A new model to predict multi-stage pyrolysis of flammable materials in standard fire tests

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Abstract. Test procedures to assess material flammability are focused on radiative heating of the examined material followed by ignition of volatiles produced by pyrolysis. In this work, a new model (Pyropolis) for predicting thermal degradation of polymer materials exposed to the external heat flux is presented. Composite materials of interest consist of a matrix polymer and a (glass or carbonized) fiber. If temperature is sufficiently high, the matrix polymer degrades thereby producing solid and/or gaseous components. Solid decomposition products may exhibit a considerable size change, which is a notable feature of intumescent materials also considered in this work. The model incorporates multi-step decomposition mechanism including two reactions in anaerobic conditions and four reactions in oxidative atmosphere. Kinetic data could be derived from TGA, DSC and PCFC/MCC measurements, which are processed by either simplified (peak value based) or comprehensive (non-linear optimization) approach suitable for both n-th order and autocatalytic reactions. The model is validated by comparing predictions of gasification rates for two distinct types of non-charring (PS) and charring intumescent (PC) polymers. Reasonable agreement has been obtained with the measured mass loss rates, which are proportional to the heat release rates if volatiles are ignited.

Nomenclature

Latin symbols

- $A$ pre-exponential factor [1/s]
- $C_{\text{eff}}$ combustion efficiency [-]
- $E$ activation energy [J/mol]
- $EF$ expansion factor [-]
- $g_{\text{surf}}$ mass flux of gas volatiles at exposed sample surface [kg/(m$^2$ s)]
- $\Delta h_c$ heat of combustion, solid sample [J/kg]
- $\Delta h_{c,g}$ heat of combustion, gas volatiles [J/kg]
- $\Delta h_g$ heat of gasification, solid sample [J/kg]
- $m$ mass [kg]
- $n$ reaction order [-]
- $q$ heat flux [W/m$^2$]
- $\dot{Q}^*$ heat release rate per unit surface area [kW/m$^2$]
- $r$ reaction rate [1/s]
- $R$ mass loss rate [kg/s]
- $R$ universal gas constant [J/(mol*K)]
- $t$ time [s]
- $T$ temperature [K]
- $V$ volume [m$^3$]
- $x$ coordinate normal to sample surface [m]

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1. Introduction

Standard flammability test procedures (such as those in OSU apparatus, cone calorimeter, or fire propagation apparatus) are focused on radiative heating of the examined material followed by ignition of volatiles produced by pyrolysis. Thus obtained measurements not only provide flammability indicators for the materials of interest, but also serve as a benchmark data for pyrolysis model validation. In its turn, a pyrolysis model is required to predict the expected outcome of the fire tests thereby reducing experimental efforts. To date, considerable experience has been gained in modeling thermal degradation of combustible materials exposed to the external heat flux. Among the published pyrolysis models, Gpyro [1] and ThermaKin [2] are most widely cited in recent literature. Specialized CFD software FDS [7] and FireFOAM [3] also include a pyrolysis model.

In this work, a new model (Pyropolis) for predicting thermal degradation of polymer materials exposed to the external heat flux is presented. The Pyropolis model is developed keeping in mind its application to the composite materials which consist of a matrix polymer and a (glass or carbonized) fiber. If temperature is sufficiently high, the matrix polymer degrades thereby producing solid and/or gaseous components. Solid decomposition products may exhibit a considerable size change, which is a notable feature of intumescent materials also considered in this work.

Developing of a practically useful, robust, computationally affordable physics-based model of thermal degradation, ignition and burning of a combustible solid material should pass a number of steps of increasing complexity. First, a single-layer configuration should be modeled and validated to demonstrate its capability to predict material gasification rates due to heating by the external heat flux. At this step, both charring and non-charring materials should be examined. Although the overall model framework is designed to allow for the virgin material and carbonaceous residue being oxidized by the air oxygen, an important step is considering thermal degradation of the material in the inert atmosphere. In the next steps, a multi-layer material configuration is to be considered, and the oxidative processes sensitive to the ambient oxygen concentration should be accounted for. The final step of model development would allow for the two-way coupling and thermal feedback between the paralyzing material and the gaseous flame produced by the volatiles. The latter option is beyond the capabilities of most of the existing models except most recent developments, e.g. [4] and [5].

The objective of this paper is to provide description of the model for predicting multi-stage
pyrolysis subject to external heat flux and to demonstrate current studies of the model validity. Validation studies include two cases for non-charring and charring polymer materials (polystyrene and polycarbonate, respectively).

2. Model description
Current version of the Pyropolis model is based on the following principles.
1. Original sample is composed of porous fiber and matrix polymer.
2. Condensed phase is represented by the solid phase only. No melting and liquid phase is considered. Phase transitions are implicitly taken into account in temperature dependencies of thermal and transport properties of the components.
3. Condensed phase is composed of fiber, matrix polymer, intermediate specie, char and (in case of aerobic pyrolysis) solid non-combustible residue (ash). The same combustible gas is produced in all pyrolysis reactions, and non-combustible gas is produced in oxidation reactions.
4. Condensed and gas phases are in local thermal equilibrium (single-temperature model).
5. Intumescence is allowed that may cause the control volumes to expand thereby shifting the exposed boundary, unexposed boundary is fixed at \( x = 0 \).
6. Gas filtration throughout the porous media obeys the Darcy’s law (not available in ThermaKin).
7. The sample is represented by 1D plane layer having thickness \( x_{surf} \).
8. Single-layer and multi-layer structures are considered.

2.1. Reaction rates and mass conservation

2.1.1. Anaerobic decomposition (two-step mechanism)
In the inert atmosphere, thermal decomposition of the matrix material is modeled by two-step reaction mechanism: (1) matrix polymer reacts producing an intermediate specie and gas, and (2) intermediate specie decomposes to char and gas. The mechanism includes the following reactions

\[
\begin{align*}
R_1 &= \frac{dm_{mp}}{dt} = \frac{m_{mp}}{k_1} (1 - \nu_{g,1}) m_{mp} + \nu_{g,1} m_{mp}, \\
R_2 &= \frac{dm_{int}}{dt} = \frac{m_{int}}{k_2} (1 - \nu_{g,2}) m_{int} + \nu_{g,2} m_{int},
\end{align*}
\]

where \( \nu_{g,1} \) and \( \nu_{g,2} \) show the mass fraction of solid reactant converting to gas. The same gas is produced in both reactions; no reactions occur in the gas phase.

2.1.2. Aerobic decomposition (four-step mechanism)
In presence of oxygen, two amendments are made to the above two-step mechanism. First, possible oxidation of the matrix material or intermediate specie is considered. Second, two more reactions are included to allow for char and, possibly, fiber oxidation. It should also be taken into account that combustible volatiles are only produced in decomposition reactions (3) and (4), while non-combustible gases are produced in oxidation reactions (5) and (6). The reaction list is given below:

\[
\begin{align*}
R_1 &= \frac{dm_{mp}}{dt} = \frac{m_{mp} + m_{O_2}}{k_{mp,1}} (1 - \nu_{g,1}) (m_{mp} + m_{O_2}) + \nu_{g,1} (m_{mp} + m_{O_2}), \\
R_2 &= \frac{dm_{int}}{dt} = \frac{m_{int}}{k_{int,2}} (1 - \nu_{g,2}) m_{int} + \nu_{g,2} m_{int}, \\
R_3 &= \frac{dm_{char}}{dt} = \frac{m_{char} + m_{O_2}}{k_{char,3}} (1 - \nu_{g,3}) (m_{char} + m_{O_2}) + \nu_{g,3} (m_{char} + m_{O_2}), \quad R_4 = \frac{dm_{inert}}{dt} = \frac{m_{inert}}{k_{inert,4}} (1 - \nu_{g,4}) m_{inert} + \nu_{g,4} m_{inert}.
\end{align*}
\]
2.2. Derivation of the kinetic model
Kinetic sub-model is derived from TGA/DSC/PCFC experiments performed at several different heating rates, presumably covering the range of heating rates occurring in fire conditions. In this paper, anaerobic thermal degradation of two simple polymers (PS and PC) is considered, for which published TGA data and the PCFC measurements by the authors are used. In TGA, relative mass loss rate \( \frac{dm}{dt} \) is recorded as a function of sample temperature (\( m_0 \) is the initial sample mass).

Relative mass loss rates simulated with the kinetic parameters recovered from TGA data are related to the reaction rates given by Eqs (1) and (2) as

\[
R_i = \Delta m_i \frac{dm}{dt},
\]

where \( \Delta m_i = m_{i,0} - m_{i,\infty} \) is the total mass of solid reactant consumed in \( i \)-th reaction. The reaction rates are modeled as

\[
r_i = A_i \varphi_i(Y_i) \exp\left(-\frac{E_i}{\Delta T}\right),
\]

where functions \( \varphi_i(Y_i) \) are introduced to allow for the dependence of the reaction rates on the progress variable, which is defined as the ratio of current mass of the reactant (matrix polymer or intermediate specie) to the range of its change in the reaction: \( Y_i = (m_i - m_{i,\infty})/\Delta m_i \). In the existing literature, these functions are frequently chosen as \( \varphi(Y) = Y \) (first order reaction). Although in some cases such an approach is successful, there are clear examples demonstrating its inadequacy. In the Pyropolis model, two reaction types are considered: n-th order reaction,

\[
\varphi(Y) = Y^n
\]

and autocatalytic reaction

\[
\varphi(Y) = Y^n (1 - Y^n + Y^a).
\]

Two approaches were used in this work to derive kinetic parameters from the measurement data. The first one is a simplified method (for example, see [6, 7]) that makes it possible to determine activation energy \( E \) and pre-exponential factor \( A \) using peak reaction rate value, \( \dot{r}_p \), (or peak heat release rate value, \( \Delta h_c \dot{r}_p \)) and corresponding temperature, \( T_p \). As such, the method (called the peak value method hereafter) is applicable to the single-peak curves, which corresponds to single-step reactions; the multi-peak curves should be split into the single-peak ones. The peak value method has been originally developed for n-th order reaction (8) provided activation energy is sufficiently high. However, with additional assumptions made for parameters \( Y^r \) and \( a \), this method can also be applied to the autocatalytic reaction (9). Numerical value of \( n \) can be derived using the measured data for \( Y_p \) at multiple heating rates; in processing data for a single heating rate, the value of \( n \) should be pre-assumed. Use of a single heating rate data is not recommended since the corresponding kinetic parameters are likely to be inappropriate for a different temperature program. Alternatively, simultaneous processing of the measured data for multiple heating rates expands validity of \( E \) and \( A \) to a wider range of heating rates and checks the adequacy of the selected kinetic function.

In the second approach used in this work, not just the peak value but also the entire reaction rate-temperature curve is approximated using pre-assumed set of reactions (n-th order, autocatalytic etc.). This approach (also called model fitting and non-linear optimization method) uses multidimensional non-linear optimization procedure to minimize deviation between measured and predicted reaction rate-temperature curves. Practical experience of using of the two above approaches have shown that both produce similar data provided that the reaction mechanism obeys the single-step reaction
approximation and the kinetic function is adequate. In its turn, significant difference between the kinetic parameters produced by the two methods is most likely an indication that the kinetic function and/or the single-step model are inadequate. To apply the non-linear optimization approach in this work, we used specialized software tools TDPro and ForK by ChemInform Ltd. (St.-Petersburg) [10].

**Figure 1.** Measured (dashed lines [8]) and simulated (solid lines, comprehensive approach) reaction rate-temperature curves of polycarbonate degradation at different heating rates: a) – n-th order reaction, $E = 186.8$ kJ/mol, $A = 2.932 \cdot 10^{10}$ s$^{-1}$, $n = 0.6918$; b) – autocatalytic reaction, $E = 166.3$ kJ/mol, $A = 5.243 \cdot 10^{9}$ s$^{-1}$, $n = 2.765$, $a = 0.7559$.

For the thermal degradation of polystyrene and polycarbonate we found that the n-th order reaction cannot provide a good approximation of reaction rate-temperature curves in a wide range of heating rates. In these cases, the autocatalytic reaction behavior is pronounced as illustrated in figure 1, which shows best fit of the measured curves for polycarbonate obtained both for n-th order and autocatalytic reactions. In fact, inadequacy of n-th order reaction model is the actual reason of high sensitivity of the kinetic parameters to the heating rate observed in [8].

2.3. Non-charring, charring, intumescent polymers
The Pyropolis model is capable of predicting thermal decomposition of both charring and non-charring polymers in anaerobic conditions. In case of charring polymers, possibility of volume expansion (intumescence) is allowed. Volume occupied by a particular component depends on its bulk density (i.e. density of the pure (non-porous) component). Volumes occupied by solid components inside the control volume $\Delta V$ and its ratios to the volume of solid fraction (solid volume fractions) are $\Delta V_j = m_j/\rho_j$ and $X_j = \Delta V_j/\Delta V_s$, where $j = mp$, fib, int, char and

$$\Delta V = \Delta V_{mp} + \Delta V_{int} + \Delta V_{char} + \Delta V_{fib}$$

is the volume occupied by the solid phase. Two types of pyrolyzing materials are considered:

1. Non-intumescent material, in which volume occupied by the gas phase is determined from $\Delta V_g = \Delta V - \Delta V_s$, where $\Delta V_s$ is obtained from Eq (10). Porosity is defined as $\phi = \Delta V_s/\Delta V$. This type of material could or could not produce char. Non-charring material is completely gasified in either first or second reaction, i.e. if $(1-v_{g1})(1-v_{g2}) = 0$. For such a material, ablation type model is applied. If at exposed boundary mass of condensed phase becomes zero, $m_j(t) = 0$, then sample boundary is translated to the nearest control volume with $m_j(t) > 0$.

2. Charring and intumescent materials are modeled by different way in calculating porosity.
Porosity of intumescent materials is calculated as
\[ \phi = \phi_{mp} X_{mp} + \phi_{int} X_{int} + \phi_{chars} X_{chars} + \phi_{fib} X_{fib}, \]
where \( \phi_{mp} \), \( \phi_{int} \), \( \phi_{chars} \), and \( \phi_{fib} \) are the porosities of pure components (given in input data). Updated value of the control volume is then calculated as
\[ \Delta V = \Delta V_i / (1 - \phi). \]
It is assumed that intumescence occurs due to increasing of the char porosity, \( \phi_{chars} \), which is related to the expansion factor \( EF \) (ratio of final and initial thicknesses of the material):
\[ \phi_{chars} = 1 - \left( 1 - \phi_i \right) \left( 1 - v_{c,d} \right) \left( 1 - v_{e,d} \right) \left( 1 - X_{fib,b} - X_{int,b} \right) \frac{\rho_{mp}(T_i)}{\rho_{chars}(T_i)}. \] (11)
The expansion ratio is pre-assigned in the input data.

2.4. Gas flow equation
Mass flux of the gas volatiles is calculated according to the Darcy’s law. Applying gas state equation and considering plane geometry, the equation for gas pressure is obtained from the gas continuity equation, which allows for gas production by pyrolysis. The gas pressure equation is solved assuming that unexposed boundary is impermeable while the exposed boundary is at atmospheric pressure. Given the pressure profile, gas flow at the sides of internal control volumes and at the exposed surface, \( g_{surf} \), are determined from the Darcy’s law. An empirical correlation coupling permeability and porosity for multiple wire mesh screens (plain or sintered) is used in the simulations.

2.5. Energy conservation
In Pyropolis model, solid and gas phase are assumed to be in local thermal equilibrium and therefore described by a single temperature. Heat flux through the sample consists of conductive, convective (gas filtration) and radiative constituents. The energy conservation equation is solved in 1D form allowing for heat consumption in endothermic pyrolysis and heat release in exothermic oxidation. The media is considered to be semi-transparent, and the radiative heat flux is assumed to be one-dimensional:
\[ q_{rad} = \varepsilon q_0 \exp(-\kappa_{abs}(x_{surf} - x)), \]
where \( q_0 \) is the external heat flux (EHF), \( \varepsilon \) is the surface absorptivity, and \( \kappa_{abs} \) is the radiative absorption coefficient.

Boundary condition at the unexposed surface approximately takes into account heat transfer to the substrate material (constant pre-assumed heat transfer coefficient, no radiative heat flux). Boundary condition at the exposed surface takes into account convective (given heat transfer coefficient) and radiative (given surface emissivity) heat exchange with the environment having ambient temperature, \( T_{amb} \). In the limit of non-transparent media \( \kappa_{abs} \to \infty \) incident heat flux in the boundary condition at the exposed surface includes absorbed portion of external radiative flux \( \varepsilon q_0 \); in case of transparent media volumetric absorption of the external heat flux becomes the source term of the energy equation.

To approximately model experimental scenarios where ignition of gas volatiles is followed by flaming combustion, it is assumed that the ambient temperature quickly (characteristic time scale \( t_{flame} \approx 3 \text{ s} \)) rises to the pre-assigned value of \( T_{flame} \):
\[ T_{amb} = \begin{cases} T_i, & t < t_{ign} \\ T_i + \left( T_{flame} - T_i \right) \left( 1 - \exp\left( -\frac{t - t_{ign}}{t_{flame}} \right) \right), & t > t_{ign} \end{cases} \] (12)
Time of ignition is determined as the time instant when volatile mass flux approaches the critical value, corresponding to the heat release rate per unit area of 20 kW/m². The heat release rate per unit area is calculated as
\[ \dot{Q}^* = C_{eff} \Delta h_{c,g} g_{surf}, \] (13)
where for combustion efficiency and heat of gas volatile combustion the following values are used after [8]: $C_{eff} = 0.84$, $\Delta h_{C,g} = 25.6$ MJ/kg. Heat of gasification is set to $\Delta h_g = -1.0$ MJ/kg for polystyrene [9] and $\Delta h_g = -0.83$ MJ/kg for polycarbonate [8].

2.6. Thermal and transport properties

Thermal conductivity and gas permeability of the multicomponent heterogeneous media are calculated as a weighted sum of thermal conductivities (permeabilities) of two extreme configurations with material layers aligned parallel and normally to the heat flux (gas flow) direction. Volumetric radiative absorption in solid material is calculated as a volume-averaged value of absorption coefficients for pure components. Specific heat of the media is obtained as a mass-weighted average of all the components. All thermal and transport properties of pure components depend on temperature. Thermal conductivity of char includes radiative contribution. Data for pure components are compiled from various sources.

3. Model validation

3.1. Non-charring polymer

This series of simulations replicates test conditions of NIST gasification apparatus in which the plane sample of high impact polystyrene 8.6 mm thick is exposed to a radiative heat flux of 52 kW/m$^2$. The test was conducted in a nitrogen atmosphere [9]. In figure 2, measured and simulated mass loss rates are compared, and the dependencies of surface temperature and sample thickness on time are shown.

![Figure 2. Mass loss rate measurements and predictions of mass loss rate, surface temperature and sample thickness. HIPS, initial sample thickness 8.6 mm. Kinetic model: a) – n-th order reaction, $E = 213.9$ kJ/mol, $A = 1.663 \times 10^{14}$ s$^{-1}$, $n = 0.6434$; b) – autocatalytic reaction, $E = 179.4$ kJ/mol, $A = 6.370 \times 10^{11}$ s$^{-1}$, $n = 0.8102$, $m = 0.3457$, $Y' = 0.0001$.](image)

Char is not produced in gasification of polystyrene; therefore, only first of two reactions (1) and (2) is activated in the model. Figure 2a presents simulation results with n-th order reaction (8), while simulations with autocatalytic reaction (9) are presented in figure 2b. Autocatalytic reaction makes it possible to obtain better fit of the measured TGA curves (not shown here) than n-th order reaction. However, comparison of figures 2a and 2b demonstrates that use of the kinetic model which provides the best fit with TGA curves may not drive predicted mass loss rates closer to the measured data. The first reason for this is that model uncertainties other than kinetic model (primarily in prescribing thermal and transport properties) are very important and should be further investigated. Secondly, the range of heating rates at which reaction rate-temperature curves were determined (in TGA or PCFC/MCC) does not cover the entire range of heating rates occurring in the heated and decomposed...
sample. Indeed, figure 3 shows that the heating rates could be much higher than those in TGA or PCFC/MCC, particularly at small times when the heating rate is of order of 10 K/s. This limits applicability of the kinetic model and data used. It can therefore be concluded that precise fit of reaction rate-temperature curves by a complicated kinetic model may not be justified, and use of reduced kinetic models with small number of reactions is sufficient.

![Figure 3](image.png)

**Figure 3.** Predicted heating rates across the polystyrene sample (initial thickness 8.6 mm, external heat flux 52 kW/m$^2$): a) – small times, b) – long times.

Keeping in mind the above comment, it can be seen in figure 1 that the pyropolis model can predict the gasification rate of the non-charring material in the inert atmosphere with a good accuracy. This makes it possible to approximately predict polymer gasification in air, with volatile ignition followed by flaming combustion. The ignition is assumed to occur when the volatile mass flux approaches its critical value, corresponding to the heat release rate per unit area of 20 kW/m$^2$ (the heat release rate per unit area is calculated using Eq (13)). As the ignition occurs, ambient temperature is assumed to quickly rise to the pre-assigned value of $T_{\text{flame}} = 800$ K. The latter quantity is considered as an adjustable parameter (the flame itself is not modeled here).

### 3.2. Charring intumescent polymer

Here we consider the experimental scenario in which bisphenol A polycarbonate (PC) was exposed to the 75 kW/m$^2$ external heat flux in the cone calorimeter. The sample produced highly intumescent char, with the expansion ratio $EF = 10$. Initial sample thickness is 5.5 mm. In the simulations, heat release rate per unit sample area was calculated as a function of time. Corresponding measurement data were taken from [8]. It can be seen in figure 4, that measured heat release rates exhibit large scatter which could be explained by highly irregular shape of the char surface.

In the simulations, anaerobic conditions are assumed, although the experiment is conducted in open air. As a result, predicted heat release rates become zero when all the volatiles are exhausted, although the measurements show steady non-zero values; the latter is attributed to slow char oxidation. Also, external heat flux in the simulations was assumed to be constant (75 kW/m$^2$) although it is expected to increase due to increased elevation of the exposed surface (due to char expansion, its surface gets closer to the radiating panels). This might be one of the reasons for the underestimated heat release rate predicted at the end of pyrolysis, when most of the expansion occurs.

To model gasification of PC sample, kinetic data were derived from TGA measurements (presented in [8]). In two-step reaction scheme, the rate of the first reaction was calculated using Eq (7) while the second reaction was assumed to be very fast. This is equivalent to the single-reaction model, which was also used in [8] (mass of the intermediate component tends to zero as the second reaction rates increases). Volatile production was assigned to the second reaction only: $V_{g,1} = 0$, $V_{g,2} = 0.79$. 


Figure 4. Heat release rate measurements and predictions of heat release rate, surface temperature and sample thickness. PC sample, initial thickness 5.5 mm. Kinetic model: n-th order reaction. Expansion factor, $EF$: a) – 10, b) – 8.

Figure 5. Predicted temperature profiles (a) and heating rates (b) across the polycarbonate sample (initial thickness 5.5 mm, external heat flux 75 kW/m$^2$).

Both measured and predicted dependences of sample gasification rate on time are qualitatively different compared to those in non-charring materials. Indeed, after rapid increase just after ignition the mass loss rate of the charring polymer decreases in time. The latter is due to expanding char layer which isolates the virgin material from the external heat flux.

A comparison of predicted and measured heat release rates are shown in figure 4 along with the transient dynamics of surface temperature and sample thickness (normalized by its initial value). The agreement is reasonable, particularly when compared to similar predictions by Thermakin in [8]. However, the model contains a number of adjustable parameters (optimised for this particular test), which may not be transferrable to alternative test conditions. To illustrate the effect of the input data which cannot be precisely defined, the expansion factor was varied, and two values of $EF = 10$ and 8 are considered in figure 4a and 4b, respectively. Transient development of temperature profiles across the sample is shown in figure 5b.

Simulations shown in figures 4 and 5 were performed with n-th order kinetic model. It was found that use of the autocatalytic kinetic model does not improve agreement of predicted and measured heat release rates, despite it does improve representation of mass loss rate-temperature curves in TGA. It means that other model uncertainties are equally or more important for the predictions, and further
refinement of the kinetic model can only be advantageous if performed jointly with the improvements to other model components. Also, consideration of heating rates in the sample (figure 5b) shows that they are normally higher than those used in the kinetic analysis which may affect reliability of the kinetic model.

4. Conclusions and future work
In this work, a new model for predicting thermal degradation of polymer materials exposed to the external heat flux is presented. The Pyropolis model incorporates the multi-step decomposition mechanism including two reactions in anaerobic conditions and four reactions in oxidative atmosphere. Kinetic data could be derived from TGA, DSC and PCFC/MCC measurements, and either peak value-based or non-linear optimization approach suitable for both n-th order and autocatalytic multi-step reactions can be applied. The model has been preliminarily validated against published experimental data for two distinct types of non-charring (polystyrene) and charring intumescent (polycarbonate) polymers. Reasonable agreement has been found with the measured mass loss rates, which are proportional to the heat release rates if volatiles are ignited.

The ongoing work is focused on enhancing predictive capabilities of the Pyropolis model by implementing multi-step kinetic models, allowing for the multicomponent and multilayered structure of the composite materials, incorporation of the oxidation reactions in presence of oxygen, and further model validation for a wider range of materials.

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