

Modeling & Simulation of Pyrolysis: Effect of Convective Heat Transfer & Orders of Reactions

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Abstract: Pyrolysis is a process by which a biomass feedstock is thermally degraded in the absence of air/oxygen. It is used for the production of solid (charcoal), liquid (tar and other organics) and gaseous products. In the present study, a mathematical model to describe the pyrolysis of a single solid particle of biomass is used to study the effect of convective heat transfer coefficient and orders of reactions. Pyrolysis rate has been simulated by a scheme consisting of two parallel primary reactions and a third reaction for secondary interactions between volatile and gaseous products and the char. Finite difference method using pure implicit scheme is used for solving heat transfer equation and Runge-Kutta 4th order method for chemical kinetics equations. The model equation is solved for cylindrical pellets, spheres and slab geometries of equivalent radius ranging from 0.00025 m to 0.013 m, and temperature ranging from 303 K to 1000 K, and the results are presented here. The work carried out in the present study is important and useful for optimal design of the biomass gasifiers, reactors, etc. It is very useful in the design of industrial pyrolysis units also.

Key Words: Pyrolysis; Biomass; Kinetics; Heat transfer; Simulation; Convection; Order

INTRODUCTION

The pyrolysis process consists of the thermal degradation of biomass feedstock, in the absence of oxygen/air, leading to the formation of solid (charcoal), liquid (tar and other organics) and gaseous products (H₂, CO₂, CO). 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. The overall process of pyrolysis can be classified into primary and secondary stages.

The pyrolysis process has a great future in the world [Srivastava and Jalan, (1994)]. The various modeling studies appearing in the literature present different versions or enrich the model suggested by Bamford *et al.*, [1946]. According to this model, the equation for heat conduction in a pyrolyzing solid is combined with those for heat generation, assuming first order kinetics. However, the heat transfer equation does not consider the effect of change of density as a function of time. The model developed by Bamford *et al.* [1946], was used by several researchers [Tinney, (1965); Roberts and Clough, (1963); Tang and Neil, (1964); Shafizadeh, (1978)] and was modified by Kung [1972] in order to incorporate the effects of internal convection and variable transport properties. Many of the above

studies have not considered the secondary reactions in pyrolysis kinetics. Kansa *et al.*, [1977] pointed out that secondary reactions are essential to match fully the experimental observations. Keeping the above drawbacks of the existing models in view, Babu and Chaurasia [2002a] presented the kinetic model, which considered the secondary reactions in pyrolysis kinetics. This kinetic model was utilized by Babu and Chaurasia [2002b] and the model was developed for pyrolysis of a single biomass particle, which includes kinetics and heat transfer effects in the particle.

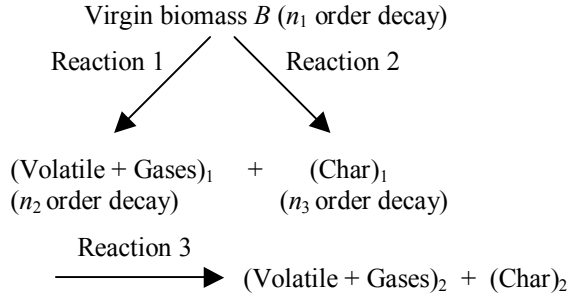
The simulated results obtained by Babu and Chaurasia's model [2002b] was in excellent agreement with the experimental data much better than the agreement with the models proposed by Jalan and Srivastava [1999] and Bamford [1946]. The model developed [Babu and Chaurasia, (2002b)] was used in the present paper to study the effect of convective heat transfer and orders of reactions on the single biomass cylindrical pellet.

MODELING

The pyrolysis reactions can be described by means of following scheme as proposed by Babu and Chaurasia [2002a]. This model 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

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(Reaction 3), resulting in modified final product distribution.



The kinetic equations for the mechanism shown above are as follows:

$$\frac{dC_B}{dt} = -k_1 C_B^{n_1} - k_2 C_B^{n_1} \quad (1)$$

$$\frac{dC_{G_1}}{dt} = k_1 C_B^{n_1} - k_3 C_{G_1}^{n_2} C_{C_1}^{n_3} \quad (2)$$

$$\frac{dC_{C_1}}{dt} = k_2 C_B^{n_1} - k_3 C_{G_1}^{n_2} C_{C_1}^{n_3} \quad (3)$$

$$\frac{dC_{G_2}}{dt} = k_3 C_{G_1}^{n_2} C_{C_1}^{n_3} \quad (4)$$

$$\frac{dC_{C_2}}{dt} = k_3 C_{G_1}^{n_2} C_{C_1}^{n_3} \quad (5)$$

The equation for heat transfer is given by,

$$\begin{aligned}
 \frac{d}{dt}(C_p \rho T) = k \left(\frac{b-1}{r} \frac{dT}{dr} + \frac{d^2 T}{dr^2} \right) \\
 + (-\Delta H) \left(-\frac{d\rho}{dt} \right) \quad (6)
 \end{aligned}$$

The equations (1)-(5) are solved by Runge-Kutta fourth order method. The equation (6) is solved by finite difference method using pure implicit scheme. The values of various parameters employed and the initial conditions and boundary conditions used in the present study are taken from the literature [Srivastava *et al.*, (1996); Jalan and Srivastava, (1999); Pyle and Zaror, (1984); Babu and Chaurasia, (2002b; 2002c)]. The notations used in the above equations have the same meaning as given by Babu and Chaurasia [2002b; 2002c].

RESULTS AND DISCUSSION

Fig. 1 shows the temperature profiles as a function of radial distance at various times of progression of

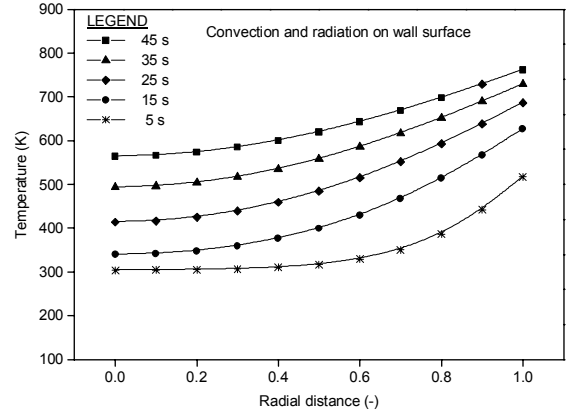


Fig. 1 Temperature profile as a function of radial distance considering both convection and radiation on wall surface ($R=0.005$ m, $T_0=303$ K, $T_f=900$ K).

pyrolysis of 5 s, 15 s, 25 s, 35 s and 45 s for the particle radius of 0.005 m, considering both convection and radiation on the wall (surface of the particle). It is observed that as pyrolysis time increases, temperature increases at a given radial position. The rate of increase is high at the radial position close to the wall compared to that at the centre of the particle. In the initial stages of pyrolysis, the temperature profile is very steep near the wall (refer the temperature profile corresponding to 5 s in Fig. 1), and as the time progresses the steepness in the temperature profile near the wall decreases. This can be explained with the fact that when the heat transfer takes place by both the mechanisms of convection and radiation from the wall surface, the resistance offered for heat transfer near the wall at initial stages of pyrolysis is very high. On the contrary when heat transfer from wall surface takes place only by convection and with no radiation, the resistance offered for heat transfer near the wall is not as much high as in the above case which is clearly demonstrated by plotting the simulation results as shown in Fig. 2. It is also observed that the increase in temperature at various radial positions at different times of progression of pyrolysis is not significant which is obvious due to the reasons mentioned above. Interestingly, to see the extent of effect of convection on temperature profile, simulations are carried out for a case where there is no radiation at the wall surface, but having ten times of convective heat transfer. The results are plotted in Fig. 3 for various times of pyrolysis progression. As expected, the results obtained are almost similar to those corresponding to combined convection and radiation case of Fig. 1. This consolidates the explanation given above in terms of

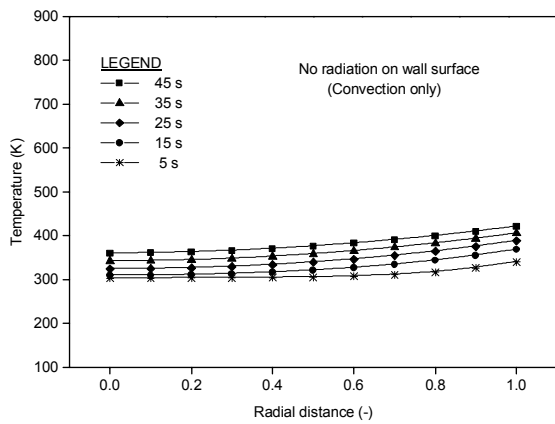


Fig. 2 Temperature profile as a function of radial distance considering convection only with no radiation on wall surface ($R=0.005$ m, $T_0=303$ K, $T_f=900$ K).

resistances offered by various heat transfer mechanisms. It means that more the resistance offered for heat transfer near the wall of the particle (either by combined convection and radiation, or by convection alone but at higher convective rate) the more will be the difference (increase) in temperature profiles. In the present case the total net resistance offered by convection and radiation is approximately equal to ten times of convective resistance with no radiation at the wall of the particle. The above results shown in Figs.

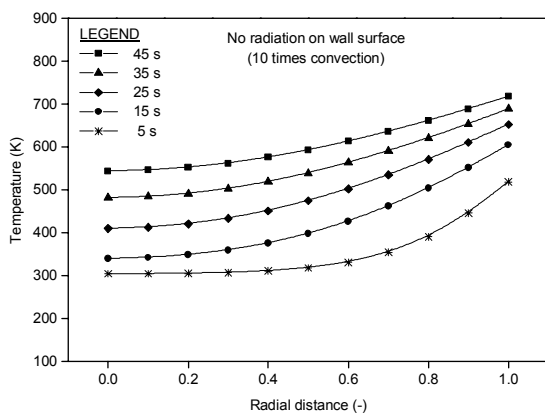


Fig. 3 Temperature profile as a function of radial distance considering ten times convection with no radiation on wall surface ($R=0.005$ m, $T_0=303$ K, $T_f=900$ K).

1-3 and the justifiable and logical explanation given therein have a lot of practical importance and physical significance in industrial pyrolysis applications. The results obtained consolidate the fact that it is possible to get the same extent of conversion of biomass and with lesser pyrolysis time under controlled conditions by increasing convective heat transfer at much lower operating temperatures which are much safer than at higher operating temperatures leading to combined convective and radiative heat transfer mechanisms which are not safe.

Figs. 4 and 5 show the temperature profile as a function of radial distance at the time of completion of pyrolysis (i.e. when biomass concentration=0) for the orders of reactions of $n_1=1$; $n_2=n_3=1.5$ and $n_1=0$; $n_2=n_3=1.5$ respectively for the particle radii of 0.005 m. It is observed that the time for completion of pyrolysis is very less (70 s) (i.e. pyrolysis is significantly faster) for the case of $n_1=0$; $n_2=n_3=1.5$, because in this case the model equations (1)-(3) become independent of the initial biomass concentration as discussed [Babu and Chaurasia, 2002a].

CONCLUSION

In the present work, the effect of convective heat transfer and orders of reactions on pyrolysis of biomass particle have been studied, utilizing the model developed by Babu and Chaurasia (2002b). The wide ranges of temperature (303-2700 K) and pellet diameters (0.0005-0.026 m) are considered. It is found that the pyrolysis is faster for zeroth order as compared to first order of reaction 1, as the rates are independent

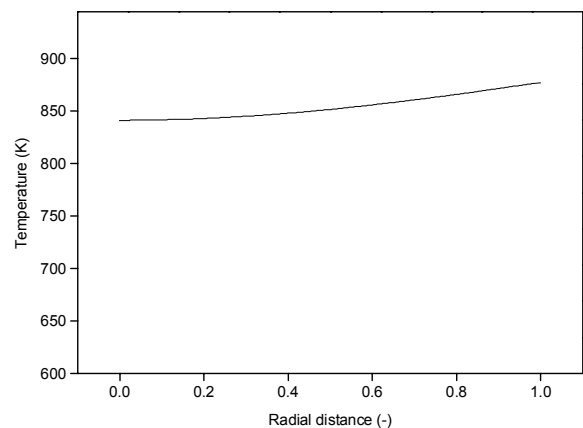


Fig. 4 Temperature profile as a function of radial distance at the time of completion of pyrolysis ($n_1=1$, $n_2=n_3=1.5$, $t_f=188$ s, $R=0.005$ m, $T_0=303$ K, $T_f=900$ K).

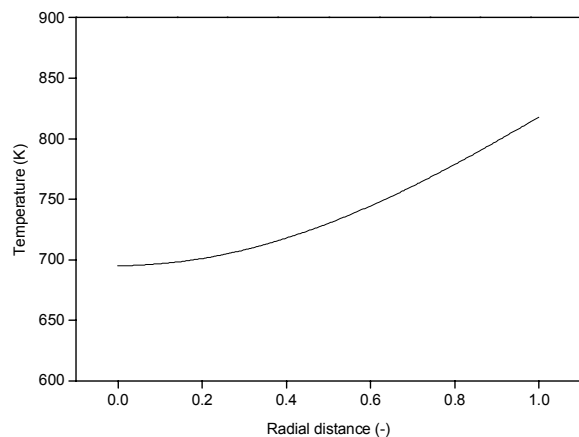


Fig. 5 Temperature profile as a function of radial distance at the time of completion of pyrolysis ($n_1=0$, $n_2=n_3=1.5$, $t_f=70$ s, $R=0.005$ m, $T_0=303$ K, $T_f=900$ K).

of initial biomass concentration for zeroth order. The work carried out in the present study is important and useful for optimal design of the biomass gasifiers, reactors, etc. It is very useful in the design of industrial pyrolysis units also. Biomass gasification and pyrolysis are the most important areas in renewable energy on which the government in general, and MNES (Ministry of Non-Conventional Energy Sources) in particular are very much focused and lot of policy decisions have been made to encourage the use of these energies. From this perspective, the results of present study would be definitely useful in policy decision-making.

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