Generalized Pyrolysis Model for Combustible Solids

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Motivation – Big Picture

- Reliable prediction of large-scale fire development
- Predictive capabilities for solid-phase pyrolysis lags gas-phase
  - "Practical" or "real-world" materials poorly understood
  - Many models specific to one class of materials

Objectives

1) Develop generalized pyrolysis model
   - Thermoplastic, charring, intumescent, smolder
   - Practical/real-world materials

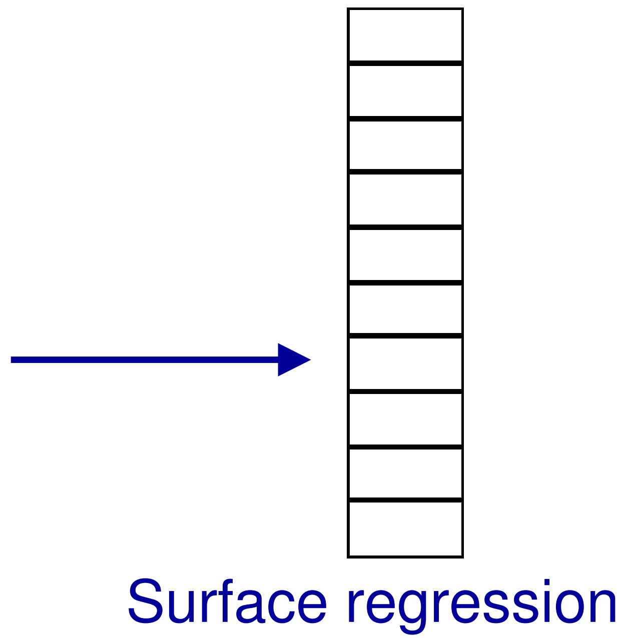
2) Develop technique to estimate model input parameters from existing laboratory tests
   - Fire tests (Cone Calorimeter, FPA)
   - Thermal analysis (TGA, DSC)

Presentation Outline

- Motivation
- Objectives
- Generalized pyrolysis model description
- Generalized pyrolysis model application
  - Oxidative pyrolysis of white pine
  - Thermal pyrolysis of polypropylene
  - Heating and swelling of intumescent coating
  - Smolder in polyurethane foam
- Concluding remarks

Generalized Pyrolysis Model

- Decomposing solid treated as coupled gaseous and condensed phases
- 1D conservation equations solved for
  - Gas and solid mass
  - Gas and solid species
  - Gas and solid energy
  - Gas momentum (Darcy's law)
- Volume change handled by variable grid spacing



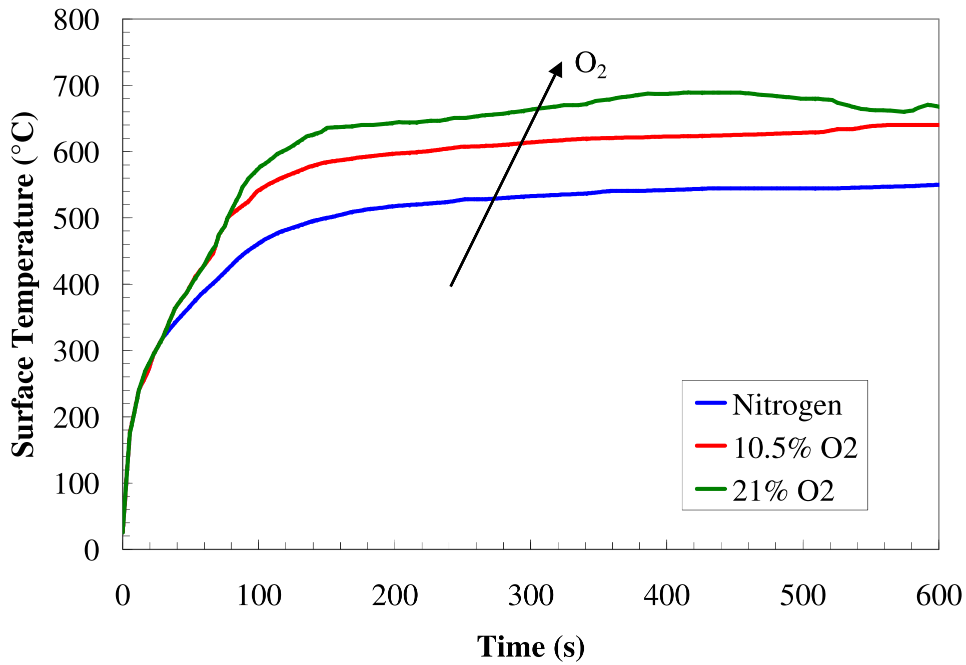
Generalized Pyrolysis Model

- User may specify any number of
  - Distinct layers
  - Solid and gaseous species
  - Solid and gaseous reactions

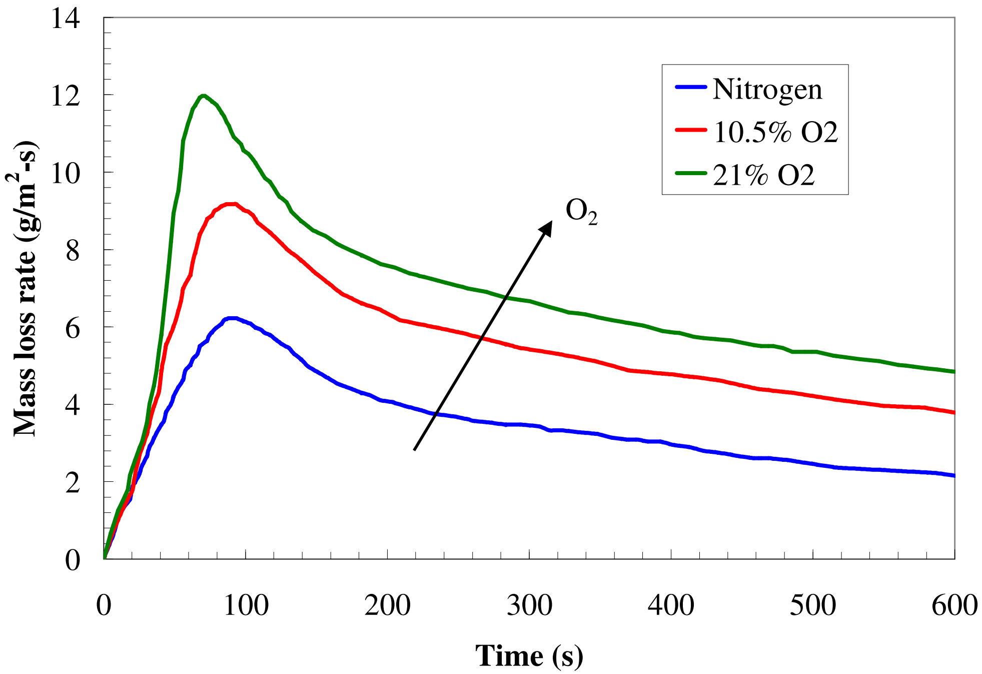
- Physics include
  - Volume change (swelling/surface regression)
  - In-depth radiation absorption, radiative transfer across pores
  - Darcy flow through porous media (pressure solver)
  - Penetration of ambient oxygen into decomposing solid and its effect on gaseous and solid reactions

White Pine Oxidative Pyrolysis – Experimental Data

- Ohlemiller, Kashiwagi, Werner - *C+F* v69 (1987)
  - 3.8 cm cubes irradiated @ 25 and 40 kW/m^2
  - O_2 ranged from 0% to 21% by volume



Surface temperature – 40 kW/m^2



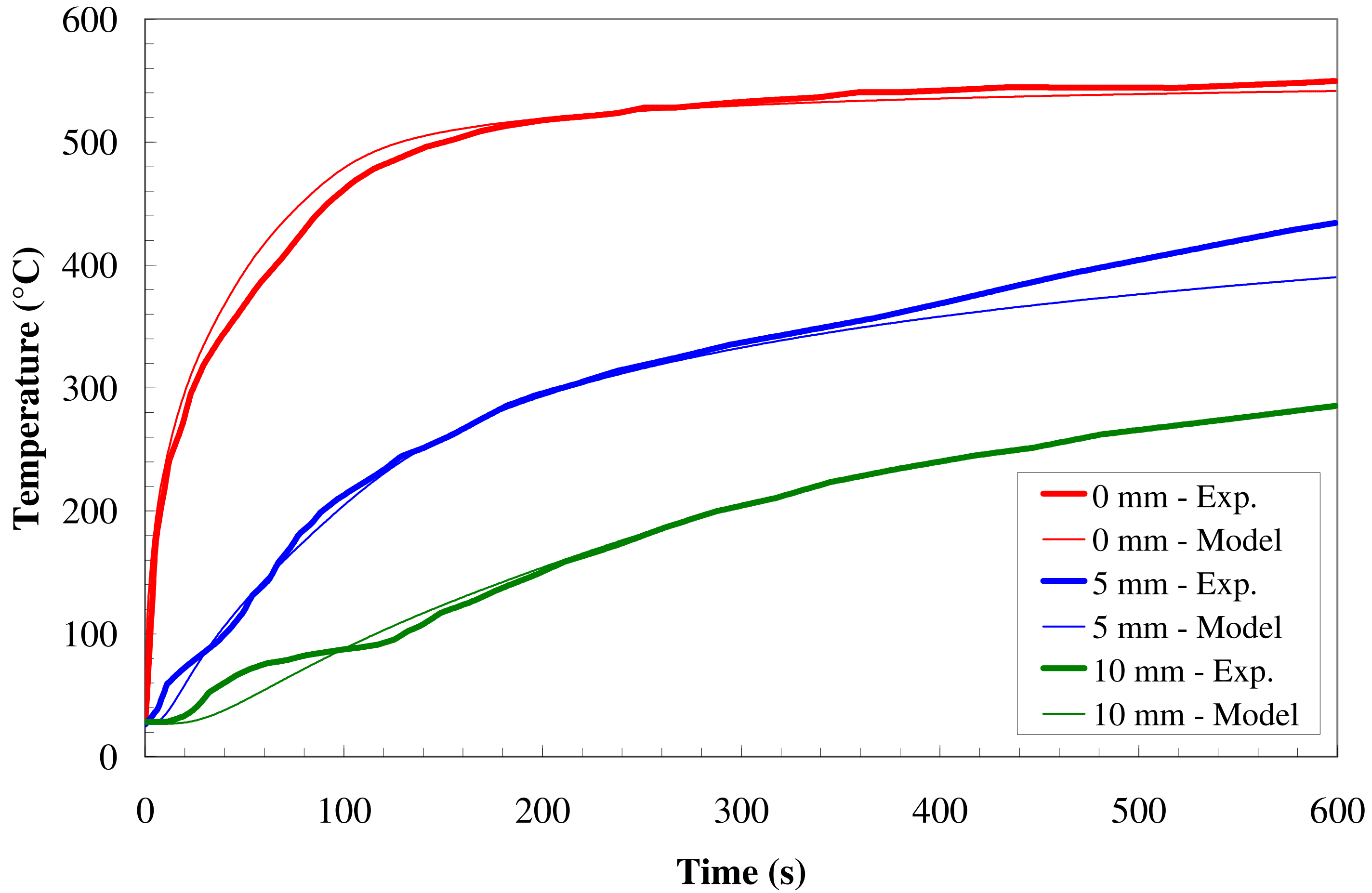
Mass loss rate – 40 kW/m^2

White Pine Oxidative Pyrolysis – Numerical Simulation

- Modeling approach
  - 4 solid species: wet wood, dry wood, char, ash
  - 4 solid reactions: drying, dry wood pyrolysis, dry wood oxidation, char oxidation
  - 1 gas-phase reaction: oxidation of pyrolysate
  - 5 gaseous species: N_2, O_2, H_2O, pyrolysate, products
- The challenge
  - At least <u>**40**</u> unknown model parameters must be specified!
- The solution
  - Parameters estimated from experimentally measured MLR and T (40 kW/m^2) using genetic algorithm optimization

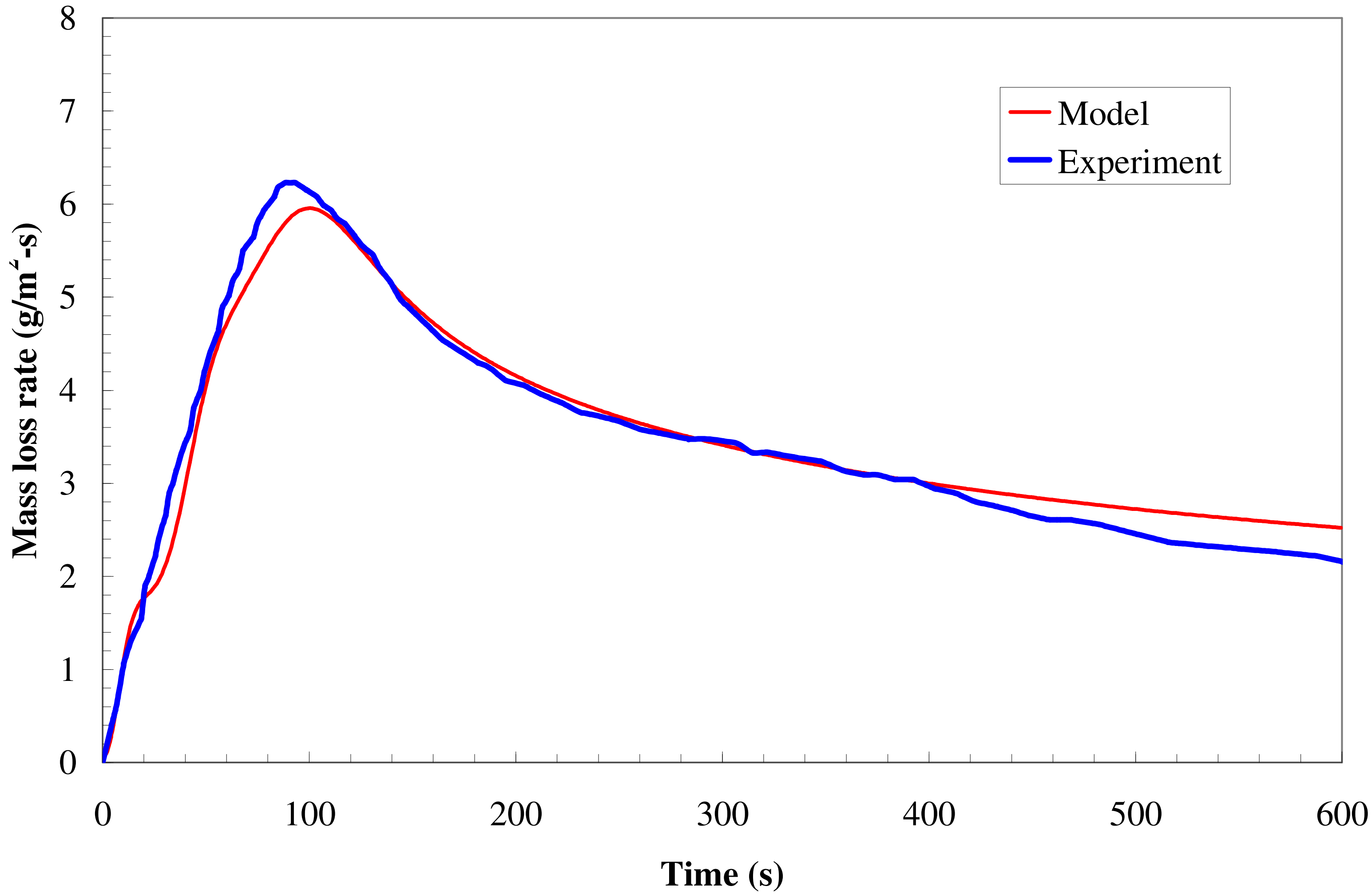
White Pine – Comparison of Measured and Modeled T

- Modeled temperatures match experimental data quite well for pyrolysis under N_2 at 40 kW/m^2:



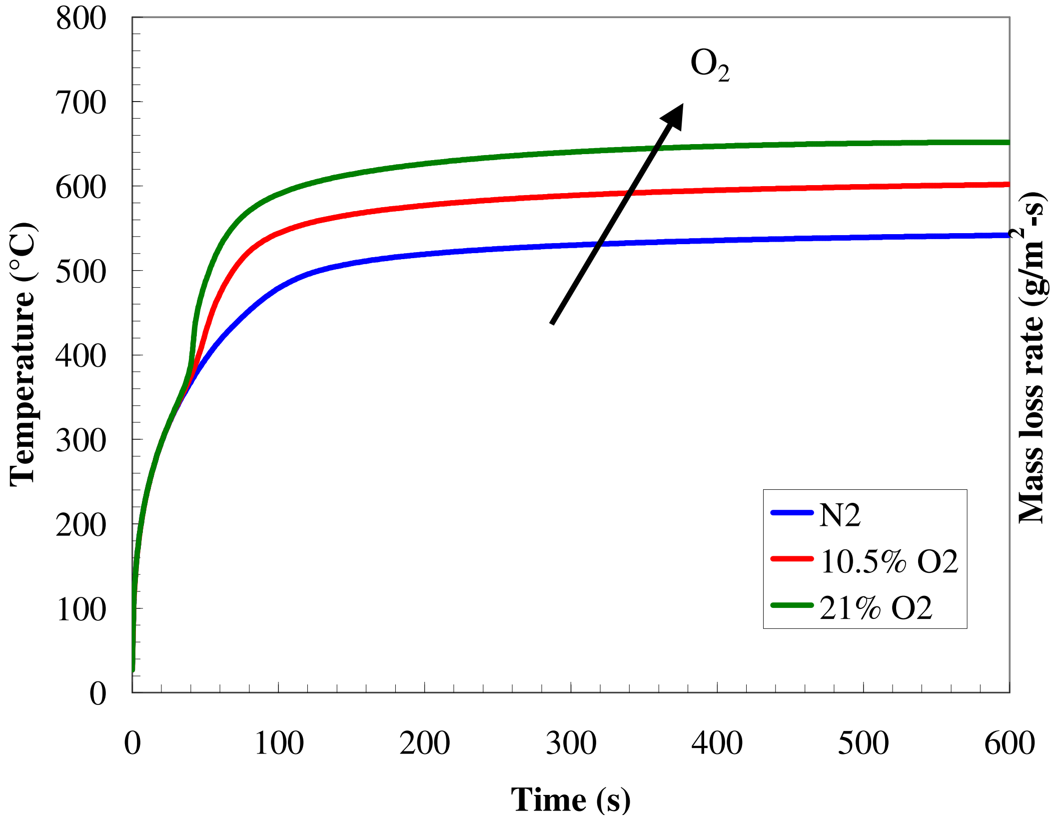
White Pine Oxidative Pyrolysis – Predictions/Measurements in N_2

- Mass loss rate under N_2 @ 40 kW/m^2:

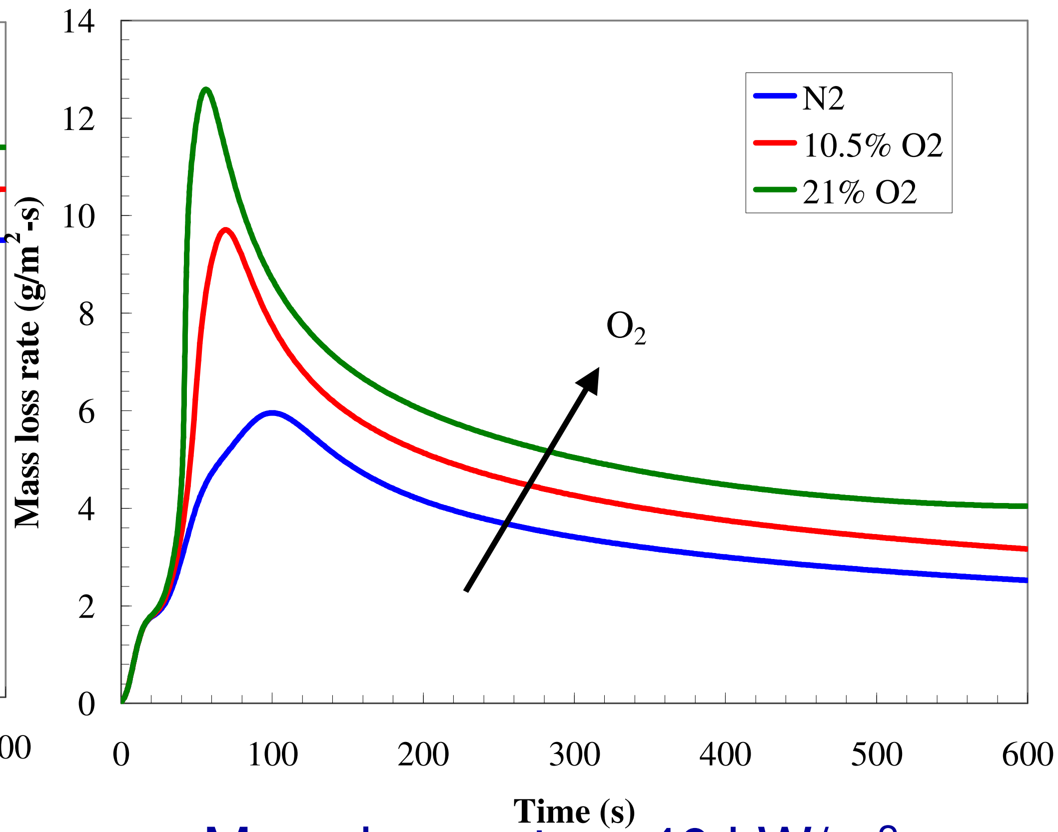


White Pine Oxidative Pyrolysis – Model Predictions

- Model captures experimentally-observed increase in MLR and surface T with increasing O_2 concentration



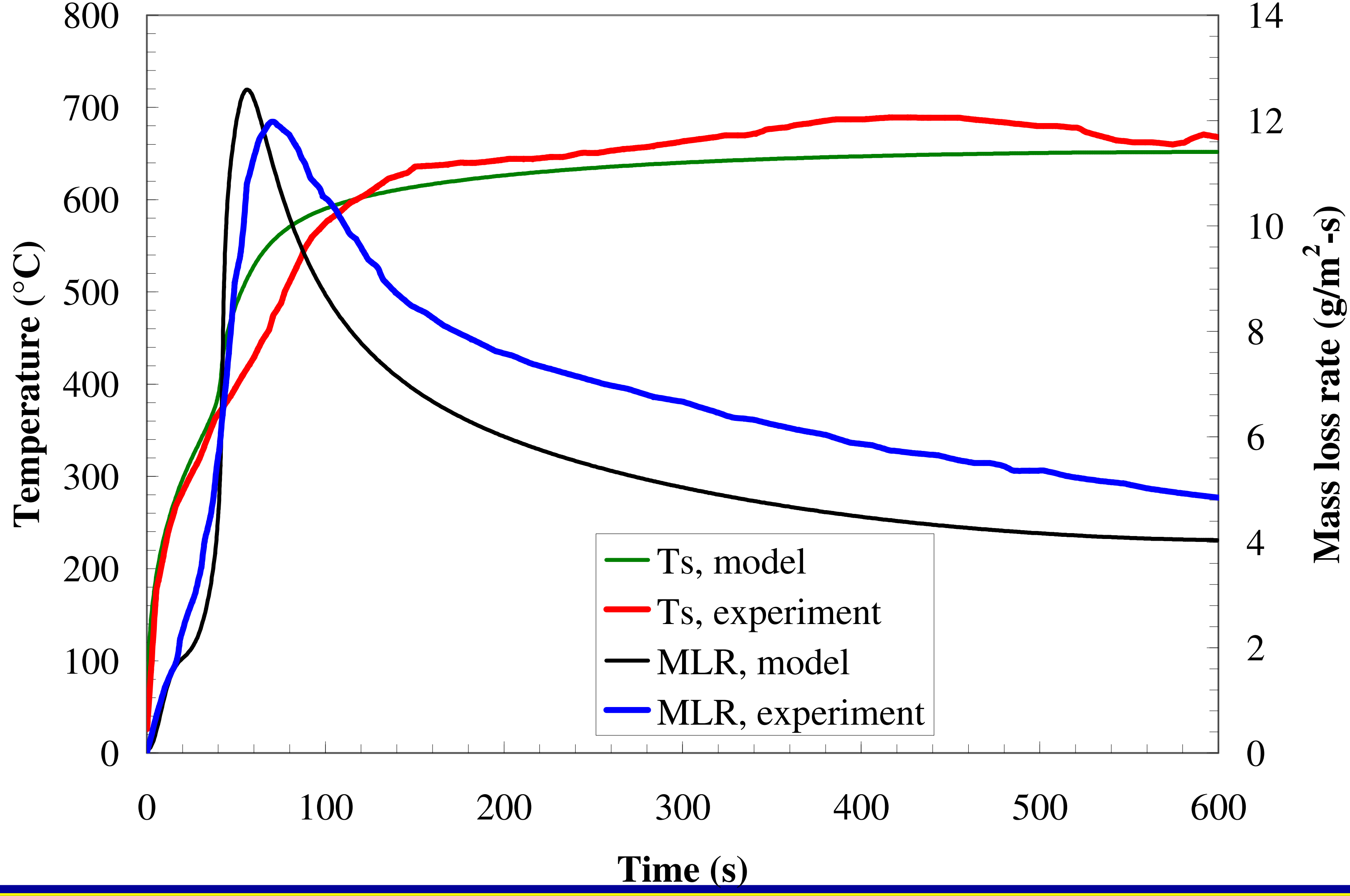
Surface temperature – 40 kW/m²



Mass loss rate – 40 kW/m²

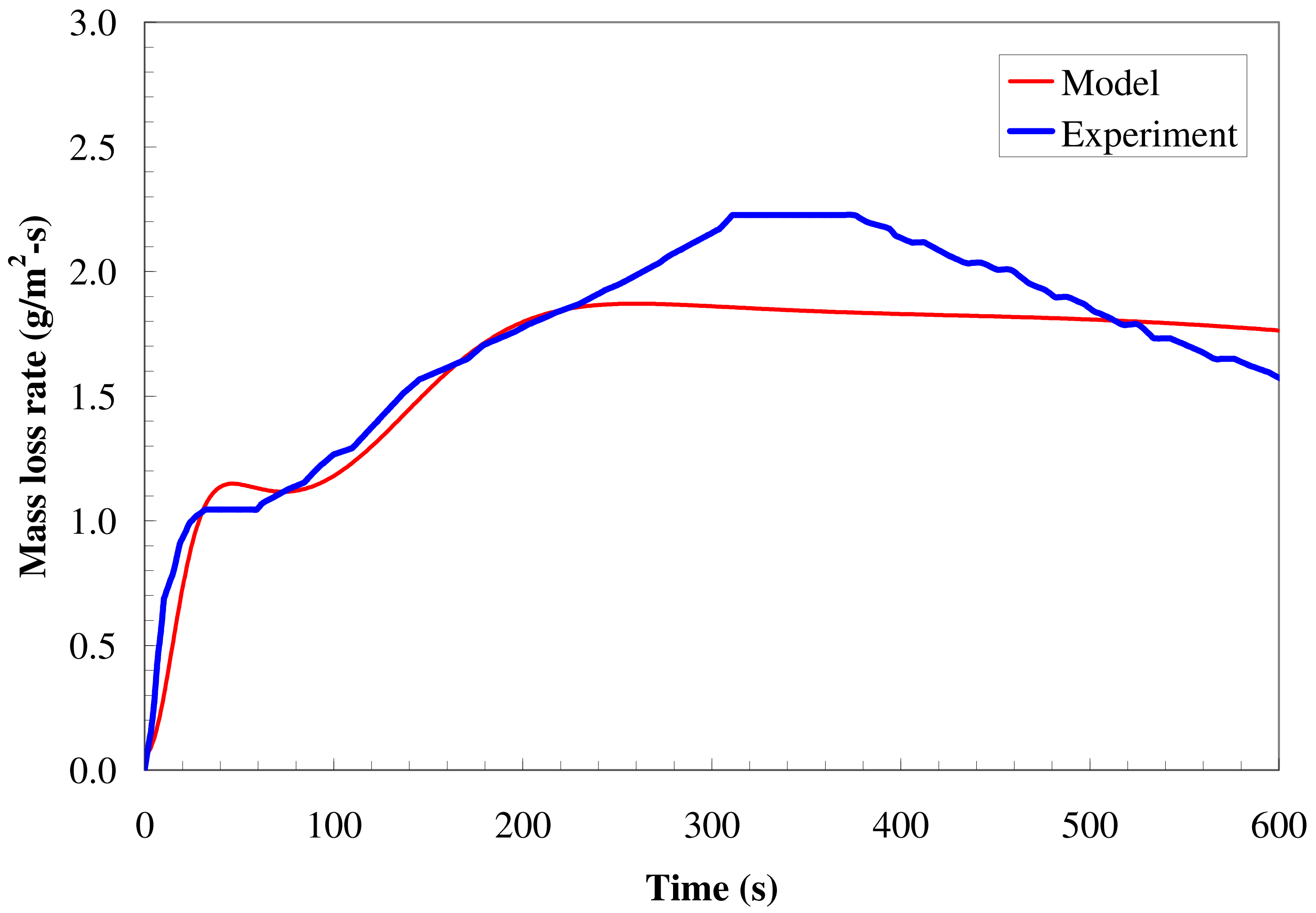
White Pine Oxidative Pyrolysis – Predictions/Measurements in Air

- Surface temperature and MLR @ 40 kW/m^2 (21% O_2)



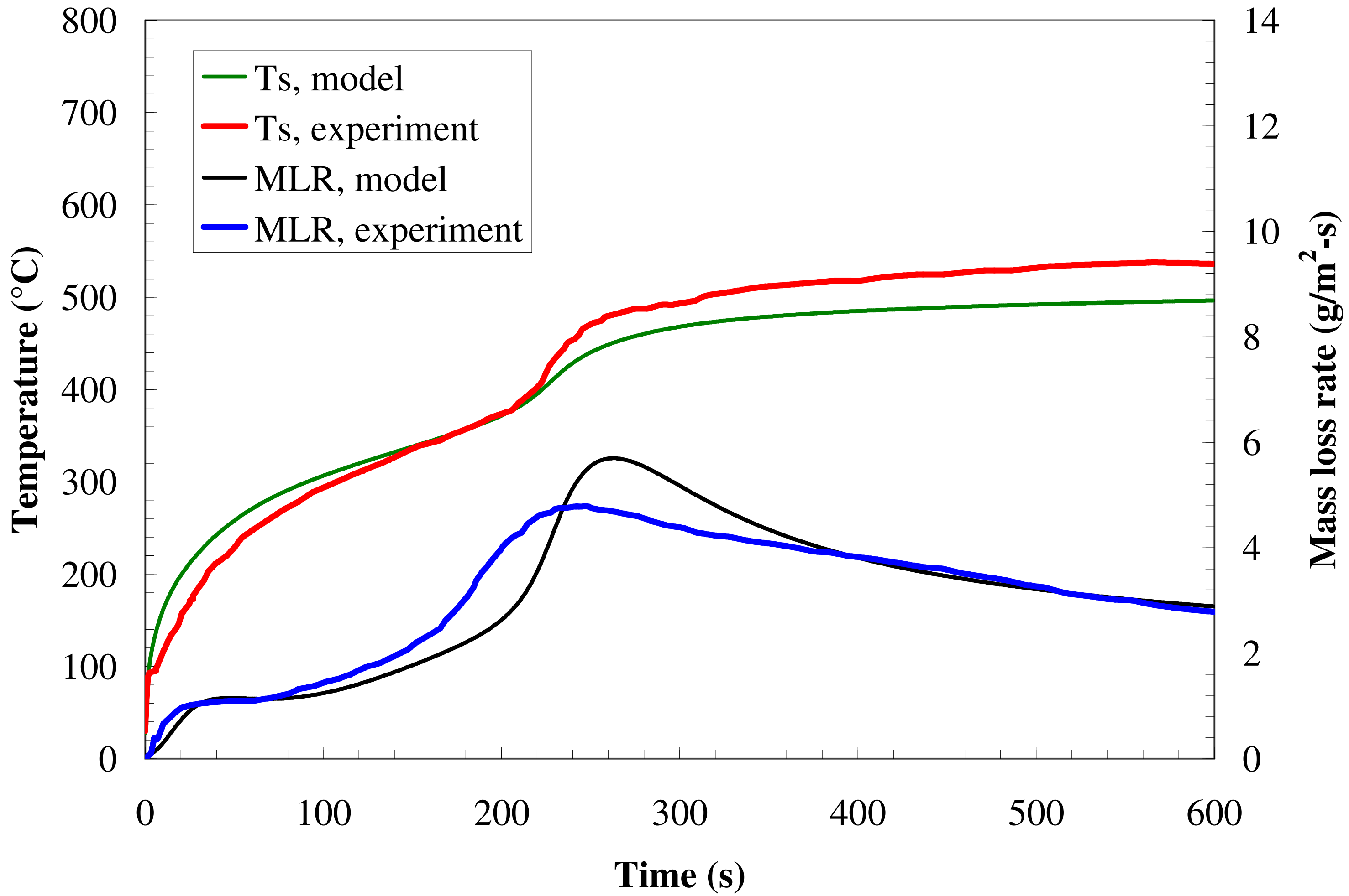
Blind Predictions
Nitrogen, 25 kW/m²

- Mass loss rate under N_2 @ 25 kW/m^2:

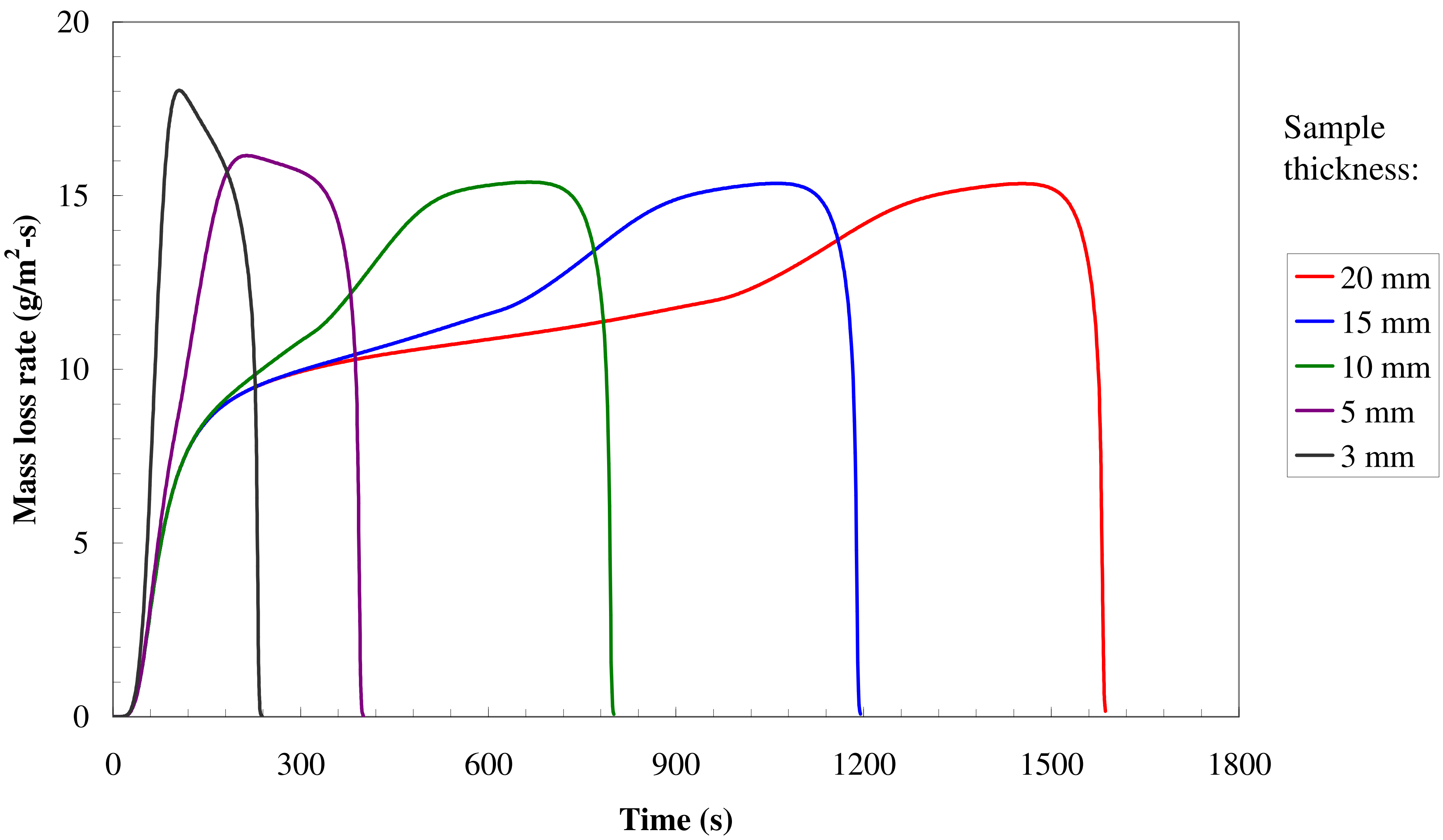


Blind Predictions
10.5% O_2, 25 kW/m^2

- MLR and surface T in 10.5% O_2 @ 25 kW/m^2:



Polypropylene Pyrolysis – Effect of Thickness

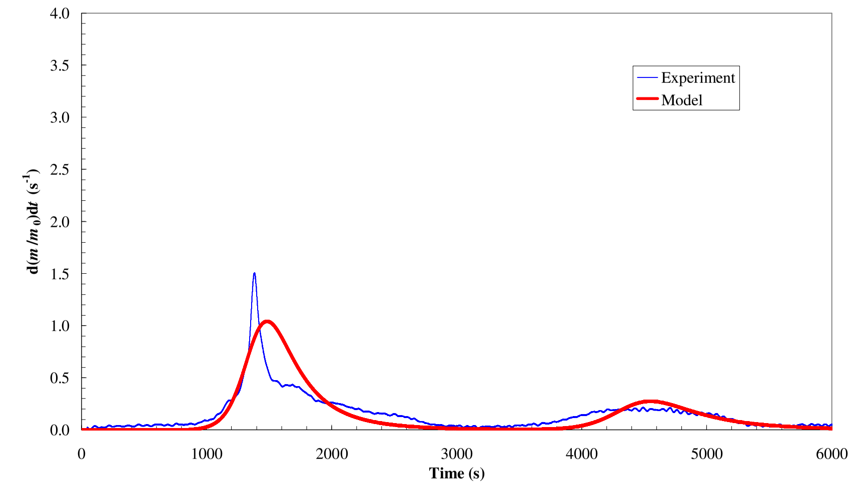


Heating and Swelling of an Intumescent Coating

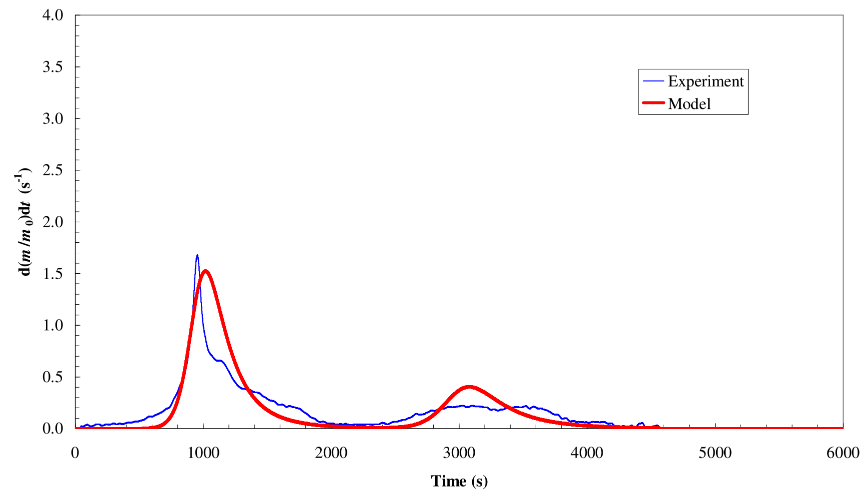
- Experiment - Griffin *et al.*, *JFS* v23 (2005)
  - Cone Calorimeter
    - 2.7 mm intumescent coating applied over steel substrate
    - Irradiated at 90 kW/m^2 (T_{subs} and δ measured)
  - Thermogravimetric analysis (TGA)

- Modeling approach
  - 5 solid species
  - 3 condensed-phase reactions, including intumescence
  - 26 model parameters determined by genetic algorithm optimization

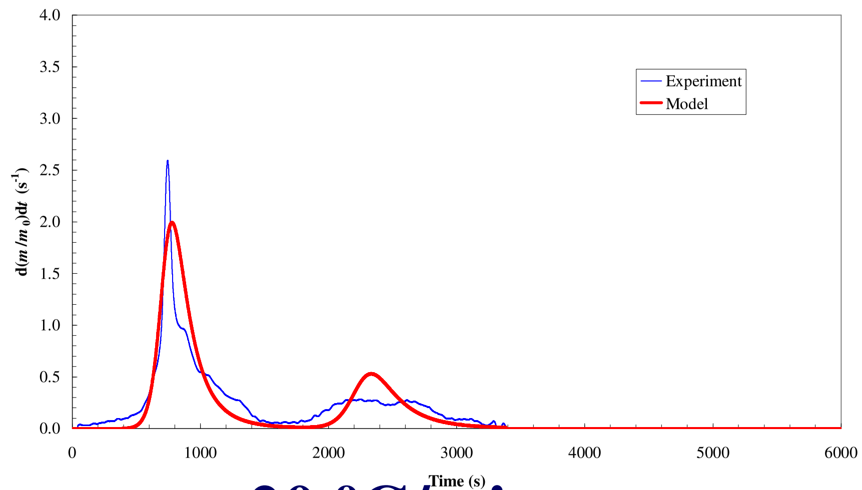
Intumescent Coating – Model Results (TGA)



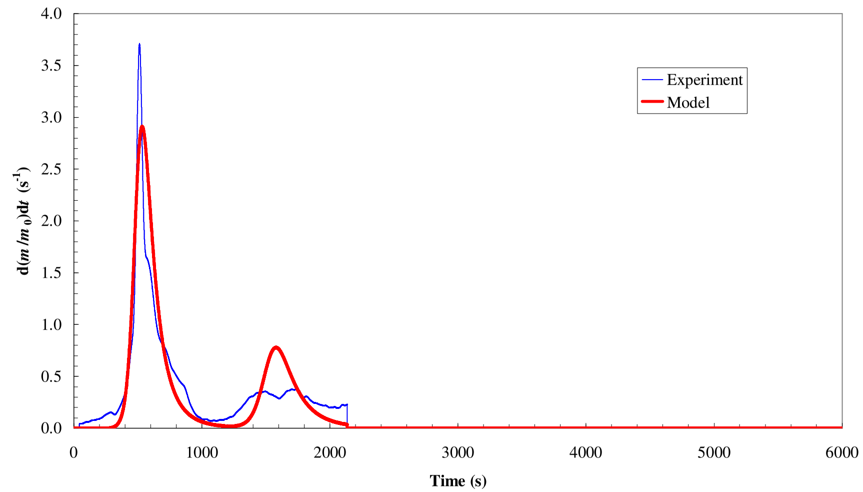
10 °C/min



15 °C/min

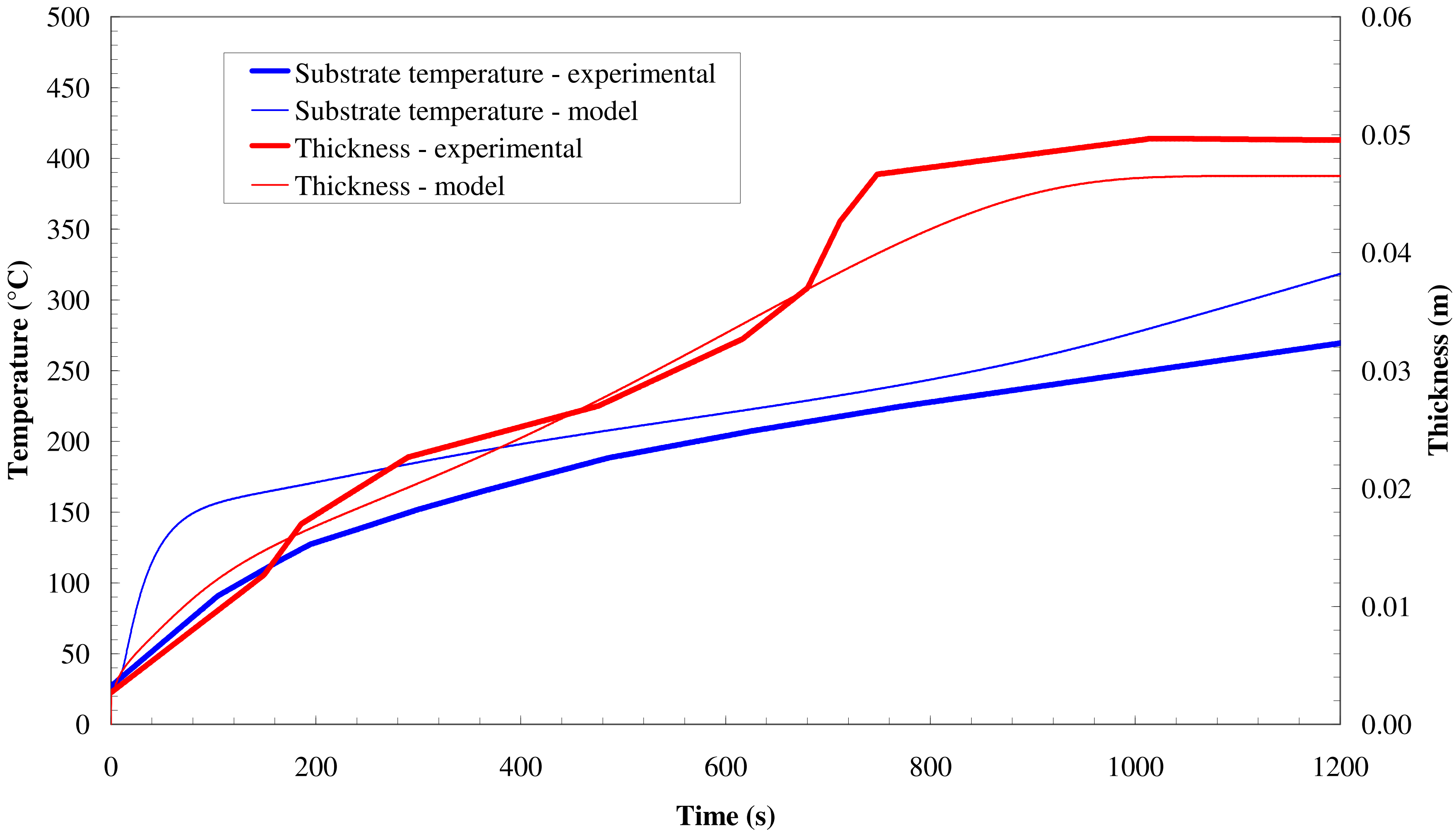


20 °C/min



30 °C/min

Intumescent Coating –
Model Results (Cone Calorimeter)

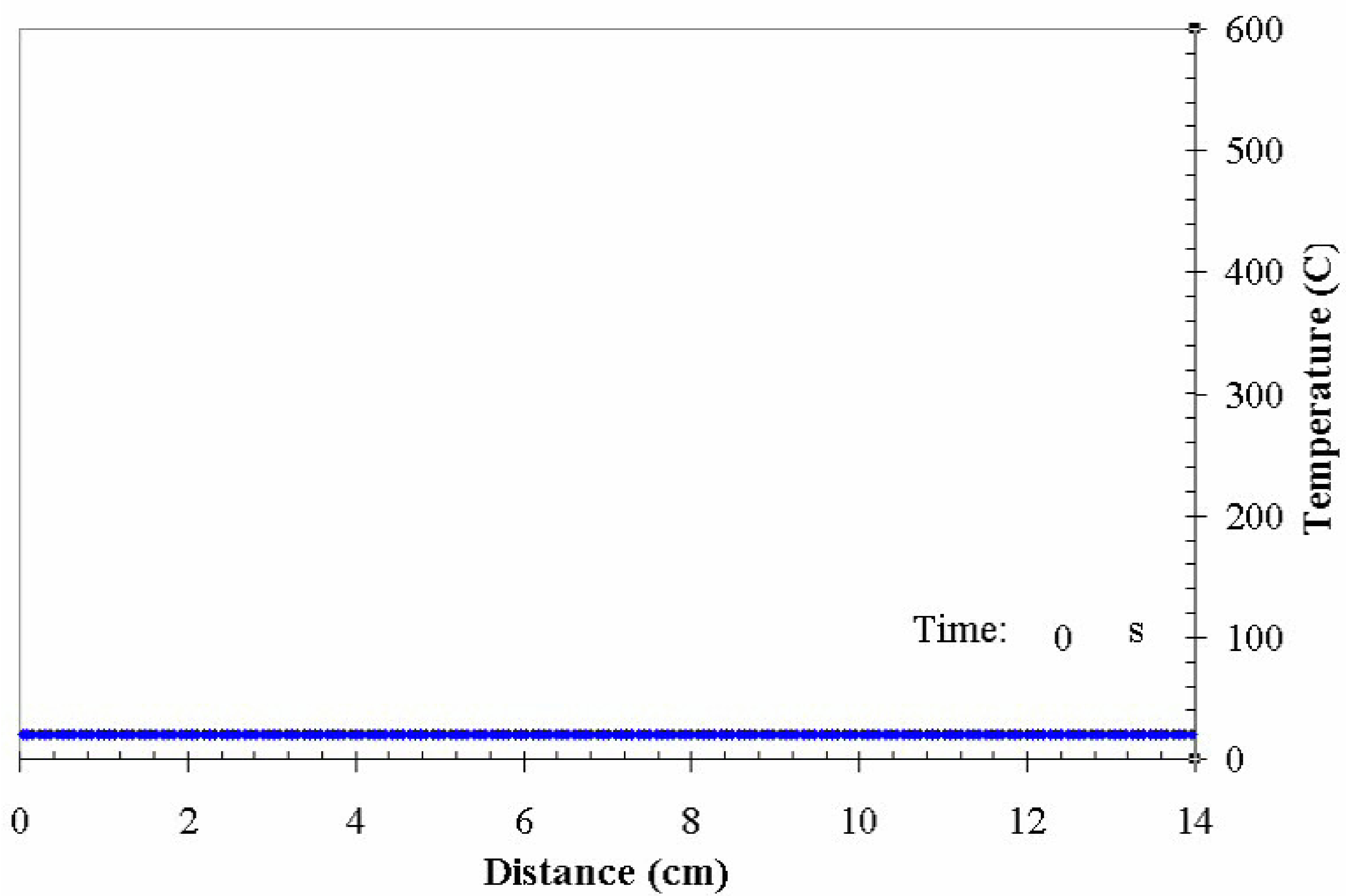


Smoldering of Polyurethane Foam

- Experiment - Bar-Ilan *et al.*, *ETFS* v28 (2004)
  - Non fire-retarded PU foam cylinders (14 cm long)
  - Space shuttle (microgravity) experiments
  - Forward smolder in air
  - 3 mm/s and 5 mm/s forced airflow velocity

- Modeling approach
  - Follows earlier smolder-specific model from our lab (Rein)
  - 2 condensed-phase species, 4 gaseous species
  - 2 condensed-phase reactions

Propagation of Smolder Wave in PU Foam



Concluding Remarks

- Pyrolysis model simulates well multiple materials
- Material property estimation via genetic algorithm optimization seems to "work" even for search spaces with 20+ adjustable parameters

- Future work
  - Additional materials (composites, charring polymers)
  - Extension to 2D (anisotropy, transition to flaming)
  - Predicting real world flame spread and fire growth via coupling to CFD code