Thermo-Kinetic Model of Burning for Polymeric Materials

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Key Long-Term Objectives

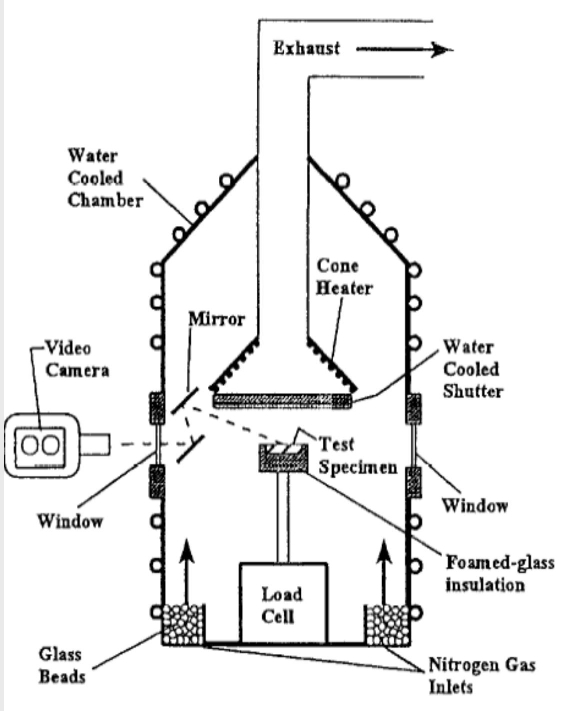
- Develop a versatile model for simulation of bench-scale flammability tests.
- Parameterize this model for various types of polymeric materials.
- Relate parameters (properties) used in the model to molecular structure.

Flammability Measurement Techniques

Cone Calorimetry
(heat release measurement)

Fire Propagation Apparatus
(heat release measurement)

Gasification Apparatus
(mass loss measurement)



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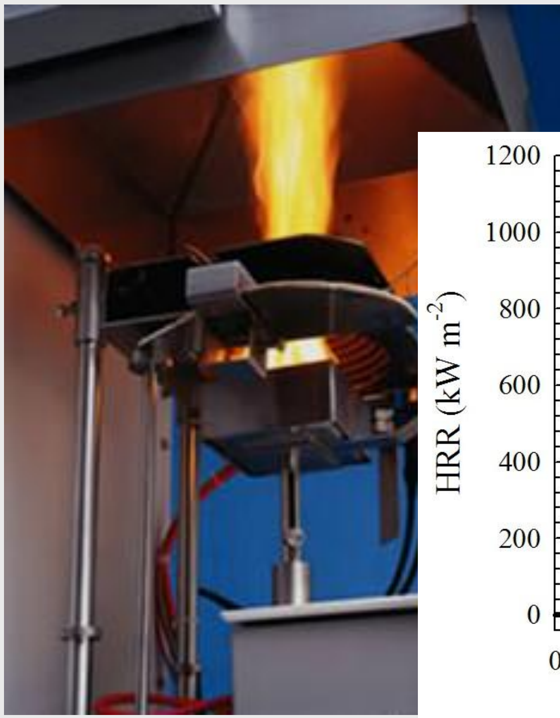
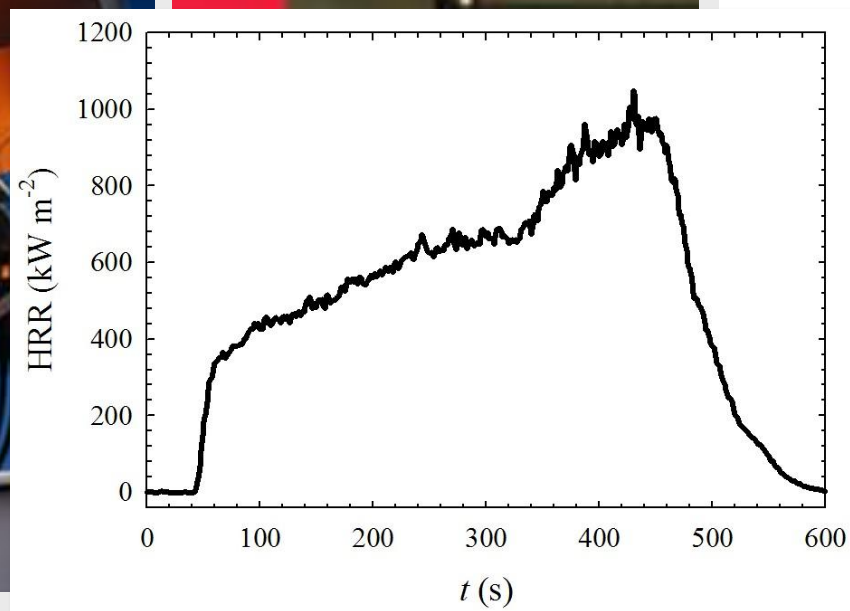
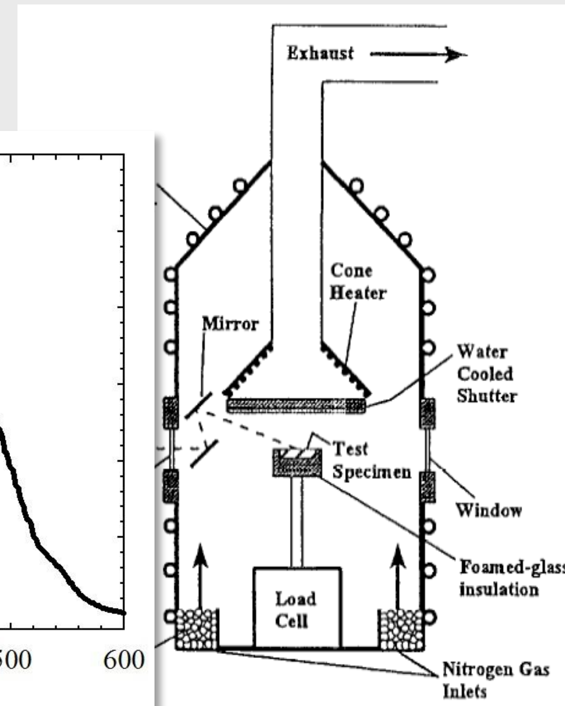
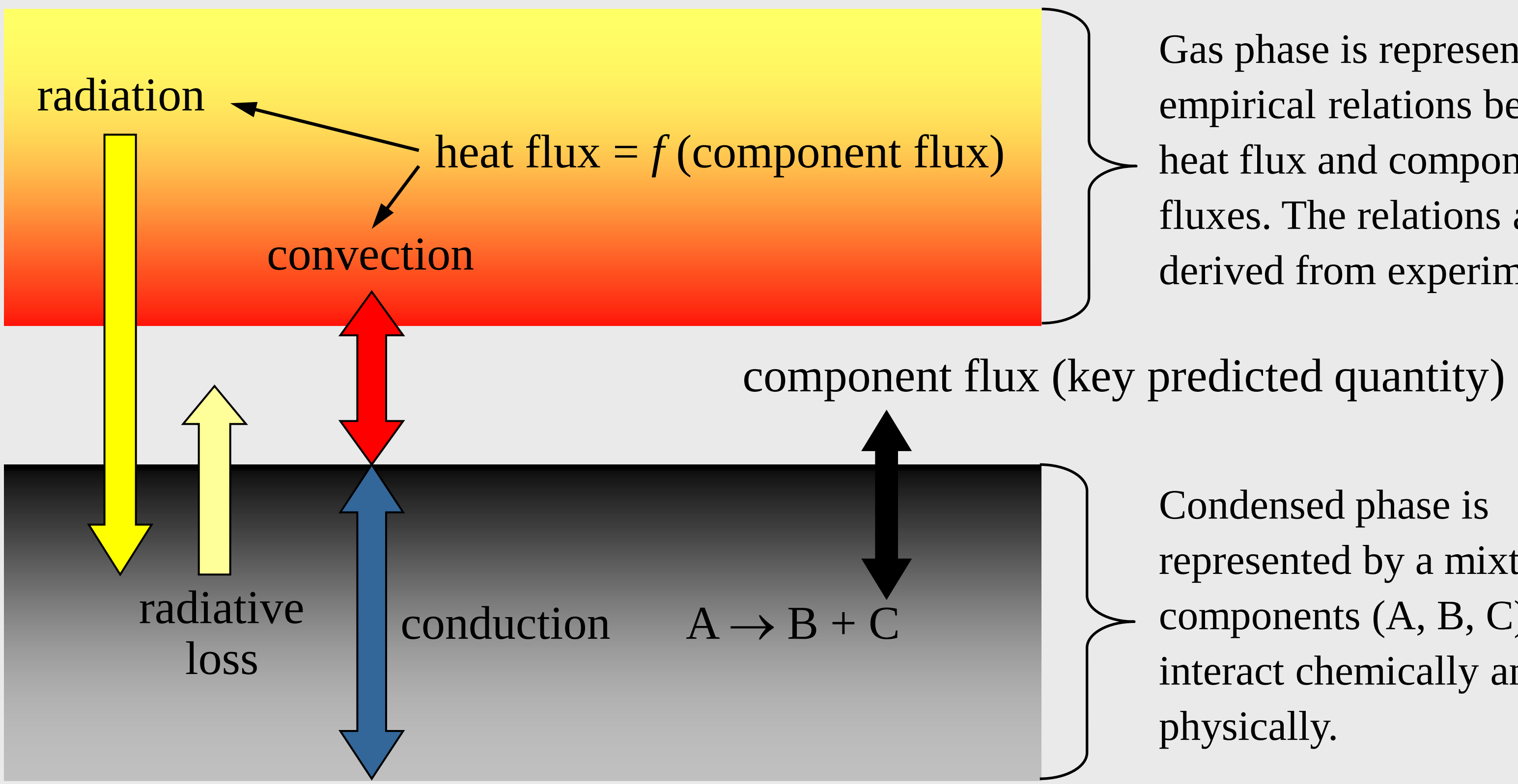






ThermaKin Model Overview



Gas phase is represented by empirical relations between heat flux and component fluxes. The relations are derived from experiments.

Condensed phase is represented by a mixture of components (A, B, C), which interact chemically and physically.

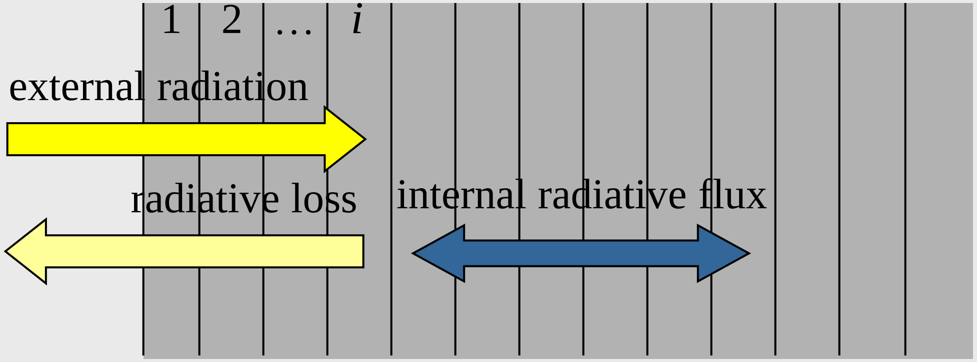
Radiative Energy Transfer

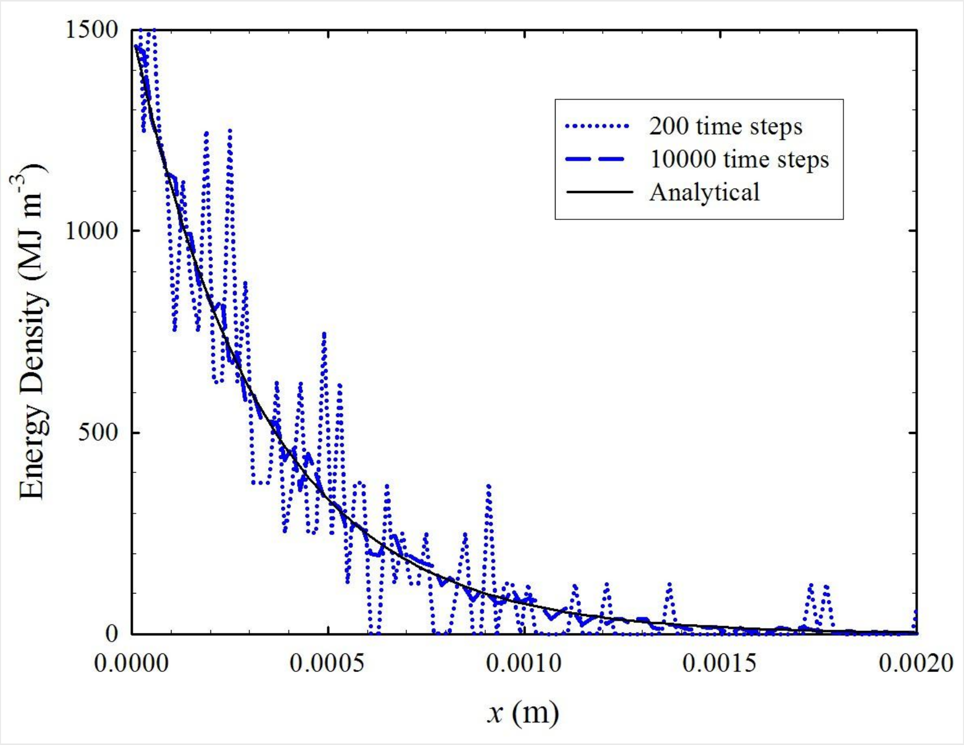
During any given time step, the external radiation is absorbed by a single element chosen at random.

$$\text{probability of absorption} = \frac{I_i \alpha_i \Delta x_i}{I_1}$$

$$\text{radiative loss} = \varepsilon_i \sigma T_i^4$$

$$\text{internal radiative flux} = -k_r \sigma T^3 \frac{\Delta T}{\Delta x}$$



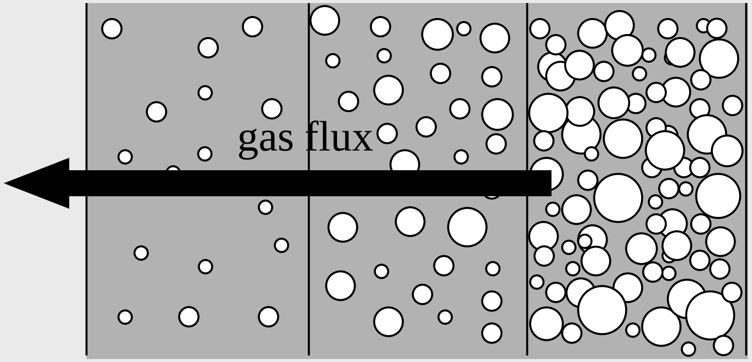


Mass Transfer

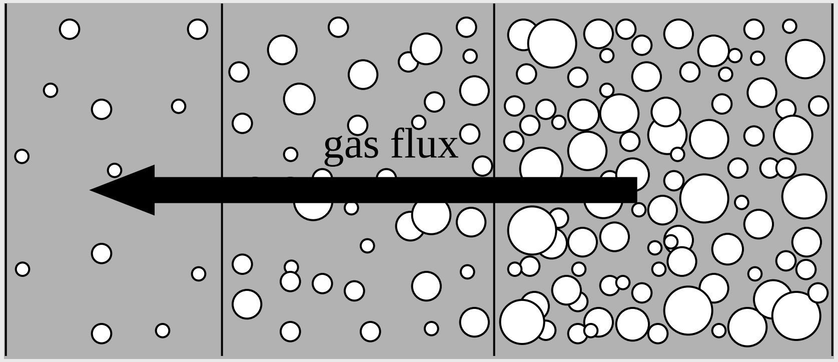
Components are categorized as solids, liquids, or gases.

$$\text{mass flux of gas} = -\lambda \rho_g \frac{\Delta\left(\frac{m_g/\rho_g}{V}\right)}{\Delta x}$$

Swelling factor γ defines volumetric reaction of the condensed phase to the presence of gases.



$\gamma = 0$



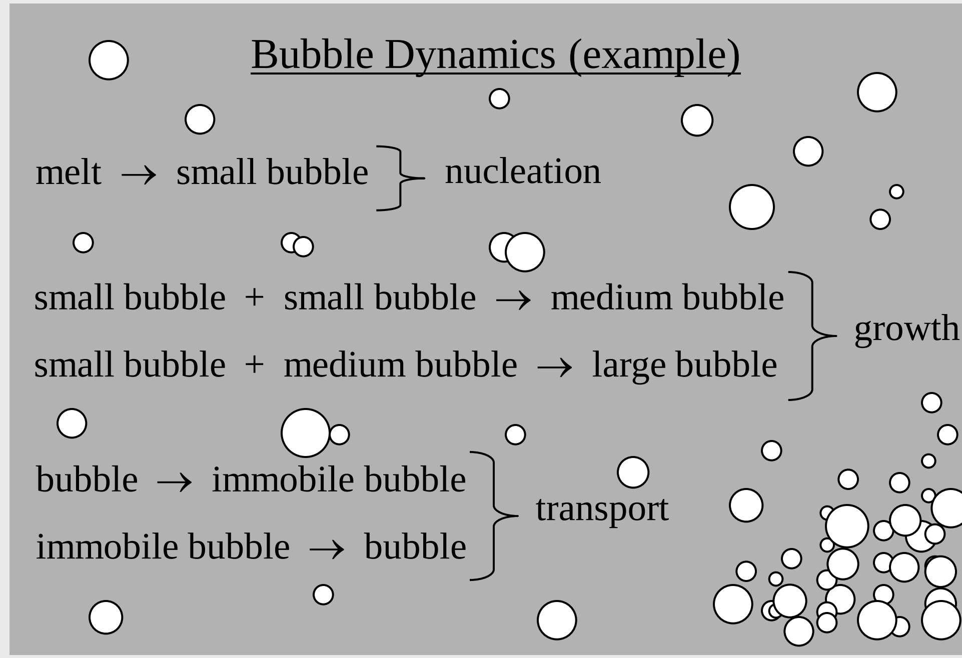
$\gamma = 1$

Chemical Reactions

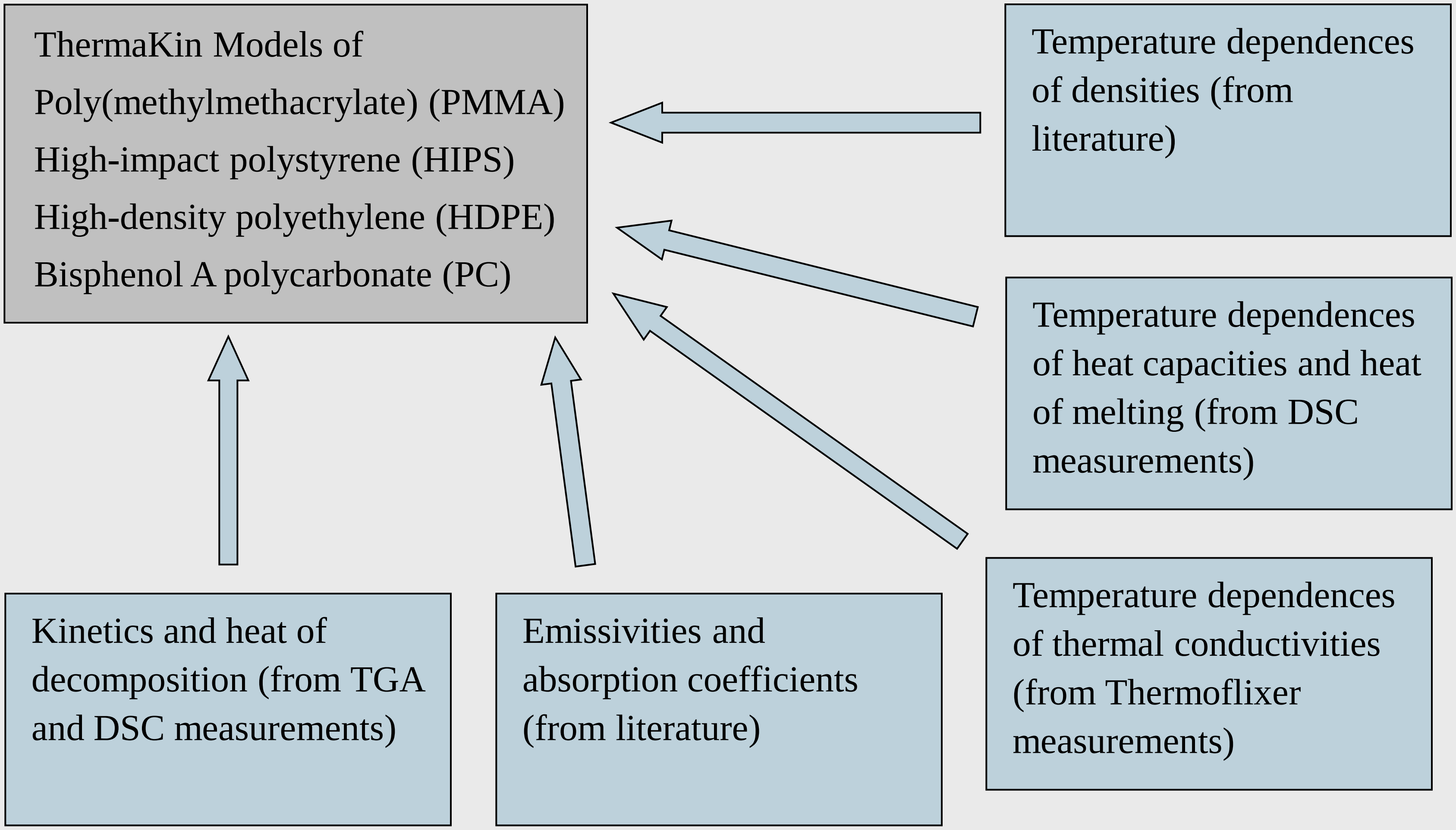
$$\theta_A \mathrm{A} + \theta_B \mathrm{B} \rightarrow \theta_C \mathrm{C} + \theta_D \mathrm{D} + \text{heat}$$

$$\text{rate} = \begin{cases} A\exp\left(-\dfrac{E}{RT}\right)\left[\dfrac{m_A}{V}\right] \\ \text{or} \\ A\exp\left(-\dfrac{E}{RT}\right)\left[\dfrac{m_A}{V}\right]\left[\dfrac{m_B}{V}\right] \end{cases}$$

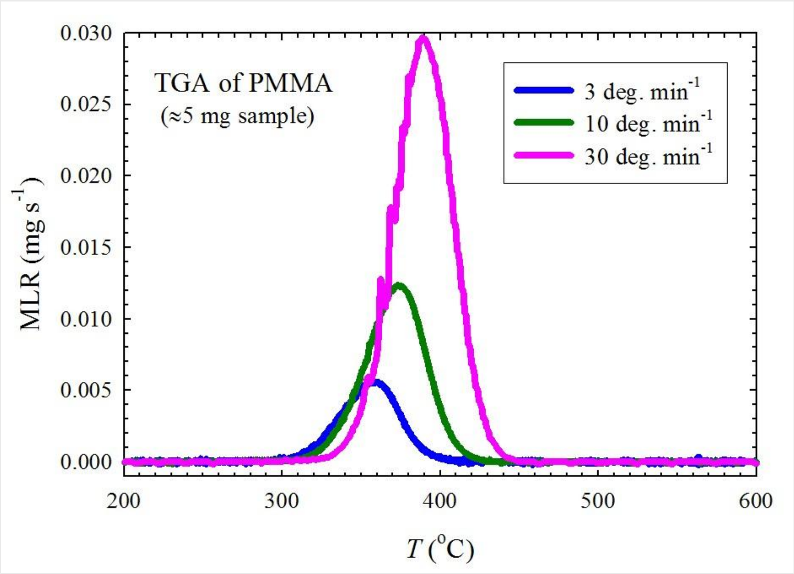
The reaction can be switched on or off at a specified temperature.



Parameterization



Kinetics of Decomposition

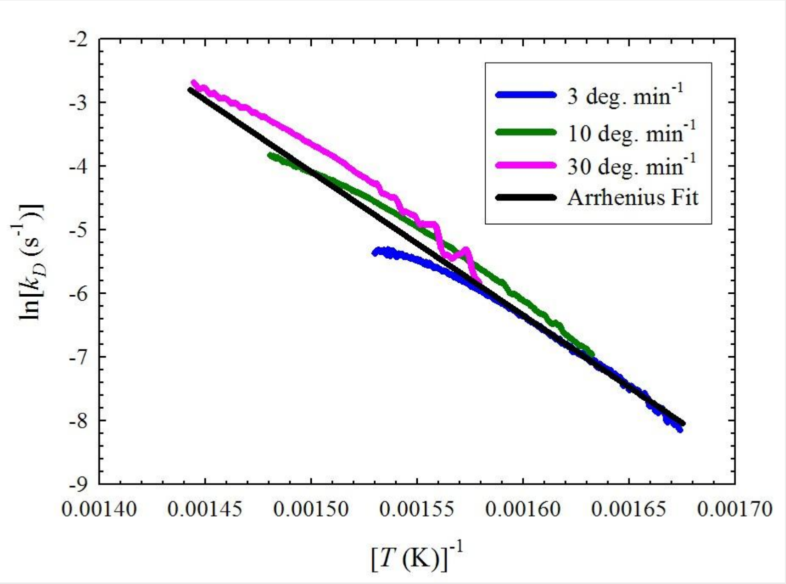


<u>Assumptions:</u>

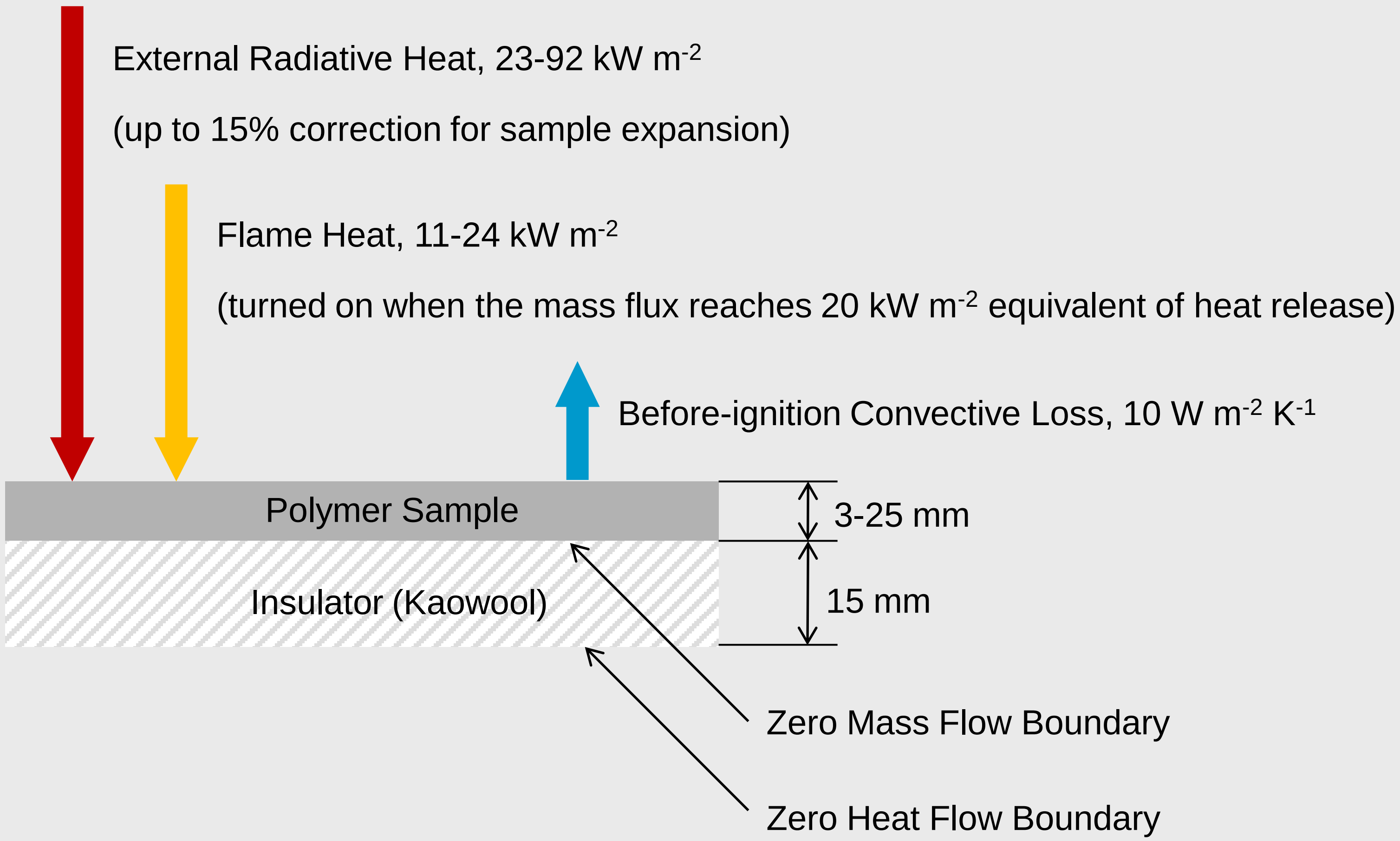
PMMA $\rightarrow$ Gas + heat

MLR = $k_D m_{\text{PMMA}}$ (first order)

Gas leaves PMMA instantaneously.



Modeling of Fire Calorimetry Experiments

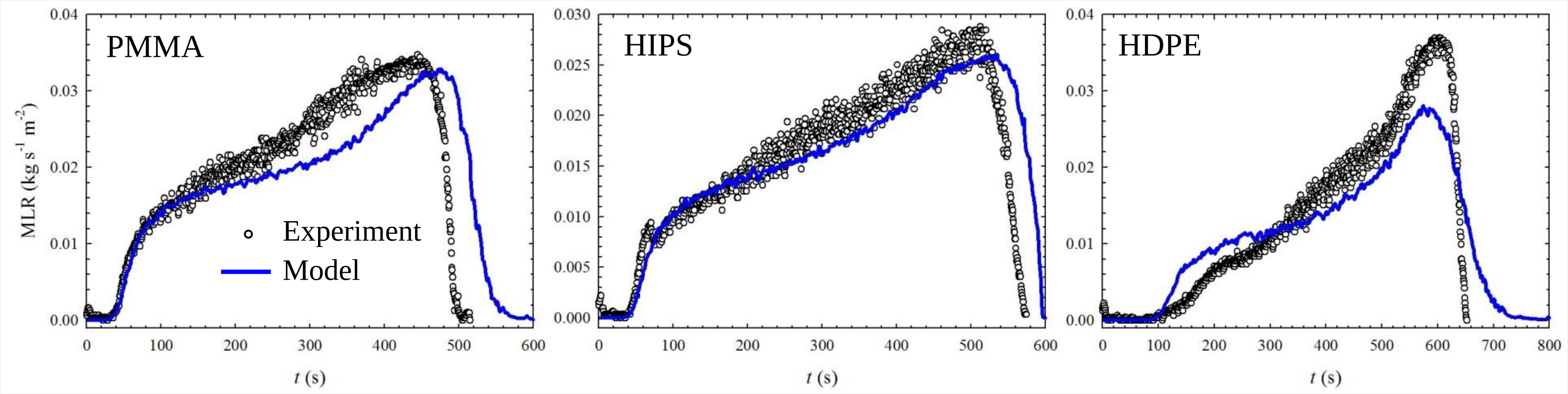


Gasification

<u>Conditions:</u>

external heat flux = 52 kW m^{-2}

initial sample thickness ≈ 9 mm

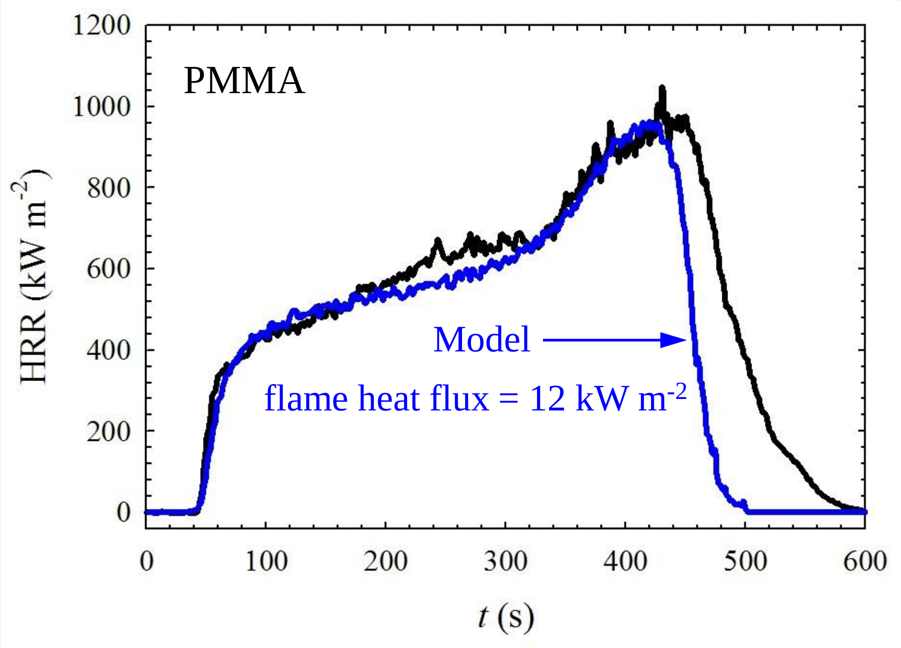


Cone Calorimetry

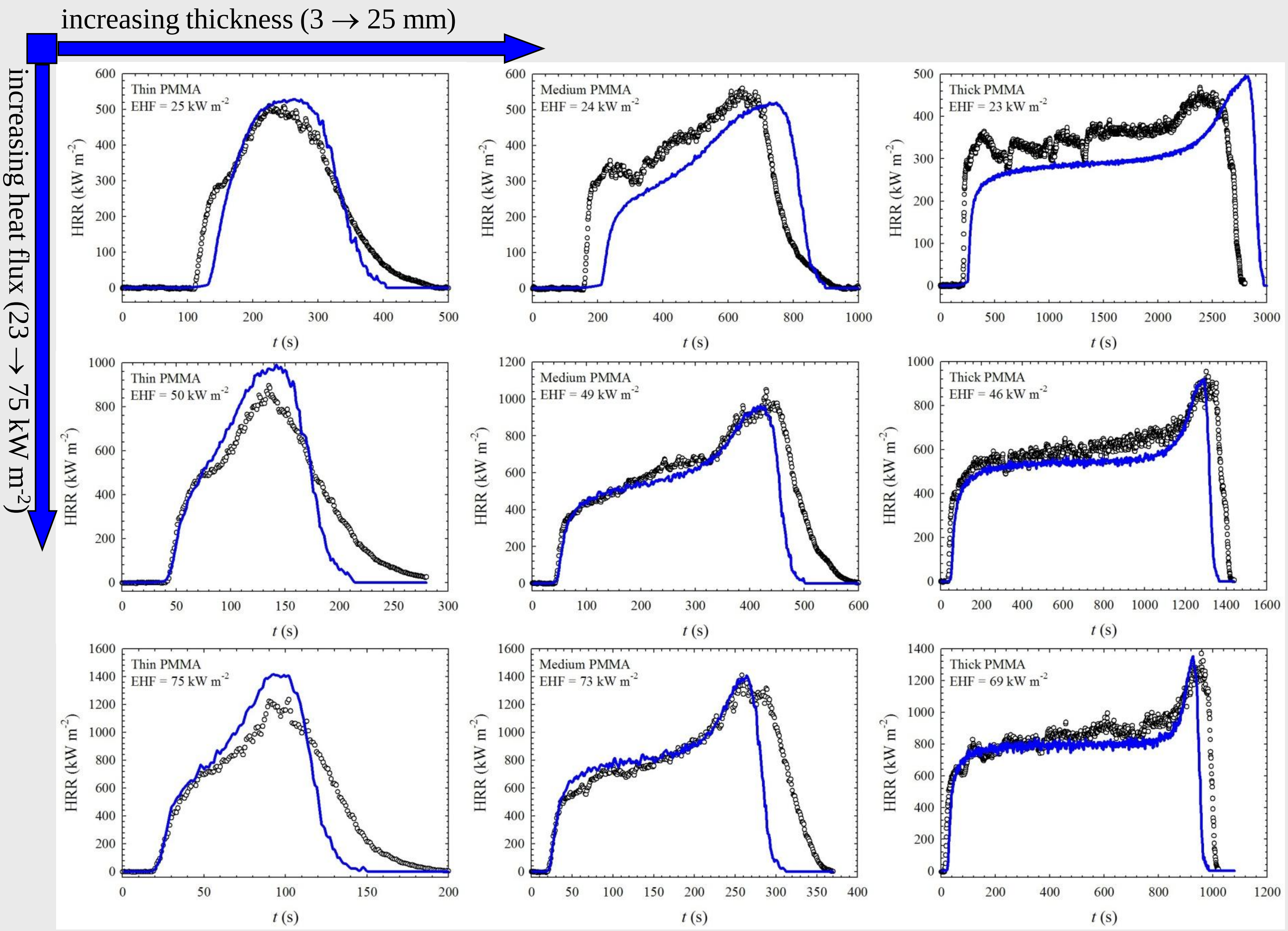
<u>Conditions:</u>

external heat flux = 49 kW m^{-2}

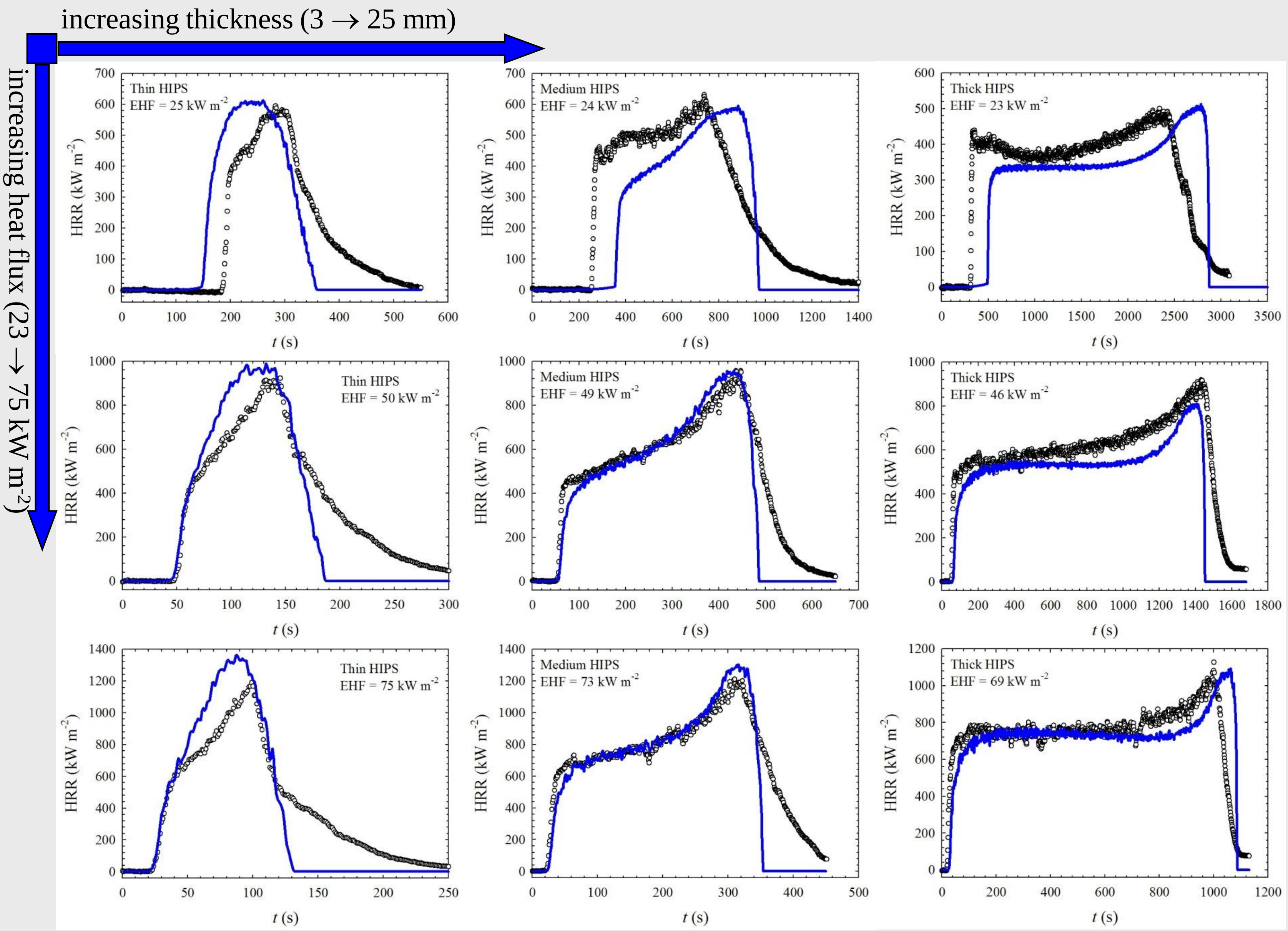
initial sample thickness ≈ 9 mm



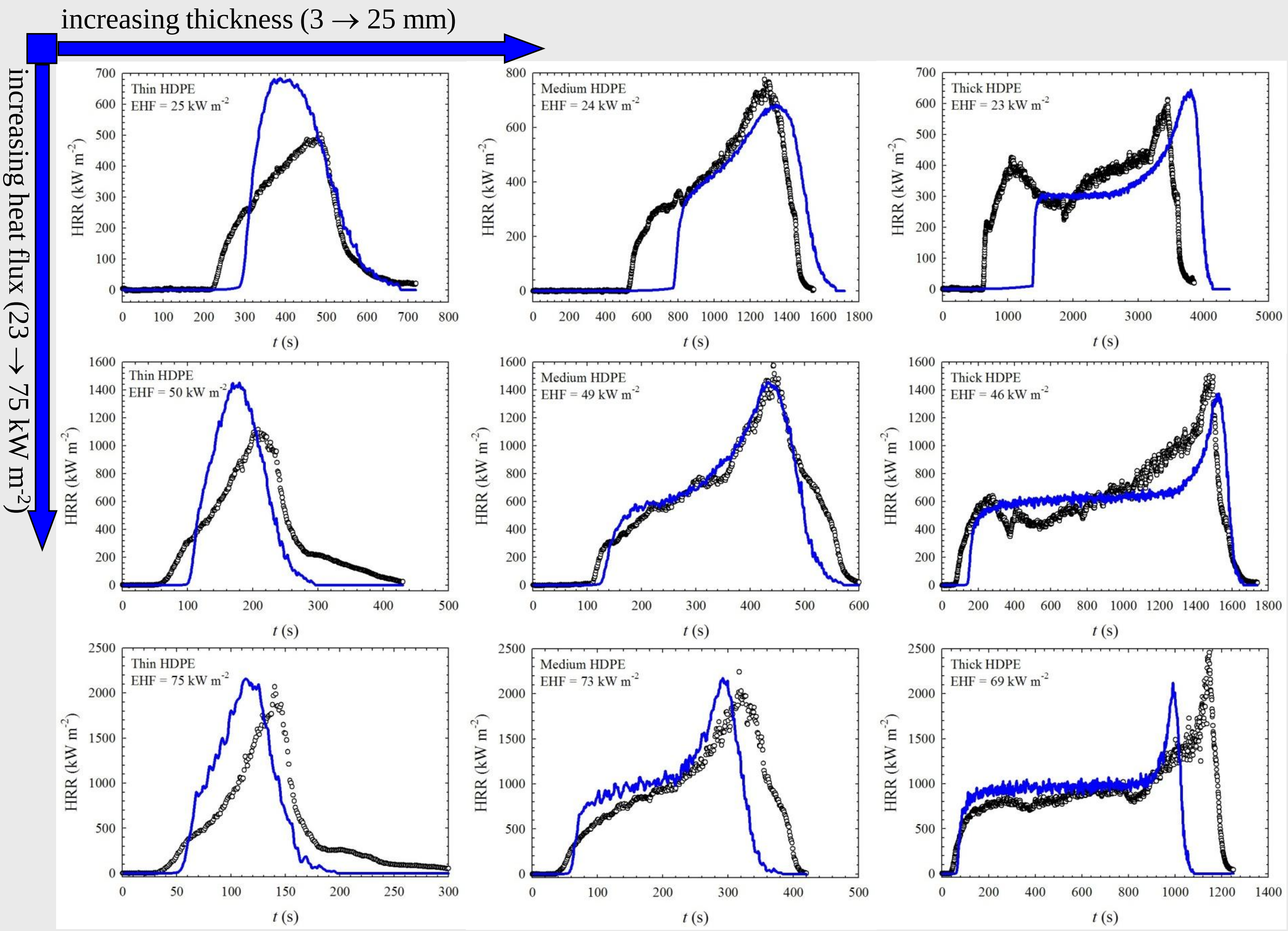
Cone Calorimetry of PMMA



Cone Calorimetry of HIPS



Cone Calorimetry of HDPE

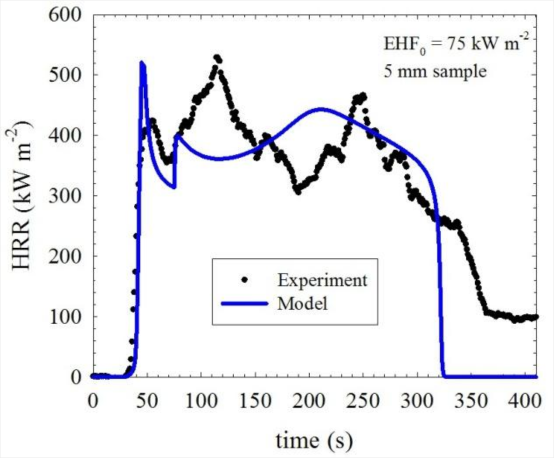


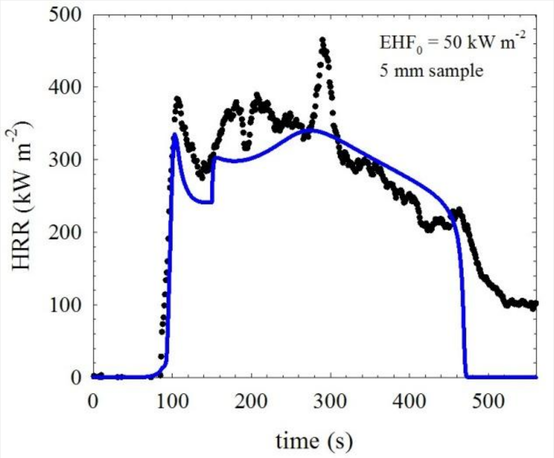
Cone Calorimetry of PC

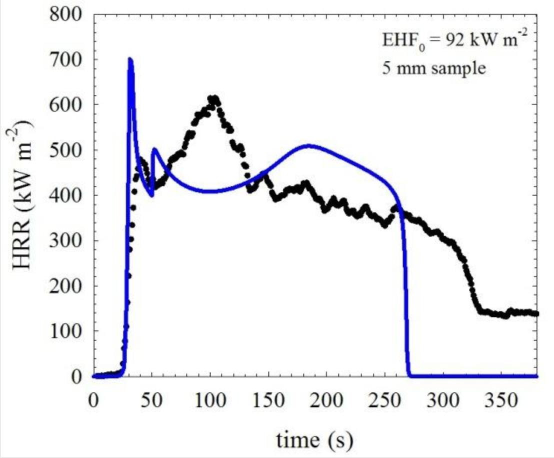
5 mm PC sample after 160 s at 75 kW m^{-2}.

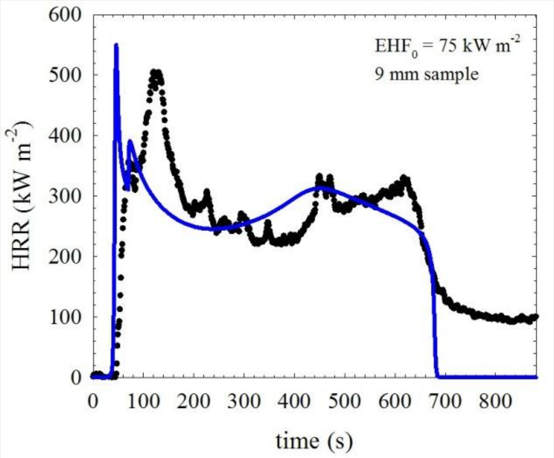
Flame heat flux = 15 kW m^{-2}.

The main mode of heat transfer inside char is radiation. The rate of transfer is defined by a single adjustable parameter.

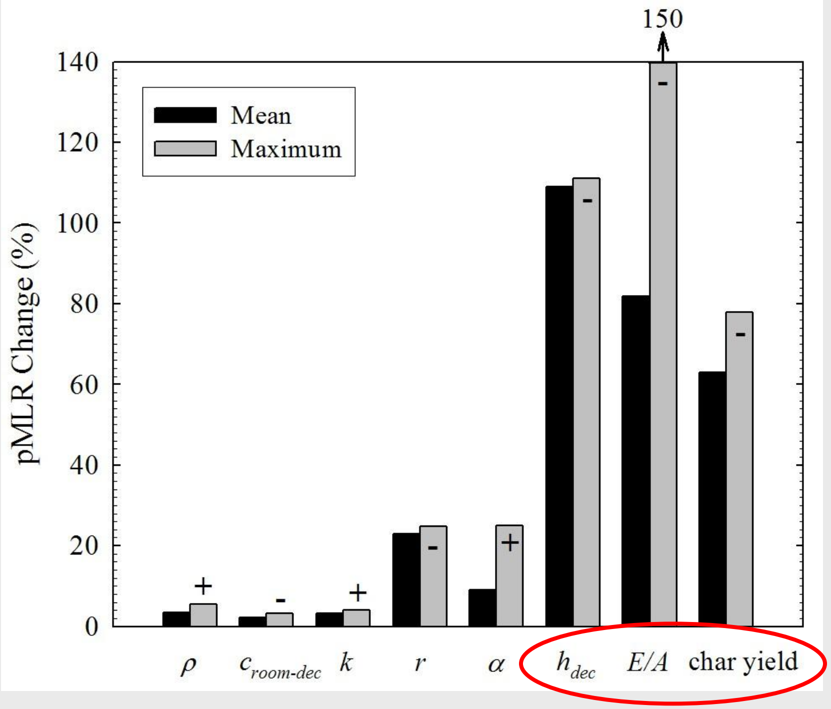


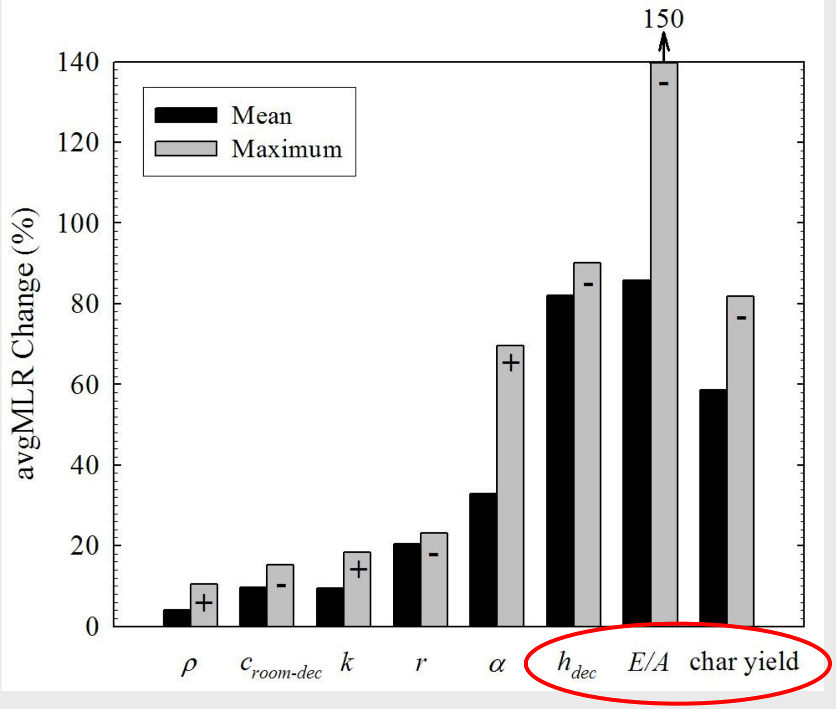






Sensitivity of Peak and Average Mass Loss Rates





Conclusions

❑ A one-dimensional numerical pyrolysis model can be used to predict the outcome of fire calorimetry experiments performed on polymeric materials.

❑ The predictions require the knowledge of chemical, thermal, and optical properties of the material. Measurement of these properties represents a challenging task.

❑ The rate of decomposition (defined by *A* and *E*), heat of decomposition, char yield and heat of combustion are the key parameters required for prediction of the peak and average heat release rates.