

CFD MODELLING OF WOOD COMBUSTION

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ABSTRACT

The modelling of extinguishment of fires still represents a significant challenge. As part of an effort to predict fire spread and extinguishment using water sprays we are developing a CFD model of fire spread. This paper deals with the description of the CFD model, the solid pyrolysis model (wood in this case) and the coupling of these models. Results are compared with experimental data from cone calorimeter tests and the model is shown to give good agreement. The sensitivity of the calculated results to uncertain parameters is also considered.

NOMENCLATURE

a	Progress variable (see eq. (8))
A_p	Pre-exponential factor
a_g	Acceleration due to gravity
E	Activation energy
f	Mixture fraction
f_v	Soot volume fraction
h	Enthalpy or heat transfer coefficient
I	Radiation intensity
k	Turbulence kinetic energy or thermal conductivity
k_g	Absorption coefficient due to gas
k_s	Absorption coefficient due to soot
l	Distance along radiation path
m_g	Mass flux of volatiles (towards surface)
p	Pressure
Q_p	Heat of pyrolysis
Q_R	Radiation source term
R	Universal gas constant
S	Mass of O_2 which reacts with 1 kg of fuel at stoichiometric conditions
S_ϕ	Source/sink term for variable ϕ
T	Temperature
t	Time
u, v, w	Velocity components in the x, y and z directions

x, y, z	Cartesian coordinates
Y_F	Fuel mass fraction
Y_O	Oxygen mass fraction
Γ_ϕ	Exchange coefficient for ϕ
ϵ	Turbulence dissipation rate or emissivity
μ_e	Effective viscosity ($\equiv \mu_t + \mu_{\text{lam}}$)
ρ	Density
ρ_{ref}	Reference density
σ	Stefan-Boltzmann constant
σ_ϕ	Turbulent Prandtl/Schmidt number
ϕ	Any variable

INTRODUCTION

The computation of the spread of fire and its extinguishment via water sprinklers still represents a considerable challenge. The University of Sydney, together with the Work-Cover Authority of New South Wales and Tyco Laboratories (formerly Wormalds) are carrying out a combined experimental and computational study of fire extinguishment. The ultimate aim of the project is the production of a validated CFD model of fire spread and fire extinguishment using water sprinklers that can be used in the design of sprinkler installations. In order to produce a validated model we have embarked upon a step by step validation process, in which each of the many submodels required in the final model are validated in turn.

Our starting point was the simulation of combustion and smoke movement for a pool fire located within a ventilated tunnel. Simulations reported in [1, 2] show that the model can successfully reproduce the measured smoke transport behaviour. The next stage in the project is the inclusion of a model of solid combustion, since in the above calculations the fuel consumption rate was specified using experimental data. The implementation of such a model, the numerical procedure used and validation of the model form the substance of this paper. We also address the important issue of model sensitivity to uncertain physical properties, such as the pyrolysis kinetics.

DESCRIPTION OF THE MODEL

In order to specify the model we present details of the CFD model, the wood pyrolysis model and a discussion of the linkage between them.

The CFD Model

The mathematical model used to perform the calculations reported in this paper is a modified version of the FURNACE code, which has been used in the study of coal-fired boilers [3] and to make calculations for tunnel fires [1, 2]. The flow is described by the three dimensional, Favre-averaged equations of transport for mass, momentum, gas species concentration and enthalpy. Turbulence is modelled using the k - ϵ closure, with the turbulent viscosity given by $\mu_t = c_\mu \rho k^2 / \epsilon$. The standard model is modified via the inclusion of extra terms (G in Table 1) in the k and ϵ equations to allow for the

production of turbulence due to buoyancy and the effect of thermal stratification on the turbulence dissipation rate. Combustion is modelled via the Eddy-Breakup (EBU) model. The nine conservation equations are cast into the following form [4]:

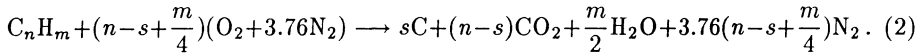
$$\frac{\partial(\rho\phi)}{\partial t} + \nabla \cdot (\rho \mathbf{u} \phi) = \nabla \cdot (\Gamma_\phi \nabla \phi) + S_\phi. \quad (1)$$

The variables, together with the exchange coefficients and source terms, are given in Table 1.

Gaseous Combustion Modelling

Gaseous combustion is modelled using the Eddy-breakup model in which conservation equations are solved for the mixture fraction and fuel mass fraction. These equations then allow the mass fractions of oxygen and products to be determined. This approach is widely used in fire modelling, as discussed by Bilger [5]. Note that in our early work we used a prescribed pdf fast chemistry model. This modelling change was made to enable us to examine situations in which fuel vapour is present but does not burn (e.g. during a pre-flashover situation) and to allow us to make the combustion rate depend on the mass fraction of water vapour present (for the extinguishment application).

The following chemical reaction is assumed



Here s is a parameter to define the amount of soot produced. If s is set to zero in the above equation, the complete combustion reaction is obtained in which fuel reacts with oxygen to give carbon dioxide and water. A non-zero value for s results in some of the carbon remaining as soot, with a consequent reduction in the mass of CO_2 formed. The soot is produced near stoichiometry and is dispersed throughout the flow, with the soot concentration being determined from the local mixture fraction. The soot is assumed to be in the form of fine particles suspended in the flow (i.e. their slip velocity is zero).

Radiation Modelling

The effect of the soot concentration on radiation is explicitly included by solving the following equation

$$\frac{dI}{dl} = -(k_g + k_s)I + \frac{\sigma}{\pi}(k_g + k_s)T^4 \quad (3)$$

for the radiant heat exchange. This equation gives the change in radiation intensity I with distance l due to absorption and emission of radiation by the gas and soot particles along the path. Scattering has been neglected because of the small size of the soot particles. The absorption coefficients are specified as follows (see [2] for details):

$$k_g = 0.32 + 0.28 \exp\left(-\frac{T}{1135}\right) \quad \text{and} \quad k_s = 1264 f_v T. \quad (4)$$

ϕ	Γ_ϕ	S_ϕ
1	0	0
u	μ_e	$-\frac{\partial p}{\partial x} + \frac{\partial}{\partial x} \left(\mu_e \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y} \left(\mu_e \frac{\partial v}{\partial x} \right) + \frac{\partial}{\partial z} \left(\mu_e \frac{\partial w}{\partial x} \right)$
v	μ_e	$-\frac{\partial p}{\partial y} + \frac{\partial}{\partial x} \left(\mu_e \frac{\partial u}{\partial y} \right) + \frac{\partial}{\partial y} \left(\mu_e \frac{\partial v}{\partial y} \right) + \frac{\partial}{\partial z} \left(\mu_e \frac{\partial w}{\partial y} \right)$
w	μ_e	$-\frac{\partial p}{\partial z} - a_g(\rho - \rho_{\text{ref}}) + \frac{\partial}{\partial x} \left(\mu_e \frac{\partial u}{\partial z} \right) + \frac{\partial}{\partial y} \left(\mu_e \frac{\partial v}{\partial z} \right) + \frac{\partial}{\partial z} \left(\mu_e \frac{\partial w}{\partial z} \right)$
k	μ_e/σ_k	$P + G - \rho\epsilon$
ϵ	μ_e/σ_ϵ	$\frac{\epsilon}{k} \{c_1[P + c_3 \max(G, 0)] - c_2\rho\epsilon\}$
f	μ_e/σ_f	0
Y_F	μ_e/σ_Y	$-c_R\rho\frac{\epsilon}{k} \min(Y_F, Y_O/S)$
h	μ_e/σ_h	$-Q_R$
$P = \mu_e \left\{ 2 \left[\left(\frac{\partial u}{\partial x} \right)^2 + \left(\frac{\partial v}{\partial y} \right)^2 + \left(\frac{\partial w}{\partial z} \right)^2 \right] + \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right)^2 \right. \\ \left. + \left(\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \right)^2 + \left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right)^2 \right\}, \quad G = a_g \frac{\mu_e}{\sigma_h} \frac{1}{\rho} \frac{\partial \rho}{\partial z}$		
$\sigma_k = 0.9, \sigma_\epsilon = 1.22, \sigma_f = 0.7, \sigma_Y = 0.7, \sigma_h = 0.7, c_\mu = 0.09$ $c_1 = 1.44, c_2 = 1.92, c_3 = 1.0, c_R = 4.0.$		

Table 1: The flux and source terms for the conservation equations.

Wood Pyrolysis Model

Wood pyrolysis and combustion is very complex, as discussed in the recent review by Di Blasi [7]. For the present calculations we make a number of simplifications and use the wood pyrolysis model based on that of Kung [8, 9]. Heat is assumed to be conducted into the wood, which releases volatiles as it transforms virgin wood (denoted v) into pre-defined amounts of char (denoted c) and volatiles (denoted g). The rate of release is controlled by a first order Arrhenius reaction. The properties of the wood are assumed to depend on the local composition. The wood is assumed to be dry and all volatiles escape to the surface as soon as they are formed. A one-dimensional treatment is used with variation normal to the surface being considered to dominate over transverse variations. At present char combustion is not included. With these assumptions conservation of energy and mass give the following equations (we adopt the usual practice of making the mass flux positive in the negative x -direction for consistency with the literature in this area):

$$\frac{\partial}{\partial t}(\rho h) = \frac{\partial}{\partial x} \left(k \frac{\partial T}{\partial x} \right) - Q_p \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} (m_g h_g) \quad (5)$$

and

$$\frac{\partial \rho}{\partial t} - \frac{\partial m_g}{\partial x} = 0. \quad (6)$$

The devolatilization rate is given by

$$\frac{\partial \rho}{\partial t} = -\rho_v a A_p \exp \left(-\frac{E}{RT} \right) \quad \text{for } \rho > \rho_c. \quad (7)$$

In the above equation the quantity a is a progress variable and is defined via

$$a = \frac{(\rho - \rho_c)}{(\rho_v - \rho_c)}. \quad (8)$$

The temperature is calculated from the enthalpy using

$$h = \int_{T_{ref}}^T c_p dT, \quad \text{where } c_p \text{ is a obtained using } c_p = a c_{p,v} + (1 - a) c_{p,c}. \quad (9)$$

A similar expression to the above is used to calculate the thermal conductivity but in this case the thermal conductivity of the char is assumed to be a linear function of temperature, so that

$$k = a k_v + (1 - a) k_c, \quad \text{where } k_c = k_c^0 + k_c^*(T - T_{ref}). \quad (10)$$

At the surface of the wood in contact with the gas phase we set

$$-k \frac{\partial T}{\partial x} = h_1 (T_{gas} - T_{surf}) + q_{rad} \quad (11)$$

and at the back surface we set

$$-k \frac{\partial T}{\partial x} = h_2 (T_{back} - T_{\infty}). \quad (12)$$

In the above expression q_{rad} contains the contributions to radiative heat transfer from the surrounding walls, the gas, the radiant heater (if used) and the re-radiation from the wood surface. The value of h_1 is calculated using the usual log-law boundary conditions and h_2 is specified from the experimental conditions. T_∞ is the ambient temperature.

Numerical Solution Procedure

The equations were solved by an iterative method which utilizes a finite volume approach. The equations were discretised on a rectangular mesh, which employed the usual staggered grid configuration [4]. All convection terms were discretised using hybrid differencing for stability. Conservation of mass was obtained by using the SIMPLER pressure correction algorithm [4]. The radiative heat transfer equation was solved using the discrete transfer method of Lockwood and Shah [6].

A fully implicit treatment is used in which the enthalpy equation is solved for the wood and the volatiles produced are released into the flow domain. Typically a finite volume cell size of 0.1 mm is used in the wood and a time-step of 0.1 s is used. At each time-step, iteration is carried out in the flow solution to ensure that a converged solution is obtained and that it is accurately coupled to the solid model.

COMPARISON OF THE RESULTS WITH EXPERIMENTAL DATA

In order to verify our numerical model we carried out two series of calculations to compare predictions with the available experimental data.

The first one dealt with thermal degradation of particle board subjected to a constant radiant heat flux in an inert atmosphere [10, 11]. Experiments were performed by Vovelle *et al.* in a chamber with dimensions of 0.3 m \times 0.45 m and a height of 0.5 m. The size of the vertically oriented sample was 0.1 m \times 0.1 m and the radiant heat flux applied to its surface was equal to 31 kW/m². The thickness of the sample was not given, but estimates made using the experimental data suggest that it was 8 mm. The experimental conditions led to a uniform heat flux on the sample, so that the thermal degradation was one-dimensional. The flow rate of nitrogen through the gas inlet at the bottom of the chamber was 3 m³/hour. The gas outlet was placed at the upper part of the chamber.

To follow the experimental setup we used a 6 \times 8 \times 10 grid to represent the chamber, with the same grid used for the flow and radiation calculations. The rate of nitrogen inflow was chosen to be the same as in experiments. The properties used in the simulation were: $\rho_v = 663 \text{ kg m}^{-3}$, $\rho_c/\rho_v = 0.2$, $c_{p,v} = c_{p,c} = 2.52 \text{ kJ kg}^{-1}\text{K}^{-1}$, $k_c^0 = k_v = 0.126 \text{ W m}^{-1}\text{K}^{-1}$, $k_c^* = 0$, $\epsilon = 0.9$, $A_p = 5.25 \times 10^7 \text{ s}^{-1}$, $E = 1.256 \times 10^5 \text{ kJ kg}^{-1}\text{mol}^{-1}$, $Q_p = 0$. Fig. 1 shows the transient behavior of the front surface temperature. The discrepancy from the experimental curve is mostly likely due to uncertainty in the properties of the sample, since we could only find data for the density of the particle board in the literature [12]. For other properties, values typical for wood materials were assumed. Also, the thermal properties of the virgin and char layers were taken to be the same due to the lack of reliable data.

Fig. 2 shows the mass loss rate per unit surface of the board as a function of time. The experimental data are for degradation in a nitrogen atmosphere, that is without combustion of volatiles released from the board. However, some calculations were made

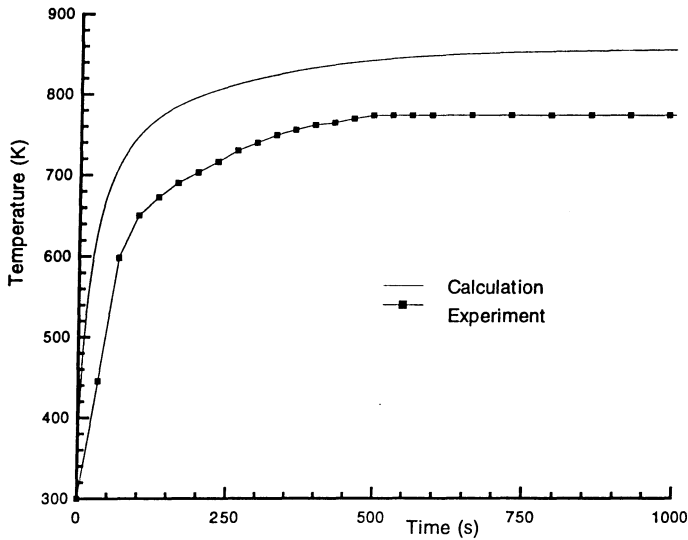


Figure 1: A comparison of the calculated and experimental front surface temperature for the particle board case.

in air to see whether the influence of the flame is important or not. In these calculations the volatiles were assumed to have the composition of methane, 2% of the carbon formed soot and the heat of combustion was 20 MJ/kg. As the results presented in Fig. 2 show, the thermal and radiant flux from the flame results in a very small increase in the mass loss rate. This suggests that the external radiant flux is much stronger than the flux generated by flame. This statement is also supported by the fact that the calculated mass loss rate was found to be independent of the orientation of the sample. This is in agreement with experimental observations [10, 13]. In these experiments a strong effect of oxygen content at low values of the radiant flux was observed compared with a much weaker effect at a flux of about 40 kW/m².

On the other hand, the convective term in equation (5) has a significant effect on the mass loss rate, as Fig. 2 clearly shows. This term results in a substantial amount of heat being extracted from the burning sample and a consequent decrease in the mass loss rate of about 20% in the region of its maximum value. Consequently, the sample burns for a longer time.

A second set of numerical experiments was carried out to make a comparison with data obtained for Pacific maple using a cone calorimeter [14]. The cone calorimeter was modelled as a rectangular prism with length and width equal to 0.4 m and a height equal to 0.5 m. The calculations were performed using a computational mesh with 8 cells along and across the calorimeter and 10 cells in the vertical direction, with the same grid used for radiation calculations. The material properties used in the simulation were: $\rho_v = 530 \text{ kg m}^{-3}$, $\rho_c/\rho_v = 0.2$, $c_{p,v} = 2.42 \text{ kJ kg}^{-1}\text{K}^{-1}$, $c_{p,c} = 1.0 \text{ kJ kg}^{-1}\text{K}^{-1}$, $k_v = 0.16 \text{ W m}^{-1}\text{K}^{-1}$, $k_c = 0.08 \text{ W m}^{-1}\text{K}^{-1}$, $k_c^* = 8.2 \times 10^{-5} \text{ W m}^{-1}\text{K}^{-2}$, $h_2 = 0$,

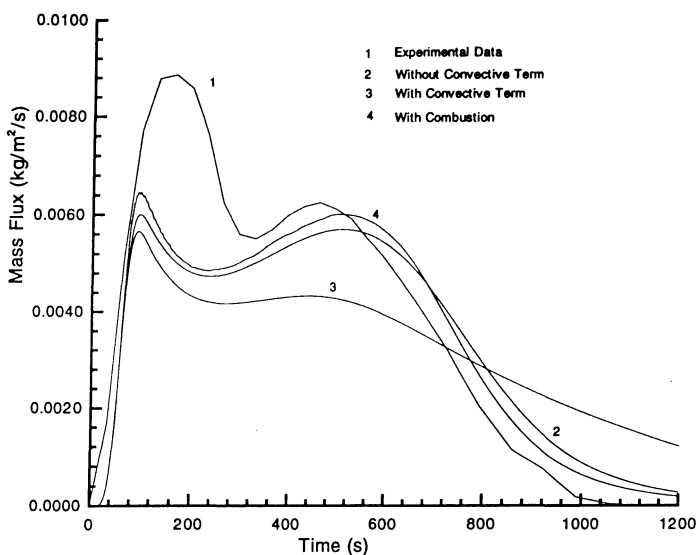


Figure 2: A comparison of the calculated and experimental mass loss rate for the vertical orientation of the particle board. The applied heat flux is 31 kW m^{-2} .

$A_p = 5.25 \times 10^7 \text{ s}^{-1}$, $E = 1.1 \times 10^5 \text{ kJ kg}^{-1} \text{ mol}^{-1}$, $Q_p = 0$. The applied heat flux was 20 kW m^{-2} .

A sensitivity analysis was performed to find the parameters which affect the pyrolysis behavior of the wood most strongly. One of these parameters appears to be the heat transfer coefficient at the back surface of the sample. As the thermal wave propagates to the depth of the sample and comes close to the back surface the mass loss rate may have a very pronounced peak provided the heat transfer coefficient is sufficiently small (see Fig. 3). The best agreement with experimental data was achieved for the adiabatic condition at the back surface. (Note that in Fig. 3 and subsequent figures there is a discrepancy between the time at which rapid pyrolysis starts in the calculations and in the experiments. This is because the calculations start with the sample at the ambient temperature whereas there was some pre-heating of the wood in the cone calorimeter tests.)

Not surprisingly, changing the activation energy has a significant effect on the mass burning rate. As Fig. 4 indicates, even a 10% change leads to a remarkable shift in the peaks of the mass loss rate curve. The dependence on pre-exponential factor is somewhat less sharp (see Fig. 4).

The results are also sensitive to the value of the heat of pyrolysis, as shown in Fig. 5. The experimental data concerning the value taken by this parameter is very uncertain. Some measurements give negative values for the heat of pyrolysis whilst others give positive values [7]. It seems that this property does not remain constant during the thermal degradation process but changes its value as well as its sign. Under these circumstances the choice of a heat of pyrolysis of zero seems to be a reasonable

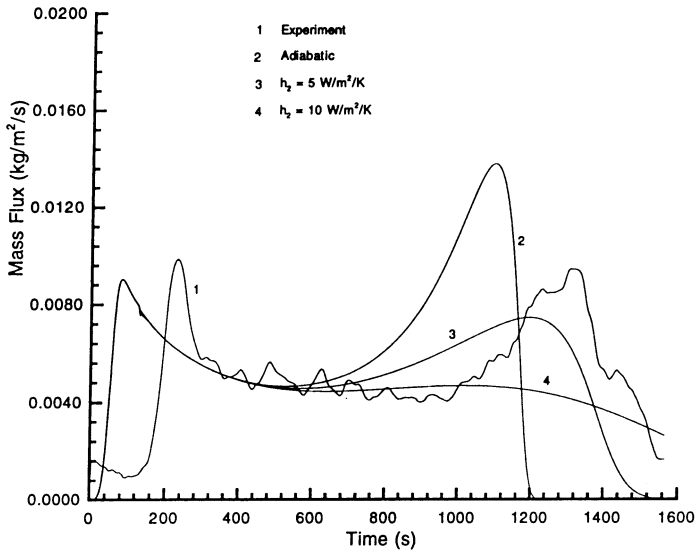


Figure 3: The effect of the back surface heat transfer coefficient (h_2) for the Pacific maple case.

approach and is also the most suitable to fit the experimental data, as can be seen in Fig. 5.

Calculations also showed the expected sensitivities to changes in the thermal conductivity and specific heat parameters. Specifically, changing the thermal conductivity of the virgin wood affects both peaks in the mass loss rate, whereas changing the thermal conductivity of the char affects only the second peak, since the char layer is very thin at the time of the first peak. Making the char thermal conductivity a factor of two lower than that for the virgin wood reduced the height of the second peak by approximately 25%.

CONCLUSIONS

In this work we have studied numerically the thermal degradation of two solid materials, particle board and Pacific maple, subjected to a constant radiant heat flux and have made a comparison with the available experimental data. To perform this analysis we have used a CFD model coupled to a detailed model of the solid phase behaviour.

The comparison of the results with the experimental data shows that the model predicts the shape of the temperature and mass loss curves for both types of combustible materials very well. The worst discrepancy between experiment and the calculations for the mass loss rate was found to be about 50% for Pacific maple in a relatively narrow time region, while for most of the time the error was less than 10% for particle board and less than 25% for Pacific maple. The calculations show that the model presented here can be used as a basis for our numerical simulation of fire extinguishment.

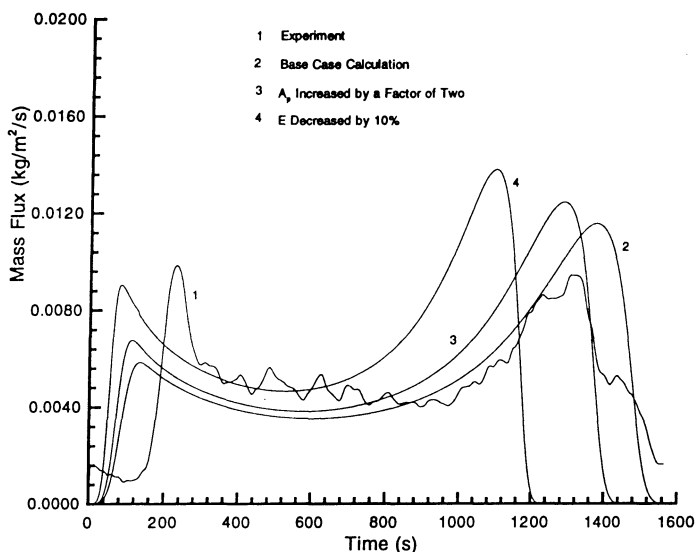


Figure 4: The effect of the activation energy (E) and the pre-exponential factor (A_p) for the Pacific maple case.

The comparison of the cases where thermal degradation occurs in an inert atmosphere with those where combustion in the gas phase takes place is interesting. Even with relatively high volatile mass fluxes and a significant amount of soot present, so that the radiative heat feedback from the flame is high, the effect of heat feedback from the flame is small. This explains why in the cone calorimeter tests the flame extinguished if the radiant heaters were turned off.

Also the sensitivity of the calculations to major input parameters has been examined and quantified. This analysis highlights the most important parameters which should be experimentally obtained for accurate combustion modelling. The results show that the back boundary condition determines to a large extent whether there is a second peak or not in the mass flux of volatiles. The results are also very sensitive to the heat of pyrolysis and there is a significant difference between the results from the calculations using a small negative (endothermic) or small positive (exothermic) reaction. The inclusion of the convective heat transport by the volatiles was also found to be very important. The present results clearly show the need to obtain thermophysical data for the material of interest if the details of the mass loss rate are required but that using best-estimate values results in reasonable agreement with the experimental data.

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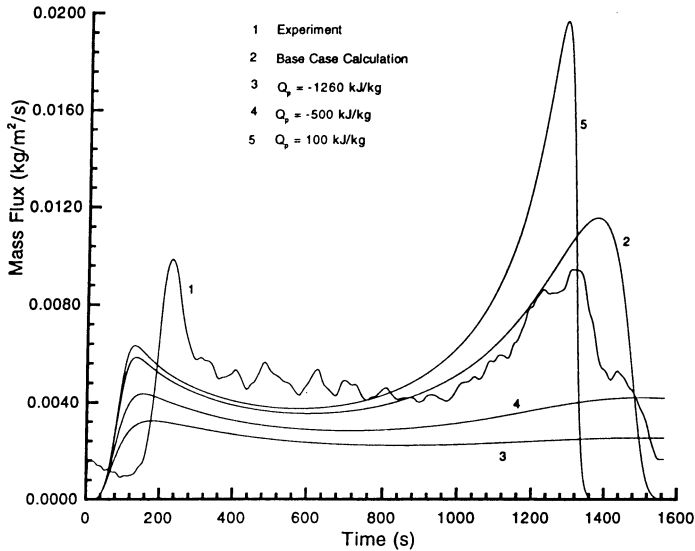


Figure 5: The effect of the heat of pyrolysis (Q_p) for the Pacific maple case.

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