The Mathematical Model for Predicting the Pyrolysis of wood particles

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1 Introduction

The ignition of a woody material is of fundamental interest to research on preventing fires and extracting energy by burning wood. There are excellent reviews of previous work on the ignition of wood. Galgano and Blasi [1] modelled decomposition of moist wood using the shrinking unreacted-core approximation for a finite rate of reaction and the effect of convective, conductive, and radiative heat transfer and different physical properties for char, dry wood, and moist wood were studied. Cetin [2] studied the gasification kinetics of chars from different biomass species. Effects of pyrolysis pressure on the chemical structure of char and char conversion reactivities were also investigated. Weng et al. [3] presented an extended integral model using char oxidation under different ambient oxygen concentrations to predict the pyrolysis of wood. Yang et al. [4] numerically and experimentally worked on the auto-ignition of wood exposed to variable heat fluxes are presented. A one-dimensional model for investigating the pyrolysis of wood subject to a linearly increasing heat flux was developed. Finally, Benkoussas et al. [5] developed a model for thermal degradation of woody fuel particles. It included drying, pyrolysis, and char oxidation processes.

In this research, the structure of laminar, one-dimensional and steady flame propagation in uniformly premixed particle-wood is analyzed. The structure of the flame is composed of three zones: a preheat zone, reaction zone and post flame zone. The analysis is performed considering the gas, tar and char combustion in the reaction zone. In this mathematical model, it is assumed that the fuel particles vaporize first to yield a gaseous fuel of known chemical structure. The analysis is performed in the asymptotic limit, where the value of the characteristic Zeldovich number and for values of $\phi > 1$.

2 Mathematical Model

In this research, as mentioned above, the flame structure is composed of three zones shown in Figure 1. In the preheat zone, the rate of reaction between fuel and oxidizer is assumed to be small. Whenever the vaporization phenomenon continues to the convection zone, a one-step overall reaction can be considered between fuel particles and oxidizer. As seen in this Figure, the reaction zone consists of three parts; gas, tar and char combustion. In this zone, the convective terms and vaporization terms in the conservation equations are presumed to be small in comparison with the diffusive and reactive terms and in the post flame zone the diffusive terms in the conservation equations are assumed to be small in comparison with other parameters.

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In order for simplifying this model, it is presumed that the temperature of gas and particle is equal. The combustion mechanism is a one-step reaction as:

$$v_F[F] + v_{O_2}[O_2] \rightarrow v_{Pyrod}[P] + \text{Char}$$  \hspace{1cm} (1)

Where $F$ and $O_2$ denote the fuel and oxygen respectively. Also the overall reaction is formulated via the Arrhenius form as:

$$K_F = B \exp\left(-\frac{E}{(RT)}\right)$$ \hspace{1cm} (2)

$$K_T = -\rho K_F \exp\left(-\frac{E}{(RT)}\right)$$ \hspace{1cm} (3)

Where $B$ represents the frequency factor, $E$ the activation energy of the reaction and $R$ is the gas constant. Subscripts $F$ and $T$ denote the gaseous fuel and tar respectively. Also the characteristic Zeldovich number, which is presumed to be large, $Z_e$ is defined as

$$Z_e = \frac{E(T_f - T_u)}{RT_f^2}$$ \hspace{1cm} (4)

It is presumed that the fuel particles vaporize first to yield a gaseous fuel, which is oxidized in gas phase. Therefore, the surface reactions are neglected in this study and the kinetics of the vaporization and Devolatilization is given by the formulas (5) and (6) respectively.

$$w_v = An_s 4\pi T^n r^2$$ \hspace{1cm} (5)

$$w_{de} = A'n_s 4\pi T^n r^2$$ \hspace{1cm} (6)

For the combustion of wood particle-cloud, the energy equation is derived as:

$$\rho u \frac{dT}{dx} = \lambda_v \frac{d^2T}{dx^2} + w_v \frac{\rho_u}{\rho} Q + w_c \frac{\rho_c}{\rho} Q + w_{fu} \frac{\rho_{fu}}{\rho} Q_{fu} - w_{de} \frac{\rho_u}{\rho} Q_{fu}$$ \hspace{1cm} (7)

The gaseous fuel conservation:

$$\rho u \frac{dY_F}{dx} = \rho_u \frac{d^2Y_F}{dx^2} - w_v \frac{\rho_u}{\rho} + w_c \frac{\rho_u}{\rho} + w_{de} \frac{\rho_u}{\rho} + w_{fu} \frac{\rho_{fu}}{\rho}$$ \hspace{1cm} (8)

The equation governing the mass fraction of the particles neglecting diffusion can be written as:

$$\rho u \frac{dY_S}{dx} = -w_v \frac{\rho_u}{\rho} - w_{de} \frac{\rho_u}{\rho} \, , \, \rho u \frac{dY_C}{dx} = w_c \frac{\rho_c}{\rho}$$ \hspace{1cm} (9)

Where $\rho_S$ and $\rho_C$ are the density of fuel particles and char, which are considered to be constant, respectively. Equation of state:

$$\rho T = cte$$ \hspace{1cm} (10)

Therefore the heat capacity correlation is evaluated from the following expression:

$$C = C_p + \frac{4\pi^3 C_S \rho_S n_s}{3\rho}$$ \hspace{1cm} (11)

Boundary conditions for governing equations are as:

$$Y_F = 0 \, , \, T = T_u \, , \, Y_S = Y_{fu} \, , \, Y_C = finite \, \text{at} \, x = -\infty$$

$$Y_F = finite \, , \, T = T_b + T_c \, , \, Y_C = finite \, \text{at} \, x = +\infty$$ \hspace{1cm} (12)

3 Nondimensionalization of the governing equations
Dimensionless parameters are defined as:

\[
y_S = \frac{Y_S}{Y_{FC}}, \quad z = \frac{P_x v_x C}{\lambda_x}, \quad x = \frac{Y_x}{Y_{FC}}, \quad \theta = \frac{T - T_u}{T_f - T_u}, \quad m = \frac{\rho v}{\rho_a v_a}, \quad y_c = \frac{Y_c}{Y_{FC}}
\]  

(13)

The quantity \( Y_{FC} \) is represented as:

\[
Y_{FC} = C(T_f - T_u)
\]

(14)

In the above equation, \( T_f \) is the maximum temperature of the reaction zone which is calculated by considering the fact that the vaporization term is negligible. This assumption causes to define the parameter \( v_u \) which is the flame burning velocity in the mixture of fuel and air. Introducing the dimensionless parameters in the governing equation yields:

\[
m \frac{d^2 \theta}{dz^2} + \omega_F \rho_u + \omega_C \rho_C + \omega_T \rho_T - \eta_T y_S \frac{\gamma}{\gamma + 1} - \eta_T y_S \frac{\gamma}{\gamma + 1} = 0
\]

(15)

\[
m \frac{d^2 y_x}{dz^2} = \omega_F \rho_u + \omega_C \rho_C + \omega_T \rho_T + \eta_T \frac{y_S}{1} + \eta_T \frac{y_S}{1} = 0
\]

(16)

\[
m \frac{d^2 y_c}{dz^2} = \omega_T \rho_T
\]

(17)

\[
m \frac{d^2 y_u}{dz^2} = \omega_u \rho_u
\]

(18)

The quantity \( y_S \) is described as:

\[
y_S = 4 \pi \rho_s r^3 n_S / (3 \rho Y_{FC}) \]

(19)

Also in order to simplify the governing equations, the Lewis number is considered unity. In the above equation, some parameters such as \( \omega_F, \omega_T, \omega_{de}, \omega_C, \gamma, q \) are defined as:

\[
\omega_F = \frac{\lambda_x \times w_F}{(\rho_u v_u)^2 \times C \times Y_{FC}}, \quad \omega_C = \frac{\lambda_a \times w_C}{(\rho_u v_u)^2 \times C \times Y_{FC}}, \quad \omega_T = \frac{\lambda_a \times w_{de} \times Y_{FC}}{(\rho_a v_u)^2 \times C^3 \times (T_f - T_u)^2}, \quad \omega_T = \frac{\lambda_a \times w_{de} \times Y_{FC}^2}{(\rho_a v_u)^2 \times C^3 \times (T_f - T_u)^2},
\]

(20)

The boundary conditions needed for solving the governing equations are represented as:

\[
\theta = \theta_b = (T_b - T_u) / (T_f - T_u), \quad y_F = finite, \quad y_c = finite \quad \text{at} \quad z \rightarrow \infty
\]

\[
\theta = 0, \quad y_F = 0, \quad y_c = 0, \quad y_S = \alpha \quad \text{at} \quad z \rightarrow -\infty
\]

(21)

Consequently solving the energy equation in the flame zone, where the rate of heat vaporization of fuel particles is presumed to be zero, and considering the boundary condition in the interface, culminate in the burning velocity correlation as:

\[
\nu_u = 2(1 + b) \lambda_a B \exp \left( - \frac{E_c}{RT_f} \right) \left( \nu_x k_F + \nu_c k_C + \nu_T k_T \right) / \rho_a C
\]

(22)

If the heat of vaporization is considered, then the equation of burning velocity can be written:

\[
\nu_u = \nu_u \exp(- q z_u / 2)
\]

(23)

4 Results

Figure 2 shows the flame temperature and adiabatic temperature as a function of equivalence ratio. As observed, the flame temperature can’t exceed the adiabatic temperature which means that for each
radius, there is an acceptable equivalence ratio and this amount of equivalence ratio changes for different radius. Also, the flame temperature drops for the larger particle size denotes that smaller particles produce higher flame temperature. The variation of burning velocity $u_b$ including the heat vaporization as a function of equivalence ratio is shown in Figure 3. As seen in this figure, shooting up the equivalence ratio increases the burning velocity. It is necessarily needed to note that when the radius of the particles decreases, the number of gaseous and solid particles in the constant control volume increases which causes to augment the burning velocity.

![Figure 2](image2.png)  
**Figure 2.** The variation of flame temperature as a function of equivalence ratio for different radius  

![Figure 3](image3.png)  
**Figure 3.** The variation of burning velocity as a function of equivalence ratio for different radius

## 5 Conclusion

In this research, the novel asymptotic analysis is used in order to investigate the effect of pyrolysis on the structure of premixed wood flame propagation. This investigation is performed in the case where the flame structure consists of three zones: a preheat zone, a narrow reaction zone and a post flame zone. The governing equations for each zone are extracted and then these equations are solved through the required boundary and matching conditions which leads to the analytical correlation for burning velocity. It is indicated that the flame temperature and burning velocity are shooting up with increasing the equivalence ratio and decreasing the radius of the particle. Also, since the flame temperature can’t exceed the adiabatic temperature, there is the acceptable range of equivalence ratio for each radius of the particle.

## References