

# Modelling of Particle Pyrolysis in a Packed Bed Combustor

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## Introduction

Biomass combustion for renewable energy production has attracted increasing attention recently. Packed bed combustion is the most common mode of biomass combustion because of its tolerance of a wide range of fuel properties and particle sizes. As with most solid fuels, combustion occurs in three distinct stages: drying, devolatilization and volatiles combustion, and char combustion. Of these, devolatilization is very important, as up to 85% of the fuel mass can be evolved as volatiles, leaving only a small fraction to be consumed in the char combustion stage.

Research in this area at the University of Ottawa has so far resulted in a detailed numerical model of packed bed combustion which treats the bed as a continuum [1,2]. This solves separate gas and solid phase energy and continuity equations, incorporating the effects of solid phase heat conduction, gas phase diffusion and heat conduction, and heat and mass transfer between the solid and the gas, together with reaction kinetics for char consumption and CO oxidation. Non-spherical particles and the effects of interstitial ash particles on heat and mass transfer are accounted for [2]. However, initial efforts to include pyrolysis were quite crude: a simple one-step global reaction was used, with the solid phase treated as a continuum of locally uniform properties [3]. Neglected in this is the role that transient heat conduction within individual fuel particles plays in devolatilization: in fact, for large fuel particles (several cm) this can be a rate-controlling process. The purpose of the work presented here is therefore to upgrade the current treatment of pyrolysis in the bed by developing a more detailed model of the heating and pyrolysis of an individual fuel particle and then incorporating this sub-model in the bed model. This paper describes the single particle model and outlines its incorporation in the bed model.

## Processes of Particle Pyrolysis

Pyrolysis (or devolatilization) is the thermal breakdown of a solid fuel into three main components: gas, tar and char. The gas component consists of light hydrocarbons, carbon dioxide and carbon monoxide. Tar is a condensable component composed of a large variety of higher molecular weight species, including hydrocarbons, organic acids, aldehydes, alcohols, phenols and other oxygenates. It can undergo secondary reactions to be further broken down into char and gas. The final component, char, is the residual solid carbon. The chemical kinetics of pyrolysis are complex, and are different for the cellulose, hemicellulose and lignin components of wood and other biomass fuels. Models for the kinetics range from a single step first order reaction to multiple step mechanisms which can include parallel reactions and secondary decomposition of products [4-9].

Fig. 1 shows the main processes involved in pyrolysis of a particle exposed to a heat flux  $q_{IN}$ . Heat conduction into the particle raises the temperature locally, initiating reaction. A reaction front

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moves radially inward, leaving a porous char layer behind it. Tar and gas move outwards from this front, finally escaping from the particle surface. Since pyrolysis is endothermic, this outward flow of volatiles constitutes a cooling convective heat flux which opposes conduction. Other processes occurring during pyrolysis include secondary reaction of the products passing through the char layer, a buildup of pressure inside the particle to overcome the flow resistance of the porous char, gas phase diffusion of different product species, and shrinkage and/or splitting of the particle. A number of single particle pyrolysis models of varying degrees of complexity are given in the literature [4-11].

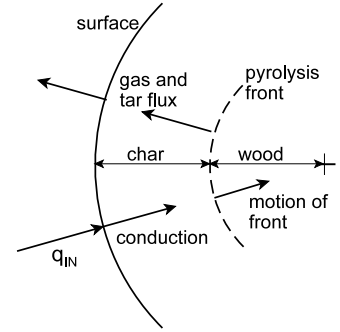


Fig. 1: Schematic of particle pyrolysis.

### Numerical Model for Particle Pyrolysis

In view of the fact that the particle model was later to be incorporated in the existing numerical model of packed bed combustion, the level of complexity of this model was to be such as to achieve a reasonable balance between complexity and accuracy. The model described here therefore includes the most important particle processes: chemical reaction, heat conduction, and convection due to the volatiles flow. Following the work of others [5], the effects of pressure, interdiffusion of different volatile components, and secondary reactions are neglected, and gas and solid are assumed to be at the same temperature locally. The particle size is assumed to remain constant during pyrolysis. However, variable solid and gas properties are included.

Pyrolysis kinetics were modelled with a one-step first order equation, giving the rate of production of volatiles as

$$\dot{r}_P = (1 - \zeta_C) \rho_W W A \exp(-E/RT) \quad (1)$$

The variable  $W$  is the local fraction of the original wood that is unconverted (ie mass of wood remaining in the partially-converted fuel / original mass of wood); it can be related to the local mass fraction of unconverted wood ( $Y_W = \text{mass of wood} / (\text{mass of wood} + \text{char})$ ) as

$$W = \frac{Y_W \zeta_C}{1 - Y_W(1 - \zeta_C)} \quad (2)$$

A solid mass balance on unconverted wood gives the local rate of change of wood fraction:

$$\frac{d(\rho_S Y_W)}{dt} = \frac{\dot{r}_P}{(1 - \zeta_C)} \quad (3)$$

where the local solid density is related to  $Y_W$  by

$$\frac{1}{\rho_S} = \left( \frac{Y_W}{\rho_W} + \frac{(1 - Y_W)}{\rho_W \zeta_C} \right)^{-1} \quad (4)$$

assuming that no shrinkage occurs on pyrolysis. A balance on the gas phase gives the volatiles flow velocity  $v_G$  as a function of radius:

$$\frac{\partial \rho_G}{\partial t} + \frac{1}{r^2} \frac{\partial (r^2 \rho_G v_G)}{\partial r} = \dot{r}_P \quad (5)$$

where for the present calculations the gas phase transient term was neglected (quasi-steady flow field). Finally, the assumption of equal gas and solid temperatures allows the energy equations for the two phases to be combined to

$$\frac{\partial (\rho_S h_S)}{\partial t} + \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \rho_G v_G h_G) = \frac{1}{r^2} \frac{\partial}{\partial r} \left( k_S r^2 \frac{\partial T}{\partial r} \right) + \frac{\dot{r}_P}{(1 - \zeta_C)} \Delta h_P \quad (6)$$

where transients and conduction in the gas phase have been assumed negligible in comparison with the solid. At the particle surface the ambient temperature  $T_\infty$  and the heat transfer coefficient  $h$  are specified. These equations were integrated numerically using a finite volume method.

Properties were allowed to vary in time and space. The solid enthalpies were calculated using mean specific heats generated by correlations given for wood by Grønli and Melaaen [4] and for char by Larfeldt *et al.* [11]. The pyrolysis products were assumed to comprise 30% CO, 30% CO<sub>2</sub> and 40% tar by mass [3], and gas enthalpies were calculated for this mixture. Tabulated specific heat correlations were used for CO and CO<sub>2</sub>, while for tar, levoglucosan was chosen as a representative compound, and specific heats for it were generated using methods from [13]. The enthalpy of pyrolysis was set at  $\Delta h_p = -420$  kJ/kg [12]. The thermal conductivity  $k_s$  was assumed to be a linear combination of those for wood and char, determined from correlations by Koufopoulos *et al.* [9] and by Larfeldt *et al.* [11] respectively. There is an extremely wide range of rate constants available for wood and biomass; those of Branca and di Blasi [8] were used here ( $A = 3.6 \cdot 10^8$  s<sup>-1</sup>,  $E = 141$  kJ/gmol). Conditions for the sample calculations shown here (Table 1) were chosen to be representative of those in earlier packed bed experiments [3].

**Table 1: Conditions for Calculations**

Particle diameter	3.4 cm
Ambient temperature	1300 K
Surface heat transfer coefficient	30 W/m K
Char fraction $\zeta_C$	0.15

## Results

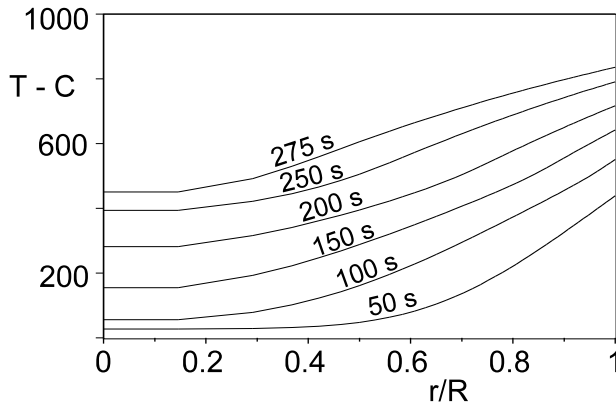


Fig. 2: Temperature profiles at various times in the pyrolyzing particle.

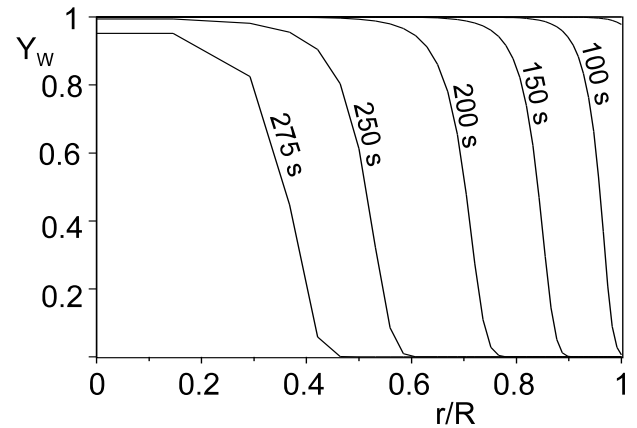


Fig. 3: Profiles of mass fraction of unconverted wood at various times.

Figs. 2 and 3 show typical temperature and wood mass fraction profiles in the pyrolyzing particle at various times. The temperatures show a fairly gentle gradient from the surface to the centre, but the profiles of  $Y_w$  by contrast show a sharply-defined pyrolysis front moving into the particle. This behaviour is the result of the high activation energy chosen for the reaction; a lower  $E$  would spread pyrolysis over a wider zone. Fig. 4 shows the overall progress of pyrolysis as reflected by the particle weight loss with time. This last is the information required for input into the packed bed model.

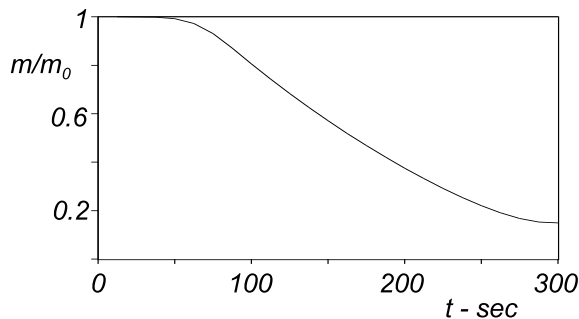


Fig. 4: Decrease of particle mass with time.

## Conclusion

The particle model is currently being incorporated into the bed model using a particle tracking and interpolation scheme. From the bed model the total heat flux to the particle surface will be input to the particle model, which will return the pyrolysis rate and particle surface temperature to the main program.

## Acknowledgement

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## Nomenclature

A pre-exponential,  $s^{-1}$   
 E activation energy, kJ/mol  
 h enthalpy J/kg  
 k thermal conductivity W/m K  
 m mass  
 r radial coordinate  
 R particle radius  
 R universal gas constant

T temperature  
 v velocity, m/s  
 W fraction of original wood remaining  
 Y mass fraction  
 $\zeta_C$  yield of char from wood  
 $\rho$  density  $kg/m^3$

### Subscripts

C char  
 G gas phase  
 S solid phase  
 W wood (unconverted)  
 0 initial

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