Presented at the COMSOL Conference 2008 Boston

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Mid-Atlantic Technology, Research & Innovation Center

COMSOL Multiphysics Conference, Boston, 2008

A Finite Element Analysis on the Modeling of Heat Release Rate, as Assessed by a Cone Calorimeter, of Char Forming Polycarbonate

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October 10, 2008

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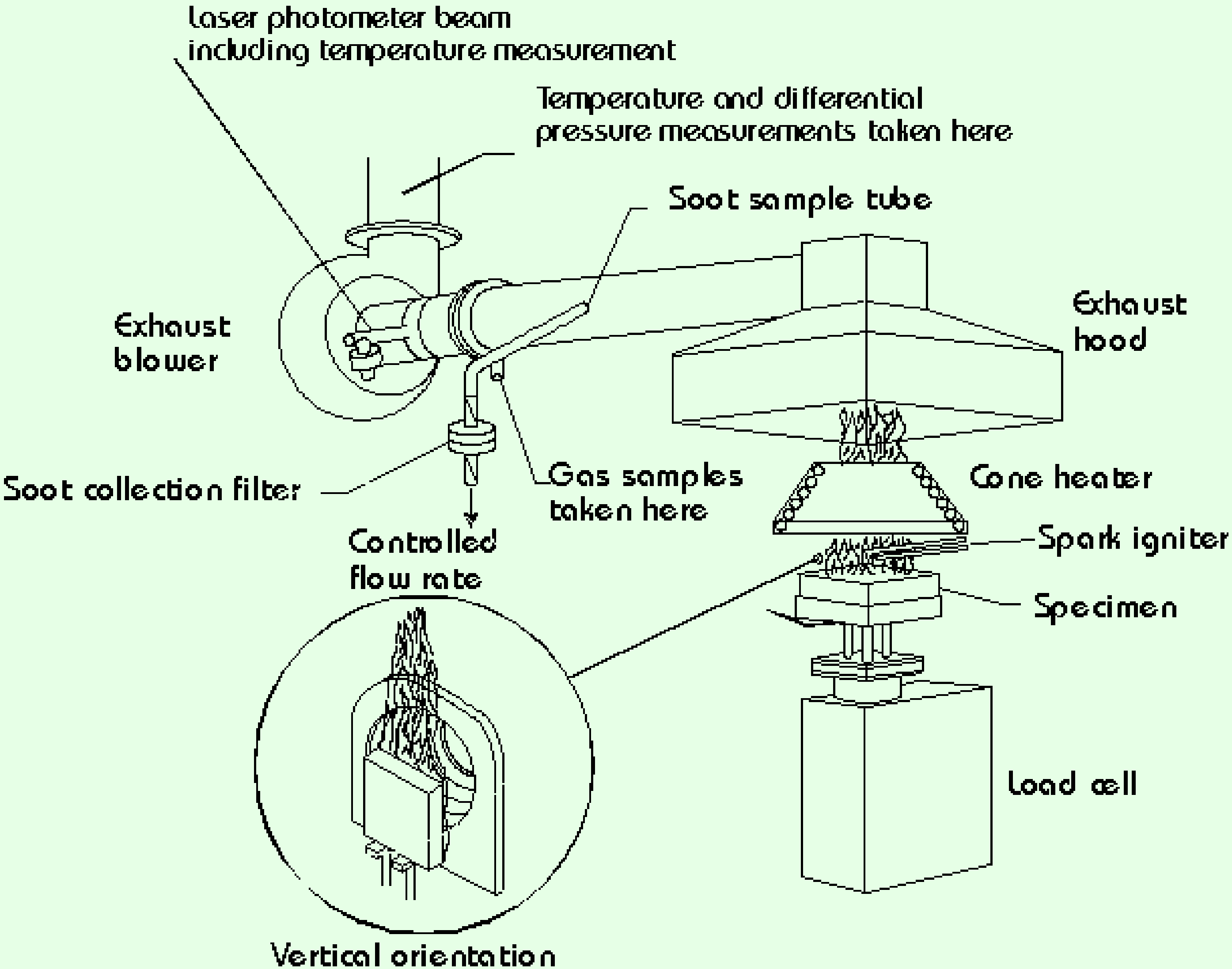
Outline

- Introduction
  - Cone Calorimeter
  - Heat Release Rate Data
- Modeling of Heat Release Rate
  - Defining the Problem
  - Solving the Problem
  - Results
- Conclusions
- Acknowledgment

Cone Calorimeter



Measures

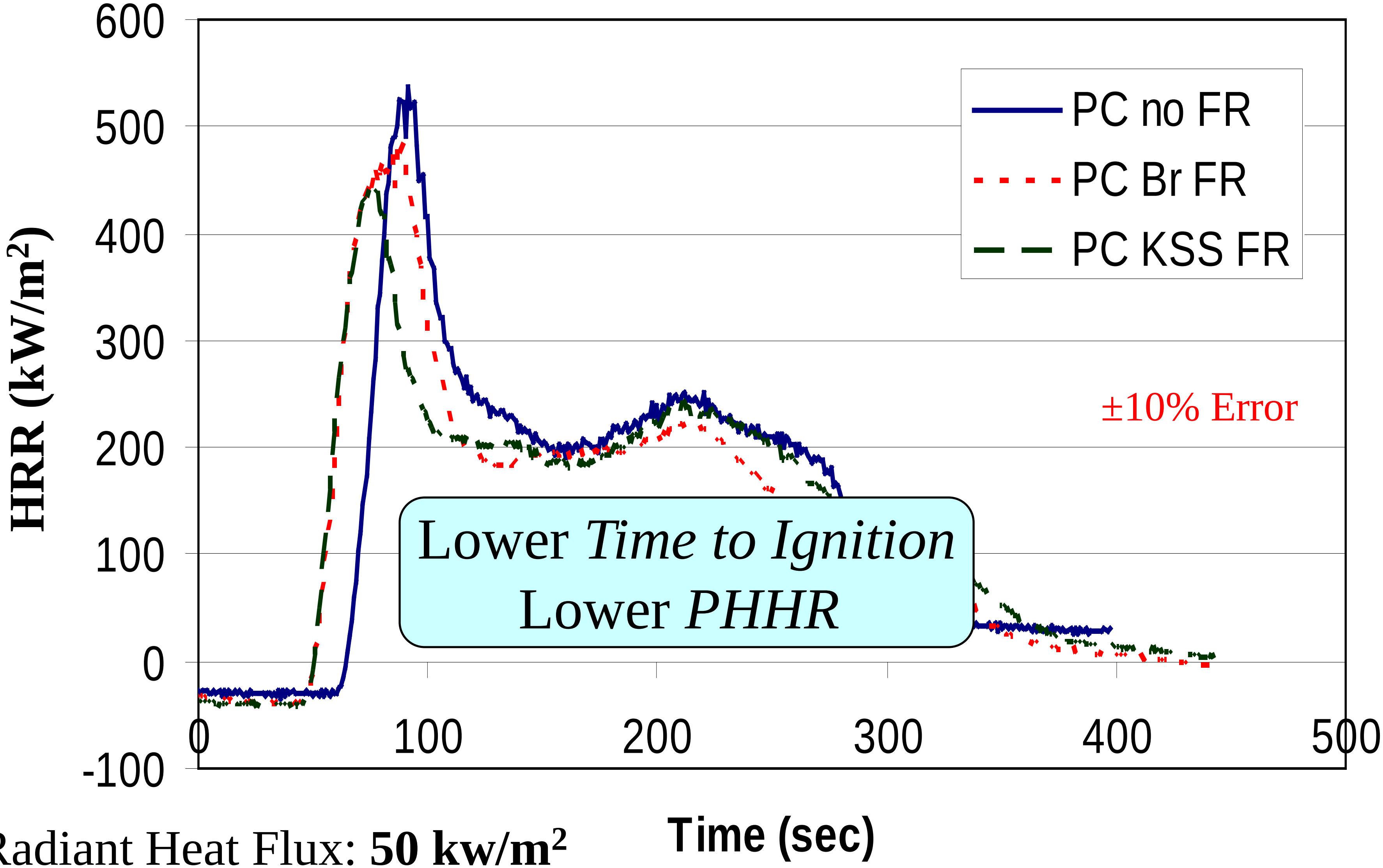
- Time to Ignition
- Heat Release Rate (HRR)
- Peak HRR
- Mass Loss Rate

Relates HRR to O_2 consumed

Performed at Marquette University

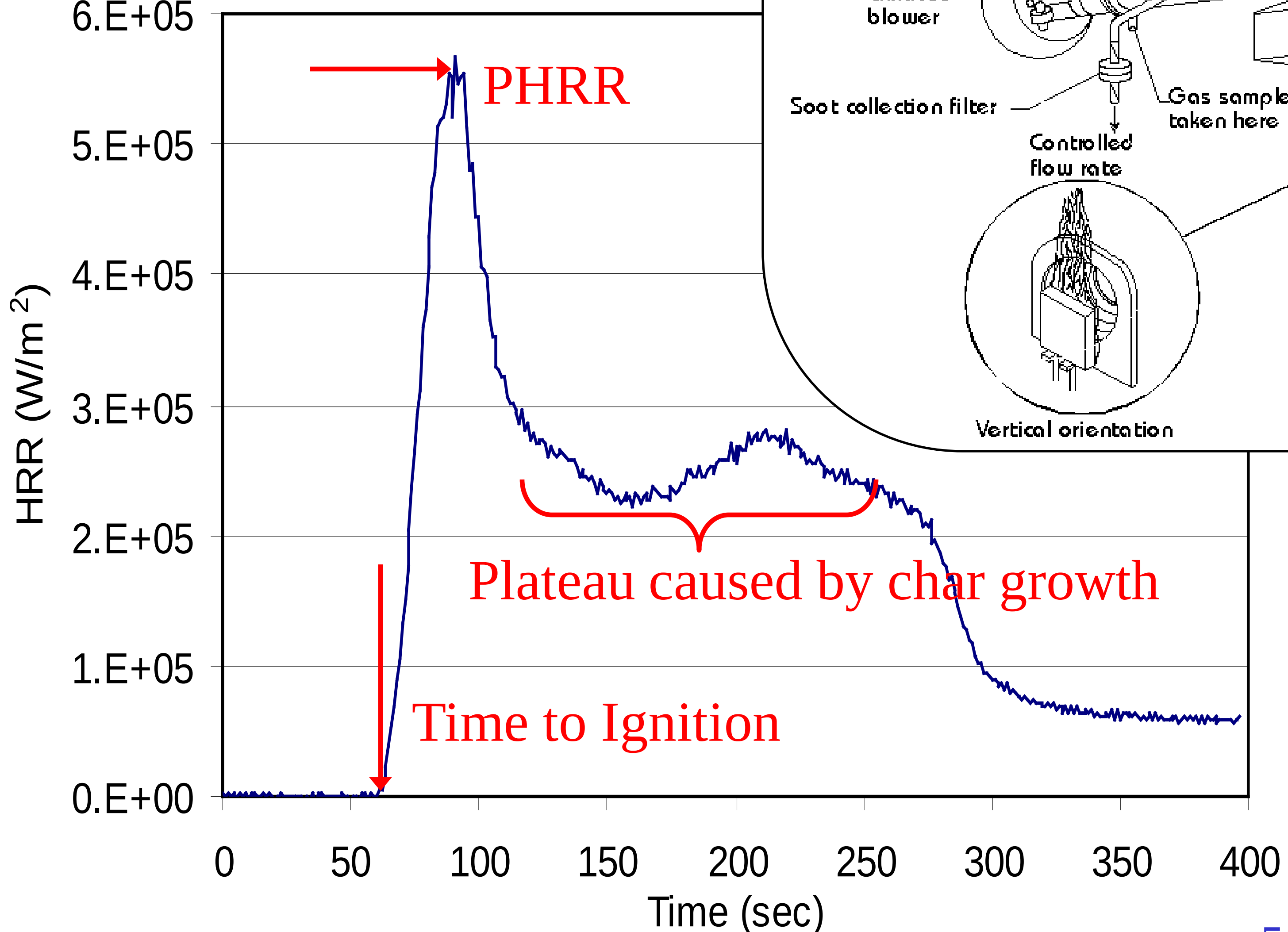
Adapted from http://www.doctorfire.com/cone.html

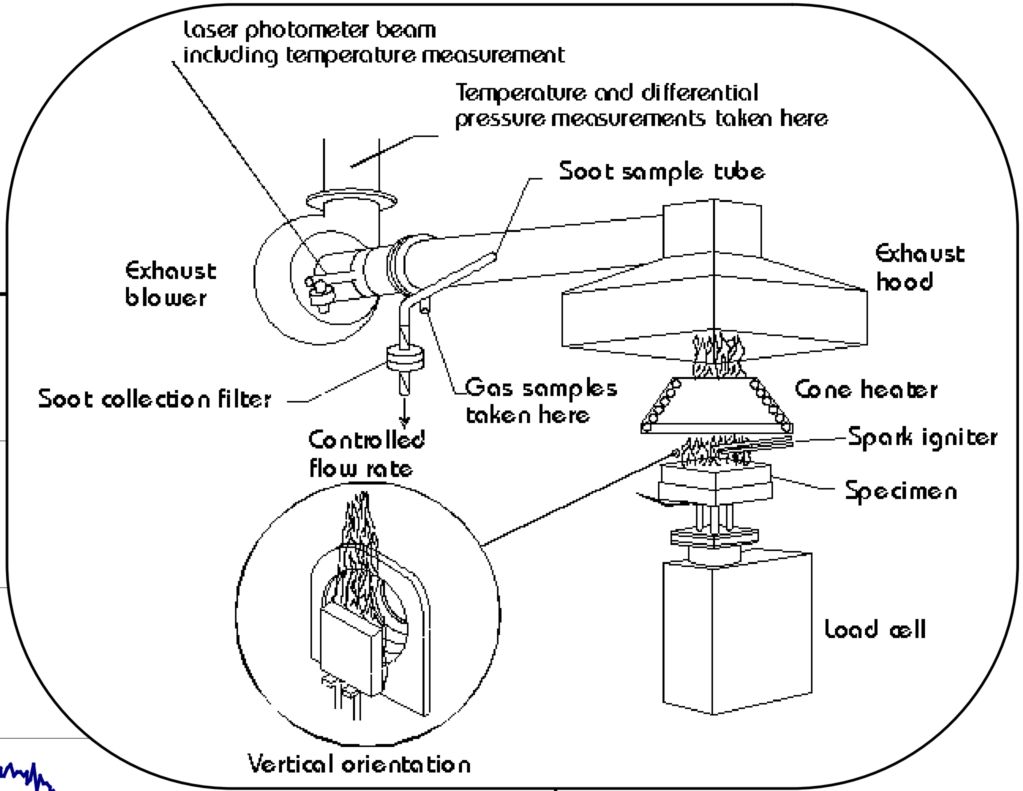
Cone Calorimeter Data



Radiant Heat Flux: **50 kw/m^2**

Cone Calorimeter





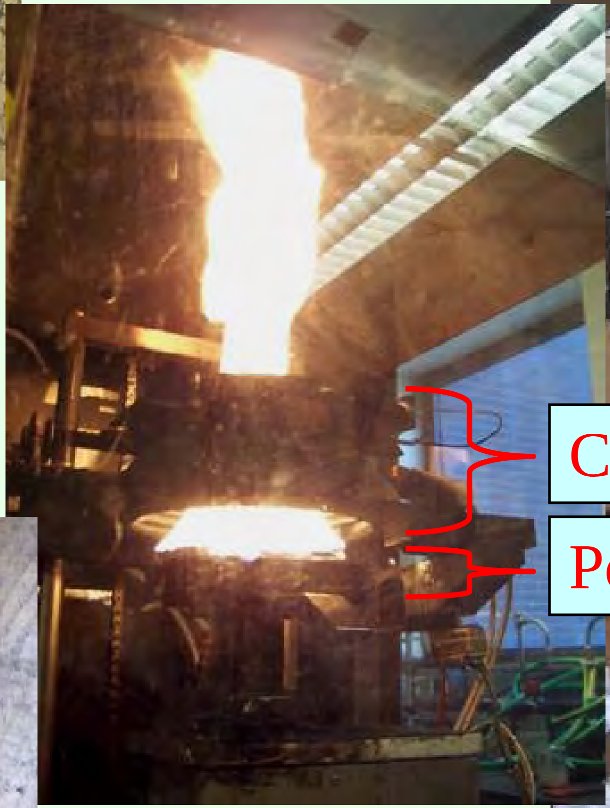
PC No FR
50 kW/m² Heat Flux

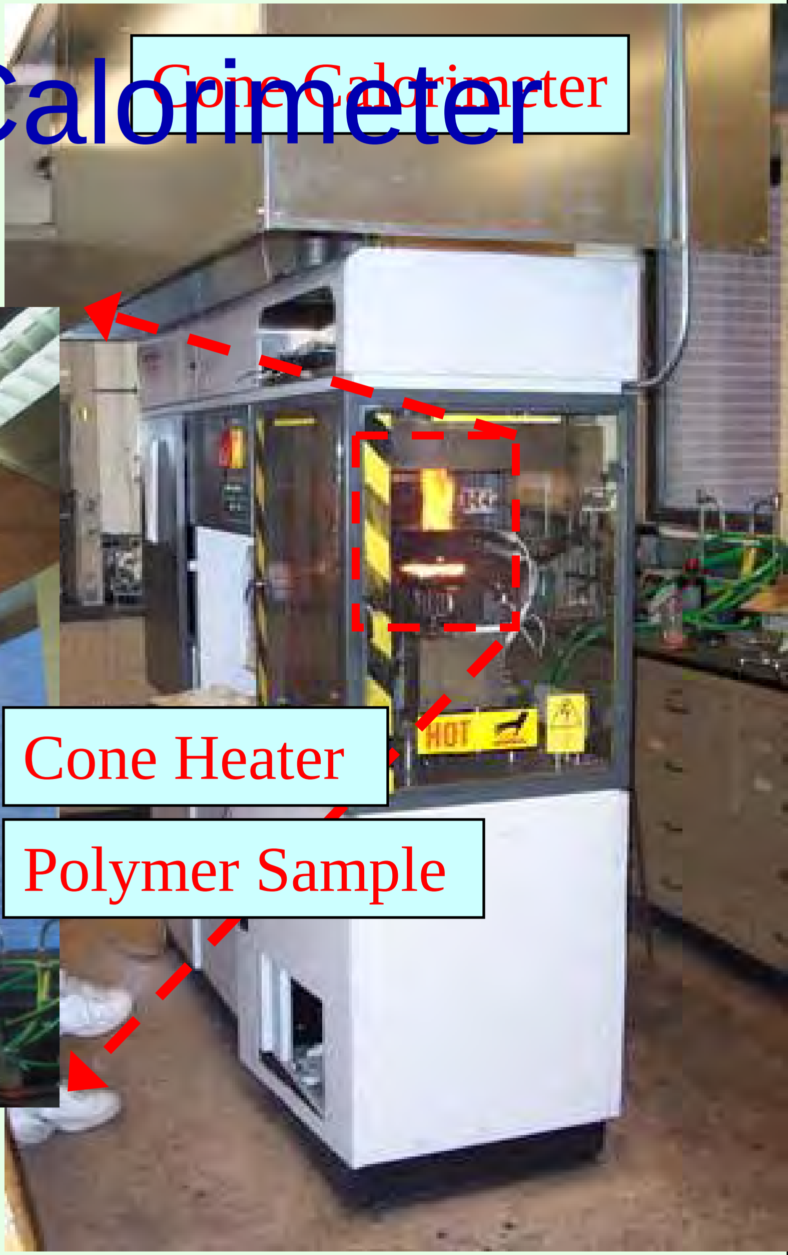
Adapted from http://www.doctorfire.com/cone.html

Cone Calorimeter

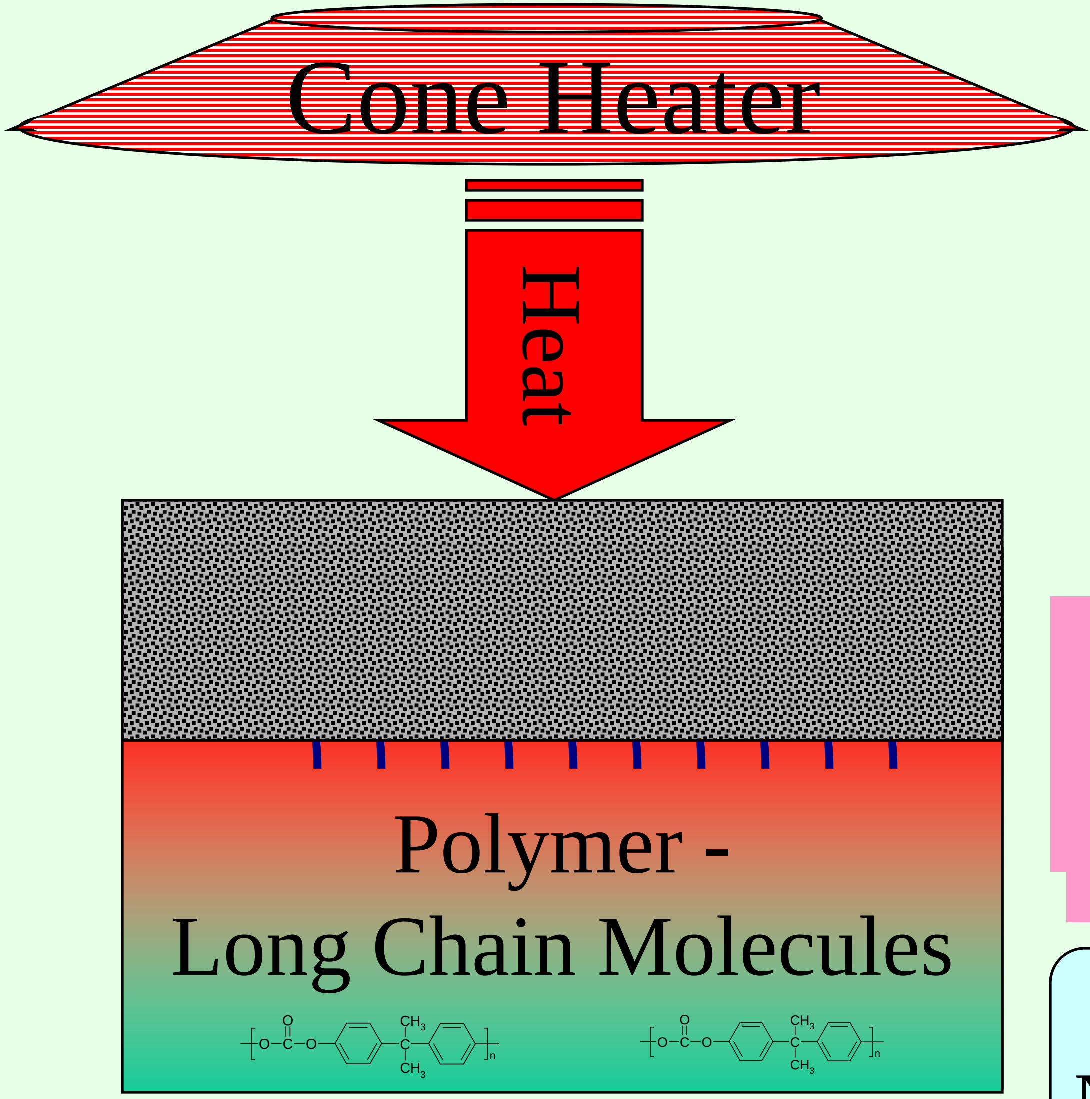
Polymer Plaque

Remaining Char





Cone Calorimeter & Polymer Combustion



FR in Condensed Phase

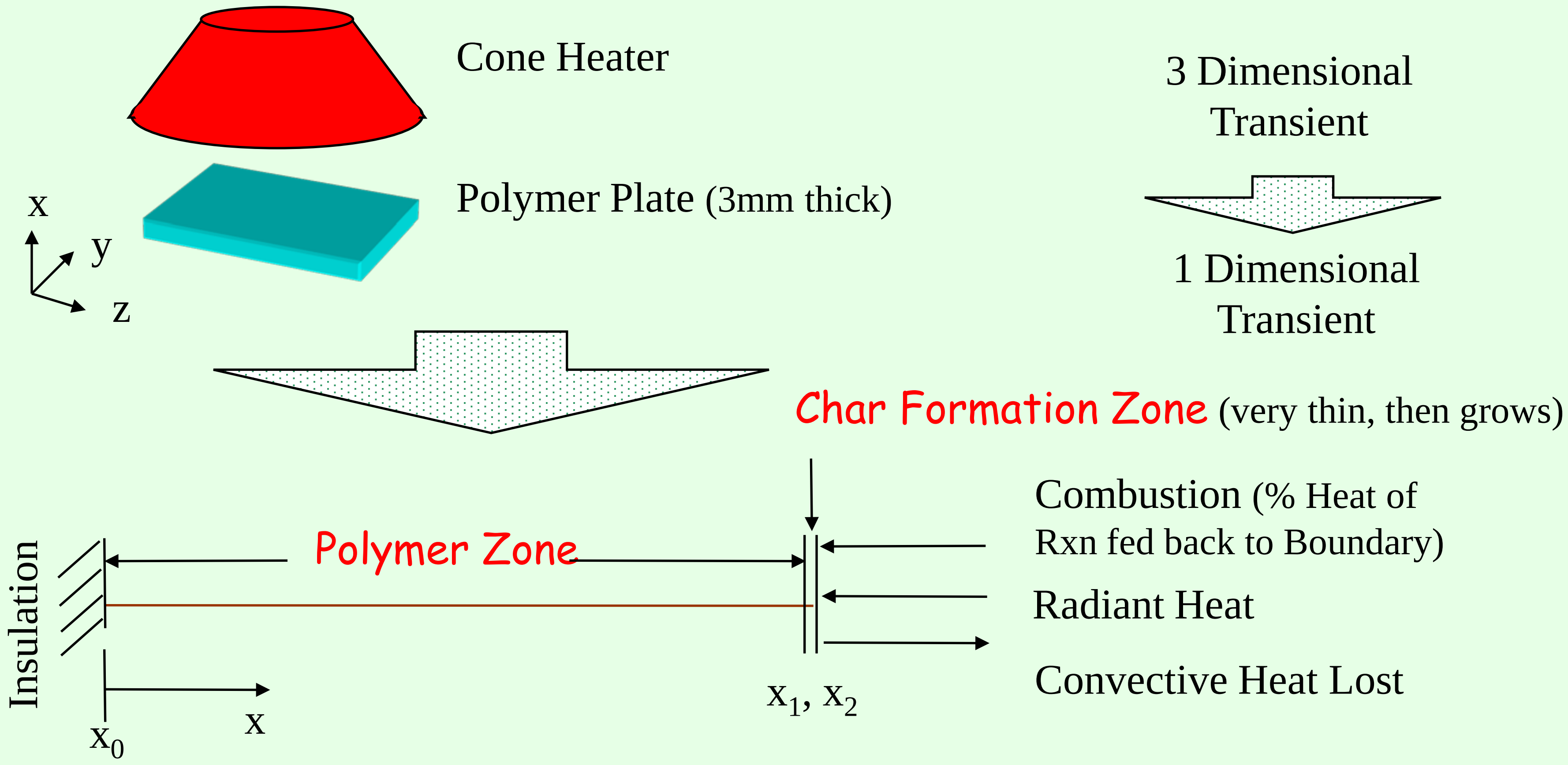
Protective Char Formation:

Barrier to Heat

and Mass Transfer

Polycarbonate is a Natural Char Former

Mathematical Modeling of Heat & Mass Transfer, along with Char Formation, to predict Heat Release Rate from Cone Calorimetry Data



Polymer Zone: Mass Transfer

- Polymer Pyrolysis

$$Polymer \xrightarrow{k0} Gas + Char$$

or

$$P \xrightarrow{k0} \alpha \cdot G + (1-\alpha) \cdot C$$

- 1st Order Rate Expression

$$\frac{\partial m_p}{\partial t} = -k_0 \cdot m_p$$

$$k_0 = A_0 \cdot \exp\left[\frac{-E_{A0}}{R \cdot T}\right]$$

- Assume Constant Volume

$$r_P = \frac{\partial c_p}{\partial t} = -k_0 \cdot c_p$$

Polymer Zone: Mass Transfer

- Gas Generation Rate Expression

$$r_{G \circ P} = \frac{\partial c_G}{\partial t} - D_{polymer} \cdot \frac{\partial^2 c_G}{\partial x^2} = \alpha \cdot k_0 \cdot c_p$$

Char Zone: Mass Transfer

- Gas Expression

$$\frac{\partial c_G}{\partial t} - D_{char} \cdot \frac{\partial^2 c_G}{\partial x^2} = 0$$

Polymer Zone: Heat Transfer

$$\rho_{polymer} \cdot Cp_{polymer} \cdot \frac{\partial T}{\partial t} - k_{polymer} \cdot \frac{\partial^2 T}{\partial x^2} = -\Delta H_0 \cdot k_0 \cdot c_P$$

Char Zone: Heat Transfer

$$\rho_{char} \cdot Cp_{char} \cdot \frac{\partial T}{\partial t} - k_{char} \cdot \frac{\partial^2 T}{\partial x^2} = 0$$

Char Growth

$$\frac{\partial m_C}{\partial t} = -(1-\alpha)\cdot\frac{\partial m_P}{\partial t} = (1-\alpha)\cdot k_0 m_P$$

- Rate of Char Production
- Rearrangements
- Defining Mesh Velocity *(smoothed step change)*

$$\frac{LHS}{\rho_{Char}} = \frac{1}{\rho_{Char}}\frac{\partial m_C}{\partial t} = \frac{\partial\left(\frac{m_C}{\rho_{Char}}\right)}{\partial t} = \frac{\partial V}{\partial t} = \frac{\partial Ax}{\partial t} = A\frac{\partial x}{\partial t}$$

$$A\frac{\partial x}{\partial t} = -\frac{(1-\alpha)}{\rho_{Char}}\frac{\partial m_P}{\partial t} = \frac{(1-\alpha)\cdot k_0}{\rho_{Char}} m_P$$

$$\frac{\partial x}{\partial t} = -\frac{(1-\alpha)\cdot\chi}{\rho_{Char}\cdot A\cdot\chi}\frac{\partial m_P}{\partial t} = \frac{(1-\alpha)\cdot k_0\cdot\chi}{\rho_{Char}}\frac{m_P}{A\cdot\chi}$$

$$mvel = \frac{\partial x}{\partial t} = -\frac{(1-\alpha)\cdot\chi}{\rho_{Char}}\frac{\partial c_P}{\partial t} = \frac{(1-\alpha)\cdot k_0\cdot\chi}{\rho_{Char}} c_P$$

$$mvel = \frac{(1-\alpha)\cdot\chi}{\rho_{Char}}\cdot\left(-\frac{\partial c_P}{\partial t}\right)\bigg|_{x_0}$$

$$mvel = flc1hs\left(\rho_{polymer} - c_P\big|_{x_0} - \min, scale\right)\cdot\frac{(1-\alpha)\cdot\chi}{\rho_{Char}}\cdot\left(-\frac{\partial c_P}{\partial t}\right)\bigg|_{x_0}$$

Variables Solved For:

- $T(x,t)$ ← Temperature Profiles
- $c_P(x,t)$
- $c_G(x,t)$

} Concentration Profiles

Heat Release Rate

- $$HRR = \Delta H_1 \cdot \left(-\frac{\partial c_G}{\partial x}\right)\Bigg|_{Surface} \cdot D_{Char}$$

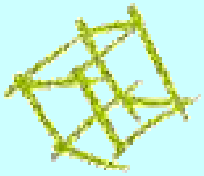
Initial & Boundary Conditions

Initial Condition (x,0)	Zone	
	Polymer $[x_0\text{-}x_1]$	Char Formation $[x_1\text{-}x_2]$
c_P	$c_P = \rho_{polymer}$	$c_P = 0$
c_G	$c_G = 0$	$c_G = 0$
T	$T = T_{initial}$	$T = T_{initial}$

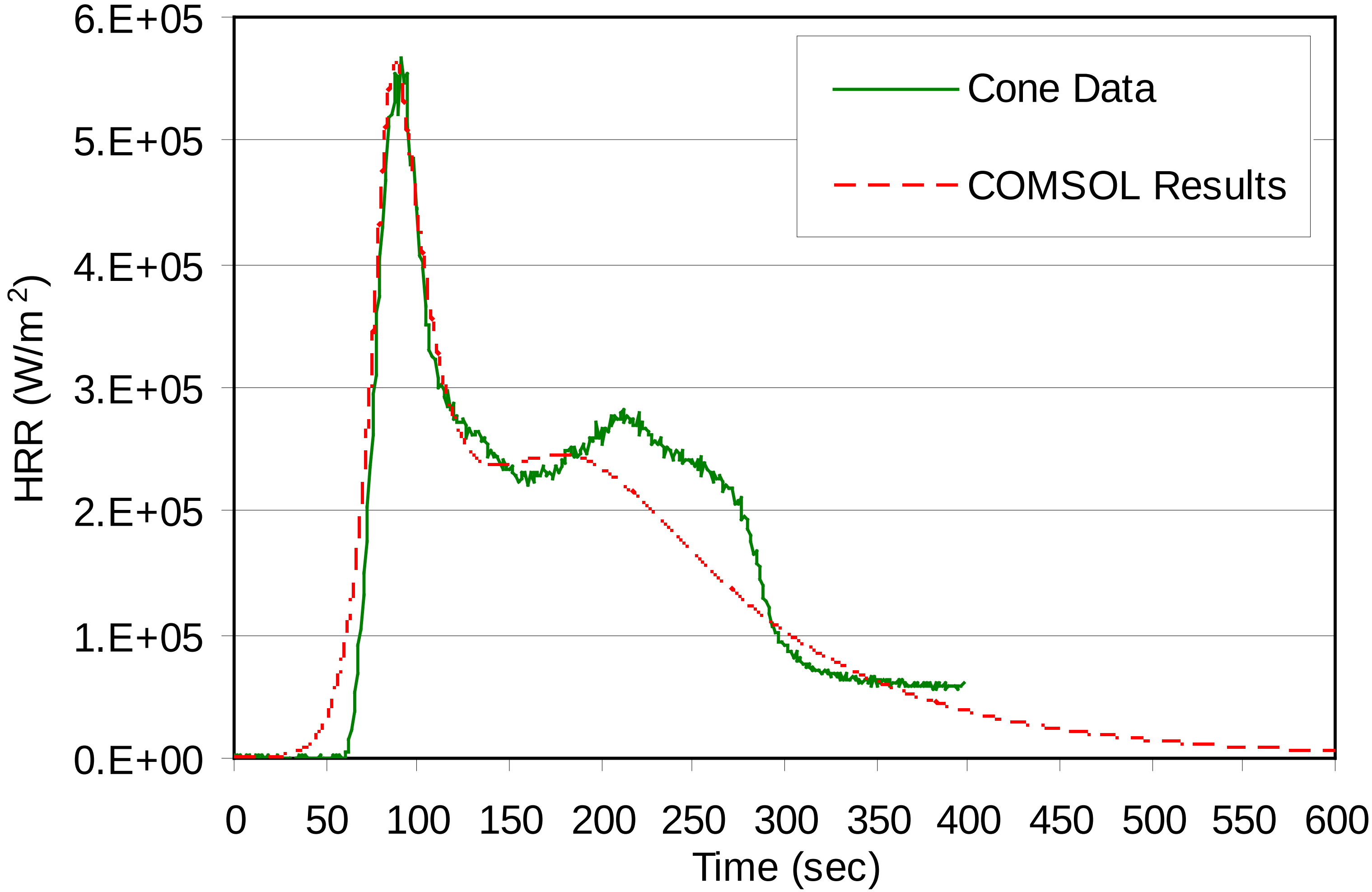
Boundary Condition $(x_0;x_2,t)$	Boundary	
	x_0	x_2
c_P	Flux=0	Flux=0
c_G	Flux=0	c_G=0
T	Flux=0	$Flux = \phi \cdot \Delta H_1 \cdot (-\frac{\partial c_G}{\partial x}) \cdot D_{Char} + \varepsilon \cdot \sigma \cdot \left(T_{cone}{}^4 - T^4\right)$

Equations are Coupled

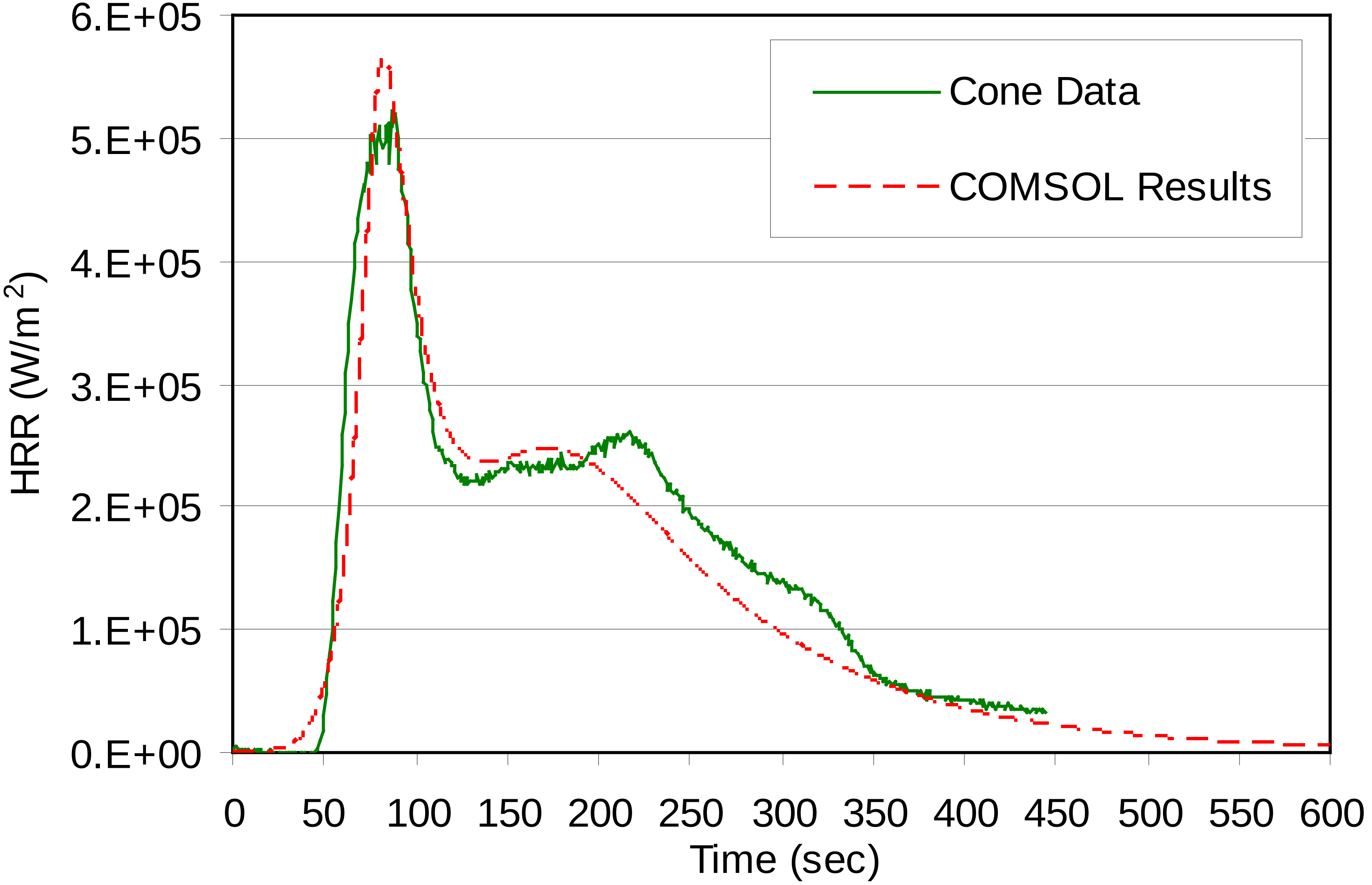
- No Analytical Solution Exists
- Numerical Solution Sought
  - Finite Element Method
  - COMSOL Multiphysics®
    - Solve Simultaneously System of Partial Differential Equations
    - Char Growth Simulated by Moving Boundary



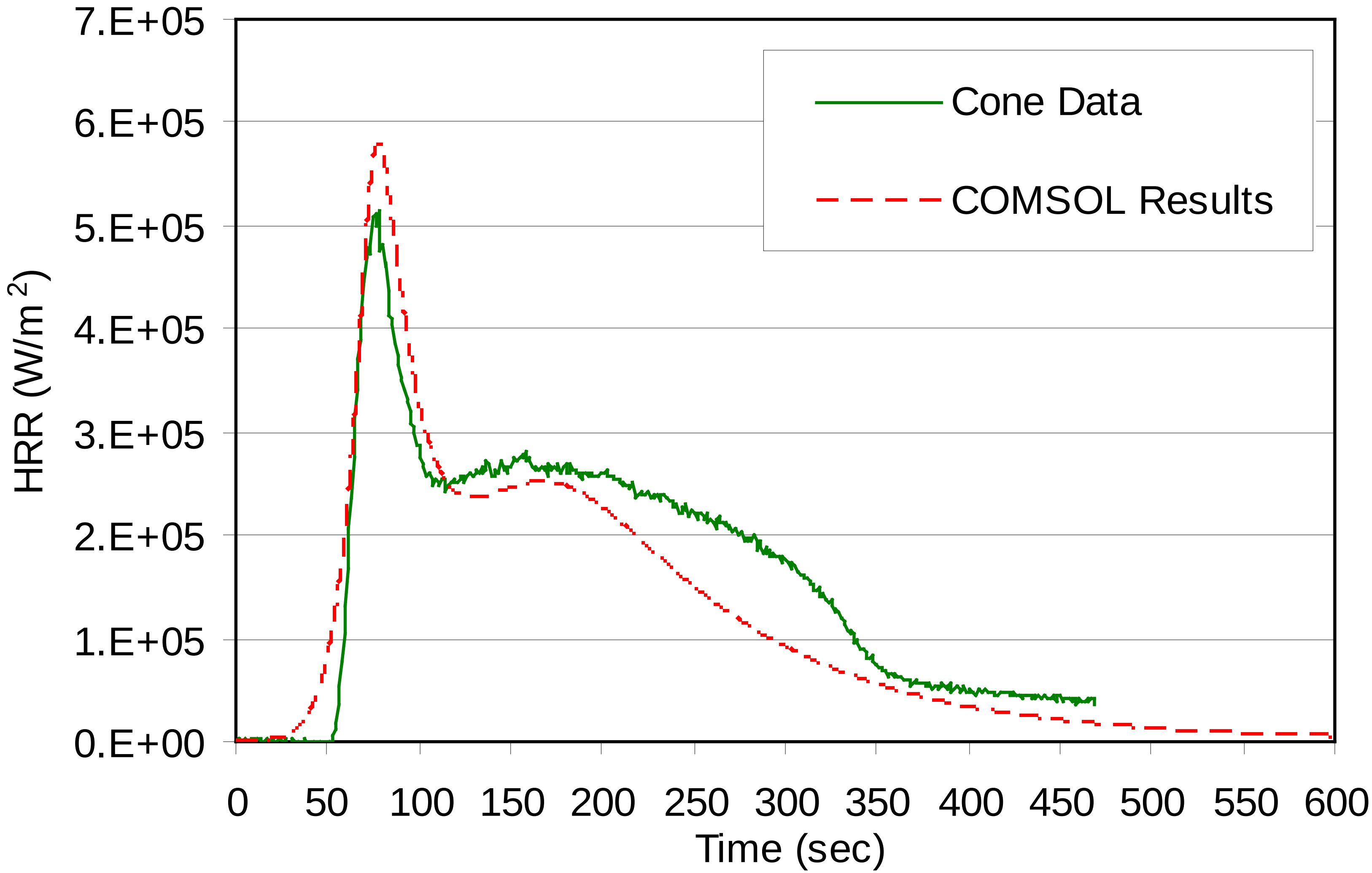
HRR Results; PC No FR



HRR Results; PC Br FR

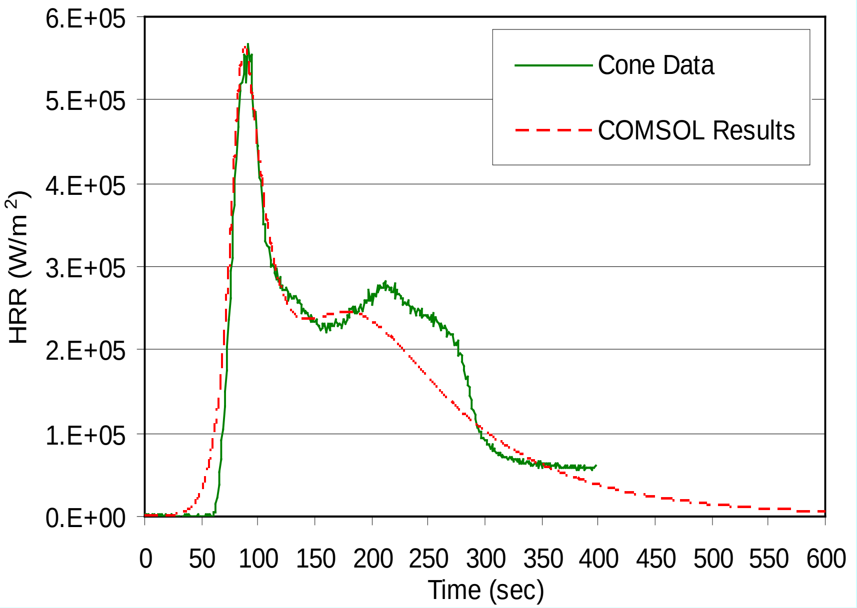


HRR Results; PC KSS FR



Modeling Conclusions

- Model predicts Heat Release Rate for Char Forming Polycarbonate with and without Flame Retardants
- All parameters in model can be found experimentally, such as, kinetics by TGA



Acknowledgments

- George and Carolyn Berry (Berry Fellowship)
- WV EPSCoR Research Challenge Grant Program (Funding)
- Department of Energy (Funding)

- Dr. Pierre Moulinie from Bayer (Makrolon® Polycarbonate)
- James Innes from Flame Retardant Associates (Sloss Industries KSS FR®)
- Dr. Sushant Agarwal from WVU (Research Assistant Professor)
- Dr. Charles Wilkie from Marquette University (FR Expert)
- Dr. Carlos Hilado from Product Safety Corp. (FR Expert)

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Thank you!

heat
flammable gases
O_2
oxygen in air
solid material
CO_2
H_2O
long-scale-molecules
short-chain and small molecules
pyrolysis
free H^+ and OH^- radicals break molecules down and enable reaction with O_2