (Shimadzu), under conditions of kinetic control. The sample temperature was measured with a thermocouple directly at the crucible, very close to the sample. Approximately 2 to 4 mg of the bagasse was placed in the pan of the TGA microbalance, which was enough to fill the pan because of the low density of the bagasse. Initially, the samples were dried for 35 min at 398 K. After that, the furnace was heated to a programmed temperature of 1173.15 K at different heating rates (1.5, 5, 10, 20 and 50 $K\ min^{-1}$), under inert atmospheres performed by N_2 with a flow rate of 50 $ml\ min^{-1}$. Residual weight of the sample and its derivative, with respect to time and temperature, were recorded using TGA software.

3 KINETIC OF PRIMARY DECOMPOSITION: THREE INDEPENDENT PARALLEL REACTION MODEL

The kinetics of pyrolysis of biomass is complicated and it involves a large number of reactions in parallel and series (Vamvuka, et al., 2003). One of the most widely used models to describe the kinetic thermal decomposition of lignocellulosic materials is the independent parallel reactions model (IRP model), or n-pseudo-component model, known to exhibit excellent fit with experimental data.

This approach assume that the main pseudo-components (in general: hemicellulose, cellulose and lignin) degrade individually and simultaneously. The primary conversion of biomass into gases and volatiles, namely devolatilization, can be expressed by:

$$X = \frac{m_0 - m}{m_0 - m_\infty} \quad (1)$$

The dependence of the conversion rate with temperature (T) can be represented by an Arrhenius relationship. The reaction rate of each subcomponent can be written individually as:

$$\frac{dX_i}{dt} = \kappa_{0i} \exp\left(-\frac{E_{ai}}{RT}\right) (1 - X_i)^{n_i} \quad (2)$$

where, X_i , κ_{0i} , E_{ai} and n_i are the conversion, the pre-exponential factor, activation energy and apparent reaction order, for each subcomponent i , t is the time, T is temperature, and R is the universal gas constant.

The overall rate of reaction is a linear combination of the rates of partial reactions, considering the mass fraction of each of the three subcomponents c_i :

$$\frac{dX}{dt} = -\sum_{i=1}^3 c_i \frac{dX_i}{dt} \quad (3)$$

Thus, the weight loss over time is determined by the following relationship:

$$\frac{dm^{calc}}{dt} = -(m_0 - m) \sum_{i=1}^3 c_i \frac{dX_i}{dt} \quad (4)$$

The unknown parameters of the model are determined by the evaluation of the experimental data using least squares non-linear methods. Therefore, the objective function ($O.F.$) to be minimized, was performed by the curve of mass loss (TG), generating the objective function described by Eq. (5). An objective function based in DTG data was defined by Eq.(6) only to calculate the fitting error on DTG curve.

$$O.F._{TG} = \sum_{j=1}^N \left(m(t)_j^{obs} - m(t)_j^{calc} \right)^2 \quad (5)$$

$$O.F._{DTG} = \sum_{j=1}^N \left((dm/dt)_j^{obs} - (dm/dt)_j^{calc} \right)^2 \quad (6)$$

In order to compare with the literature results, the deviation between the observed and the calculated TG and DTG curves at the optimal set of parameters was given in percentage of the highest measured:

$$FIT_{TG} (\%) = 100 \sqrt{(O.F._{TG})/N} / \max(|m_j^{obs}|) \quad (7)$$

$$FIT_{DTG} (\%) = 100 \sqrt{(O.F._{DTG})/N} / \max(|(dm/dt)_j^{obs}|) \quad (8)$$

For make the estimates, the hemicellulose and cellulose decomposition reactions were approximated as first-order, but the pyrolysis of lignin cannot be modeled by first-order kinetics (Li et al., 2008). Several works report a better fit to experimental data when the behavior of the last subcomponent, lignin, is described by a third-order reaction (Lee, 2007; González et al., 2003; Hu et al., 2007; Li et al., 2008).

4 DIFFERENTIAL EVOLUTION ALGORITHM

The DE algorithm is an evolutionary optimization technique proposed by Storn and Price (1995) to solve the Chebyshev polynomial fitting problem. This approach differs from other evolutionary algorithms in the scheme for mutation and recombination phase used. According to Storn et al. (2005) the main advantages of their method are the following: simple structure, easiness of use, speed and robustness. Moreover, the main disadvantage is the high number of objective function evaluations.

The control parameters in DE are the following: N, the population size, CR, the crossover constant and, D, the weight applied to random differential (perturbation rate). According to Storn and Price (1995), N should be about 5–10 times the dimension (number of parameters in a vector) of the problem, D and CR should be in the range 0.4–1.0.

A generic DE algorithm is presented bellow (Storn et al., 2005).

Differential Evolution

```

Initialize and evaluate population P
while (not done)
{ for (i = 0 ; i < N ; i++)
  { Create candidate C[i]
    Evaluate C[i]
    if (C[i] is better than P[i])
      P'[i] = C[i]
    else
      P'[i] = P[i]
  }
P = P'
}

```

where P is the population of the current generation, and P' is the population to be formed for the next generation. The routine Create candidate C[i] is listed bellow.

Create candidate C[i]

Randomly select parents P[i₁], P[i₂], and P[i₃] where i, i₁, i₂, and i₃ are different.

Create initial candidate C₁[i] = P[i₁] + D × (P[i₂] - P[i₃]).

Create final candidate C[i] by crossing over the genes of P[i] and C₁[i] as follows:

```

for (j = 0 ; j < N ; j++)
{ if (r < CR)
  C[i][j] = C1[i][j]
  else
  C[i][j] = P1[i][j]
}

```

where $C[i]$ is the candidate solution with population index i , $C[i][j]$ is the j -th entry in the solution vector of $C[i]$, r is a random number between 0 and 1.

The general convention used for different configurations of DE is DE/ α / β / γ . Here DE stands for DE algorithm, α represents a string denoting the vector to be perturbed; β is the number of difference vectors considered for perturbation of α ; and γ is the type of crossover being used (exp-exponential and bin-binomial). Here the perturbation can be made either in the best vector of the previous generation (best) or in any randomly chosen vector (rand). Similarly, for perturbation, either single or two vector differences can be used. For perturbation with a single vector difference, out of the three distinct randomly chosen vectors, the weighted vector differential of any two vectors is added to the third one. Similarly, for perturbation with two vector differences, five distinct vectors other than the target vector are chosen randomly from the current population. Out of these, the weighted vector difference of each pair of any four vectors is added to the fifth one for perturbation. In the binomial crossover, this operator is performed on each one of the decision variables whenever a randomly picked number between 0 and 1 is within the crossover constant value.

DE has been successfully applied to various fields such as digital filter design (Storn, 1995), batch fermentation process (Chiou and Wang, 1999), estimation of heat transfer parameters in a bed reactor (Babu and Sastry, 1999), synthesis and optimization of heat integrated distillation system (Babu and Singh, 2000), optimization of an alkylation reaction (Babu and Gaurav, 2000), parameter estimation in fed-batch fermentation process (Wang et al., 2001), optimization of thermal cracker operation (Babu and Angira, 2001), engineering system design (Lobato and Steffen, 2007), economic dispatch optimization (Coelho and Mariani, 2007), identification of experimental data (Maciejewski et al., 2007), apparent thermal diffusivity estimation during the drying of fruits (Mariani et al., 2008), estimation of drying parameters in rotary dryers (Lobato et al, 2008), solution of inverse radiative transfer problems in two-layer participating media (Lobato et al, 2010), and other applications (Storn et al., 2005).

5 RESULTS AND DISCUSSIONS

5.1 Pyrolysis Characteristics

The Figure 1 and Figure 2 show the TG and DTG curves, respectively, at heating rates of 1.5, 5, 10, 20 and 50 K min⁻¹ for all sets of particles. The degradation of lignin remaining is clearly noticeable only for the lower heating rate (1.5 K min⁻¹) for all particle sizes, as demonstrated in Figure 1. Lignin decomposition occurs slowly over a very broad range of temperature, because at lower heating rates the reactions minimize the overlapping of events that are shifted to lower temperatures (Manyà J. Araùzo, 2008; Riegel et al., 2008). The weight loss rate curves consist of two visible peaks, which represent the decomposition of hemicellulose and cellulose, respectively (Hu et al., 2007). Three peaks can be visualized on DTG curve at high heating rates (50 K min⁻¹), being the former two are related to the degradation of hemicellulose (Varhegyi et al., 1989).

The maximum pyrolysis rate increases with increasing heating rate for the three sets of particles, as demonstrated in the Figure 2. The peak temperature in DTG curve for larger particles (S_3) also increases directly with heating rate (Figure 2 (c)): 598 K to 1.5 K min⁻¹, 613 K to 5 K min⁻¹, 631 K to 10 K min⁻¹, 642 K to 20 K min⁻¹ and 657 K to 50 K min⁻¹. Manyà and Araùzo (2008) found a similar value of activation energy for bagasse pyrolysis (643 K, to 20 K min⁻¹).

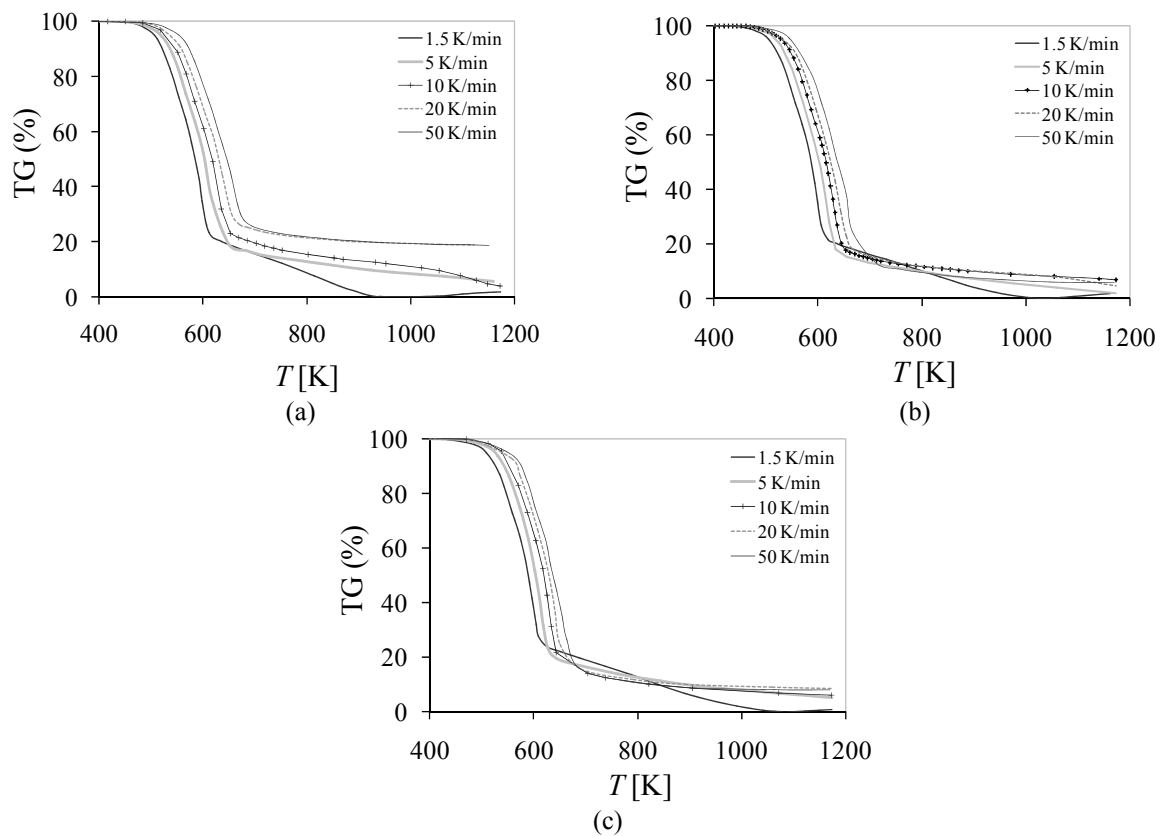


Figure 1– Mass fraction of non-reacted bagasse as a function of temperature, at different heating rates: (a) S_1 ; (b) S_2 and (c) S_3 .

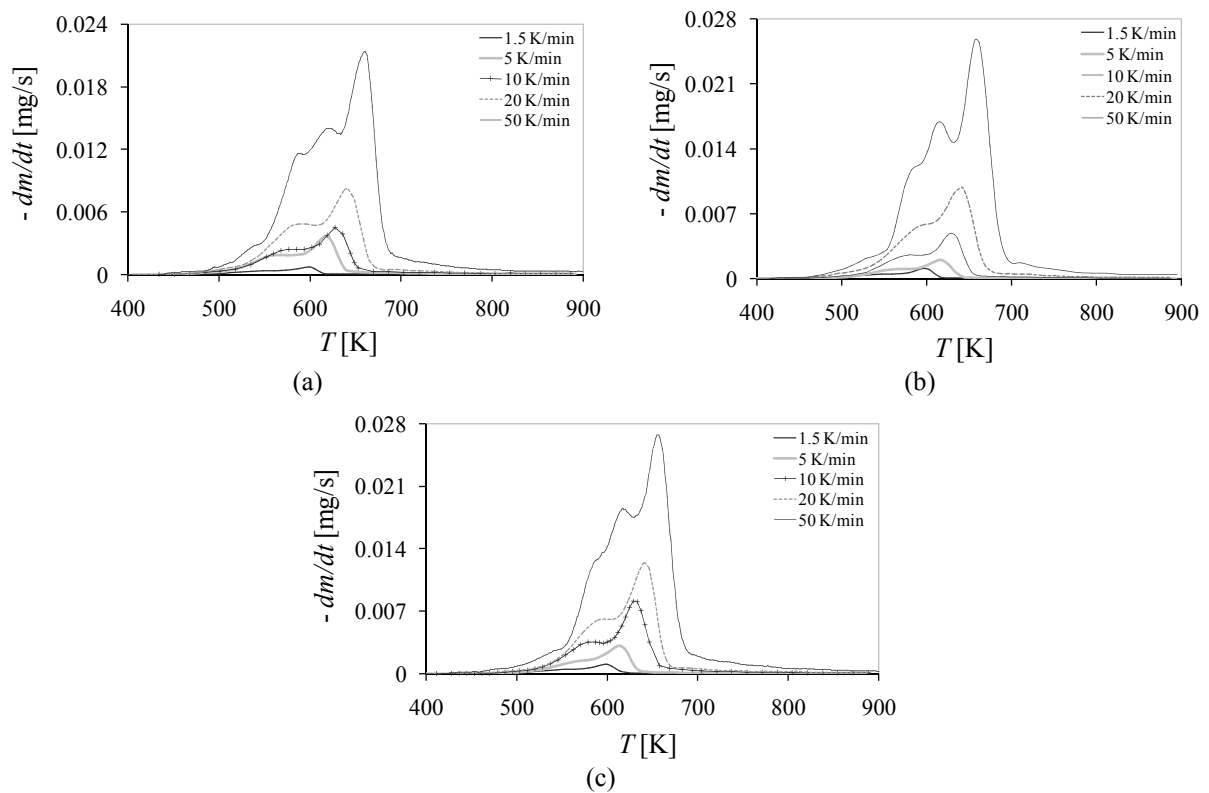


Figure 2– DTG curves of bagasse pyrolysis at different heating rates: (a) S_1 ; (b) S_2 and (c) S_3 .

The samples with lower ash content showed higher total weight loss (Munir et al., 2009). This effect is demonstrated in Figure 3 (a), which shows a lower conversion for the particle set with higher ash content set, S₁. According to Di Blasi (2008), highest ash content, especially potassium, sodium and calcium, can acts as catalysts for the pyrolysis process promoting secondary reactions of the volatile decomposition and char formation.

Figure 3 (b) compares the heating rates of 1.5 and 50 K min⁻¹ and shows a shift of 70 K at a temperature which starts the decomposition of hemicellulose. The final temperature of the second step (cellulose decomposition) also shows a shift of 70 K.

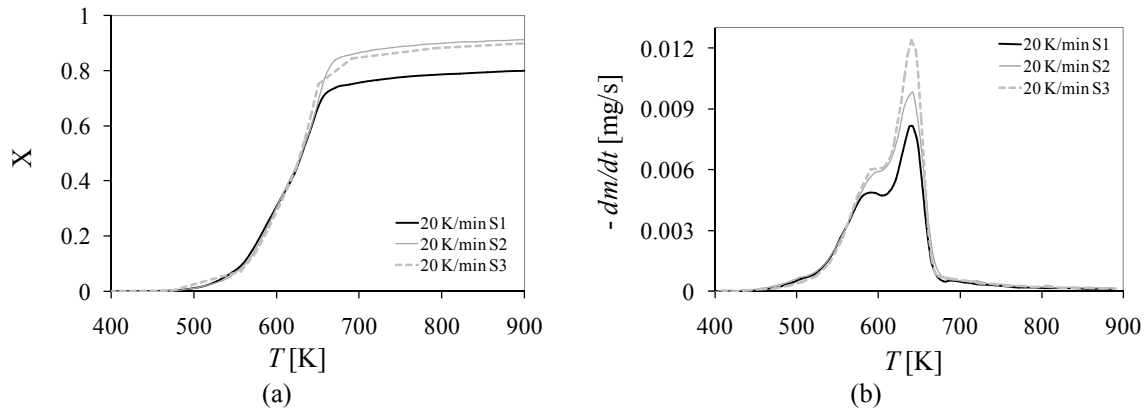


Figure 3– Comparison between experimental data of the three sets of particles, for $\beta = 20 \text{ K min}^{-1}$: (a) TG curves; (b) DTG curves.

5.2 Kinetic Study

The Differential Evolution method was used to solve an inverse problem formulated to estimate the kinetic parameter of biomass pyrolysis, employing the three independent parallel reactions model. The reaction order for each subcomponent was kept constant: first-order to hemicellulose and cellulose and third-order to lignin decomposition. The mass fraction of subcomponents (c_1 , c_2 and c_3), as the parameters of Arrhenius equation for each subcomponent ($k_{0,1}$, $k_{0,2}$, $k_{0,3}$, Ea_1 , Ea_2 and Ea_3) were calculated for each run, as summarized in Table 2.

β	S ₁				S ₂				S ₃			
	k_0	Ea	c_i	FIT	k_0	Ea	c_i	FIT	k_0	Ea	c_i	FIT
1.	$1.80 \cdot 10^6$	97	0.38	0.58 ^a	$3.07 \cdot 10^6$	99	0.35	0.31 ^a	$1.58 \cdot 10^7$	107	0.33	0.44 ^a
	$2.73 \cdot 10^{17}$	231	0.40	1.82 ^b	$9.44 \cdot 10^{16}$	225	0.43	1.40 ^b	$6.30 \cdot 10^{17}$	236	0.43	1.83 ^b
	$1.40 \cdot 10^2$	77	0.22		$3.14 \cdot 10^1$	70	0.22		$2.73 \cdot 10^1$	72	0.24	
5	$1.17 \cdot 10^7$	103	0.37	0.29 ^a	$3.14 \cdot 10^7$	108	0.36	0.21 ^a	$1.61 \cdot 10^7$	106	0.33	0.19 ^a
	$2.55 \cdot 10^{17}$	232	0.41	1.16 ^b	$2.12 \cdot 10^{17}$	231	0.44	1.52 ^b	$1.36 \cdot 10^{18}$	239	0.43	0.93 ^b
	$8.39 \cdot 10^{-2}$	32	0.22		$2.55 \cdot 10^{-1}$	35	0.20		$7.88 \cdot 10^{-2}$	30	0.24	
10	$4.98 \cdot 10^7$	109	0.33	0.37 ^a	$3.11 \cdot 10^7$	107	0.36	0.29 ^a	$6.00 \cdot 10^7$	111	0.34	0.64 ^a
	$2.70 \cdot 10^{16}$	222	0.42	2.64 ^b	$1.93 \cdot 10^{17}$	232	0.43	1.32 ^b	$1.72 \cdot 10^{19}$	256	0.46	1.22 ^b
	$1.09 \cdot 10^{-2}$	21	0.25		$5.08 \cdot 10^{-2}$	26	0.21		1.61	41	0.21	
20	$1.91 \cdot 10^7$	103	0.32	0.33 ^a	$2.48 \cdot 10^7$	106	0.36	0.34 ^a	$2.51 \cdot 10^8$	116	0.34	0.33 ^a
	$2.49 \cdot 10^{14}$	199	0.40	2.00 ^b	$6.02 \cdot 10^{16}$	227	0.41	1.40 ^b	$1.28 \cdot 10^{19}$	255	0.45	1.37 ^b
	$1.14 \cdot 10^{-2}$	21	0.28		$2.18 \cdot 10^{-1}$	28	0.23		$2.01 \cdot 10^{-1}$	29	0.21	
50	$3.65 \cdot 10^{14}$	90	0.13	0.56 ^a	$7.25 \cdot 10^{13}$	166	0.08	0.33 ^a	$7.90 \cdot 10^{13}$	169	0.08	0.32 ^a
	$7.14 \cdot 10^{11}$	152	0.23	4.50 ^b	$3.96 \cdot 10^{12}$	163	0.26	1.78 ^b	$5.31 \cdot 10^{13}$	176	0.26	1.57 ^b
	$1.78 \cdot 10^{19}$	257	0.33		$3.80 \cdot 10^{15}$	213	0.44		$1.91 \cdot 10^{17}$	233	0.42	
	6.04	35	0.26		1.88	32	0.22		1.08	29	0.24	

Table 2 – Kinetic parameters using the three independent parallel reaction model, for different heating rates and

set of particles (β in kJ mol^{-1} ; k_0 in s^{-1} ; Ea in kJ mol^{-1}).

The two hemicellulose peaks present in runs with 50 K min^{-1} can indicate a different mechanism of hemicellulose decomposition or different hemicellulose materials (Varhegyi et al., 1989). Due to individual calculation of hemicellulose peaks and their interference in the estimation of other parameters, only the intermediary heating rates were analyzed together.

The mass fraction estimated was comprised in a range of 0.32–0.38 for hemicellulose, 0.40–0.46 for cellulose and 0.20–0.28 for lignin. These values agree well with the composition of bagasse reported in literature: 14–35 % for hemicellulose, 26–54 % for cellulose and 18–30 % for lignin (Rao and Sharma, 1998; Williams and Besler, 1993; Gómez, 2006).

The values of activation energy were between 97–116 kJ mol^{-1} for hemicellulose and 199–256 kJ mol^{-1} for cellulose. The activation energy of lignin at lower heating rate (1.5 K min^{-1}) was overestimated for all sets of particles (70 to 77 kJ mol^{-1}). This can indicate a different decomposition mechanism for lignin in this heating rate. For others heating rates, the activation energy of lignin was between 21 and 41 kJ mol^{-1} . The activation energy estimated in this work for individual subcomponents agrees well with literature data, as showed in Table 3.

*	Biomass	Hemicellulose				Cellulose				Lignin				FIT
		k_0	Ea	c_i	n	k_0	Ea	c_i	n	k_0	Ea	c_i	n	
a)	Cotton straw	$3.6 \cdot 10^{15}$	191	0.20	1.7	$3.8 \cdot 10^{16}$	173	0.38	1.3	$2.1 \cdot 10^3$	65	0.32	3.5	1 ^b
	Rice straw	$5.4 \cdot 10^7$	102	0.05	1	$2.6 \cdot 10^9$	130	0.45	1	0.54	31	0.23	1	2 ^b
b)	Cotton Residue	$7 \cdot 10^6$	95	0.13	1	$2.0 \cdot 10^{10}$	145	0.36	1	25	31	0.25	1	0.8–2 ^b
c)	bagasse	$4.7 \cdot 10^{15}$	198	0.14	1	$1.0 \cdot 10^{18}$	246	0.43	1	380	57	0.19	3	1.17 ^a
d)	Pine Wood	$3.2 \cdot 10^{18}$	88	0.23	1	$4.0 \cdot 10^{18}$	201	0.33	1	0.94	18	0.44	1	2–2.1 ^b

Table 3 – Kinetic parameters using the IPR model, for different heating rates and set of particles. *References: a) Hu et al. (2007); b) Vamvuka et al. (2003); c) Manyà and Araúzo (2008); d) Órfão et al. (1999).

Figure 4 shows experimental and simulated curves of TG and DTG for a constant heating rate of 5 K min^{-1} , for all sets of particles. It can be seen a good agreement between the experimental data and the predictions of the model. The fitting error was less than 0.64% for TG curves and 4.50% for DTG curves as presented in Table 2, which shows the great capability of Differential Evolution Method to nonlinear estimation of parameters.

6 CONCLUSIONS

The knowledge of kinetics of chemical reactions is a requisite to understand the reaction mechanisms and find out the optimum reaction conditions. In this work, the pyrolysis of sugarcane bagasse was carried out in order to investigate the kinetic of primary decomposition of this biomass. The kinetic model used was the three independent parallel reaction model, which are based on single-step reactions to model the individual decomposition of main subcomponents of lignocellulosic materials: hemicellulose, cellulose and lignin. Weight loss data with time/temperature were obtained by thermogravimetric experiments. The kinetic parameters were estimated using the Differential Evolution Algorithm. From experimental data and simulated results, the following conclusions can be drawn:

- The maximum rate of pyrolysis increases with increasing heating rate, for all sets of particles.

- The particle set with higher ash content set (S_1) showed a lower final devolatilization and a higher residual mass of char, probably due to the action of ash as catalyst.

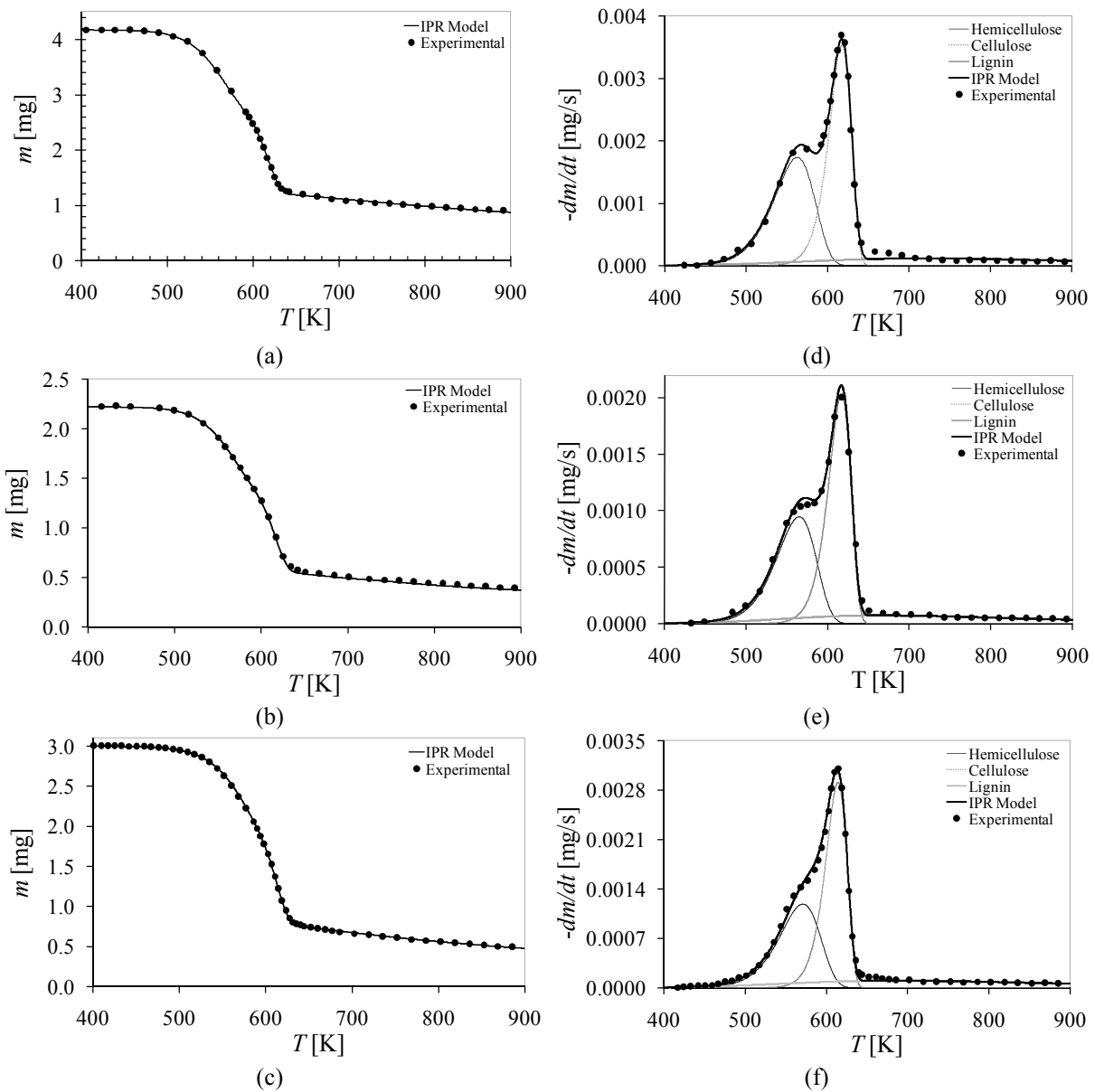


Figure 4 – Experimental and simulated curves for the different sets of particle, for $\beta = 5 \text{ K min}^{-1}$: TG: a) S_1 ; b) S_2 , c) S_3 and DTG: d) S_1 ; e) S_2 , f) S_3 .

- The two hemicellulose peaks present in runs with 50 K min^{-1} can indicate a different mechanism of decomposition at higher heating rates.
- The mass fraction estimated was comprised in a range of 0.32–0.38 for hemicellulose, 0.40–0.46 for cellulose and 0.20–0.28 for lignin, which agree well with the composition of bagasse reported in literature (Rao and Sharma, 1998; Williams and Besler, 1993; Gómez, 2006).
- The values of activation energy were between 97–116 kJ mol^{-1} for hemicellulose; 199–256 kJ mol^{-1} for cellulose and 21–41 kJ mol^{-1} for lignin.

- The activation energy of lignin at lower heating rate (1.5 K min^{-1}) showed higher values (70 to 77 kJ mol^{-1}), which can indicate a different decomposition mechanism for lignin in this heating rate.
- The simulated TG and DTG data showed good agreement with experimental data and literature works, with fitting error less than 0.64% for TG and 4.50% for DTG data.
- The results obtained for the DE algorithm was considered satisfactory and performing a smaller number of objective function evaluations.
- The knowledge of kinetic parameters for pyrolysis of sugarcane bagasse can improve the design of reactor for slow pyrolysis and facilitate the future application of CFD studies to pyrolysis of sugarcane bagasse.

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