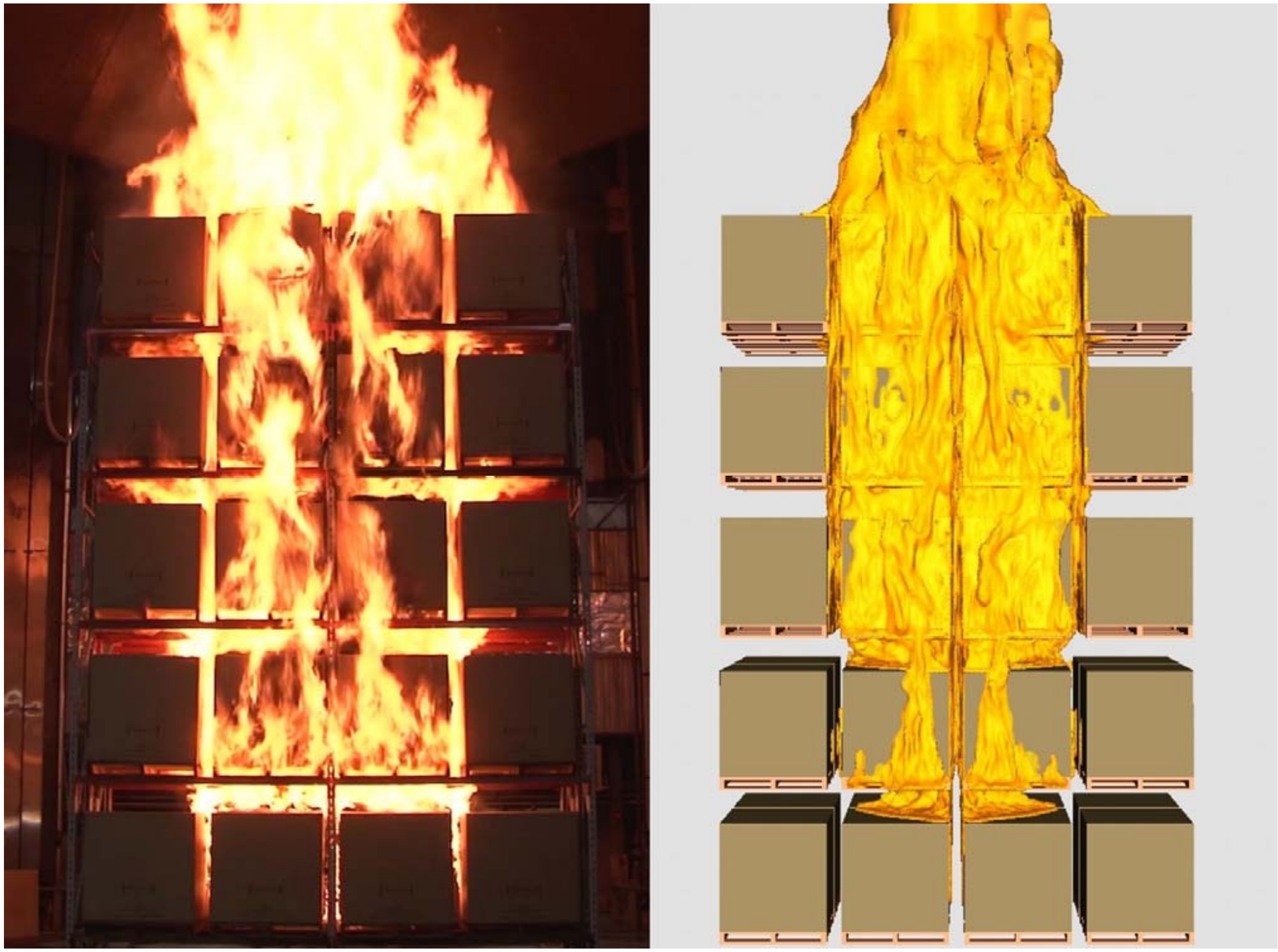
# From Pyrolysis to Industrial Fire Protection -- Coupling with CFD

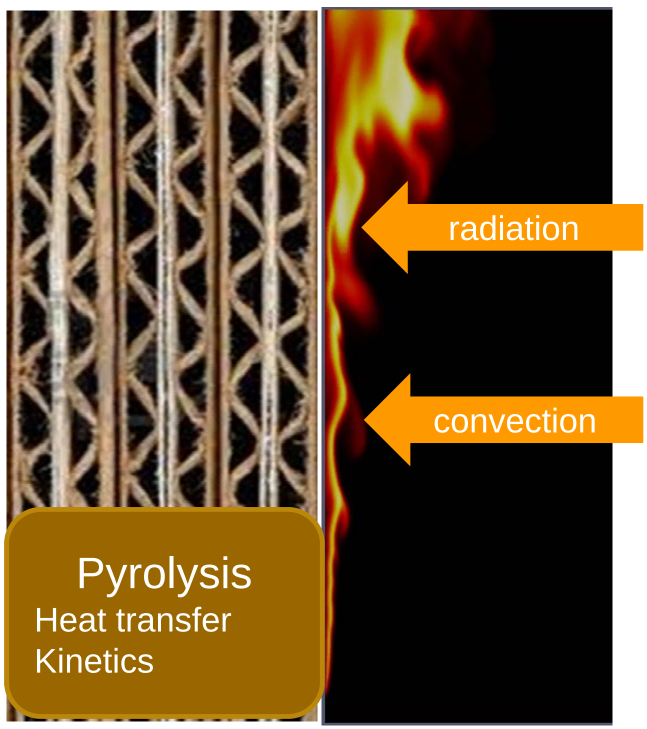
Yi Wang, FM Global

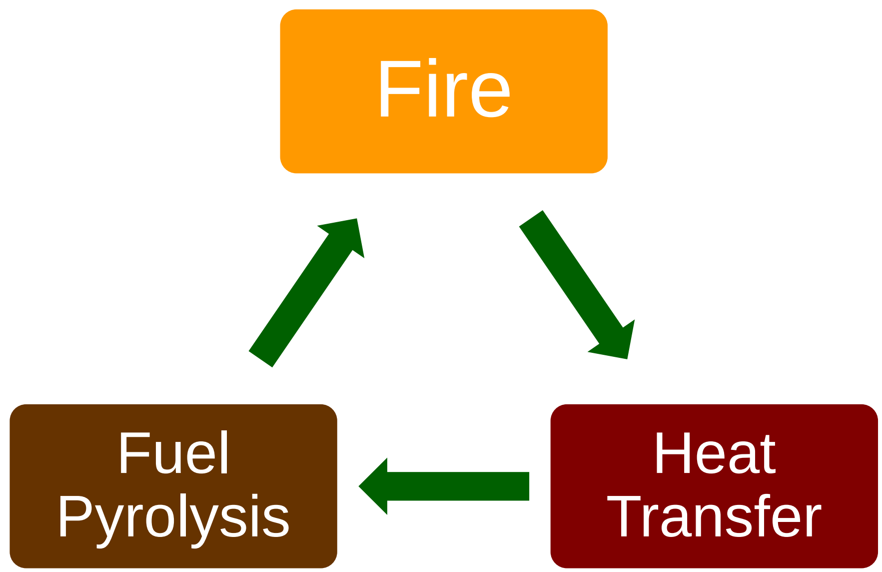
Measurement and Computation of Fire Phenomena – MaCFP
Lund University, 06/10/2017

# Objective – Predicting Fire



# Flame Spread – Coupling



# Pyrolysis Model – Fuel Specific

# Outline

- Methodology used at FM Global
- Validation
- Scale up
- Complex fuels
  - Cartoned unexpanded plastic commodity
  - Roll papers

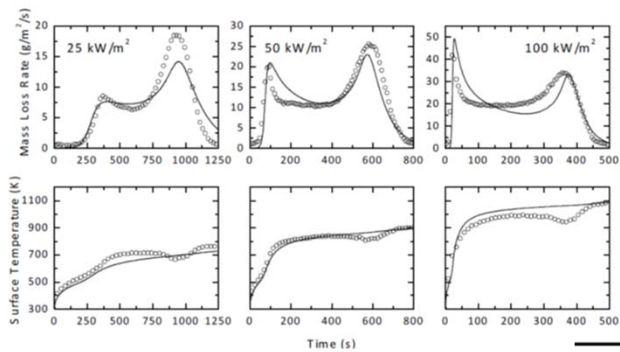
# Modeling Methodology

# Inverse Modeling/Optimization

Constant heat flux FPA Pyrolysis Experiments

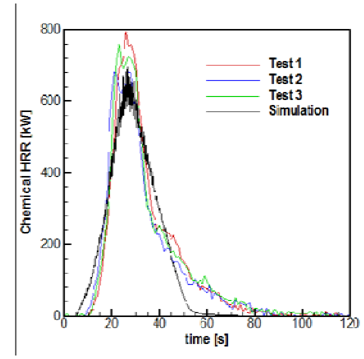
Inverse Modeling & Optimization using SCE

1D Pyrolysis model with single step Arrhenius reaction.

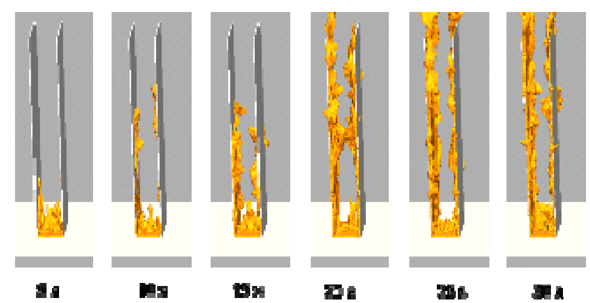



Model effective Material Properties

| Property | Value |
|---|---|
| Thermal Conductivity (W/m²/K) | 0.26 |
| Density (kg/m³) | 660[a] |
| Heat Capacity (J/kg/K) | 2533 |
| Emissivity/Absorptivity | Varies[b] |
| Thermal Conductivity (W/m²/K) | 0.36 |
| Density (kg/m³) | 100 |
| Heat Capacity (J/kg/K) | 1450[c] |
| Emissivity/Absorptivity | 0.85[d] |
| Pre-exponential Factor ($s^{-1}$) | $5.13\times10^{14}$ |
| Activation Energy (J/mol) | $1.63\times10^{5}$ |
| Heat of Pyrolysis (J/kg) | -6.8 |
| Reaction Order | 6.02 |

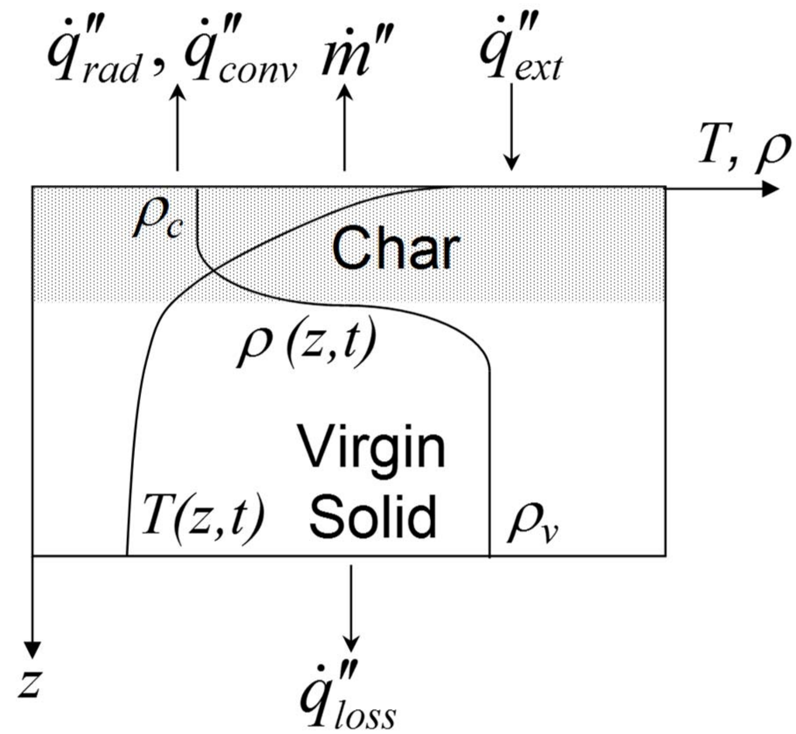



FireFOAM applications



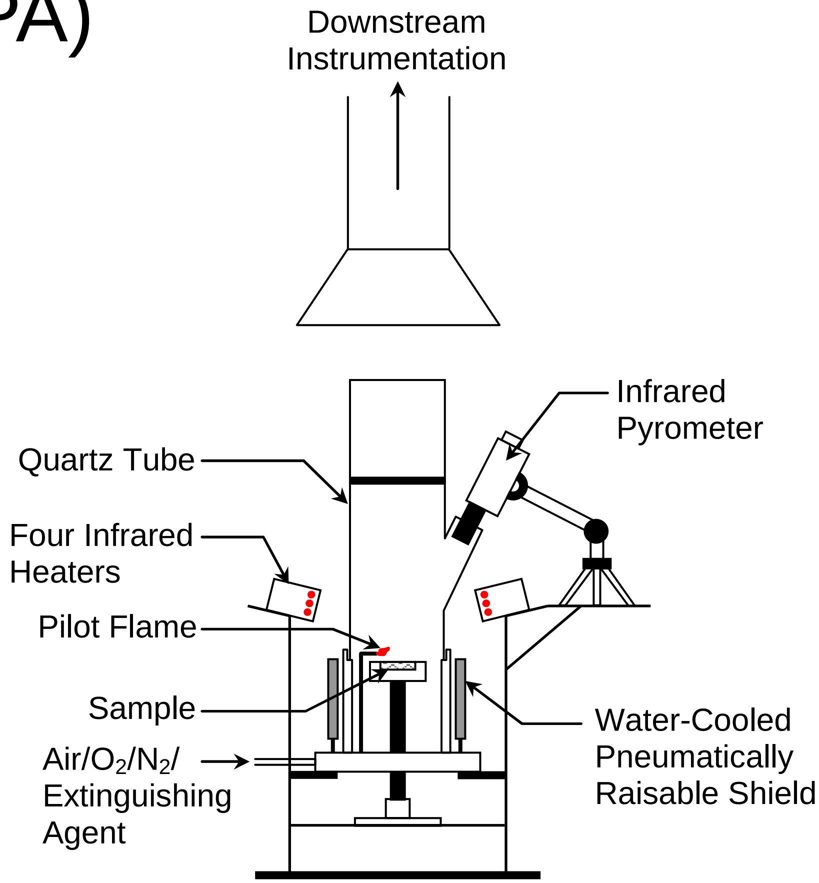
# Pyrolysis Model

- 1-D, CV approach
- T-independent properties
- Virgin, char, and gas species
- Arrhenius decomposition reaction
- Thermal equilibrium
- No pressure build-up



# Bench-Scale Experiment

- Fire Propagation Apparatus (FPA)
  - Anaerobic tests (100% $N_2$)
  - 25, 50, 100 $kW/m^2$
  - Relative humidity (50%RH)
  - Surface temperature pyrometry
  - Targets: ML, MLR, $T_s$



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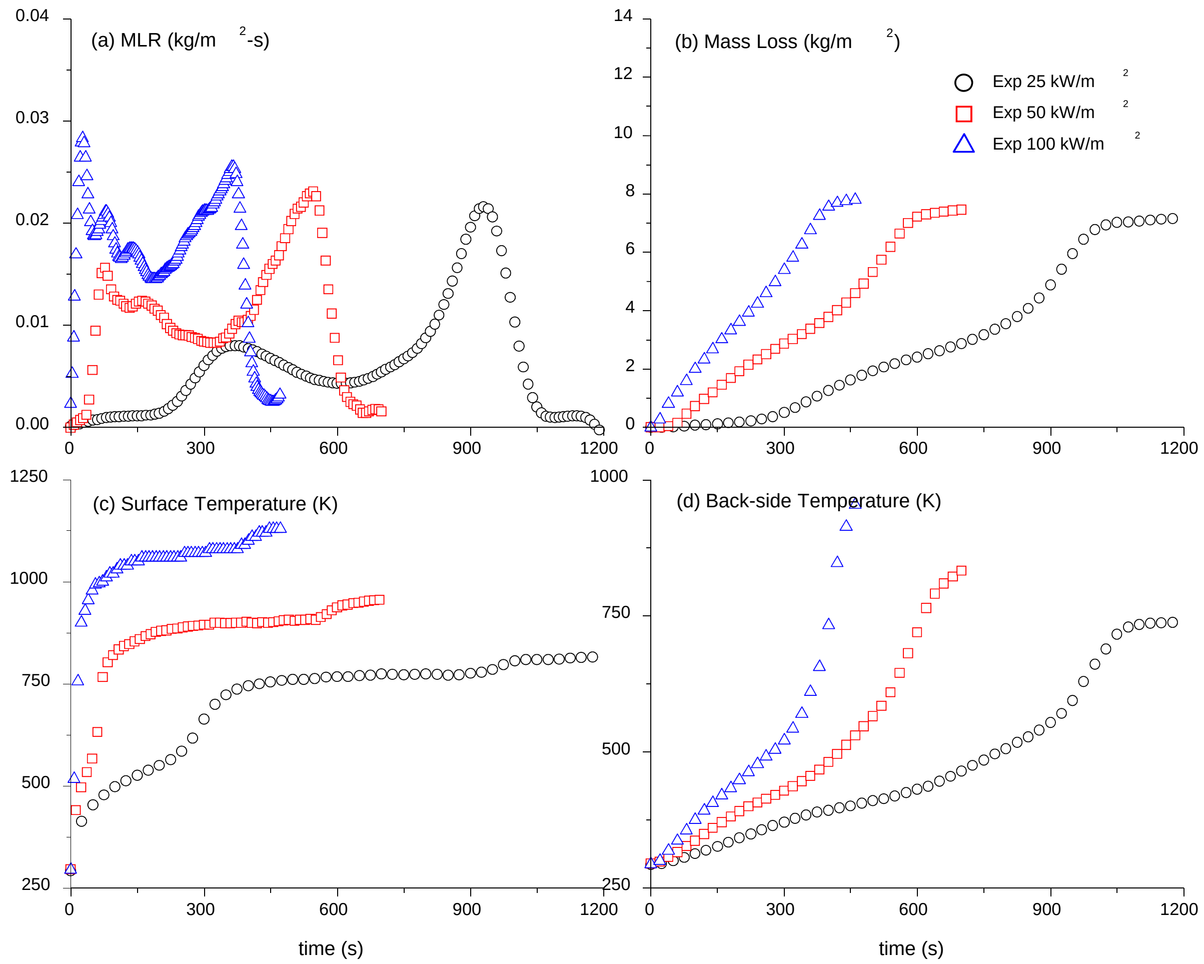
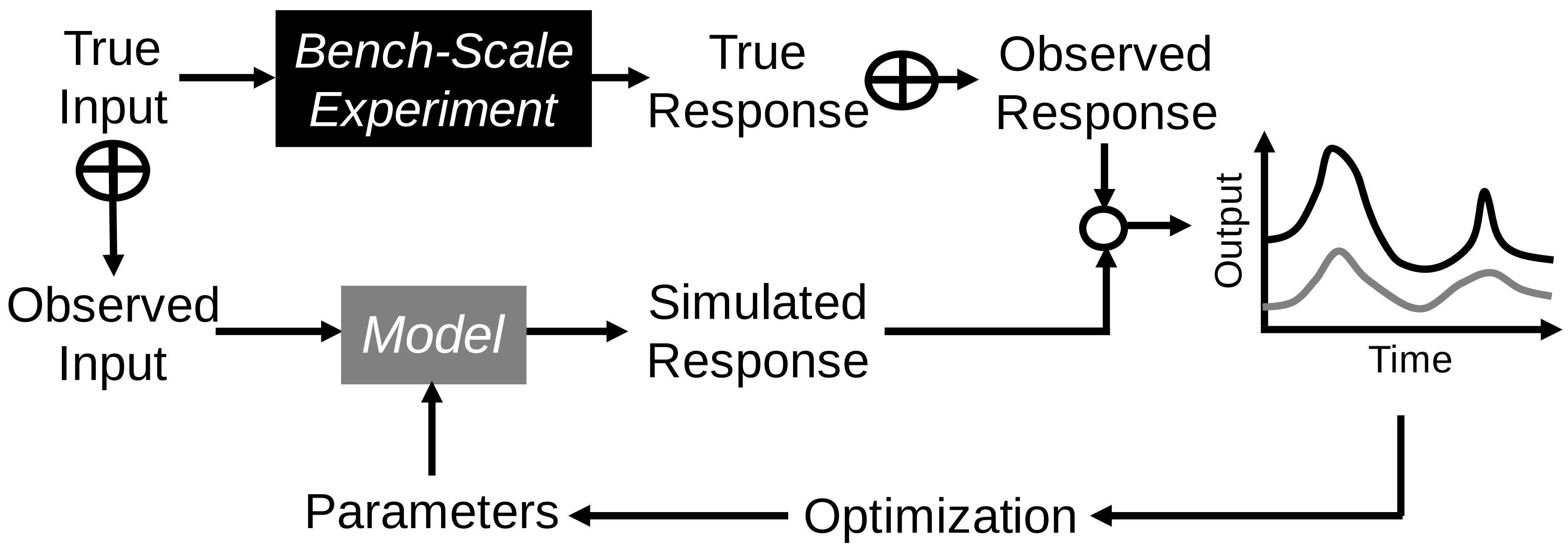
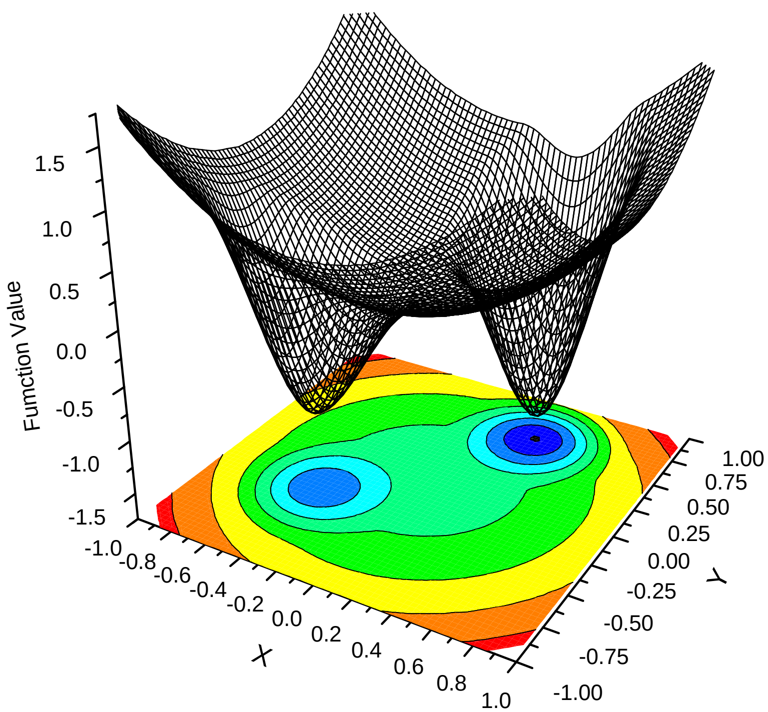
# Experimental Results

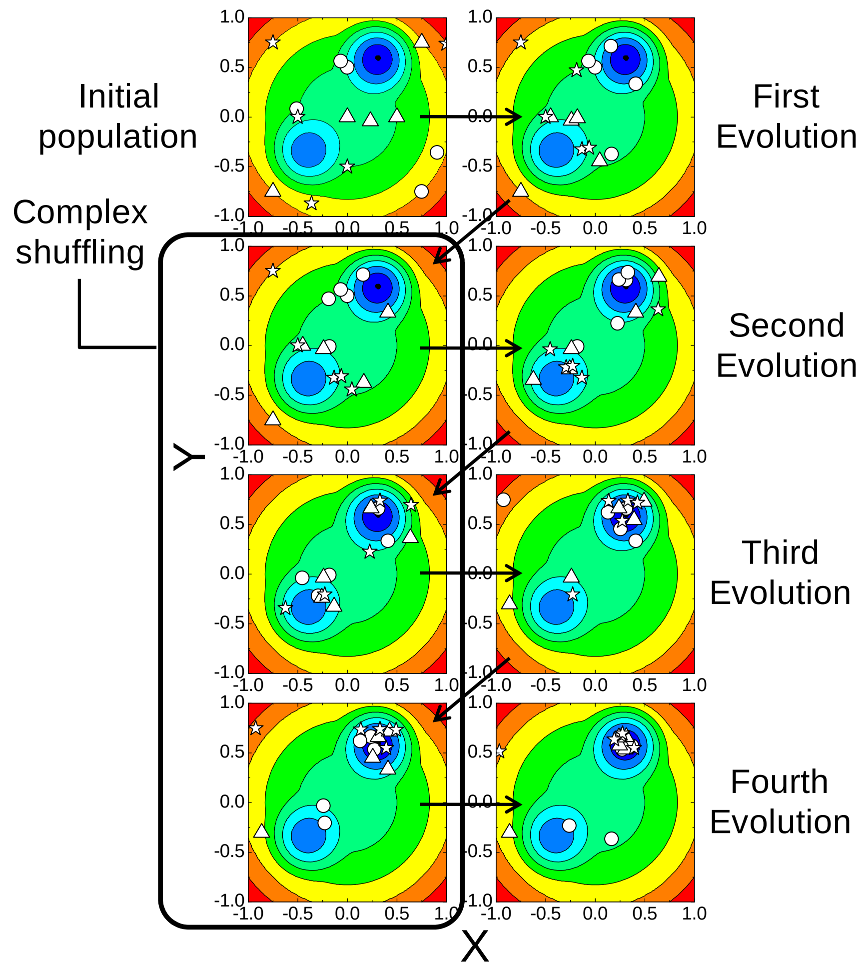


# Optimization: Material Properties

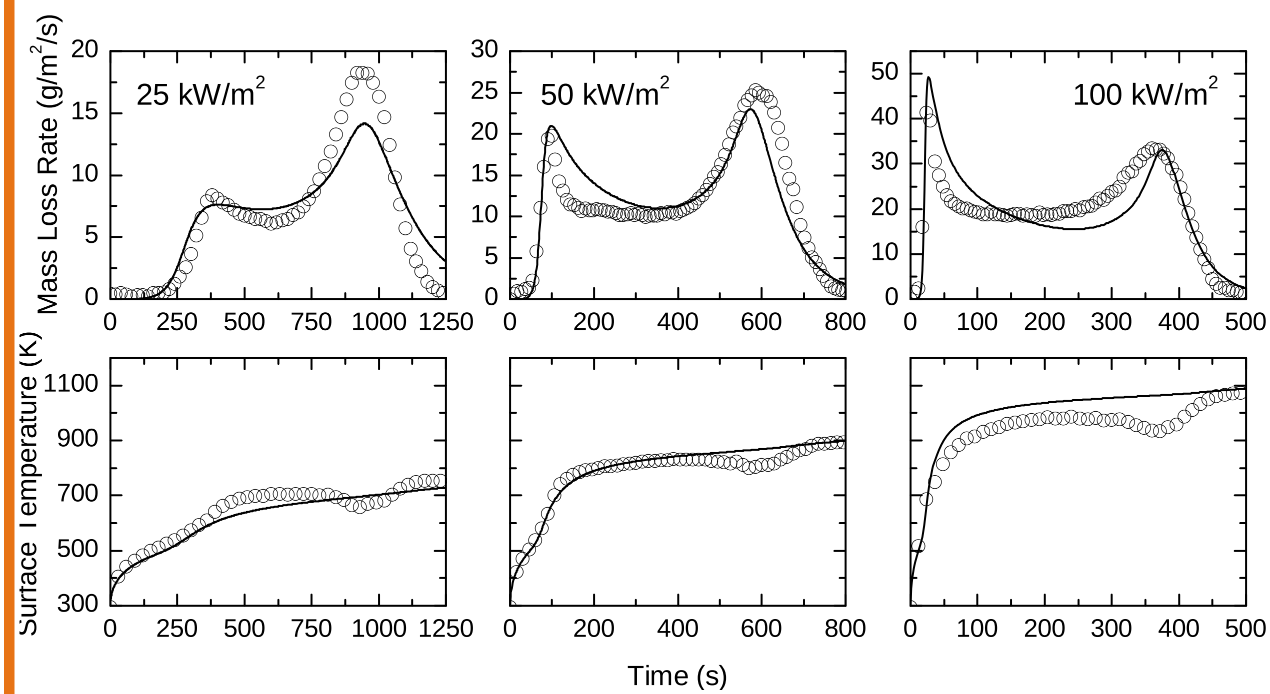


# Shuffled Complex Evolution (SCE)



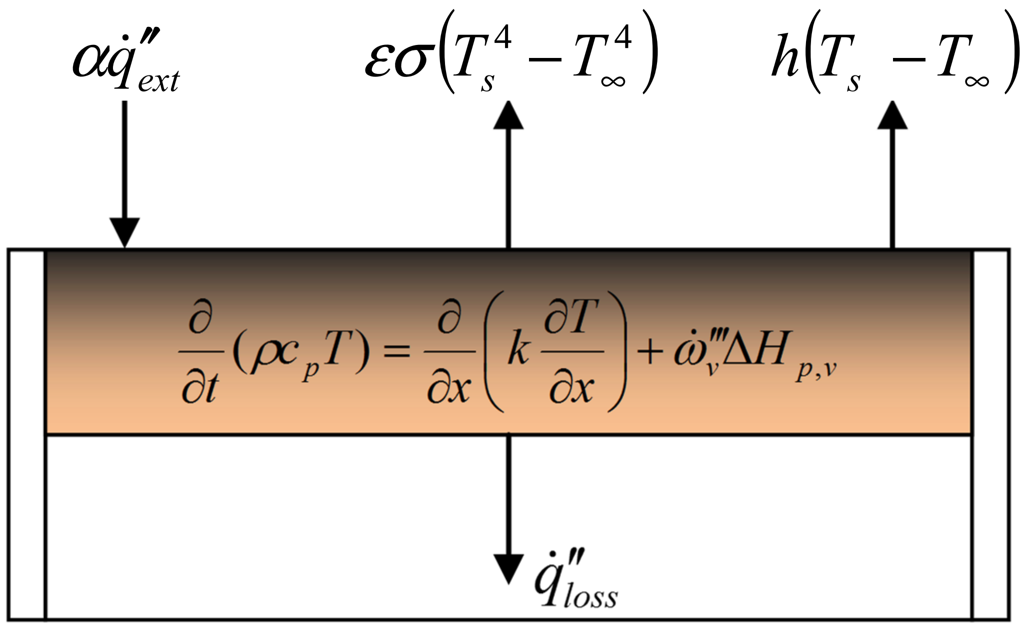



# Results – Model Specific Properties

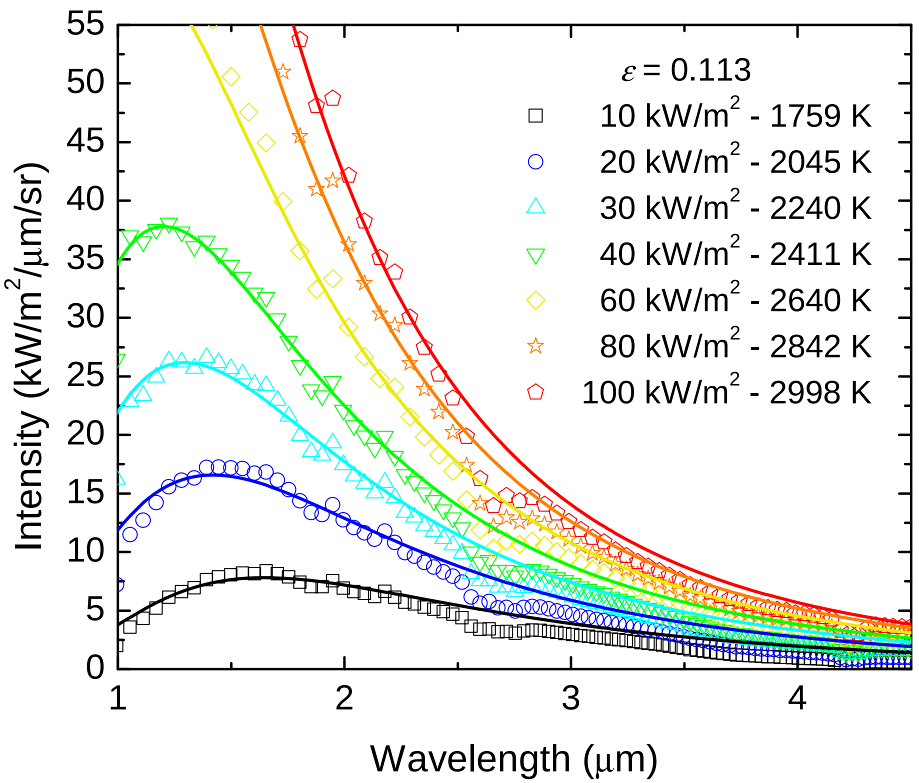



| | Property | Value |
|---|---|---|
| *Virgin* | Thermal Conductivity (W/m²/K) | 0.26 |
| | Density (kg/m³) | ***660*** |
| | Heat Capacity (J/kg/K) | 2533 |
| | Emissivity/Absorptivity | Varies |
| *Char* | Thermal Conductivity (W/m²/K) | 0.36 |
| | Density (kg/m³) | 100 |
| | Heat Capacity (J/kg/K) | ***1450*** |
| | Emissivity/Absorptivity | ***0.85*** |
| *Reaction* | Pre-exponential Factor ($s^{-1}$) | $5.1 \times 10^{14}$ |
| | Activation Energy (J/mol) | $1.63 \times 10^{5}$ |
| | Heat of Pyrolysis (J/kg) | -6.8 |
| | Reaction Order | 6.02 |

# Importance of Boundary Condition



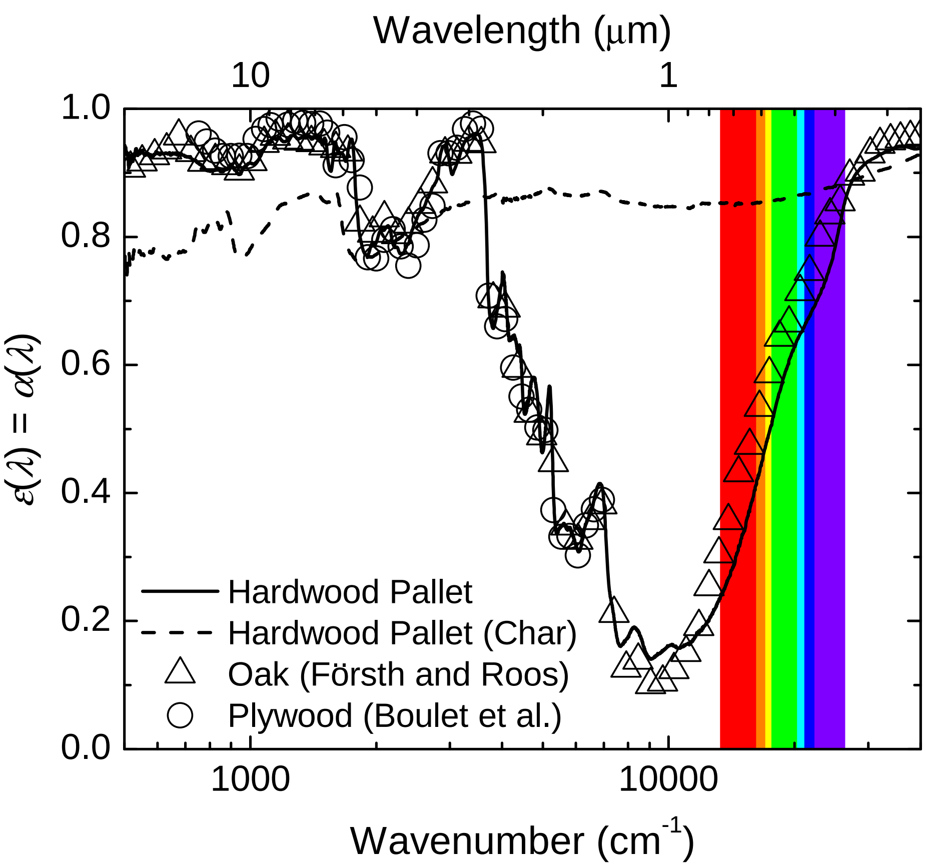
# Spectral Distribution of Heating Source




$$\varepsilon_l I(\lambda, T) = \varepsilon_l \frac{h_p c^2}{\lambda^5}\left[\exp\left(\frac{h_p c}{\lambda k_B T}\right) - 1\right]^{-1}$$

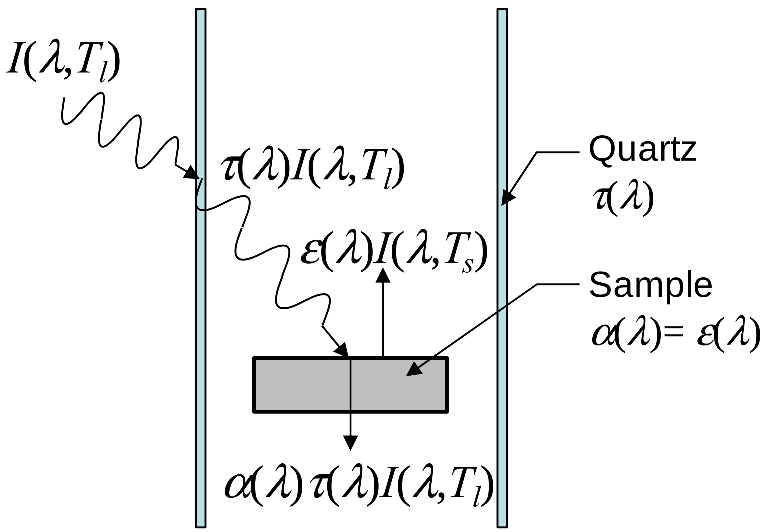
- Gray body behavior
- Emissivity within reported ranges (Touloukian & DeWitt)

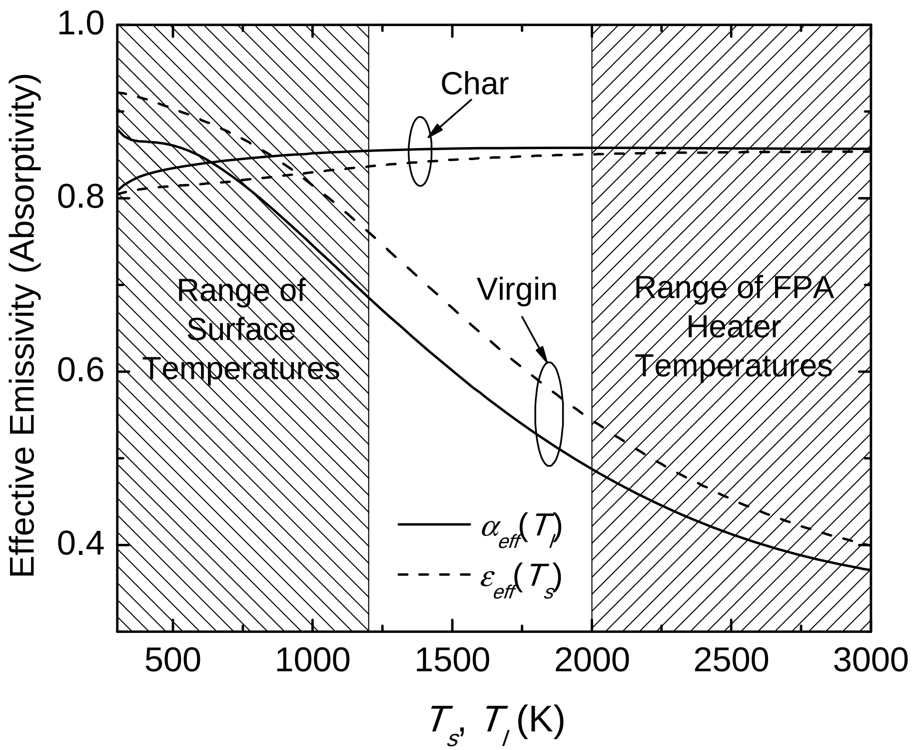
# Sample Surface Absorptivity/Emissivity




- Highly non-gray behavior
- Same features in NIR and MIR for several cellulosic materials

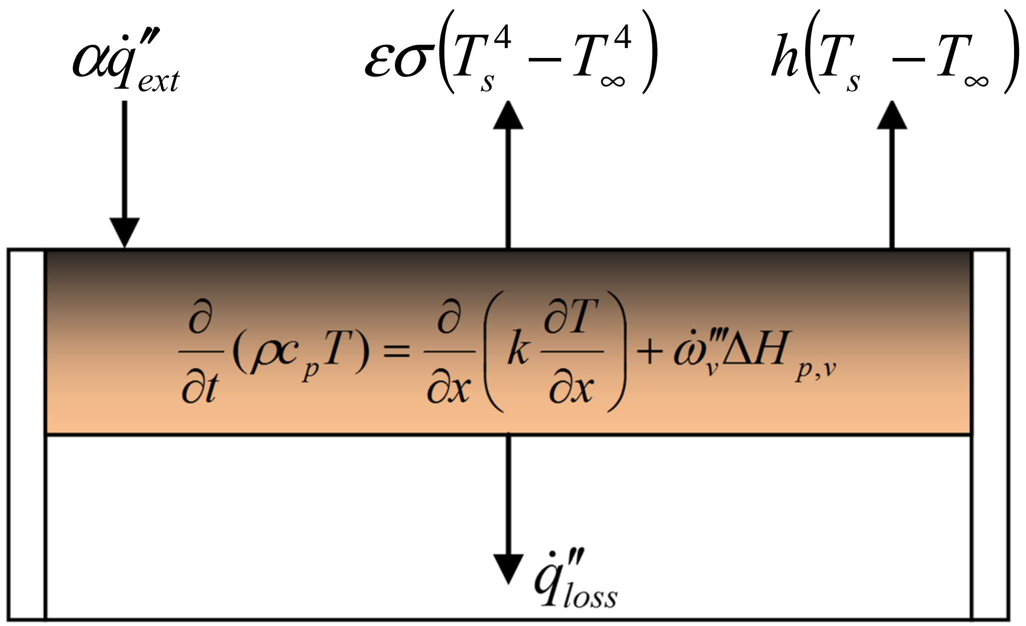
# Effective Emissivity/Absorptivity



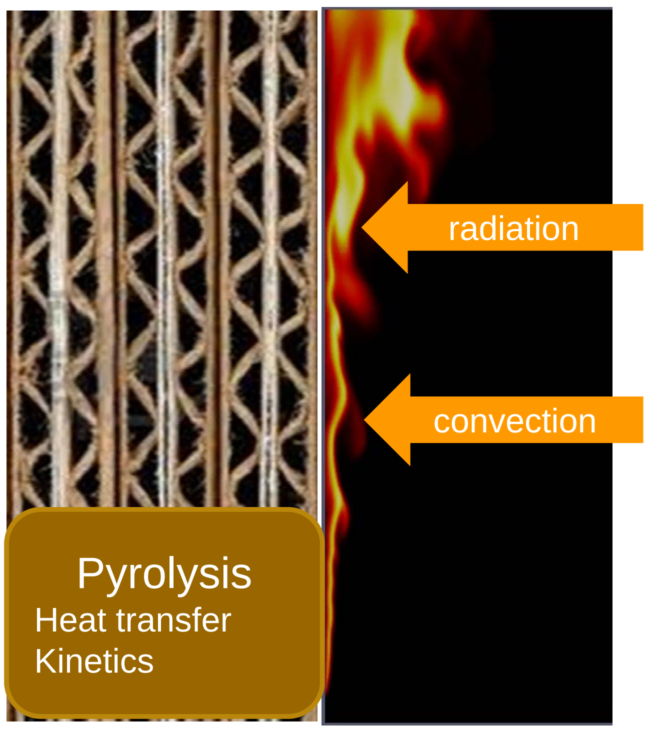

$$\alpha_{eff}(T_l) = \frac{\int \alpha(\lambda)\tau(\lambda)I(\lambda,T_l)d\lambda}{\int \tau(\lambda)I(\lambda,T_l)d\lambda} \quad \varepsilon_{eff}(T_s) = \frac{\int \varepsilon(\lambda)I(\lambda,T_s)d\lambda}{\int I(\lambda,T_s)d\lambda}$$

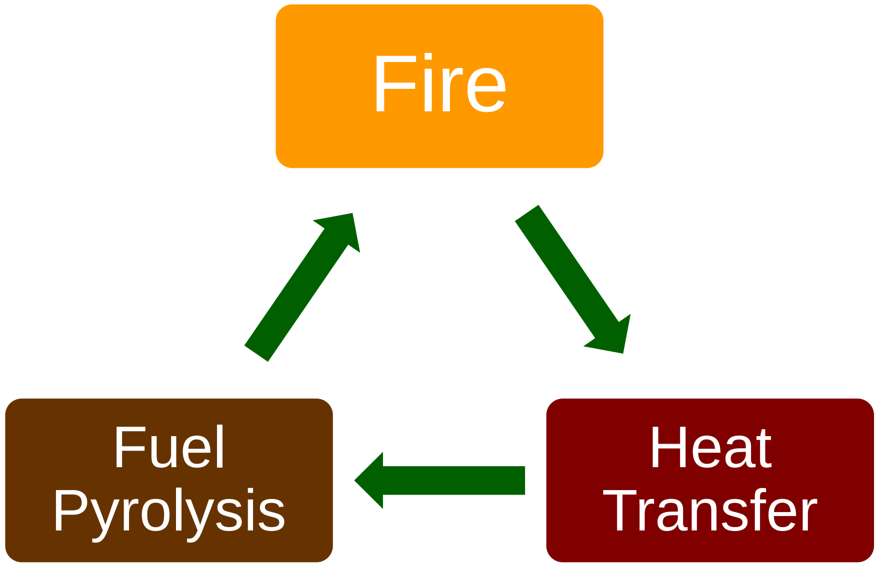
# Importance of Boundary Condition



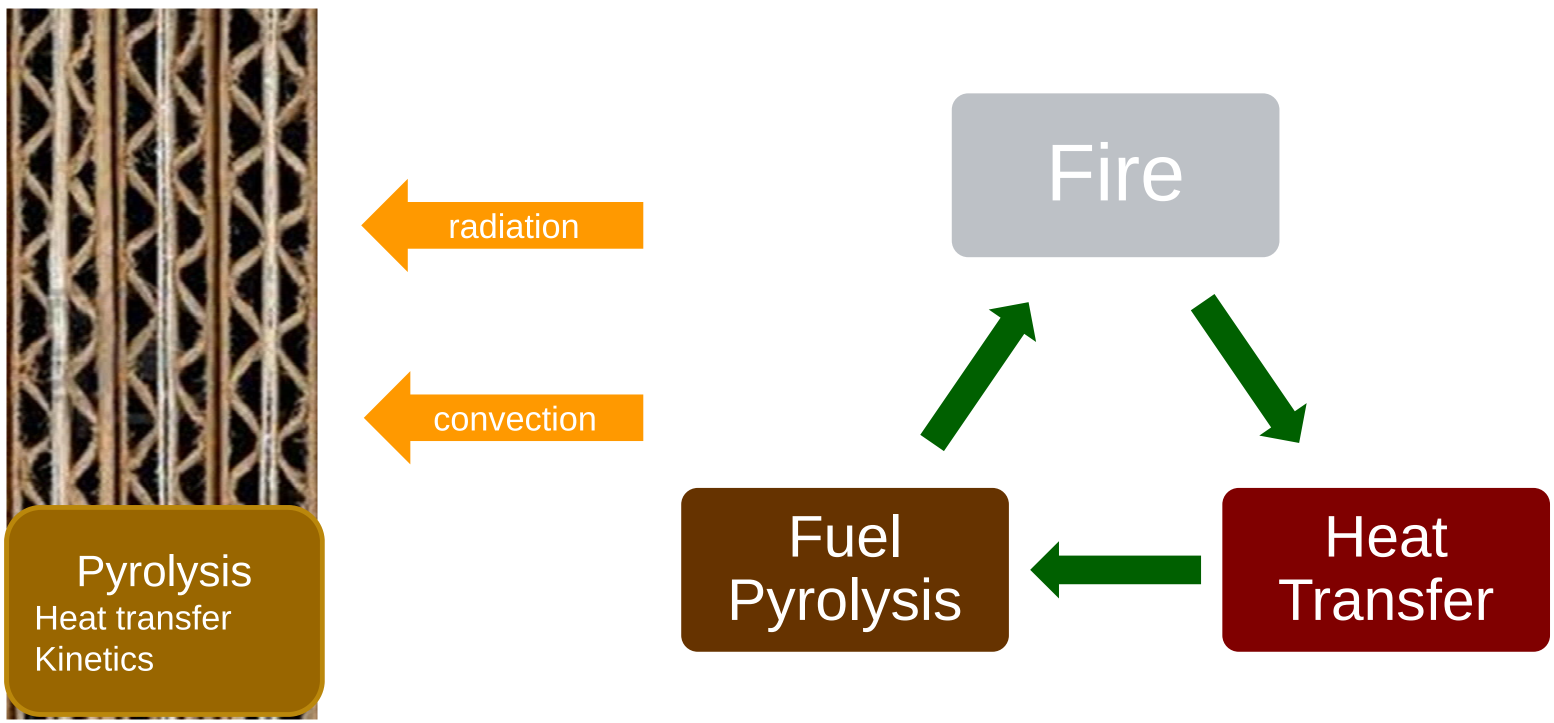
# Model Validations

# Flame Spread – Coupled Problem



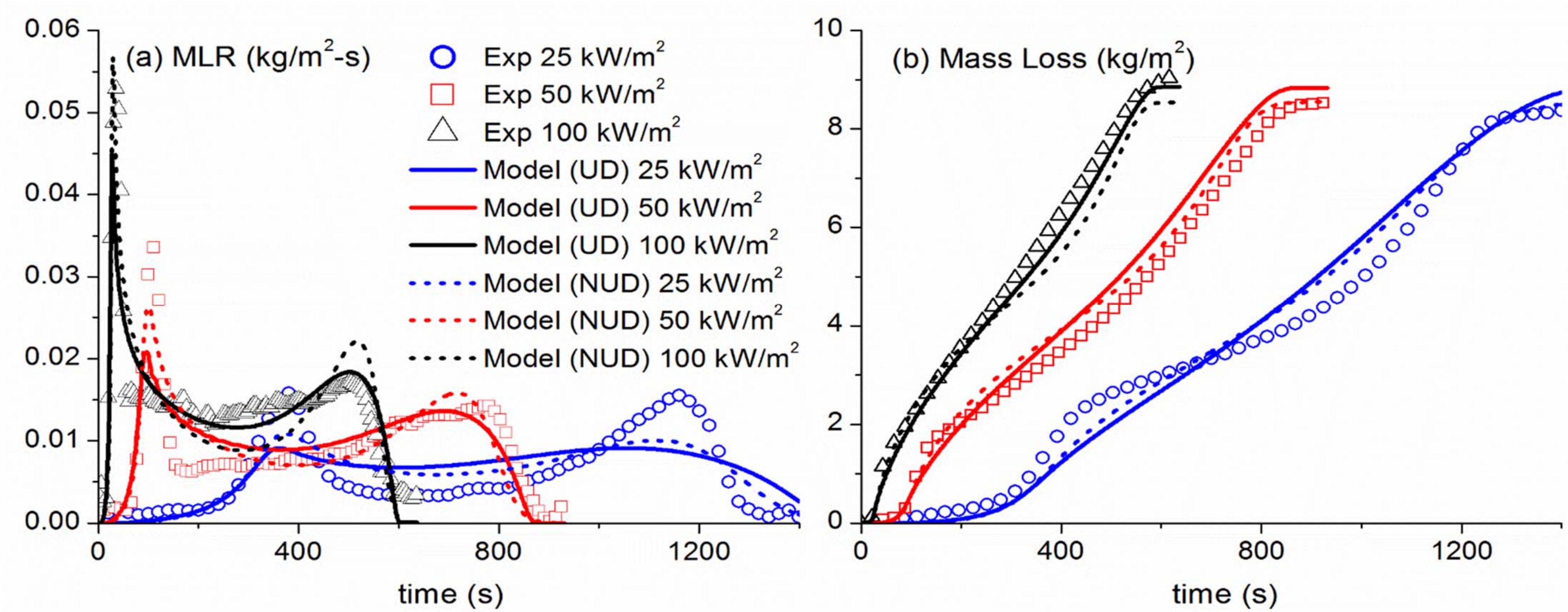



# Separate Effect Validation



# Separate Effect Validation

- MDF, optimization result



# Validation Experiments

- Relevant to real fire
- Different from cases used in optimization
  - Case 1:
    - Samples coated with high absorptivity coating and constant heat flux
  - Case 2:
    - Uncoated samples. Step changes in heat flux during pyrolysis
  - Case 3:
    - Uncoated samples. Linear (dynamic) change in heat flux during material pyrolysis

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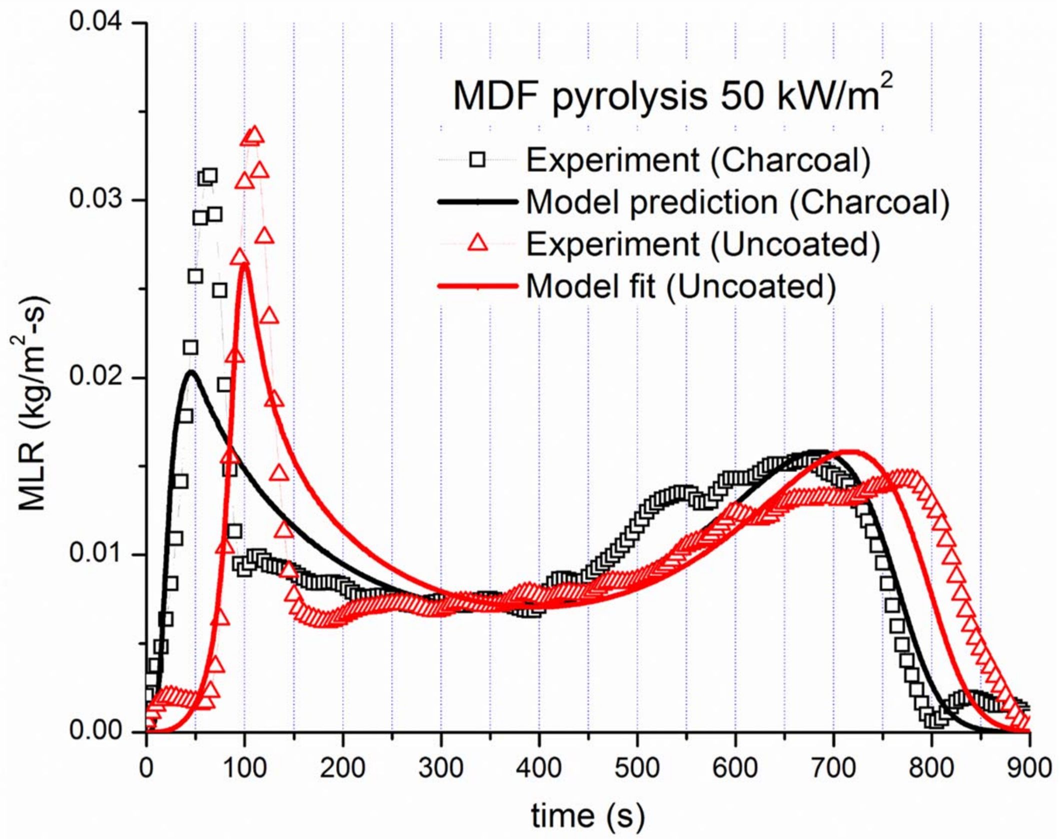
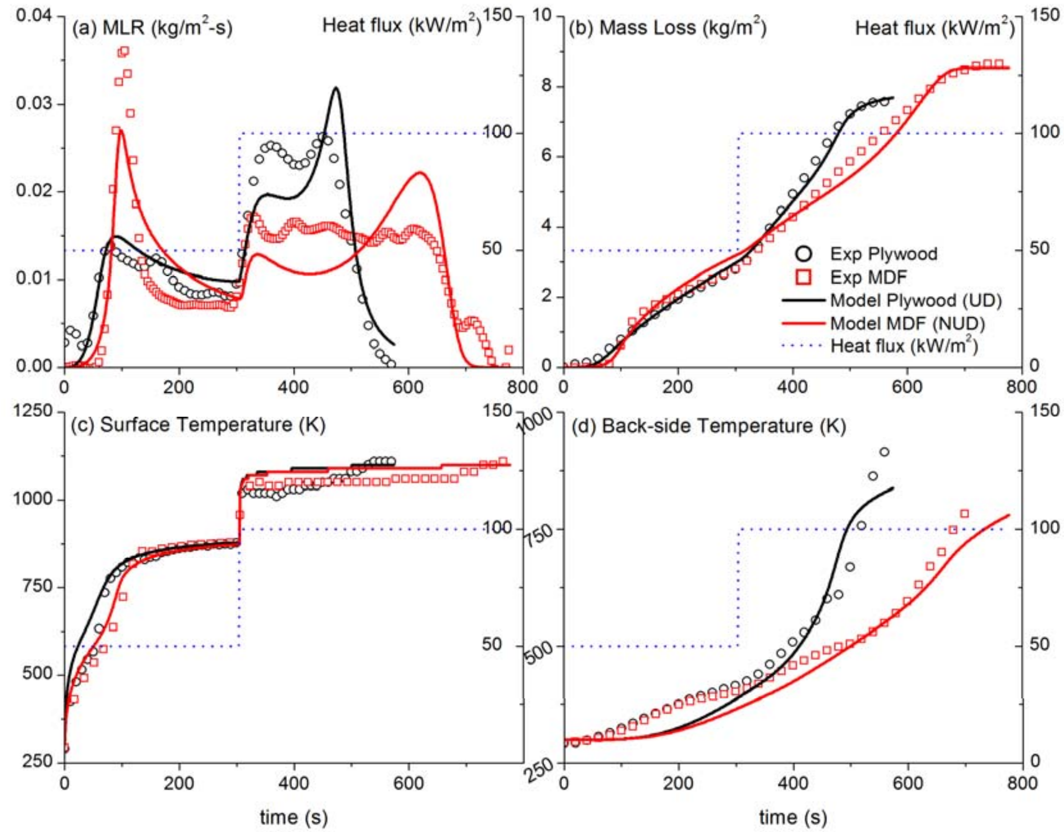
# Validation Test Case - 1

- Surface coated with Activated charcoal. $\alpha_{eff} = \varepsilon_{eff} = 0.93$
- 50 kW/m$^2$ constant heat flux
- Charcoal increases the net heat flux absorbed by surface
- Model properties relevant for heat fluxes beyond those tested and independent of BCs



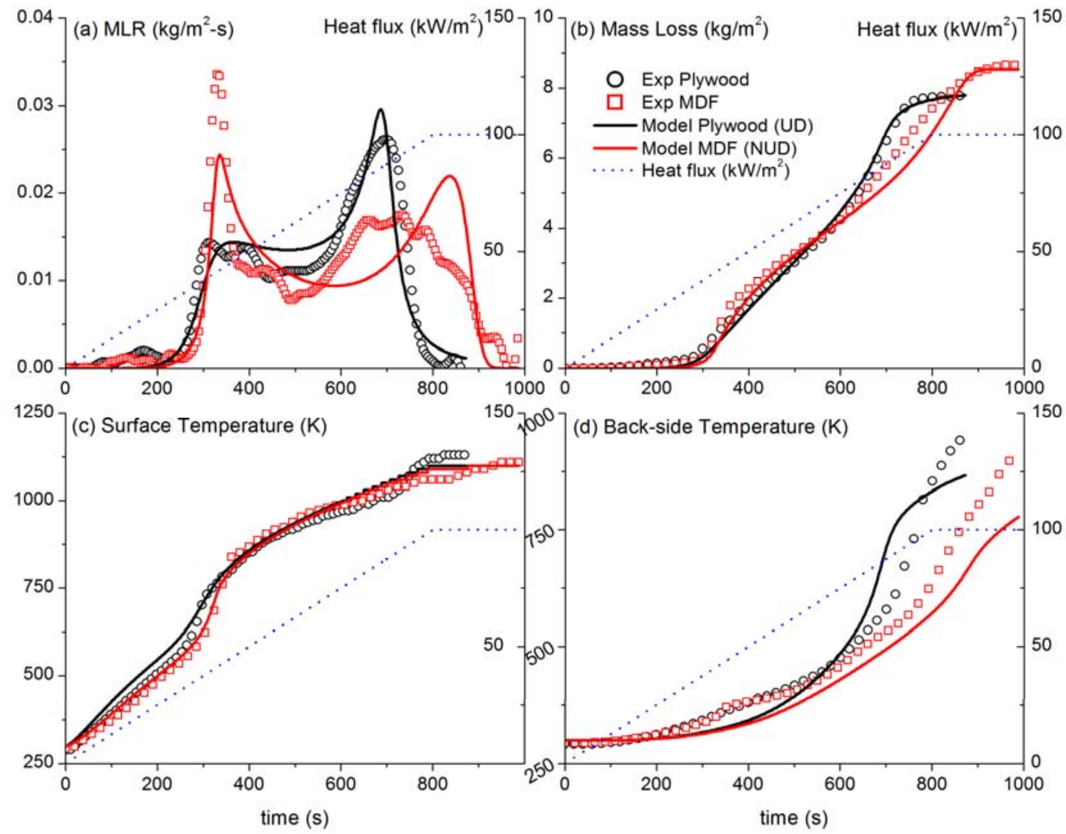
# Validation Test Case - 2

- Uncoated sample
- 50 to 100 kW/m² heat flux step
- Step change, subsequent pyrolysis process and termination is well predicted



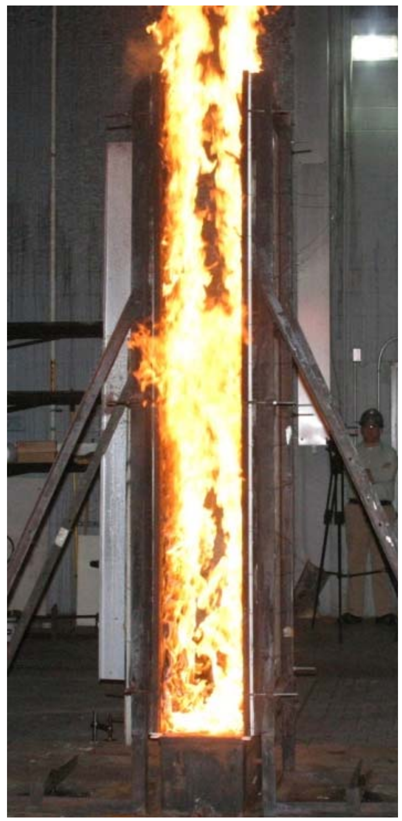
# Validation Test Case - 3

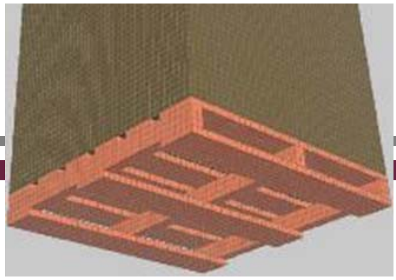
- Uncoated sample
- 0-100 kW/m$^2$ linearly varying
- More stringent validation with thermally thick and thin heating scenarios
- Onset well predicted
  - Simulation of an ignition event



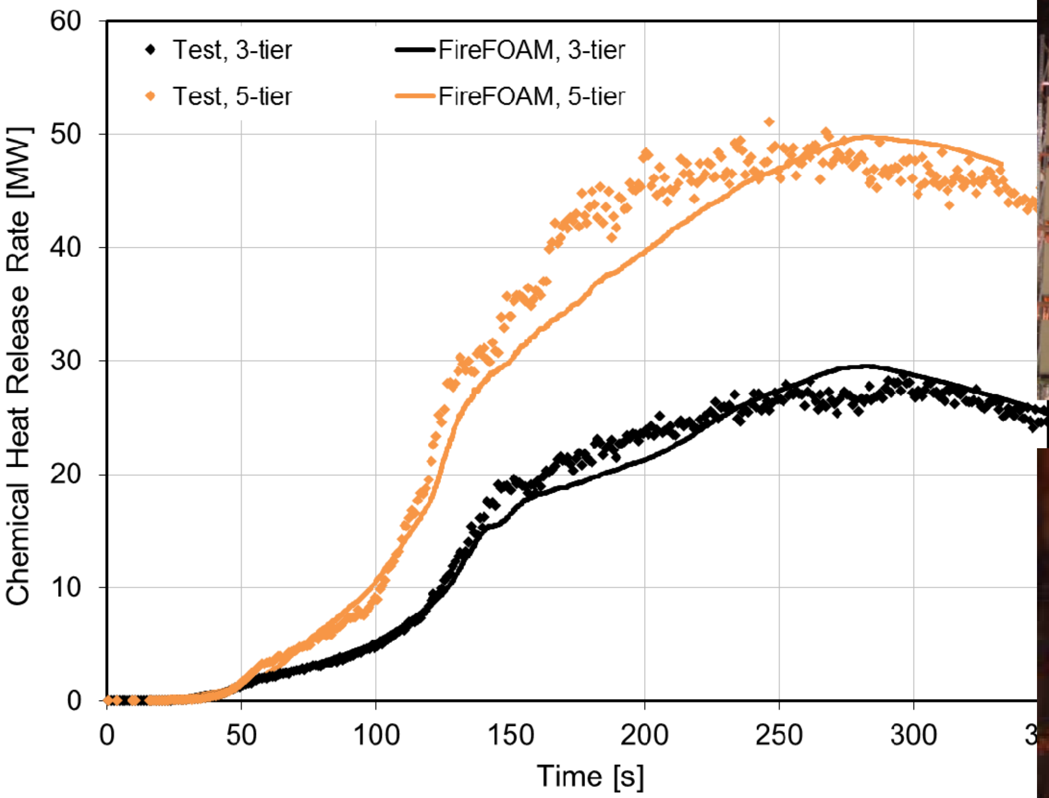
# Coupling – Scale Up

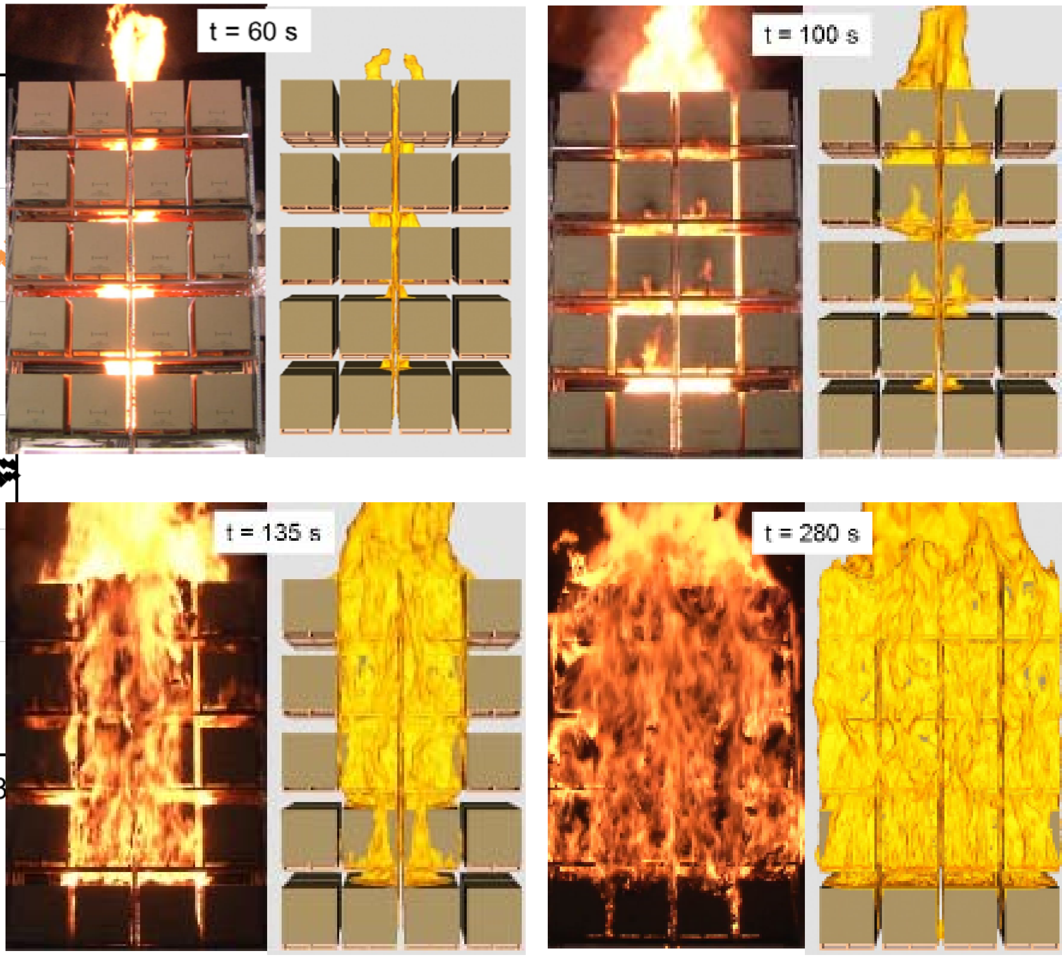
# Scale Up



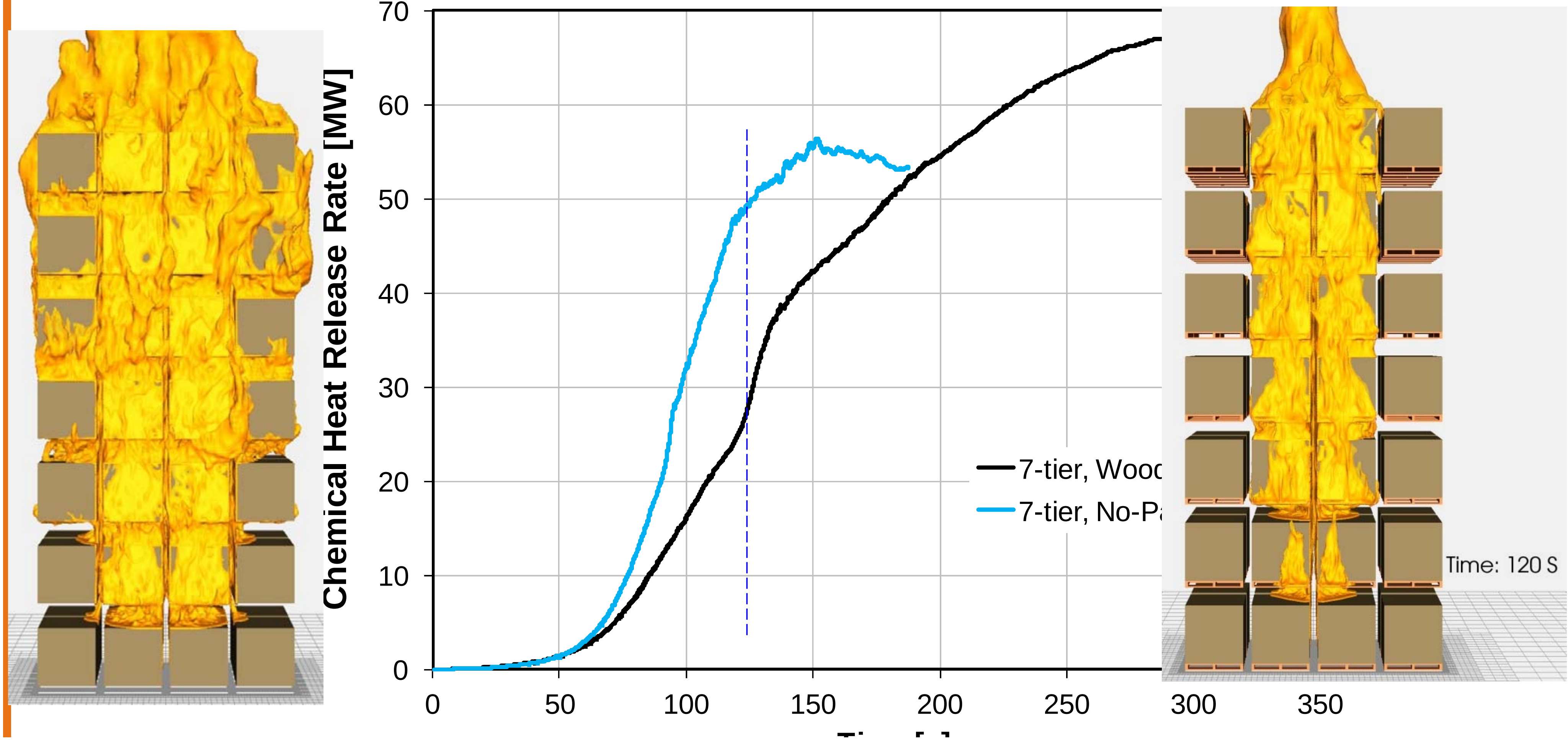


# Rack Storage



# Scale Up


Chemical Heat Release Rate [MW]
70
60
50
40
30
20
10
0
0
50
100
150
200
250
300
350
7-tier, Wood
7-tier, No-P
Time: 120 S

# Other Fuels

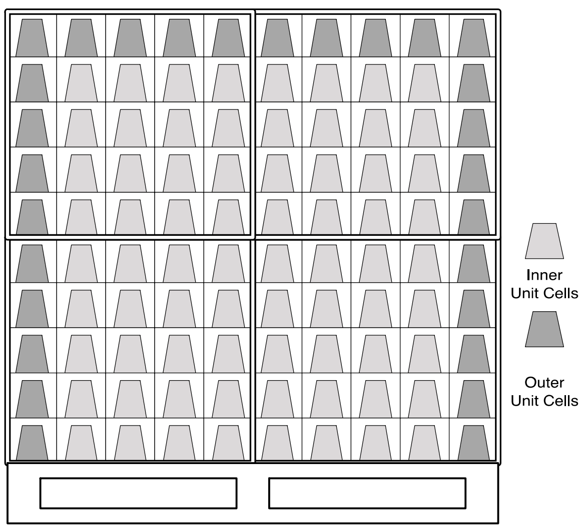
# Cartoned Unexpanded Plastic (CUP)

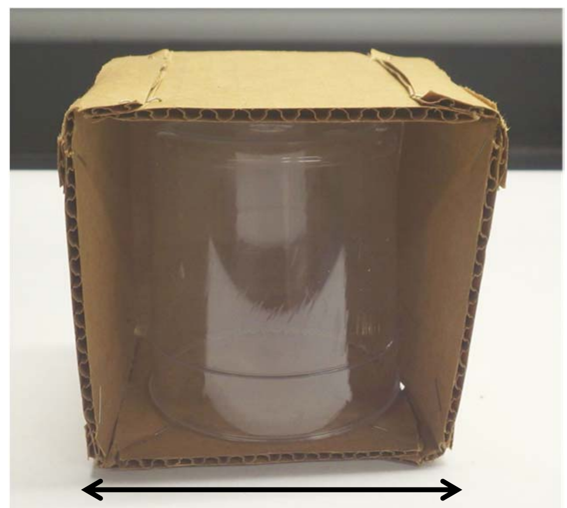
Pallet load – 8 cartons on a hardwood pallet


Carton – 125 characteristic cells

# Layered Approach

- CUP outer unit cell
  – Represents an outer cell of CUP commodity for which outer liner board has burnt through



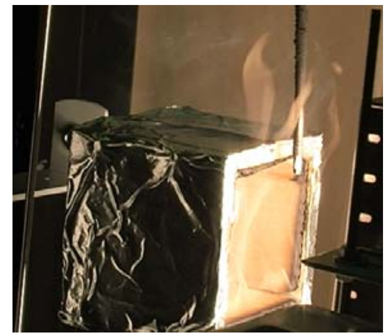



10.7 cm

# Experiment

Initiation ($t$ = 0)

Pyrolysis



Ignition

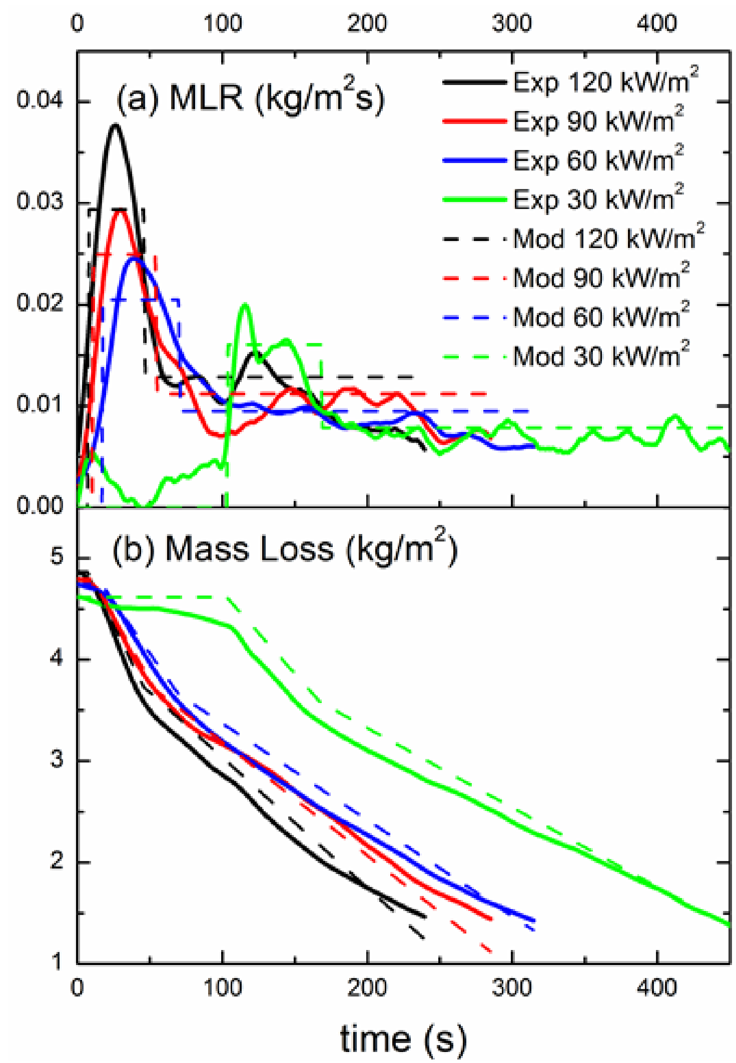
Cardboard burning

Co-combustion

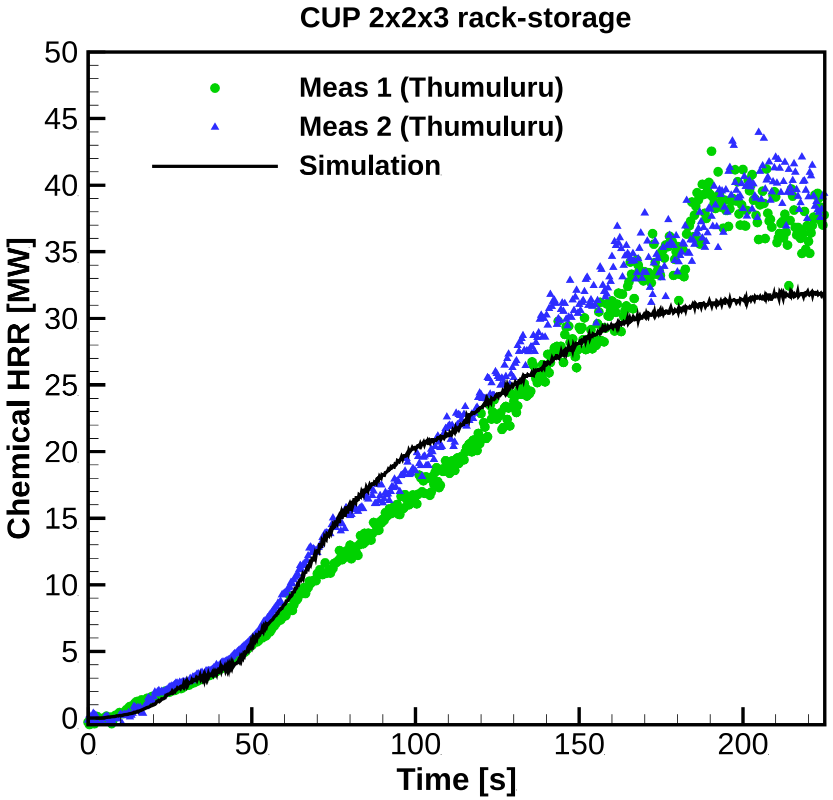
Post combustion

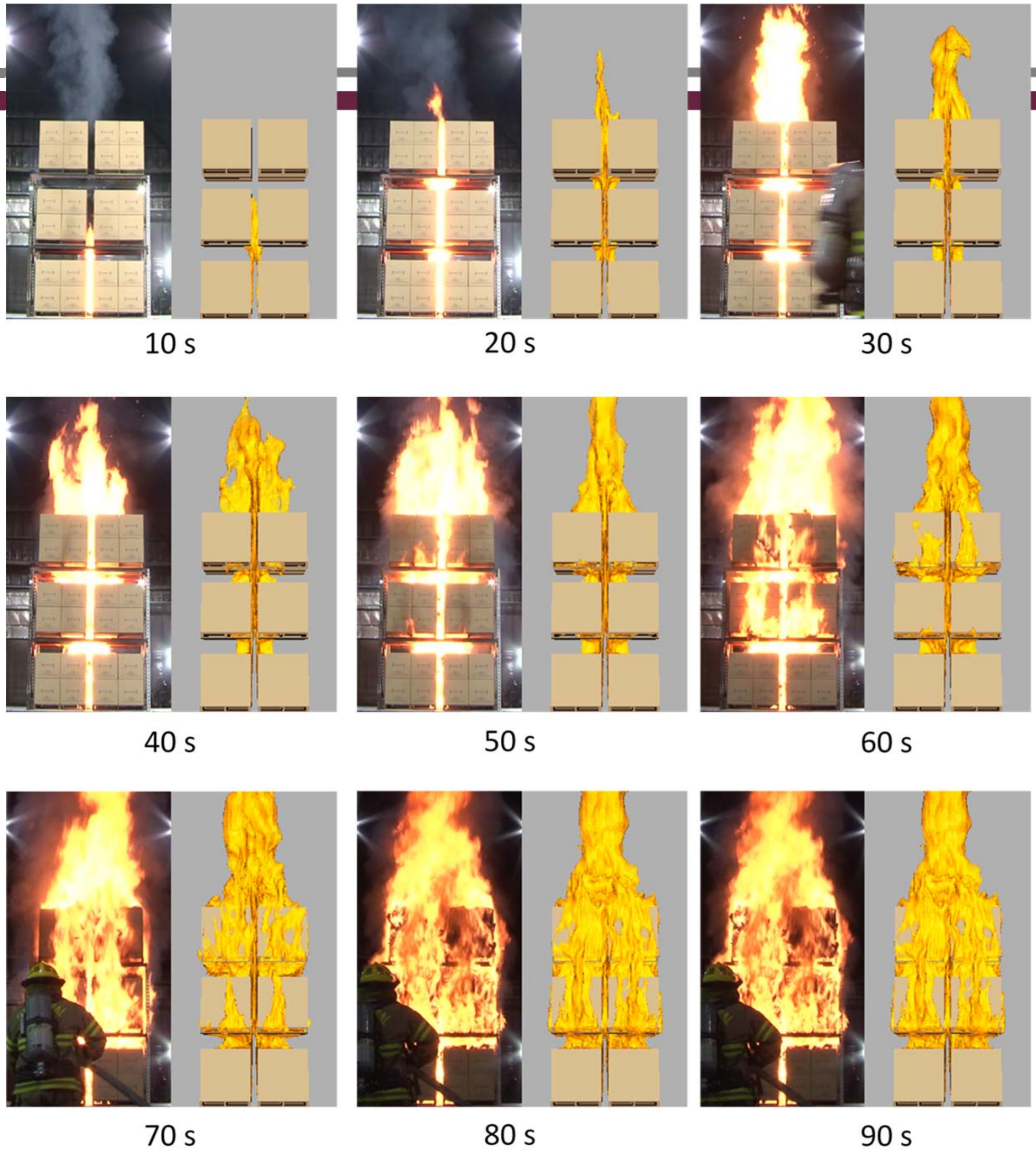
# Optimized Results

| Property | Optimized Values |
|---|---|
| $T_{ig}$ | 770 K |
| $C_p$ | 280 J/kg-K |
| $\alpha_l$ | 0.75 |
| $\varepsilon_l$ | 0.90 |
| $\chi_{cr}$ | 0.77 |
| $Q_{fl,1}$ | 20.1 kW/m² |
| $\alpha_{ll,1}$ | 0.26 |
| $\Delta H_{c,1}$ | 12.1 kJ/g |
| $Q_{fl,2}$ | 9.9 kW/m² |
| $\alpha_{ll,2}$ | 0.09 |
| $\Delta H_{c,2}$ | 19.7 kJ/g |



# Model Prediction



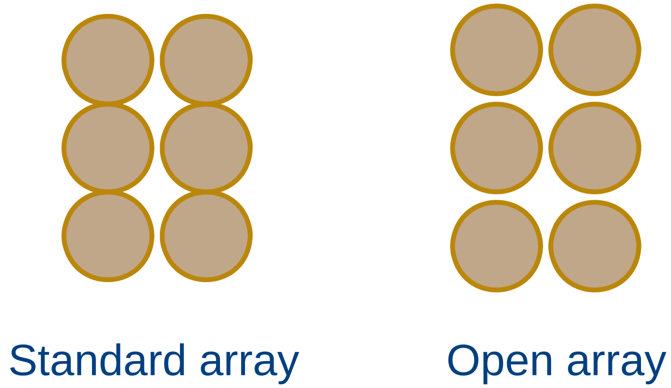



# Roll Paper

- Storage height increase
  – 15-20 meters or more
- Open array

# Fire Hazard – Test Experience

- >20MW, 1-5MW/s
  - Paper type: weight based
  - Storage Height
  - Storage configuration




# Roll-paper Pyrolysis: Thick & Thin

- Thermally thick to thin transition
  - 1D -- Delamination
  - 2D – Peeling
- Fast burning of single paper sheet
  - Transition back to thick material
  - No char layer buildup, and heat transfer blockage

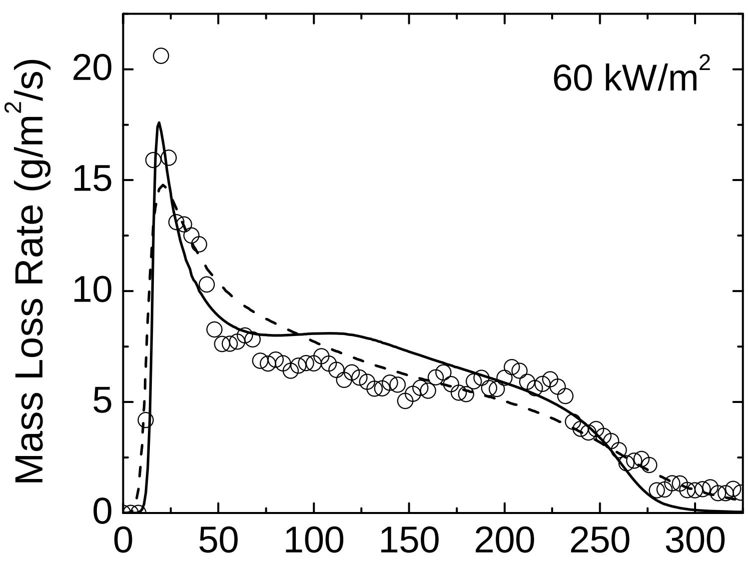
26lb paper, FPA, Bench scale

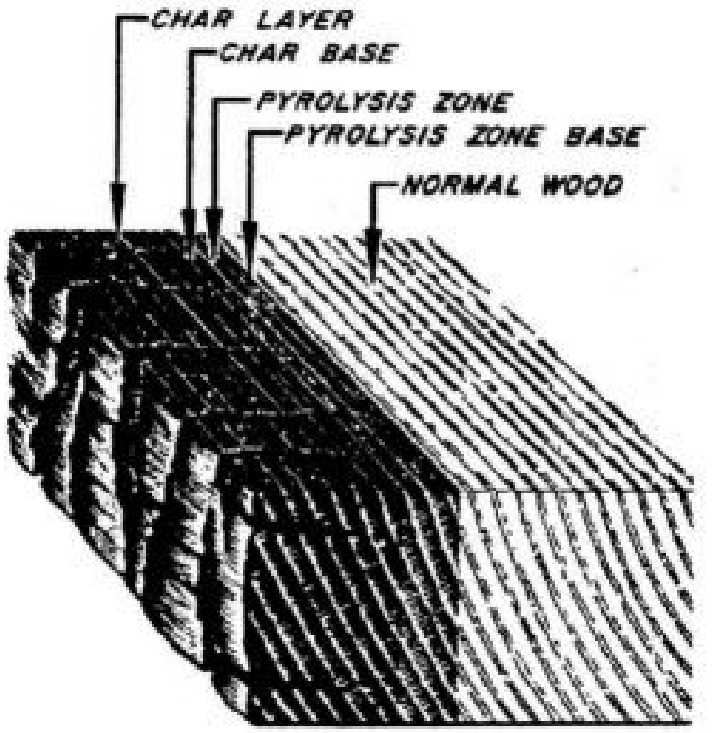
Zeng D., Chaos, M., Wang, Y., and Dorofeev S.B., “Experimental and Pyrolysis Modeling Study of Delaminating Materials” Proceedings of the 14th International Conference on Fire and Materials, San Francisco, (2015) 285-299.

# In Contrast to Charring Material

- Thermally thick
- Char layer buildup

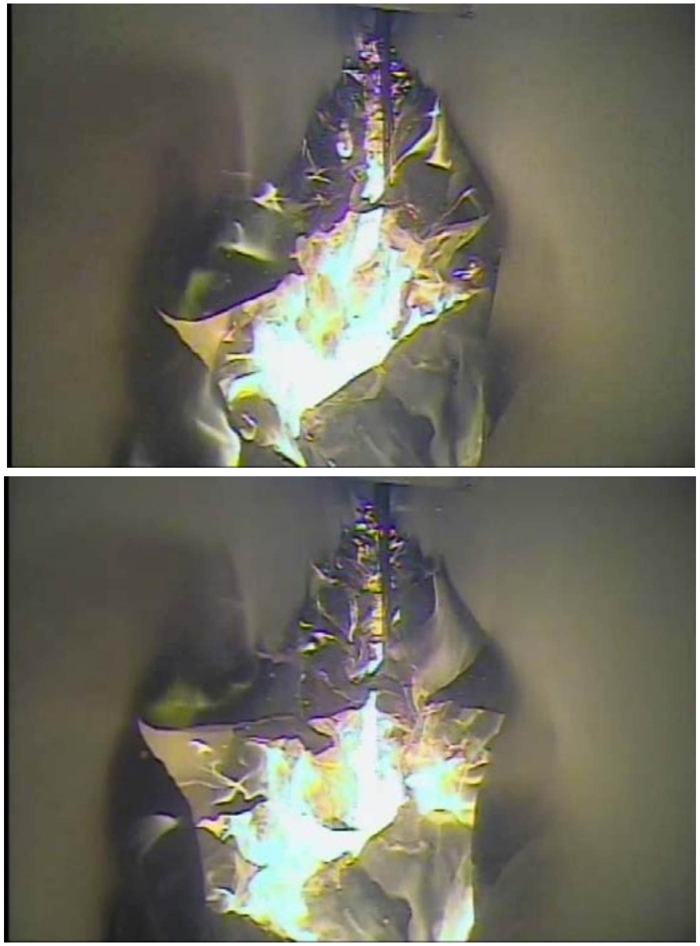
$$\rho c_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(k \frac{\partial T}{\partial x}\right) + \dot{\omega}_v''' \Delta H_{p,v}$$



# Roll-paper Pyrolysis: 2D Effect

- 1D -- Delamination
  - # of sheets burning
- 2D – Peeling
  - Propagation of delaminated front
  - Accelerate surface flame spread

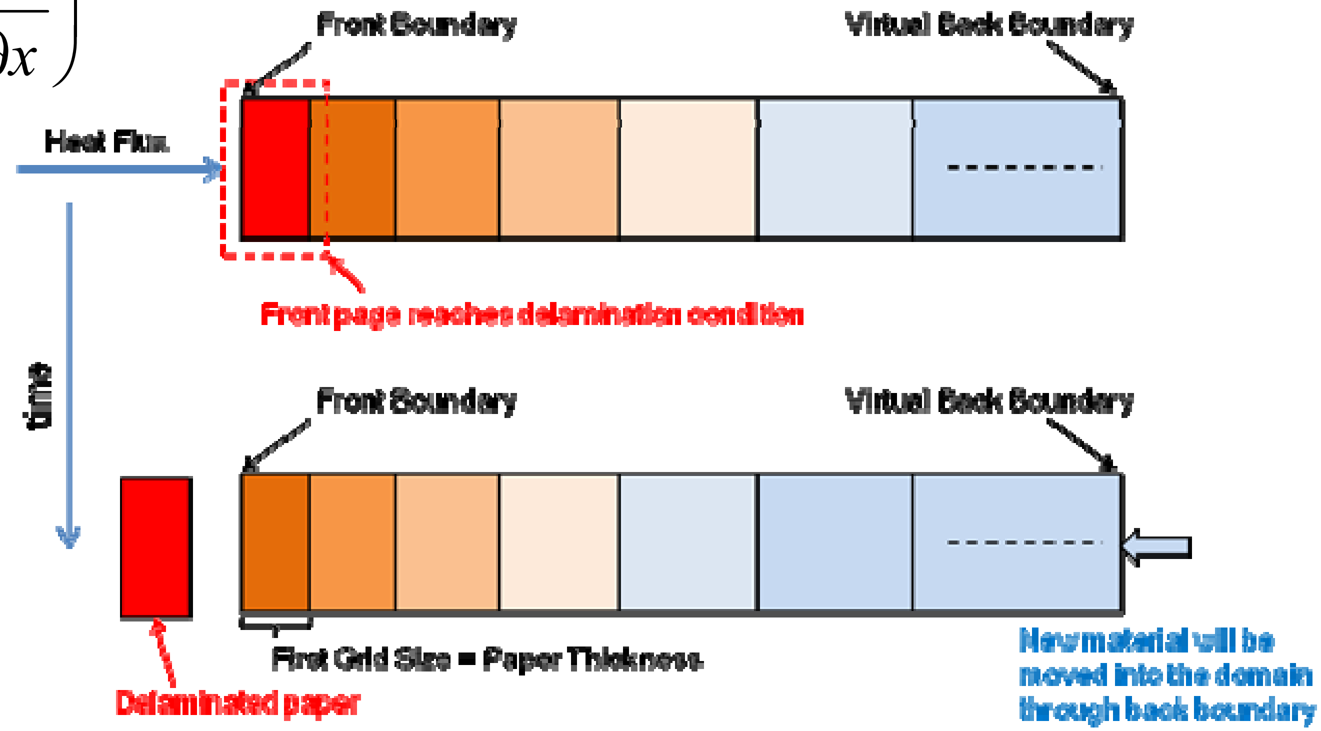


37lb paper, large scale testing

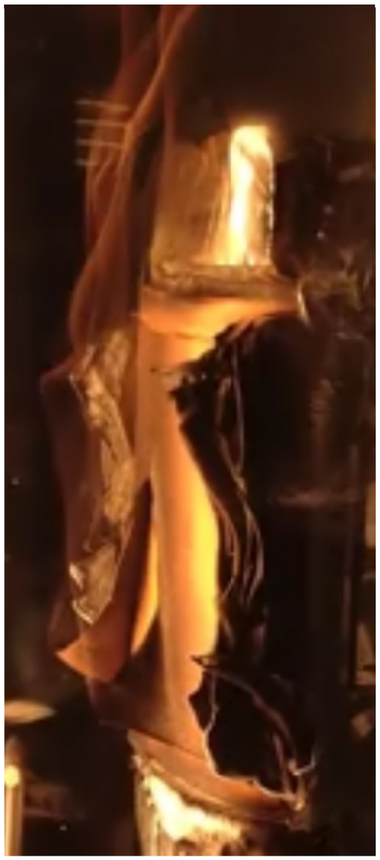
# Delamination: Material Advection

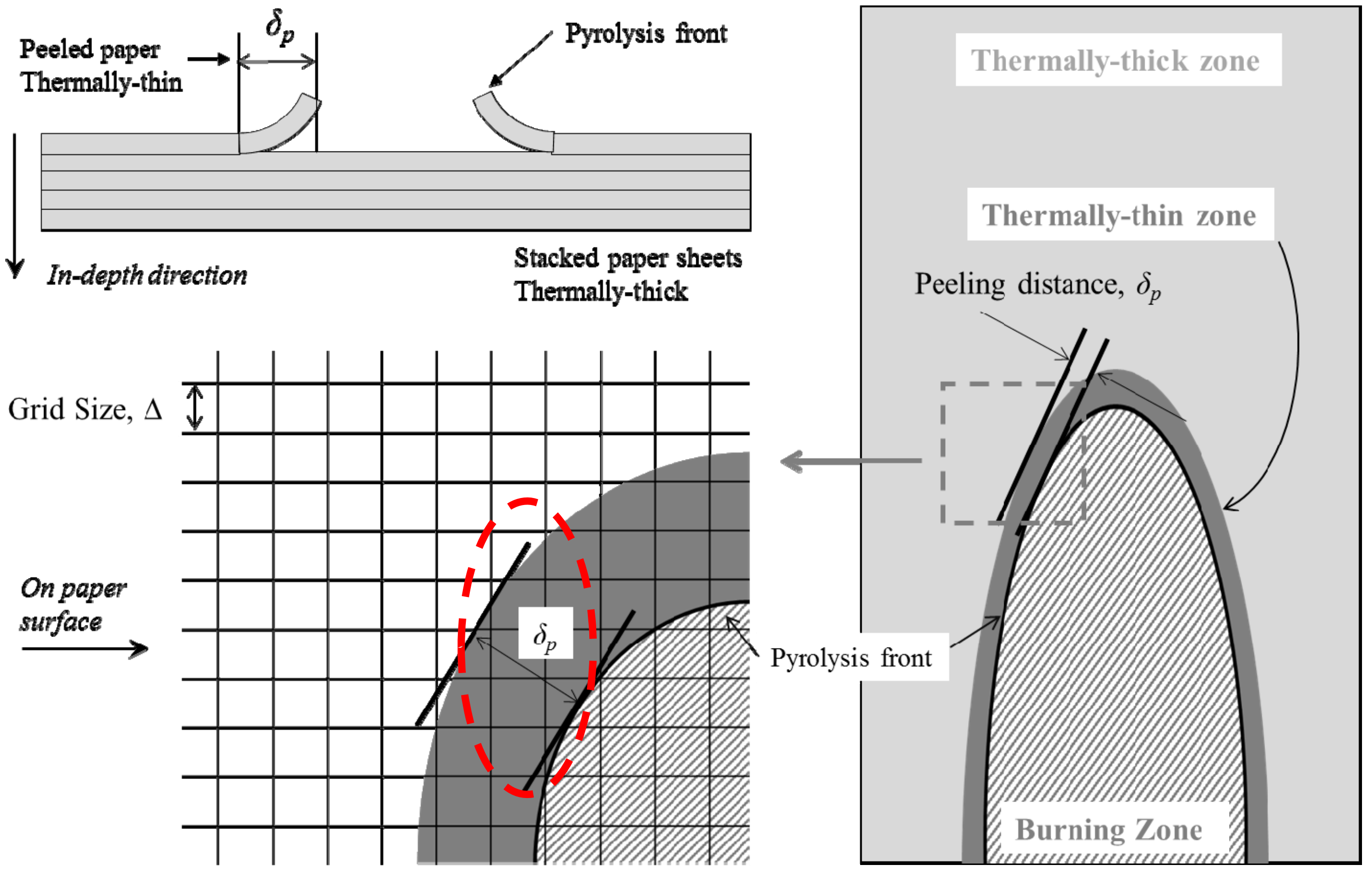
$$\frac{\partial(\rho h)}{\partial t} + \nabla \cdot (\rho U h) = \frac{\partial}{\partial x}\left(k \frac{\partial T}{\partial x}\right)$$

$$U = \frac{\delta_{paper}}{\Delta t}$$



# 2D Peeling Model





# Calibration → Validation → Prediction

- 26-lb paper test matrix
  - Intermediate-scale parallel roll
    - 2.13m (1-roll high)
  - Open Array
    - 4.26 m (2-roll high)
    - 6.39 m (3-roll high)
    - 8.52 m (4-roll high)
  - Standard Array
    - 6.39 m (3-roll high)

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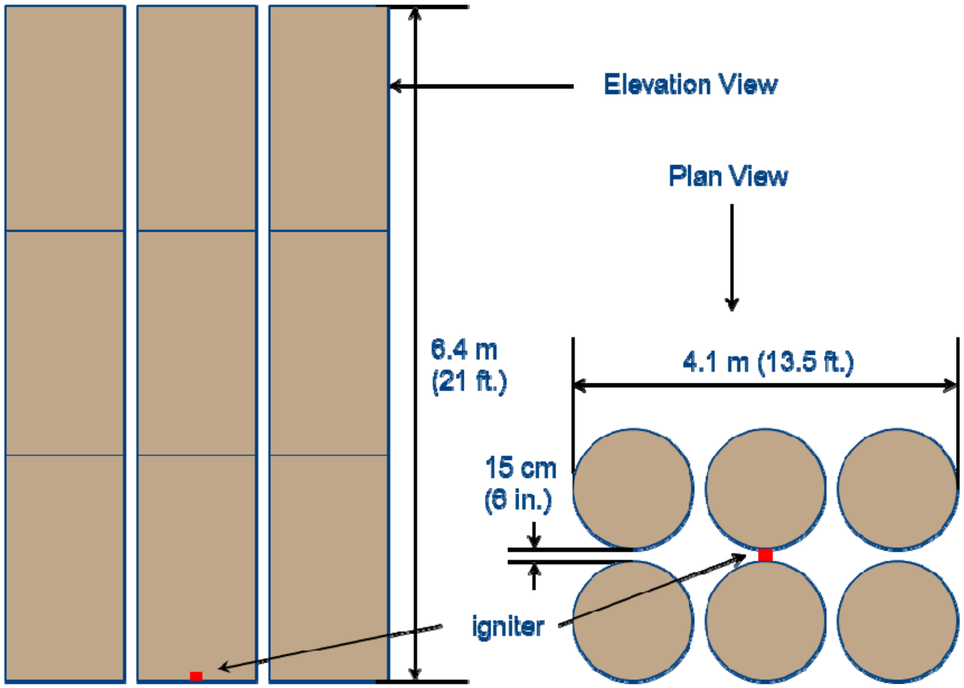
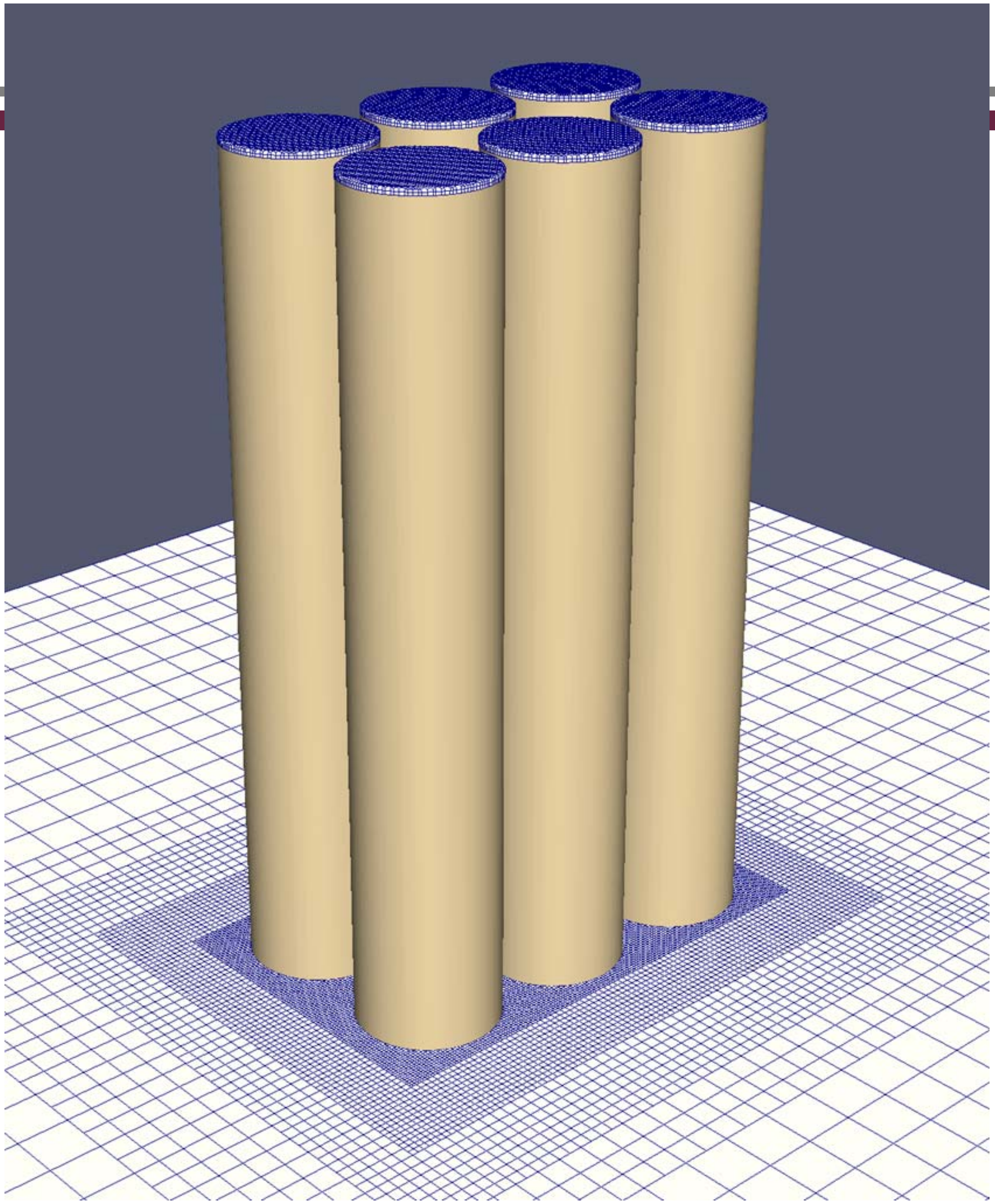
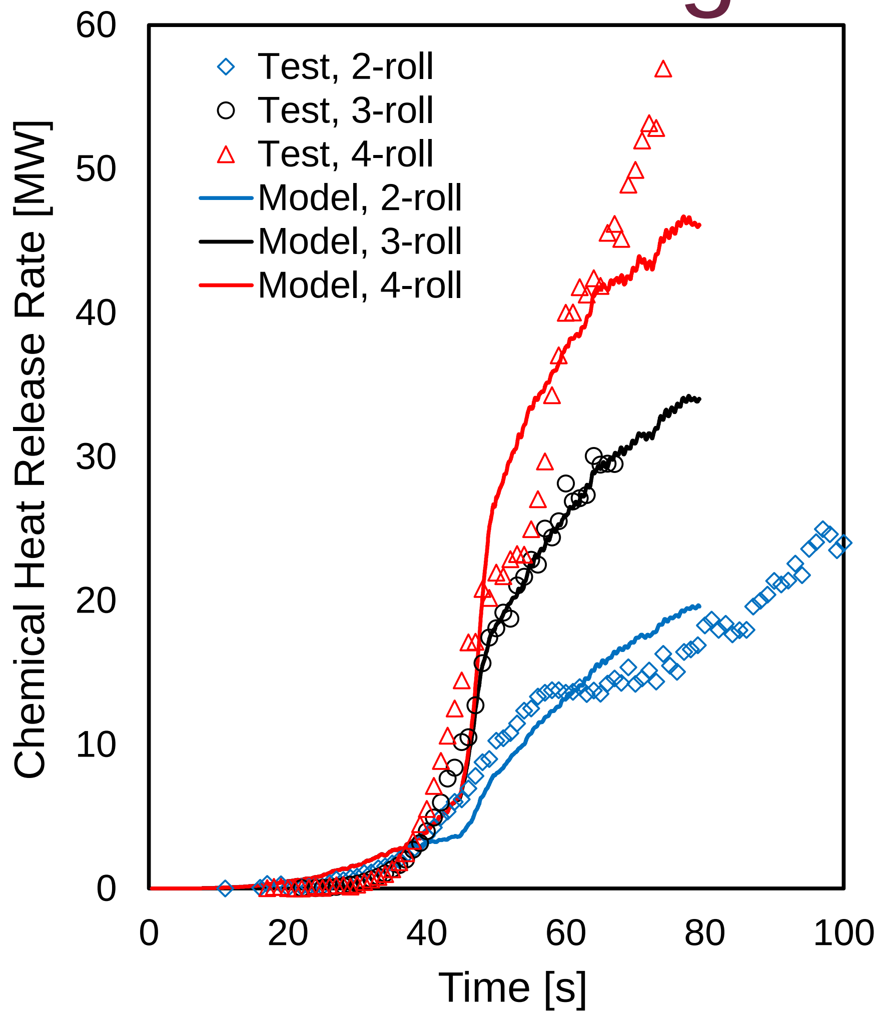
# Mesh

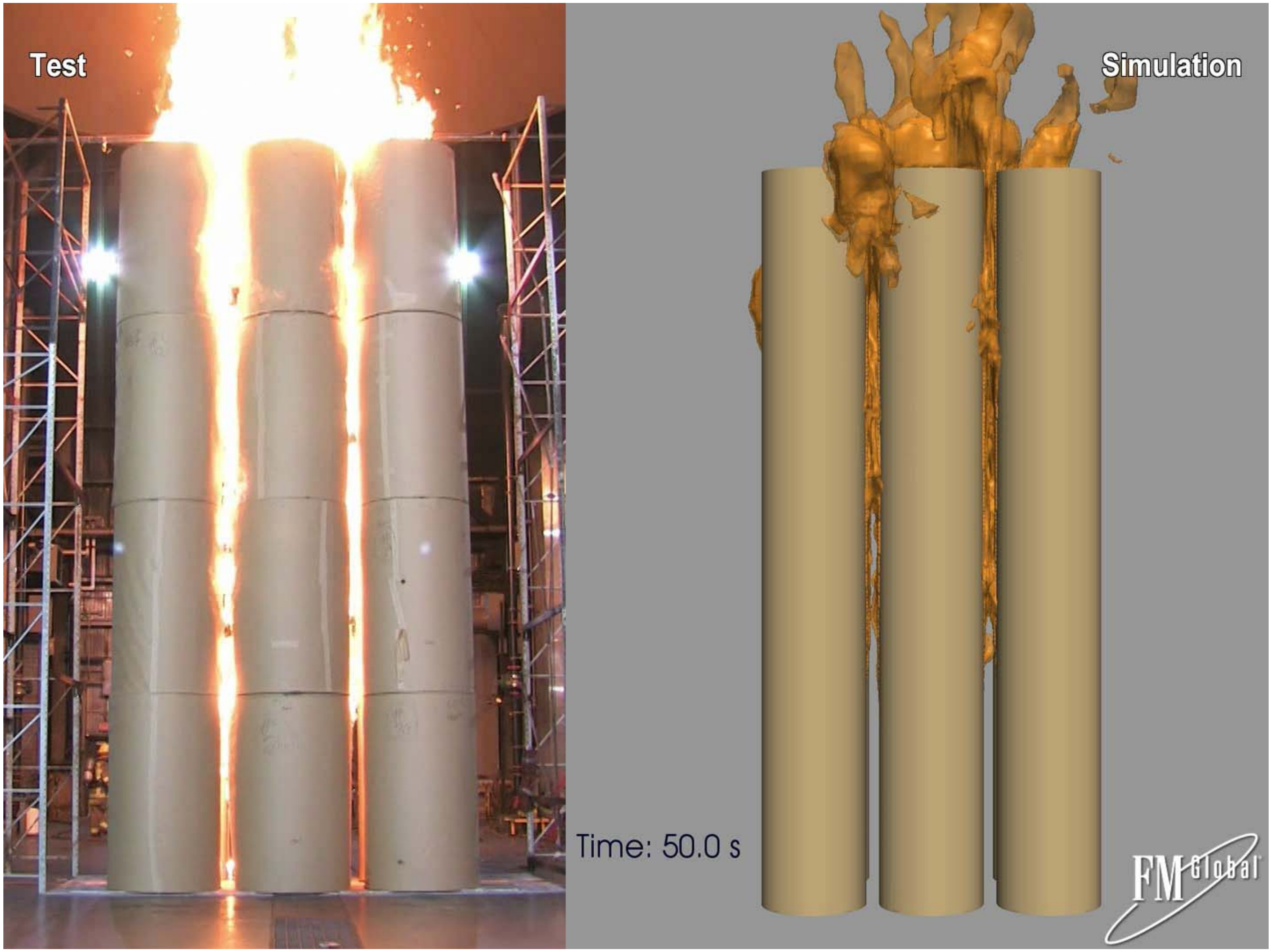


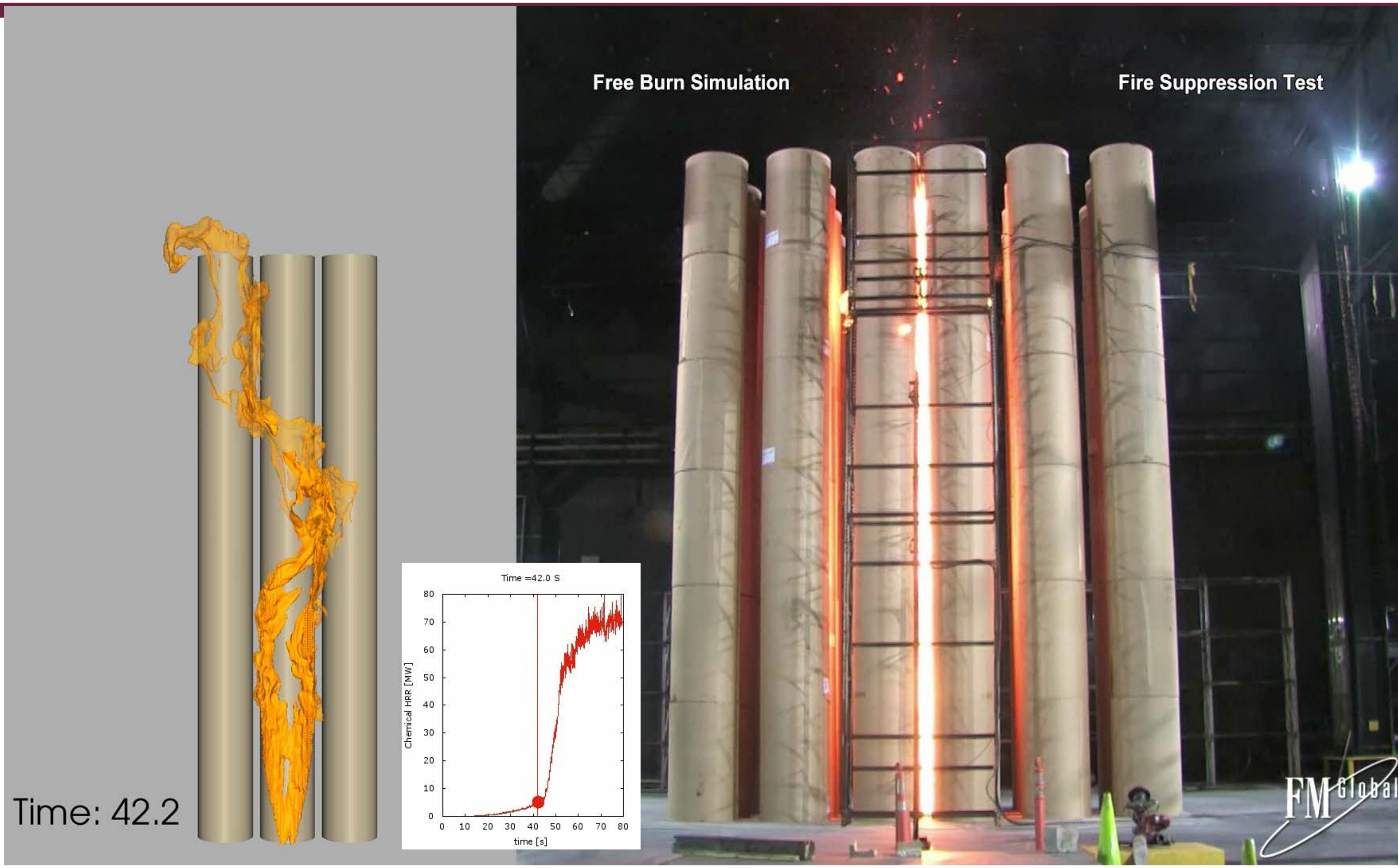
# HRR Prediction for Different Heights

| Peak Fire Growth Rate (MW/s) 5 seconds average | | |
|---|---|---|
| **H** | **Model** | **Test** |
| **4.26 m** | **0.81** | **0.67** |
| **6.39 m** | **2.1** | **1.7** |
| **8.52 m** | **3.5** | **2.78** |

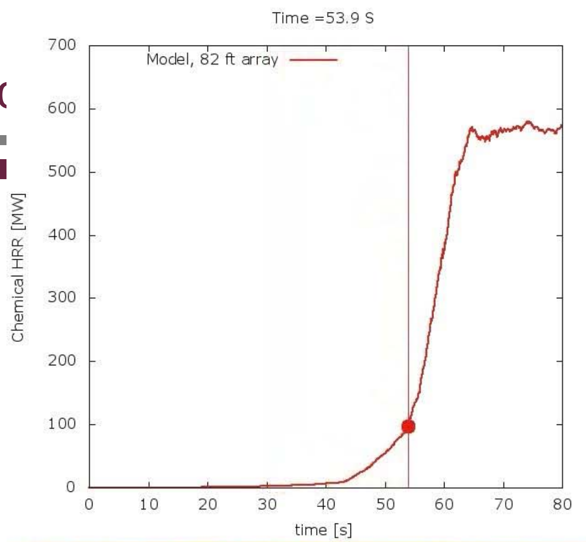



Test
Simulation
Time: 50.0 s
FM Global

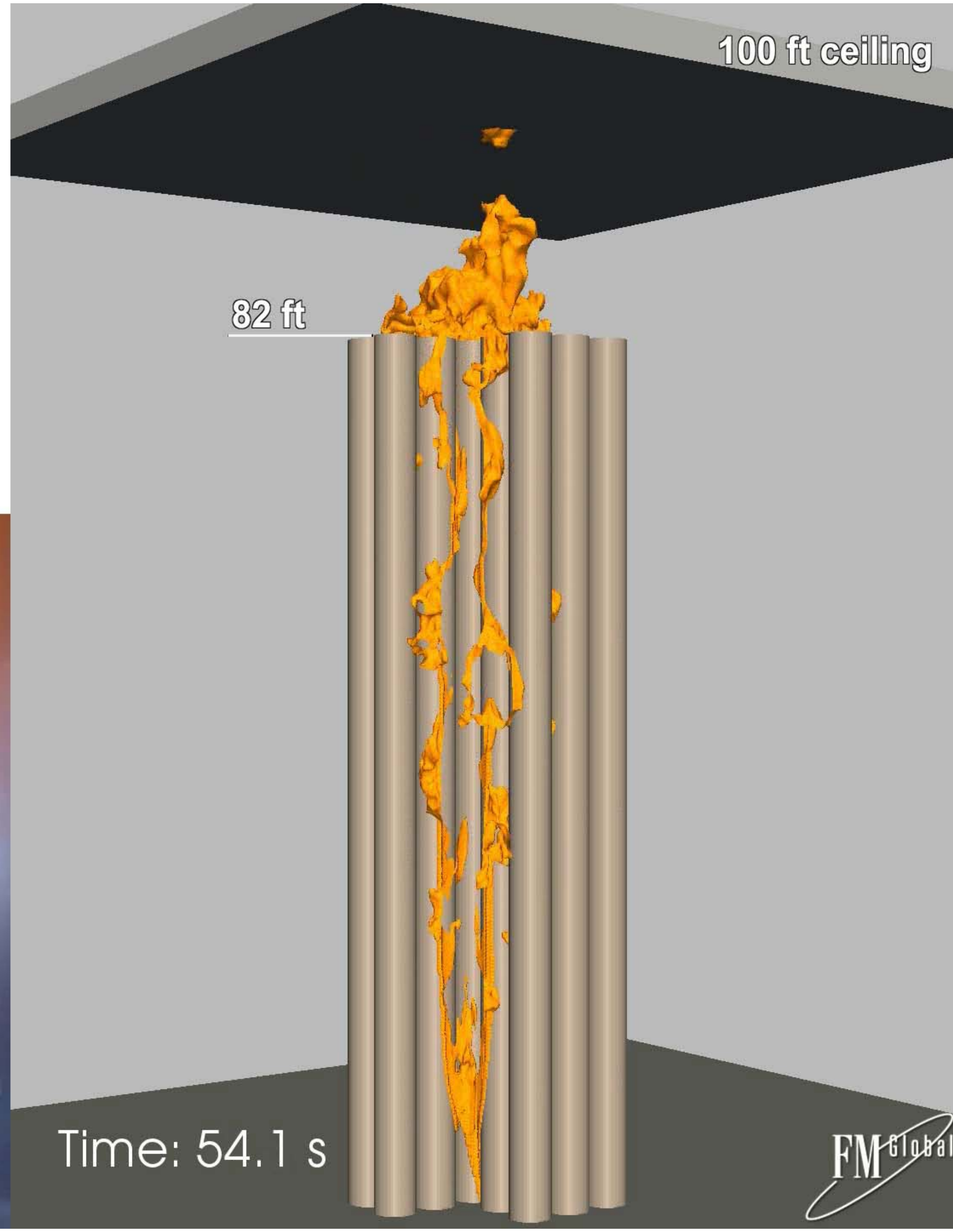
# FM Global


Free Burn Simulation
Fire Suppression Test
Time: 42.2
Time =42.0 S
Chemical HRR [MW]
time [s]
0 10 20 30 40 50 60 70 80

FM Gl


Time =53.9 S
Model, 82 ft array
Chemical HRR [MW]
time [s]
0
100
200
300
400
500
600
700
0
10
20
30
40
50
60
70
80


60 ft ceiling
42 ft


100 ft ceiling
82 ft
Time: 54.1 s
FM Global

# Key Messages

- Pyrolysis coupled with CFD, solve real-world problem
- Level of model complexity determined by problem
- Decoupled validation is needed
- Pyrolysis model and validation target need to capture large scale physics
- Coupled simulation needs to be validated with different scales

# Team

- Marcos Chaos
- Dong Zeng
- Gaurav Agarwal
- Sergey Dorofeev
- Ning Ren
- Prateep Chatterjee
- Ankur Gupta
- Karl Meredith