



## Prediction of the burning rates of charring polymers<sup>☆</sup>

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### ARTICLE INFO

#### Article history:

Received 16 December 2009

Received in revised form 2 February 2010

Accepted 23 March 2010

#### Keywords:

Material flammability

Pyrolysis model

Cone calorimetry

Charring polymer

Intumescence

ThermaKin

### ABSTRACT

A quantitative understanding of the processes that take place in the condensed phase of a burning material is critical for prediction of ignition and growth of fires. In the current study, a model of burning of two widely-used charring and intumescent polymers, bisphenol A polycarbonate and poly(vinyl chloride), was developed and validated. The modeling was performed using a flexible computational framework called ThermaKin, which had been developed in our laboratory. ThermaKin solves time-resolved energy and mass conservation equations describing a one-dimensional material object subjected to external heat. Most of the model parameters were obtained from direct property measurements. The model was validated against the results of cone calorimetry experiments performed under a broad range of conditions. Potential sources of uncertainties in the model parameterization were analyzed.

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### 1. Introduction

It is recognized that the processes that take place in the condensed phase of a burning polymer play an important role in the overall combustion [1]. Quantitative understanding of these processes is critical for prediction of ignition and growth of fires. During the past decade, a significant effort has been made to develop mathematical models of polymer pyrolysis. The principal objective of this effort is to provide the means for extrapolation of the results of a bench-scale fire test to a large scale fire scenario. Typically, the model parameters, which describe thermal and chemical properties of a given material, are obtained by fitting the results of cone calorimetry [2] or fire propagation apparatus experiments [3]. The parameterized pyrolysis model is subsequently used in conjunction with a model of gas phase combustion to predict the development of a large scale fire. The main drawback of this approach is that the problem of deriving material properties from the results of fire calorimetry tends to be underdefined (i.e., there is more than one set of property values that gives an equally good fit). Consequently, this approach provides only a limited understanding of the physics and chemistry of pyrolysis.

In the current study, a one-dimensional numerical model of burning called ThermaKin [4,5] was used to simulate cone calorimetry tests performed on widely-used charring and intumescent

polymers – bisphenol A polycarbonate (PC) and poly(vinyl chloride) (PVC). Most of the model parameters were obtained from the results of direct property measurements, which is the key distinguishing aspect of this work. This is the second study in a series; the first one [6] was focused on non-charring polymers (poly(methylmethacrylate), high-impact polystyrene and high-density polyethylene). The results of both studies indicate that a combination of material properties describing energy transport and thermally-induced gasification reactions defines polymer burning behavior in a wide range of conditions. The charring polymers clearly represent a more challenging case for modeling. This study is an attempt to address these challenges.

The paper is organized as follows. Section 2 contains an overview of the numerical and experimental techniques employed in this study and a specification of the polymeric materials that were investigated. Section 3 contains a detailed description of the model parameterization and set up and a comparison of the modeling results with the cone calorimetry experiments. This section also includes analyses of two important questions. What is the best way to represent intumescent char within the framework of the model? And how sensitive is the model output to uncertainties in the input parameters? Section 4 summarizes the key findings.

### 2. Methods and materials

#### 2.1. ThermaKin

ThermaKin is a flexible computational framework that solves energy and mass conservation equations describing a one-dimen-

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**Nomenclature**

PC	bisphenol A polycarbonate	HCC	heat of complete of combustion
PVC	poly(vinyl chloride)	HRR <sub>MCC</sub>	heat release rate obtained by MCC
$r$	reaction rate	HRR <sub>cone</sub>	heat release rate obtained by cone calorimeter
$J$	mass flux	$\mu$	yield of non-volatile product
$\xi$	concentration	$\gamma$	reflectivity
$c$	heat capacity	EHF	incident external radiative heat flux
$\rho$	density	EHF <sub>0</sub>	initial value of EHF
$T$	temperature	EHF <sub>t</sub>	time-dependent correction of EHF
$t$	time	CE <sub>cone</sub>	efficiency of cone calorimetry combustion
$x$	Cartesian coordinate	CHR	critical heat release rate
$h$	heat of reaction	TTI	time to ignition
$\theta$	stoichiometric coefficient	$\omega$	radiative heat transfer coefficient
$A$	Arrhenius pre-exponential factor	$\tau_p$	areal density of plate
$E$	Arrhenius activation energy	$l$	distance between plates
$R$	gas constant	$\tau_L$	areal density of layer
$k$	thermal conductivity	$N_p$	number of plates in layer
$\lambda$	gas transfer coefficient	ChBE	char thermal barrier efficiency
$\alpha$	absorption coefficient	AHRR	average heat release rate
$I$	radiative heat flux		
$\sigma$	Stefan–Boltzmann constant	<i>Subscript</i>	
$H$	convective heat flux	S	surface boundary
$\nu$	convection coefficient	$c$	component
$\zeta$	critical mass flux	$g$	gaseous component
TGA	thermogravimetric analyzer	$r$	reaction or reactant
$\beta$	heating rate	$M$	mixture
MLR <sub>TGA</sub>	mass loss rate obtained by TGA	$A$	ambient
MCC	microscale combustion calorimeter		

sional material object subjected to external heat. Only a brief description of the framework is given here; a complete description can be found in earlier publications [4,5]. In this framework, the material is represented by a mixture of components, which may interact chemically and physically. The components are assigned individual properties and categorized as solids, liquids or gases. The governing equations can be summarized as follows:

$$\sum_c^{\text{comp}} \xi_c c_c \frac{\partial T}{\partial t} = \frac{\partial}{\partial x} \left( k_M \frac{\partial T}{\partial x} \right) + \sum_r^{\text{reac}} r_r h_r - \sum_g^{\text{gases}} J_g \frac{\partial}{\partial x} \left( \int_0^T c_g dT \right) + \alpha_M I \left( 1 - \frac{\sigma T^4}{I_S} \right) \quad (1)$$

$$\frac{\partial \xi_g}{\partial t} = \sum_r^{\text{reac}} \theta_r^g r_r - \frac{\partial J_g}{\partial x} \quad (2)$$

$$r_r = A_r \exp \left( -\frac{E_r}{RT} \right) \xi_r \quad (3)$$

$$J_g = -\rho_g \lambda_M \frac{\partial}{\partial x} \left( \frac{\xi_g}{\rho_g} \right) \quad (4)$$

Eq. (1) is the energy conservation statement; Eq. (2) is the mass balance for a gaseous component. Eq. (3) is an expression of the first order reaction rate,  $r$  (second order reactions between components can also be defined within the ThermaKin framework). Eq. (4) is the definition of a gaseous component mass flux ( $J$ ). Only gaseous components are assumed to be mobile, which means that, for a liquid or solid component, the last right-hand-side term in the mass balance equation is 0.

$\xi$ ,  $c$  and  $\rho$  are concentration, heat capacity and density of a component.  $T$  is temperature;  $t$  is time; and  $x$  is the Cartesian coordinate.  $h$  is the heat of reaction;  $\theta$  is a stoichiometric coefficient,

which is negative when the corresponding component is a reactant and positive when it is a product.  $A$  and  $E$  are the Arrhenius parameters; and  $R$  is the gas constant.  $k$ ,  $\lambda$  and  $\alpha$  are thermal conductivity, gas transfer and radiation absorption coefficients.  $I_S$  is the flux of infrared radiation from an external source incident onto the material surface.  $I$  is the flux of the radiation inside the material, which is computed using a generalized form of Beer–Lambert law and corrected for the material reflectivity.  $\sigma$  is the Stefan–Boltzmann constant. Subscript or superscript  $g$  is used to refer to a gaseous component; subscript  $c$  is used for all types of components (including gaseous). Subscript  $r$  is used to refer to a reaction and the corresponding reactant. Subscript  $M$  indicates a property of mixture (rather than that of an individual component).

The material's volume is defined as a sum of component masses divided by the corresponding densities. The volumetric contribution of gaseous components can be scaled by a user defined factor (which can be related to the local composition). The boundary conditions are defined separately for the two surfaces of the material object. These definitions include radiative ( $I_S$ ) and convective ( $H_S$ ) heat fluxes. The convective heat flux into the material is expressed as:

$$H_S = \nu(T_A - T_S) \quad (5)$$

where  $\nu$  is the convection coefficient;  $T_S$  is the material surface temperature; and  $T_A$  is the temperature outside of material. Both  $I_S$  and  $T_A$  can be defined as a piecewise linear function of time. The radiative and convective heat fluxes can also be related to gaseous component fluxes out of the material ( $-J_S$ ). These relations are based on the following criterion:

$$CI = \sum_g^{\text{gases}} \frac{-J_S^g}{\zeta_g} \quad (6)$$

where  $\zeta_g$  are critical mass fluxes specified for gaseous components. When CI reaches 1, a constant value can be added to  $I_S$  and the

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