

Optimization of Pyrolysis of Biomass Using Differential Evolution Approach

B.V. Babu and A.S. Chaurasia
Department of Chemical Engineering,
Birla Institute of Technology & Science,
Pilani-333031 (Rajasthan) India
{bvbabu, aschaurasia}@bits-pilani.ac.in

Abstract

Differential Evolution (DE) is an evolutionary optimization technique, which is exceptionally simple, significantly faster & robust at numerical optimization and is more likely to find a function's true global optimum. Pyrolysis of biomass is an important and promising chemical process in the area of renewable energy sources. In the present study, the modeling and simulation of the above process is coupled with the optimization of a non-linear function using Differential Evolution. The objective in this problem is to estimate optimal time of pyrolysis and heating rate under the restriction on concentration of biomass. It serves as the input to the coupled ordinary differential equations to find the optimum values of volatiles and char using Runge-Kutta fourth order method.

1. Introduction

Biomass has either been processed to increase its energy content or burned directly in furnaces. The processes such as pyrolysis, gasification, anaerobic digestion and alcohol production, have been widely applied to biomass in order to increase its energy content. The pyrolysis of biomass is a promising route for the production of solid (charcoal), liquid (tar and other organics), and gaseous products (H_2 , CO_2 , CO). These products are of interest as they are possible alternate sources of energy. Pyrolysis is a process by which a biomass feedstock is thermally degraded in the absence of oxygen/air. The study of pyrolysis is gaining increasing importance, as it is not only an independent process, but it is also a first step in the gasification or combustion process.

Extensive studies have been carried out on pyrolysis of biomass by Babu & Chaurasia [1-10], Chaurasia & Babu [11-12] and Chaurasia *et al.* [13] in their earlier work. The actual reaction scheme of pyrolysis of biomass is extremely complex because of formation of over

hundred intermediate products. Pyrolysis of biomass is, therefore, generally modeled on the basis of apparent kinetics. Ideally, the chemical kinetics model should account for primary decomposition reactions as well as secondary reactions.

It is generally accepted that the most important parameters affecting the process of pyrolysis of biomass are temperature, concentration, time and heating conditions. Recently, Babu and Chaurasia [4] estimated the optimum parameters in the pyrolysis of biomass. They considered that by varying the temperature or heating rate (in an optimal fashion) during the heating process it is possible to increase the yield of the pyrolysis products beyond what is possible with isothermal or non-isothermal heating respectively. Furthermore, they found that as temperature or heating rate increase, the pyrolysis time decreases up to certain extent and then start increasing with further increase in temperature or heating rate. This point appears to be rather interesting and provided motivation to examine the problem in greater detail. The purpose of this work is to find the optimum values of these parameters for non-isothermal heating conditions by using differential evolution.

2. Differential evolution

Differential Evolution (DE) is an evolutionary optimization technique, which is exceptionally simple, significantly faster & robust at numerical optimization and is more likely to find a function's true global optimum. DE [14] is an improved version of GA [15] for faster optimization. Unlike simple GA that uses binary coding for representing problem parameters, DE uses real coding of floating point numbers. Among the DE's advantages are its simple structure, ease of use, speed and robustness. Price & Storn [14] gave the working principle of DE with single strategy. Later on, they suggested ten different strategies of DE [16]. A strategy that works out to be the best for a given problem may not work well when applied for a different problem.

Also, the strategy and key parameters to be adopted for a problem are to be determined by trial & error. The key parameters of control are: NP-the population size, CR-the crossover constant, F-the weight applied to random differential (scaling factor). The detailed Differential Evolution algorithm used in the present study is given below:

- Choose a strategy
- Initialize the value of D (Number of independent parameters), NP, CR, F & gen_max.
- Initialize all the vector population randomly in the given upper & lower bound.
For I=1 to NP
{For j=1 to D
 $x_{ij} = \text{random Number}$
- Evaluate the cost of each vector.
- Find out the vector with the lowest cost.
- Repeat.
- Perform mutation & recombination.
 - a) For each vector x_t (target vector), select three distinct vectors x_a , x_b & x_c (select five, if two vector differences are to be used) randomly from the current population (primary array) other than vector x_t .
 - b) Perform crossover for each target vector with its noisy vector to create a trial vector.
- After the mutation & recombination, if the bound (i.e. lower & upper limit of a variable) is violated then it can be brought in the bound range (i.e. between lower & upper limit) either by forcing it to lower/upper limit (forced bound) or by randomly assigning a value in the bound range (without forcing).
- Perform selection for each target vector, x_t by comparing its cost with that of the trial vector. Vector with lower cost is selected for next generation.
- Till termination criteria do not meet.
- Print results.

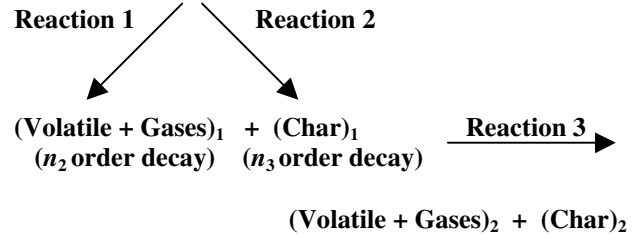
The crucial idea behind DE is a scheme for generating trial parameter vectors. Basically, DE adds the weighted difference between two population vectors to a third vector. Price & Storn [14] have given some simple rules for choosing key parameters of DE for any given application. DE has been successfully applied in various fields. The various applications of DE are: digital filter design [17], batch fermentation process [18, 19], dynamic optimization of continuous polymer reactor [20], estimation of heat transfer parameters in trickle bed reactor [21], optimal design of heat exchangers [22, 23], synthesis & optimization of heat integrated distillation system [24], optimization of an alkylation reaction [25], scenario-integrated optimization of dynamic systems [26], optimization of non-linear functions [27],

optimization of thermal cracker operation [28], optimization of non-linear chemical processes [29, 30], optimization of MINLP problems [31], etc.

3. Problem formulation

The pyrolysis reactions can be described by means of following scheme as used by Babu and Chaurasia [4]:

Virgin biomass B (n_1 order decay)



This kinetic scheme indicates that the biomass decomposes to volatiles, gases and char. The volatiles and gases may further react with char to produce different types of volatiles, gases and char where the compositions are different. Therefore, the primary pyrolysis products participate in secondary interactions (Reaction 3), resulting in modified final product distribution. The kinetic equations for the mechanism shown above along with heat transfer model equation and initial and boundary conditions are as follows:

$$\frac{\partial C_B}{\partial t} = -(k_1 + k_2)C_B^{n_1} \quad (1)$$

$$\frac{\partial C_{G1}}{\partial t} = k_1 C_B^{n_1} - k_3 C_{G1}^{n_2} C_{C1}^{n_3} \quad (2)$$

$$\frac{\partial C_{C1}}{\partial t} = k_2 C_B^{n_1} - k_3 C_{G1}^{n_2} C_{C1}^{n_3} \quad (3)$$

$$\frac{\partial C_{G2}}{\partial t} = k_3 C_{G1}^{n_2} C_{C1}^{n_3} \quad (4)$$

$$\frac{\partial C_{C2}}{\partial t} = k_3 C_{G1}^{n_2} C_{C1}^{n_3} \quad (5)$$

where,

$$k_1 = A_1 \exp[(D_1/T) + (L_1/T^2)]$$

$$k_2 = A_2 \exp[(D_2/T) + (L_2/T^2)]$$

$$k_3 = A_3 \exp[(-E_3 / R_c T)]$$

and

$$A_1 = 9.973 \times 10^{-5} \text{ s}^{-1}; A_2 = 1.068 \times 10^{-3} \text{ s}^{-1};$$

$$A_3 = 5.7 \times 10^5 \text{ s}^{-1}; D_1 = 17254.4 \text{ K};$$

$$D_2 = 10224.4 \text{ K}; L_1 = -9061227 \text{ K}^2;$$

$$L_2 = -6123081 \text{ K}^2; E_3 = 81 \text{ kJ/mol}$$

It is assumed that in thermo-gravimetric analysis, temperature and time have a linear relationship, and consequently it is appropriate to describe the above phenomenon as follows:

$$T = (HR)t + T_0 \quad (6)$$

The goal is to find the minimum value of pyrolysis time and the other optimum parameters corresponding to the optimum value of pyrolysis time. The objective function in dimensionless form is given by:

$$\begin{aligned} \text{Min } \tau = & 2.4617 \overline{HR}^4 - 8.886 \overline{HR}^3 \\ & + 12.583 \overline{HR}^2 - 7.7199 \overline{HR} + 3.4088 \end{aligned} \quad (7)$$

$$\text{Subject to } 0.2 \leq \overline{HR} \leq 1.2$$

Dimensionless groups:

$$\tau = \frac{\alpha t}{R^2} \quad (8)$$

$$\overline{HR} = \frac{HR \times t}{T_0} \quad (9)$$

4. Method of solution

The optimum values of pyrolysis time and heating rate are found by using the differential evolution. It serves as the input to the coupled ordinary differential equations to find the optimum parameters using Runge-Kutta fourth order method. The initial condition is given by

$$\text{At } t = 0, C_B = 1.0, C_{G_1} = C_{C_1} = C_{G_2} = C_{C_2} = 0.$$

The final concentration of biomass was assumed to be equal to 0.03, because beyond that concentration, pyrolysis is found to be very slow and of little practical importance. So, the iterations are continued till $C_B \leq$

0.03. The optimum values of the parameters are found using $n_1=1, n_2=n_3=1.5$ for non-isothermal condition. The problem is solved considering particle radius of $R=0.001$ m and initial temperature of $T_0=773$ K. Thermal diffusivity is taken to be a constant ($\alpha=1.79 \times 10^{-7}$ m²/s) and based on the initial temperature of wood, which is a representative value in pyrolysis.

5. Results and discussion

The final pyrolysis time vs. heating rates are plotted and shown in Fig. 1. It is found that final pyrolysis time first decreases with increasing heating rate, reaches the optimum value and then increases as heating rate is further increased. The key parameters used in differential evolution are CR=0.7, F=0.5, NP=10, seed = 9, accuracy = 0.000001%. For the orders of reactions considered, the optimum values of heating rate & final pyrolysis time are found to be 50.7165 K/s and 9.5268 s respectively after eighteen generations.

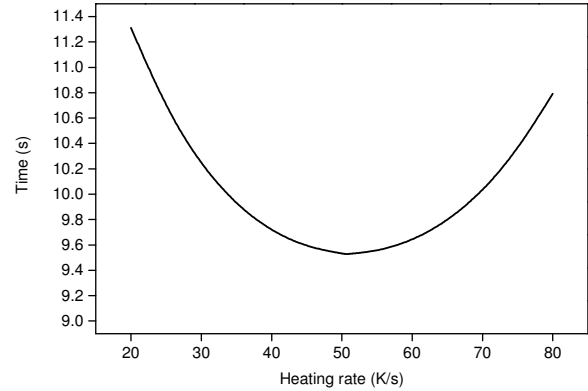


Figure 1 Pyrolysis time as a function of heating rate for pyrolysis under non-isothermal condition ($n_1=1, n_2=n_3=1.5$).

This interesting decreasing and increasing trend in final pyrolysis time with heating rate can be explained physically by comparing optimum heating rate value (50.7165 K/s) with a value slightly greater than it (say 70 K/s). It is well known that as the pyrolysis proceeds (i) temperature increases, (ii) concentration of biomass decreases and reaches the final value, (iii) concentration of (volatile)₁ increases, (iv) concentration of (char)₁ increases up to certain value of time and then decreases, and (v) concentrations of (volatile & char)₂ increase as discussed by Babu & Chaurasia [4]. The rate of decrease in concentration is more for higher value of heating rate as compared to optimum value up to certain value of

time. The concentration of $(\text{char})_1$ will reach to its maximum value earlier for higher heating rate. After attaining the maximum value, the concentration of $(\text{char})_1$ starts decreasing for both heating rates. The rate of decrease in concentration of biomass is less for higher heating rate as compared to optimum value, because the $(\text{char})_1$ left for higher value of heating rate is less. So the reaction between $(\text{volatile})_1$ and $(\text{char})_1$ is slow for higher value of heating rate as compared to optimum value, and hence it takes more time to reach the desired final concentration of biomass. Hence the final pyrolysis time is more for high value as compared to optimum value of heating rate.

The optimum values of the parameters are shown in Table-1. The maximum concentration is obtained for $(\text{volatile})_1$ as compared to other products. The rate heating influences the reaction pathway and hence, the final products. The char yield is supported at low heating rates whereas the yield of volatiles increases markedly at fast heating rates. At low heating rates, particularly those involving large samples, the residence time of all primary products within the pyrolysing matrix would dominate, accounting for large char yields.

Table 1 Optimum parametric values for pyrolysis under non-isothermal condition

Optimum Parameters	$n_1=1;$ $n_2=n_3=1.5$
Heating rate (K/s)	50.7165
Final pyrolysis time (s)	9.5268
Final pyrolysis temperature (K)	1256.1614
Final concentration of initial biomass (-)	0.030047
Final concentration of $(\text{char})_1$ (-)	0.000709
Final concentration of $(\text{volatile})_1$ (-)	0.685714
Final concentration of $(\text{char})_2$ (-)	0.141765
Final concentration of $(\text{volatile})_2$ (-)	0.141765

6. Conclusions

The modeling and simulation of the pyrolysis of biomass process coupled with the optimization of a non-linear function using Differential Evolution (an evolutionary computation method) approach has been presented. The best key parameters for the present problem are: NP=10, CR=0.7, F=0.5. This successful application of DE indicates that DE has great potential and can be applied to advantage in all the highly non-linear & complex engineering problems. The work carried out in the present study is important and useful for optimal design of the biomass gasifiers, reactors, etc. It is also important in industrial pyrolysis applications.

Nomenclature

B	= virgin biomass
G_1	= (gases and volatiles) ₁
C_1	= $(\text{char})_1$
G_2	= (gases and volatiles) ₂
C_2	= $(\text{char})_2$
C_B	= concentration of B (dimensionless)
C_{G_1}	= concentration of G_1 (dimensionless)
C_{C_1}	= concentration of C_1 (dimensionless)
C_{G_2}	= concentration of G_2 (dimensionless)
C_{C_2}	= concentration of C_2 (dimensionless)
t	= time (s)
n_1, n_2, n_3	= orders of reaction (dimensionless)
R	= radius of the particle (m)
T	= temperature (K)
T_0	= initial temperature (K)
HR	= heating rate (K/s)
\overline{HR}	= heating rate (dimensionless)
k_1, k_2, k_3	= rate constant (s^{-1})
α	= thermal diffusivity, m^2/s
τ	= dimensionless time

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