Analysis of Sensitivity of Vertical Corner Flame Spread Dynamics to Uncertainties in the Model Input

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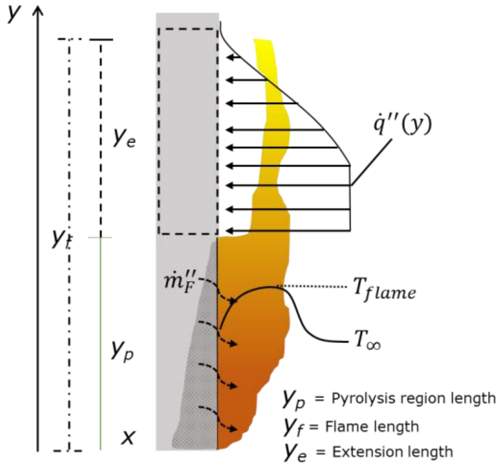
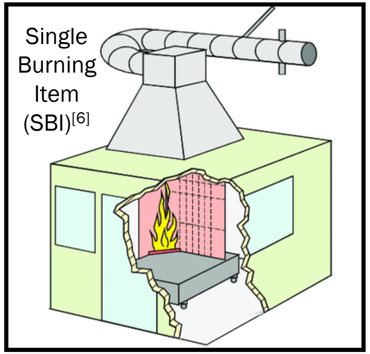
Dushyant M. Chaudhari[1,2] and Stanislav I. Stoliarov[2]

[1] Fire Safety Research Institute, UL Research Institutes, Columbia, Maryland, U.S.A
[2] Department of Fire Protection Engineering, University of Maryland, College Park, Maryland, U.S.A

Flame Spread Problem

- Fire hazard parameters, obtained from reaction-to-fire standardized tests, have limited ability to scale between fires of different scales [1,2]
- Modelling presents a cost-effective alternative to expensive standardized tests
- IAFSS working group on Measurement and Computation of Fire Phenomena (MaCFP) highlighted the need to have data from well instrumented standardized tests for modelling target [3]
- A corner scenario is of interest [4,5]



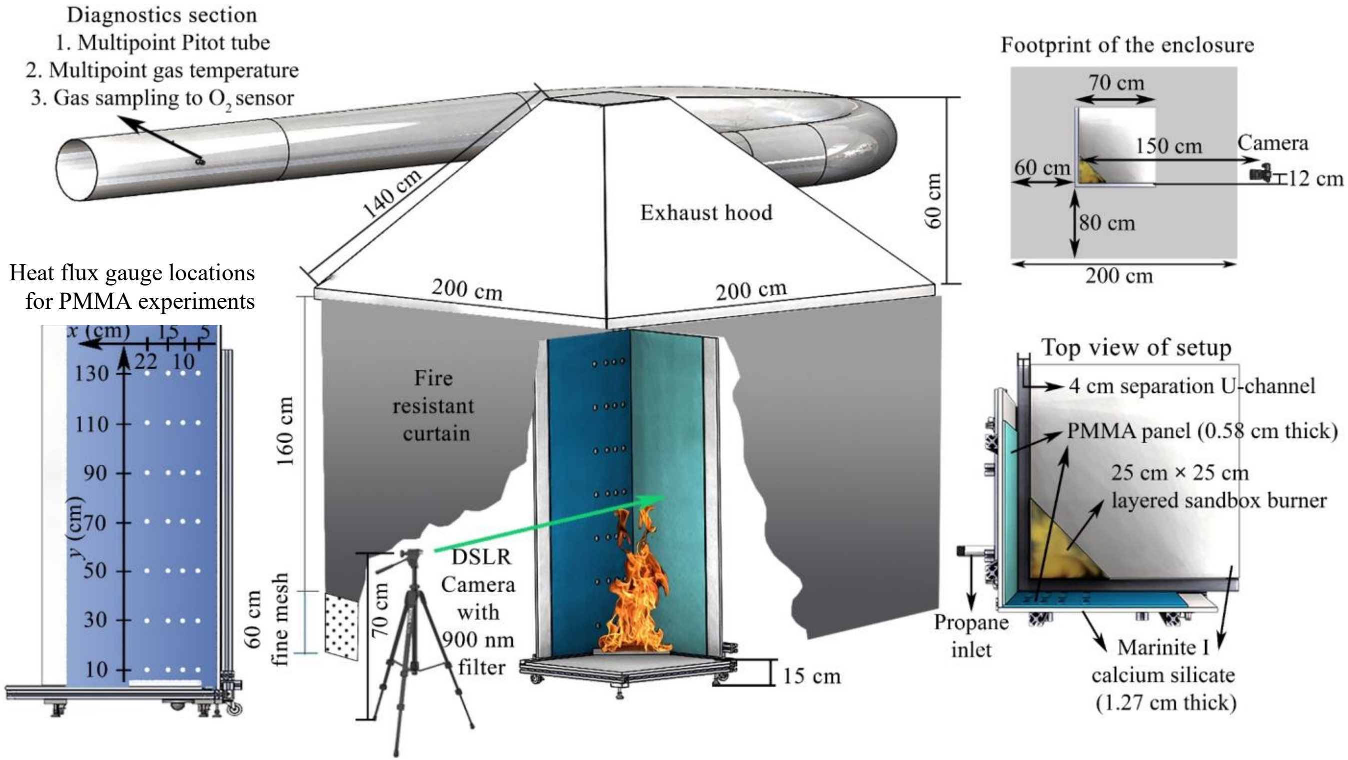


[1] R.G. Bill, P.A. Croce, Fire Safety Journal. 41 (2006) 536–538.
[2] B. Karlsson, G. North, D. Gojkovic, Journal of Fire Protection Engineering. 12 (2002) 93–108
[3] Brown A., Bruns M., Gollner M., Hewson J., Maragkos G., Marshall A., Mcdermott R., Merci B., Rogaume T., Stoliarov S., Torero J., Trouvé A., Wang Y., Weckman E, Fire Saf. J. 101 **2018** 1–17. https://doi.org/10.1016/j.firesaf.2018.08.009.
[4] Poreh M., Garrad G., Fire Saf. J. 34 2000 81–98. https://doi.org/10.1016/S0379-7112(99)00040-5.
[5] Lattimer B.Y., Heat transfer from Fires to Surfaces, in: SFPE Handb. Fire Prot. Eng., 5th ed., 2016: pp. 745–798. https://doi.org/10.1007/978-1-4939-2565-0.
[6] EN-13823 - Reaction to fire tests for building products - Building products excluding floorings exposed to the thermal attack by a single burning item, 2004.

Objective

- Understand if pyrolysis properties derived from small-scale experiments can be used to predict large-scale fires
  - Use a previously developed empirical flame spread model to predict flame spread for three materials
- Determine sensitivity of the model to the uncertainties in the input parameters
- Perform simulations using Fire Dynamics Simulator (FDS) to determine the effect of including gas-phase calculations in addition to condensed-phase calculations on flame spread predictions

Experimental setup



Our previous study [1]

- Measured flame heat flux at 28 locations over Poly (methyl methacrylate) (PMMA)
- Developed empirical flame heat feedback model and coupled it with pyrolysis model to develop a flame spread model

[1] D.M. Chaudhari, G.J. Fiola, S.I. Stoliarov, Experimental analysis and modeling of Buoyancy-driven flame spread on cast poly(methyl methacrylate) in corner configuration, Polym. Degrad. Stab. 183 (2021) 109433.

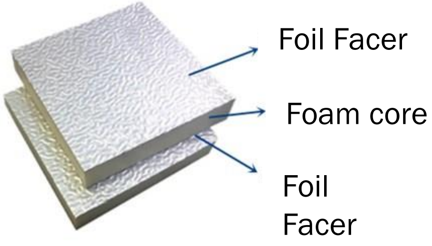
Research Institutes

Materials

- **Poly(methyl methacrylate) (PMMA)**
  - Black Cast Acrylite GT ™ manufactured by Evonik
  - Used for the development of empirical flame heat feedback model

PMMA

- Wall-lining materials:
  - Closed-cell **Dow Tuff-R™ polyisocyanurate (PIR) foam** supplied by DuPont Nemours Inc.
  - **Oriented Strand Board (OSB)**
    - Ps2-10 compliant Georgia-Pacific Blue Ribbon



Tuff-R™ foam

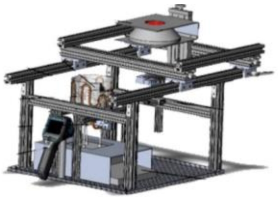
OSB

Pyrolysis model development overview

Simultaneous Thermal Analysis (STA)

Microscale Combustion Calorimeter (MCC)

Controlled Atmosphere Pyrolysis Apparatus (CAPA)



Inverse analysis using ThermaKin [1]

Reaction kinetics, thermodynamics

Heat of combustion of evolved gases

Thermo-physical properties

Optical properties

Comprehensive pyrolysis model

[1] Stoliarov S.I., Li J., Parameterization and Validation of Pyrolysis Models for Polymeric Materials, Fire Technol. 52 **2016** 79–91. https://doi.org/10.1007/s10694-015-0490-1.

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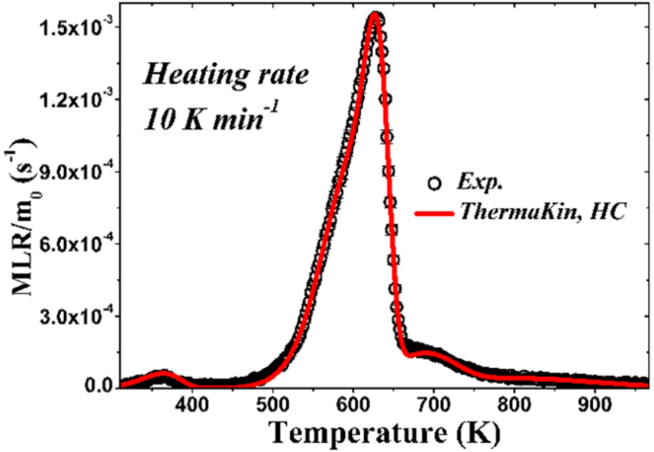
Characterization of thermal decomposition

- Developed in separate studies using inverse analysis of small-scale (milligram and gram-scale) experiments

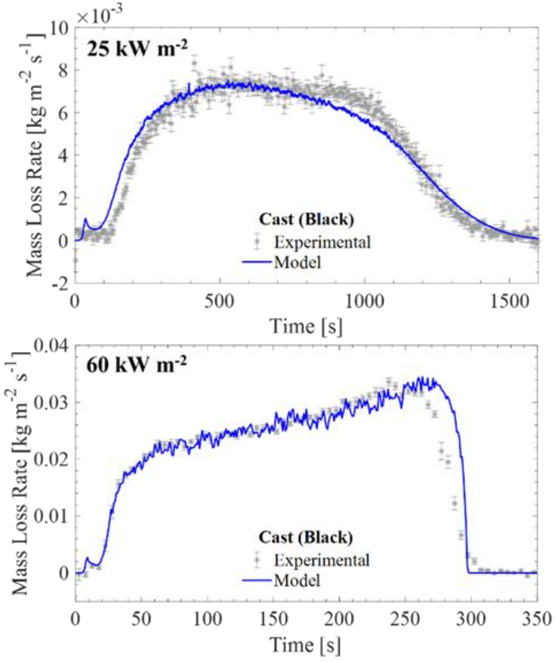


Material	Decomposition mechanism
PMMA[1]	Two first-order reactions in series
PIR foam[2]	Seven first-order reactions in series and consideration of blowing agent component contribution
OSB[3]	Five first-order reactions in series

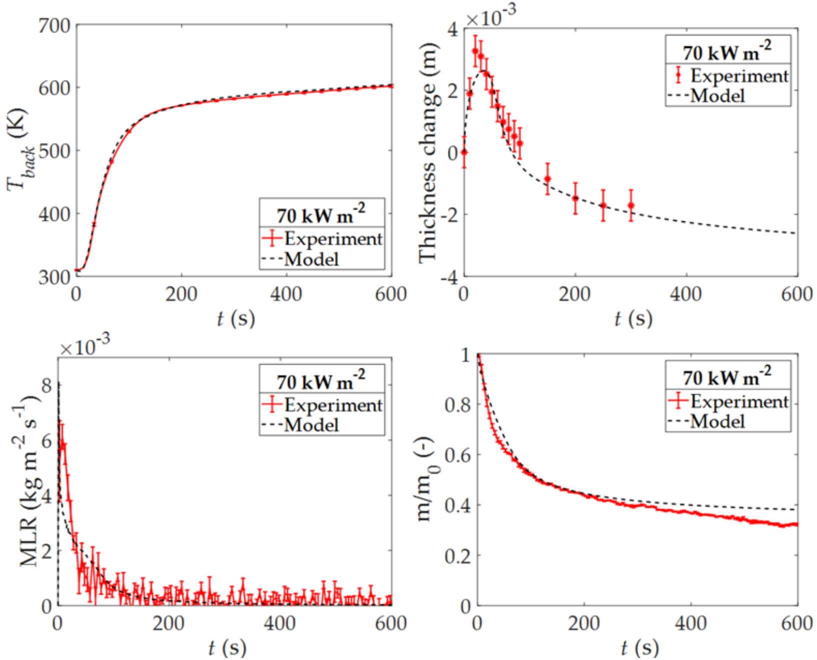
[1] Fiola G.J., Chaudhari D.M., Stoliarov S.I., *Comparison of Pyrolysis Properties of Extruded and Cast Poly(methyl methacrylate)*, Fire Saf. J. **2020**. https://doi.org/10.1016/j.firesaf.2020.103083.
[2] Chaudhari D.M., Stoliarov S.I., Beach M.W., Suryadevara K.A., *Polyisocyanurate foam pyrolysis and flame spread modeling*, Appl. Sci. 11 **2021**. https://doi.org/10.3390/APP11083463.
[3] Gong J., Zhu H., Zhou H., Stoliarov S.I., *Development of a pyrolysis model for oriented strand board. Part I: Kinetics and thermodynamics of the thermal decomposition*, Orig. Artic. J. Fire Sci. 39 **2021** 190–204. https://doi.org/10.1177/0734904120982887.

Pyrolysis model validation

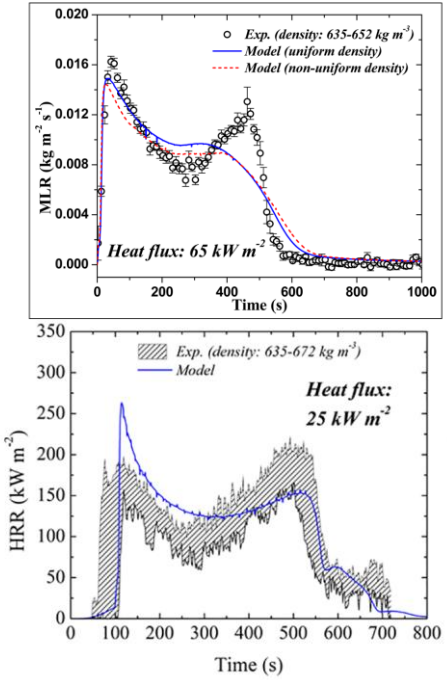
PMMA



PIR foam



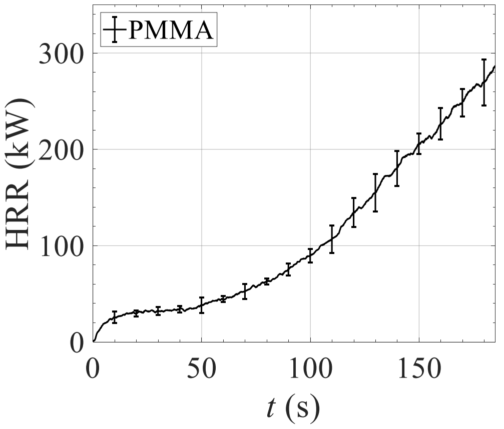
OSB



Can pyrolysis properties derived from small-scale experiments be used to predict large-scale fire scenarios?

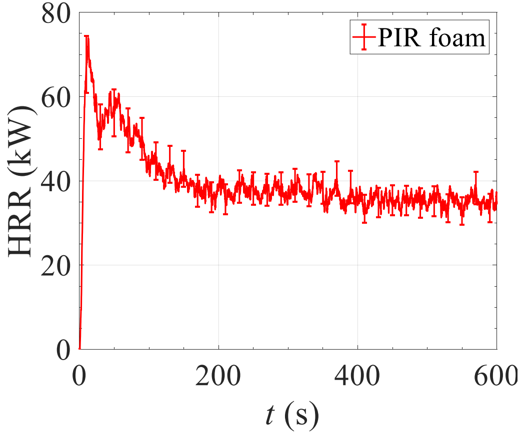
Large-scale experiments

7 tests with PMMA



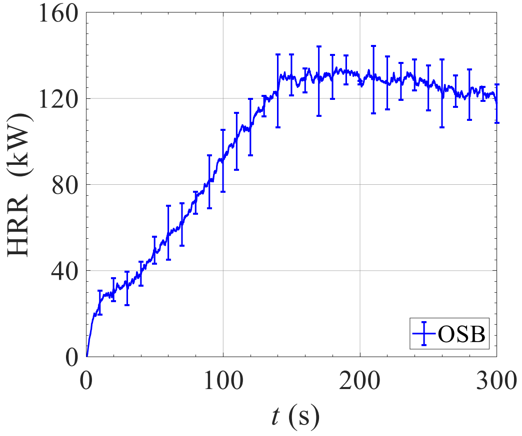
- Largest fire size
- 280 kW HRR peak HRR

2 tests with PIR foam



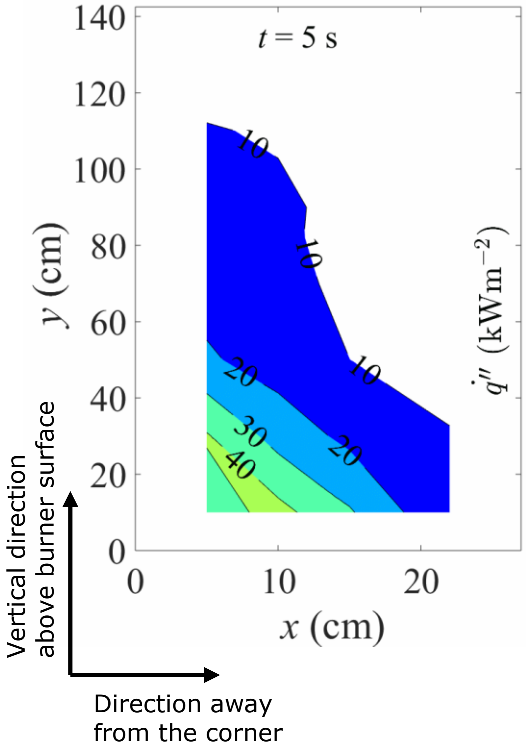
- Does not support significant flame spread
- Around 80 kW peak HRR

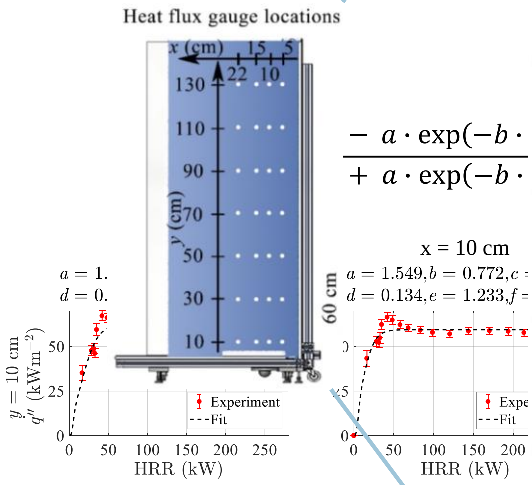
3 tests with OSB

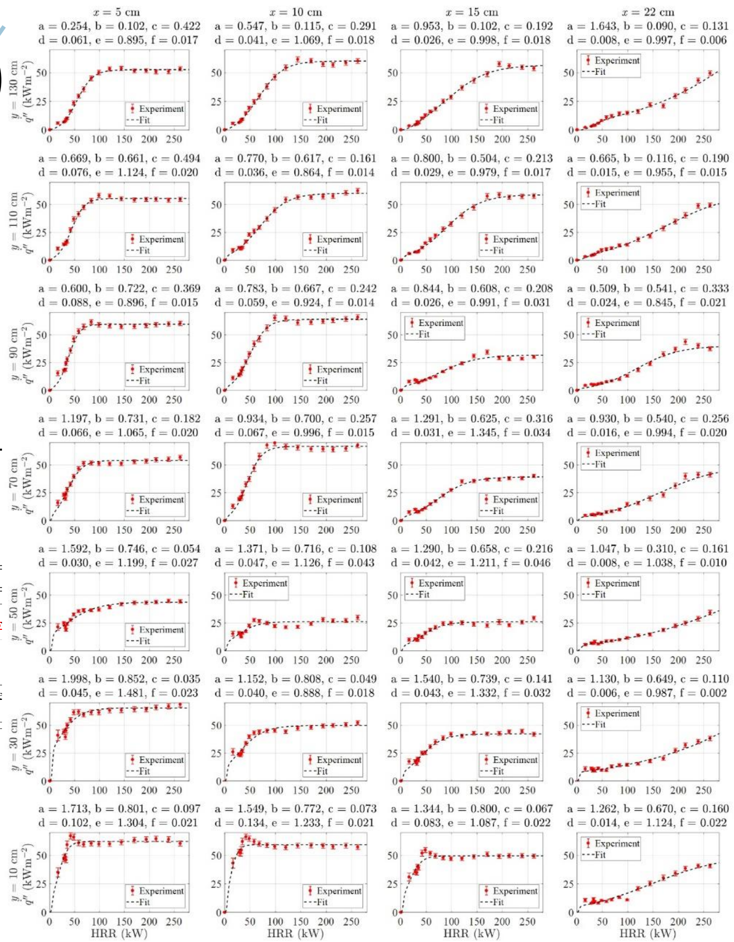


- Largest fire size
- 130 kW HRR peak HRR

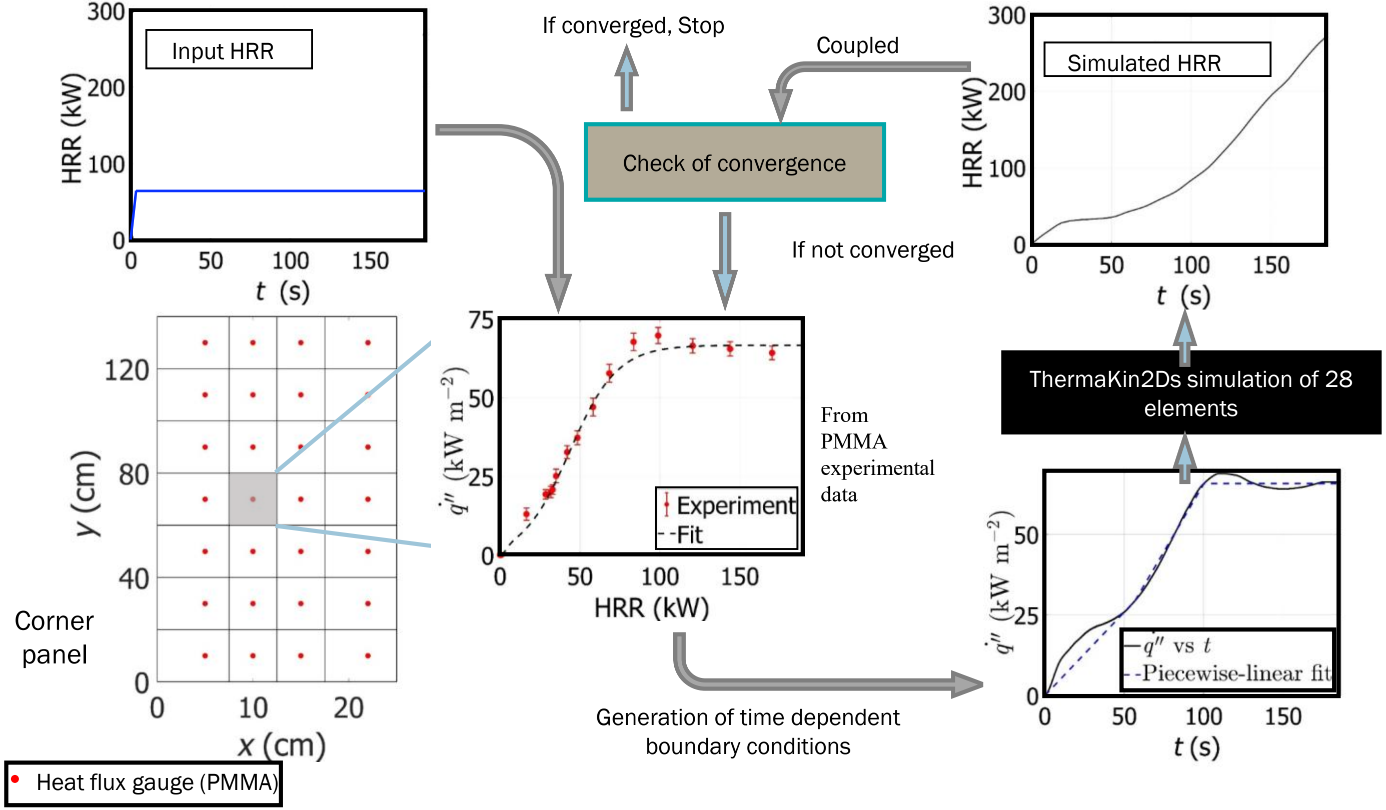
Flame heat feedback model (PMMA)







Semi-empirical Flame Spread Model



$$\text{Simulated HRR}(t) = \mathrm{HRR_b}(t) + 2\sum_{j=1}^{28} A_j \left[\sum_{i=1}^{Ng} \dot{m}''_{ij}(t)\,\Delta H_c^i\right]$$

Ng : number of gaseous pyrolyzates

j : index of element

i : index of the gaseous pyrolyzate

$\dot{m}''_{ij}(t)$: mass of gas *i* from element *j*

Aj : Area of element *j*

ΔH_c^i : heat of combustion of gas *I*

$\mathrm{HRR_b}$(t) *:* HRR contribution from propane burner

Flame heat flux representation

Radiation

$$\dot{q}''_{net} = \dot{q}''_{flame} - \underbrace{\varepsilon\left(\sigma T_{surf}^4\right)}_{II}$$

II = Calculated by ThermaKin

Hybrid

If $\dot{q}''_{flame}$ < 30 kW m^{-2}; convection expression

If $\dot{q}''_{flame}$ > 30 kW m^{-2}; radiation

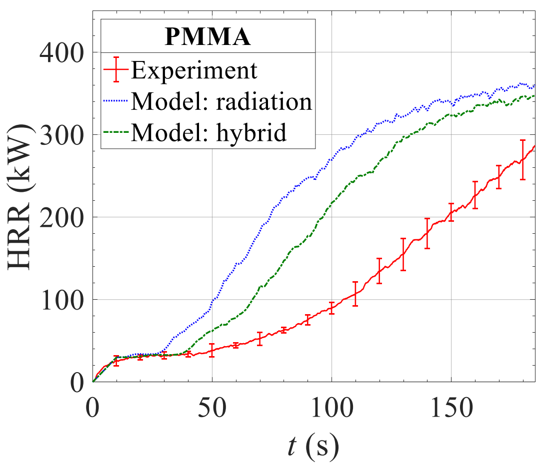
30 kW m^{-2} is 2.5 times convection heat flux estimate

Heat flux (radiative or convective) is a function of time and changes with location

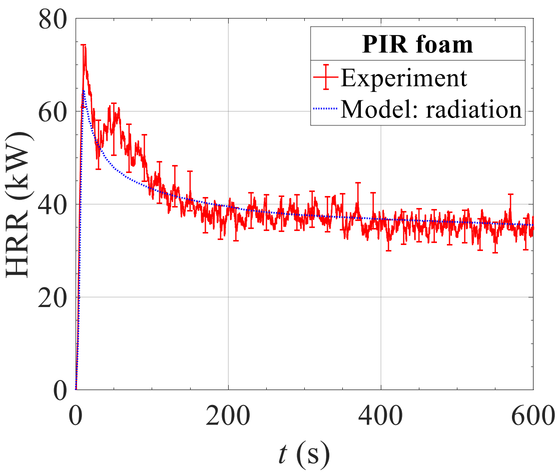
Convection expression

$$\dot{q}''_{net} = \underbrace{h\left(T_{flame} - T_{surf}\right)}_{\dot{q}''_{flame}} - \underbrace{\varepsilon\left(\sigma T_{surf}^4\right)}_{II}$$

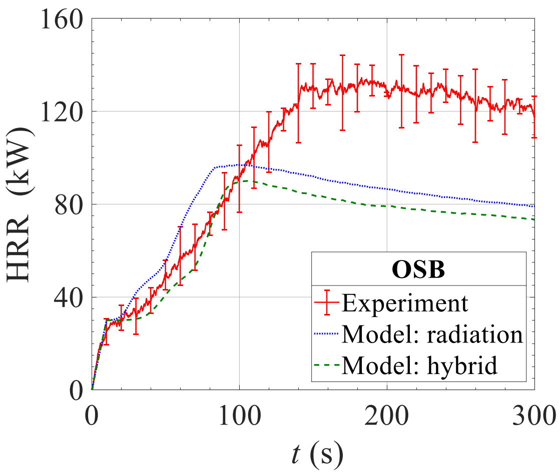
Impact of heat flux representation on model predictions



Average HRR error : 33% (hybrid heat flux)



HRR predicted within the experimental uncertainty



Average HRR error : – 28% (hybrid heat flux)

Contribution of convection and radiation to total heat flux important for PMMA than OSB

How sensitive are model predictions to the uncertainties in the model input parameters?

Sensitivity analysis

$$S_{HRR} = \frac{\Delta \mathrm{HRR}_{\mathrm{error}}}{\delta P}$$

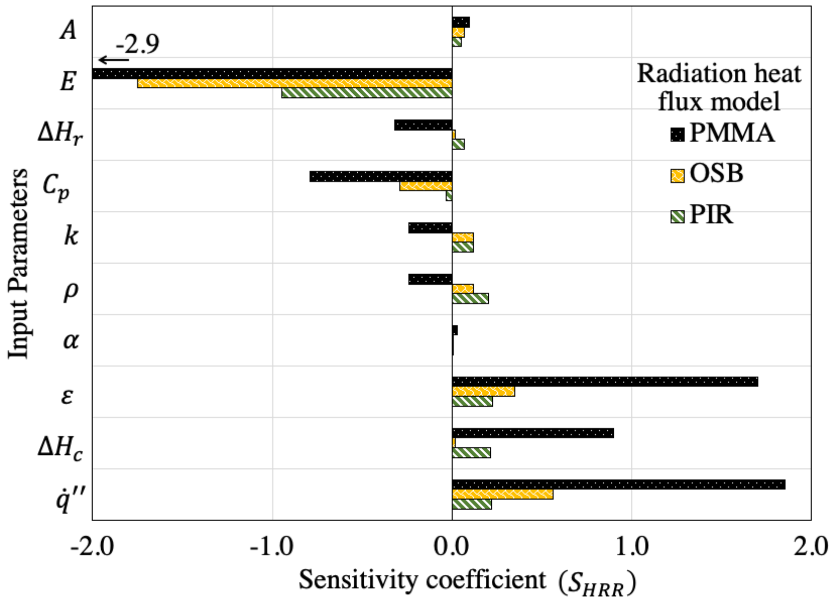
$$\Delta \mathrm{HRR}_{\mathrm{error}} = HRR_{error}^{P+\delta P} - HRR_{error}^{P}$$

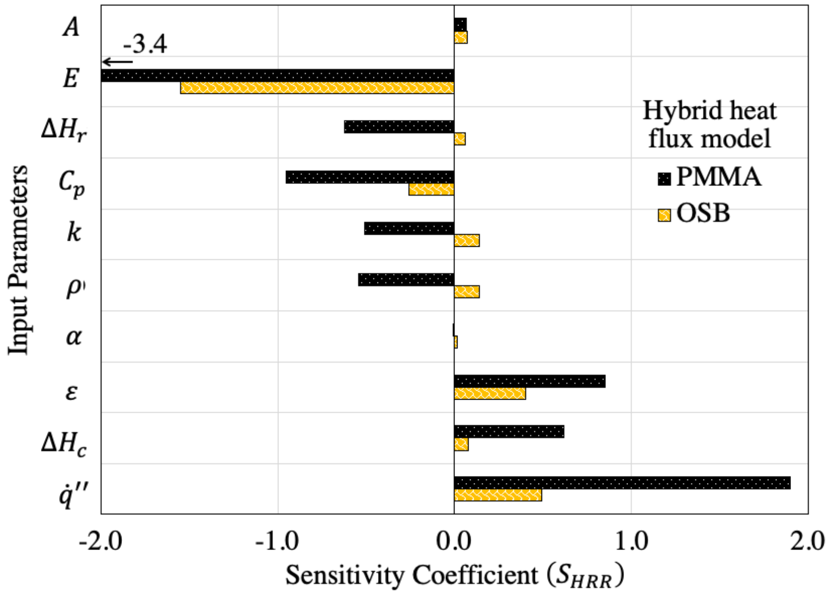
P: Baseline parameter value

δP: Fractional change corresponding to the uncertainty

Type	Parameter	Variable (P)	Uncertainty (δP)
Reaction kinetics and thermodynamics	Pre-exponential factor	A	40%
	Activation energy	E	2%
	Heat of decomposition	ΔH_r	5%
Thermo-physical	Specific heat capacity	C_p	10%
	Thermal conductivity	k	10%
	Density	ρ	5%
Optical	Absorption coefficient	α	30%
	Emissivity	ε	2%
Gas-phase combustion	Heat of combustion	ΔH_c	5%
Heat feedback	Heat flux	$\dot{q}''$	10%

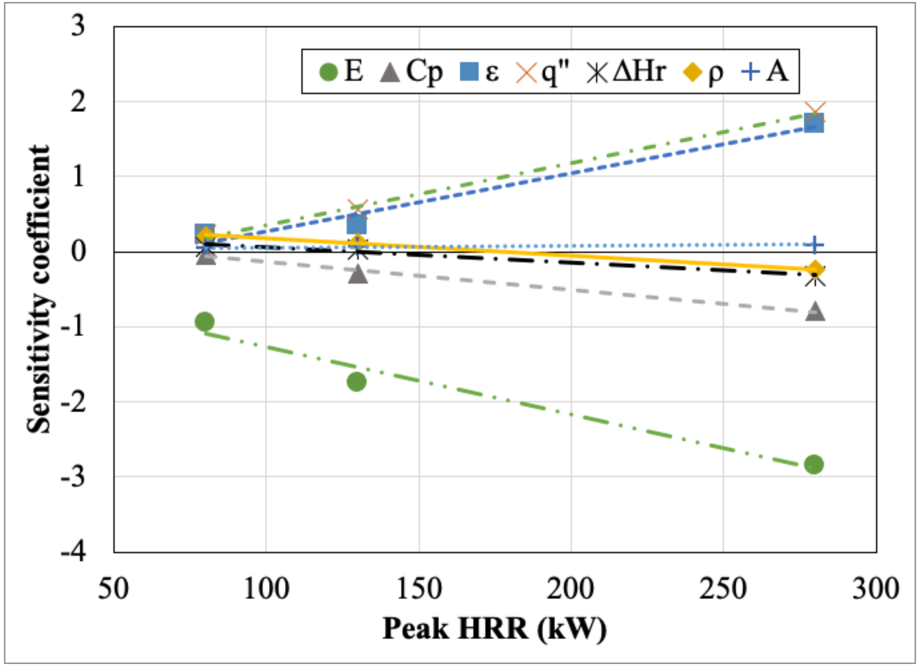
Sensitivity to parameters





- Activation energy, followed by flame heat flux has the highest sensitivity coefficient

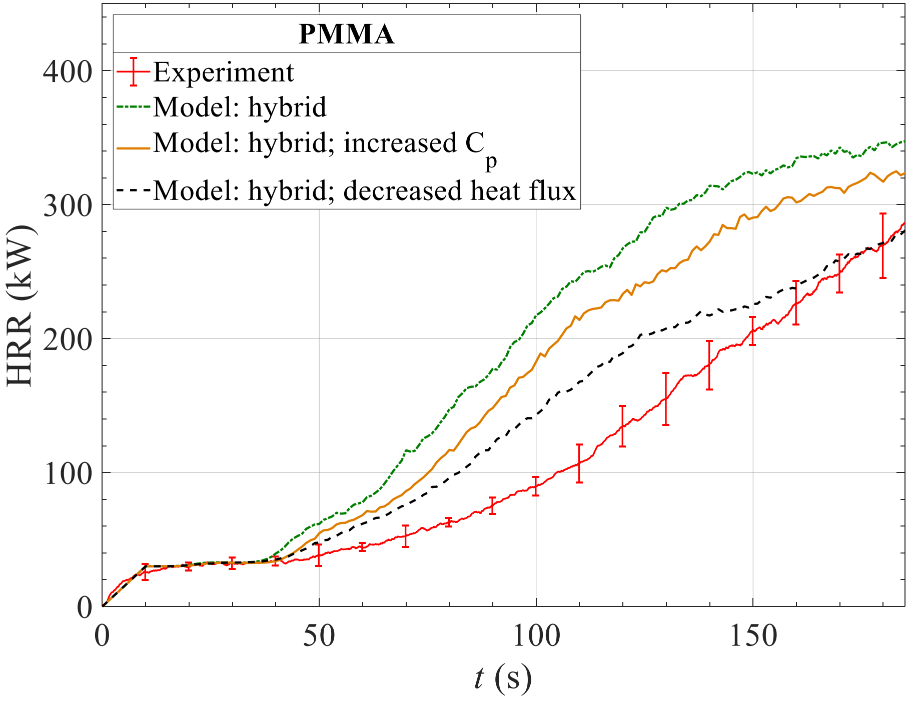
Sensitivity to parameters



- Magnitude of sensitivity coefficient increases with the fire size
- Highest sensitivity coefficient ≠ most impact on the model predictions

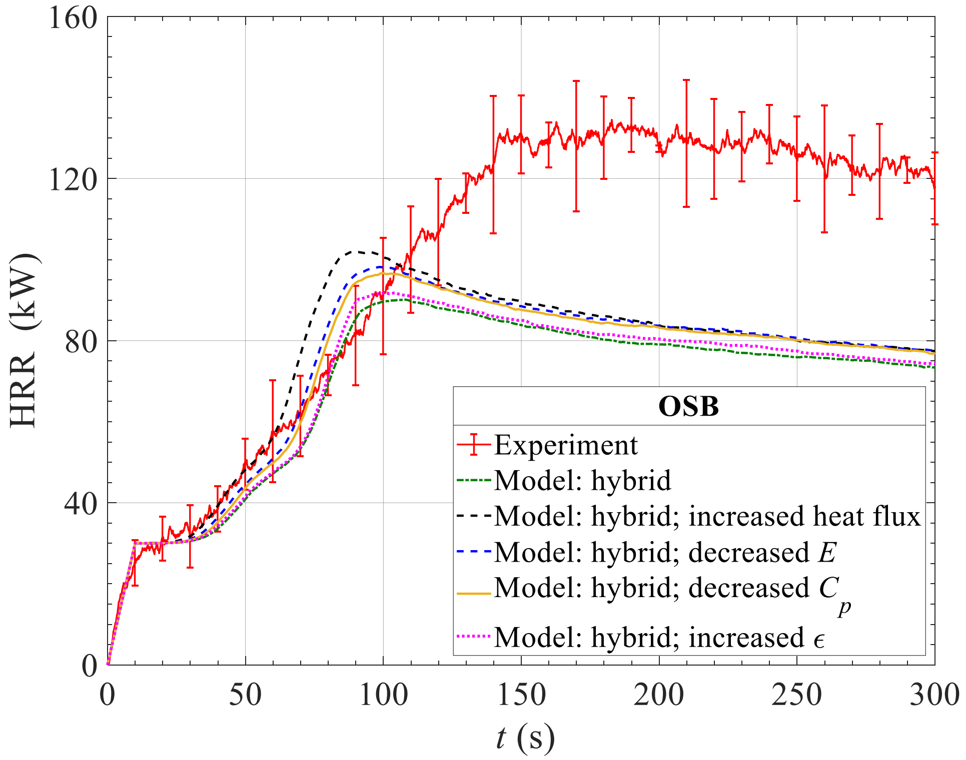
Can the uncertainty in input parameter explain the differences in the model prediction and the experimental HRR?

Effect of parameter uncertainty for PMMA



- Average HRR error for simulation with decreased heat flux : 11% (hybrid heat flux)
- Reduced from 33% average error of the simulation with original parameters
- Uncertainty in the flame heat flux explains the discrepancy between the model predictions and experimental observations for PMMA

Effect of parameter uncertainty for OSB



- Uncertainty in emissivity have low impact on predictions
- Average HRR error for OSB simulation with increased heat flux : –28% (hybrid heat flux)
- The 10% increase for heat flux assumed here (based on uncertainty of PMMA data) may not be representative of the differences in flame heat flux between OSB and simulated by the flame feedback model

Radiation intensities for OSB and PMMA flame

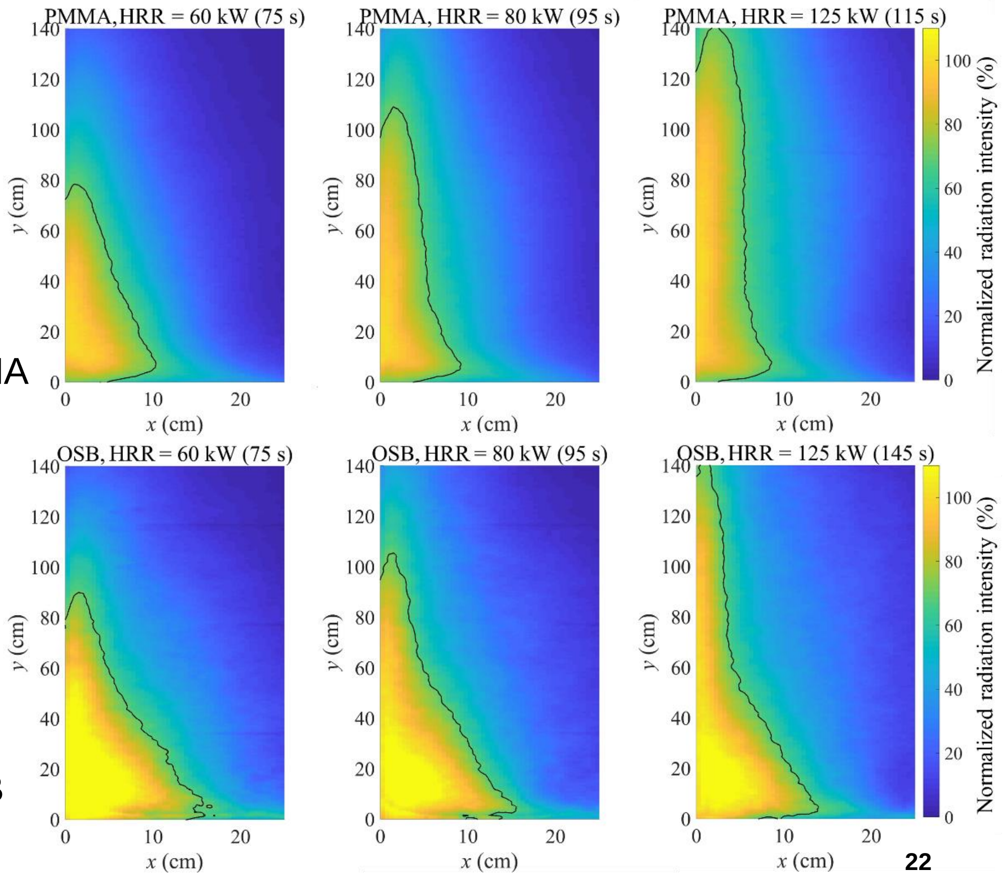
- Radiation intensity for the flame over OSB is higher than for the flame over PMMA
- The discrepancy in prediction is likely due to differences in flame heat flux

Flame feedback model developed using PMMA data cannot be assumed to be directly applicable to OSB

Flame heat feedback model can be calibrated on materials with different radiative fractions

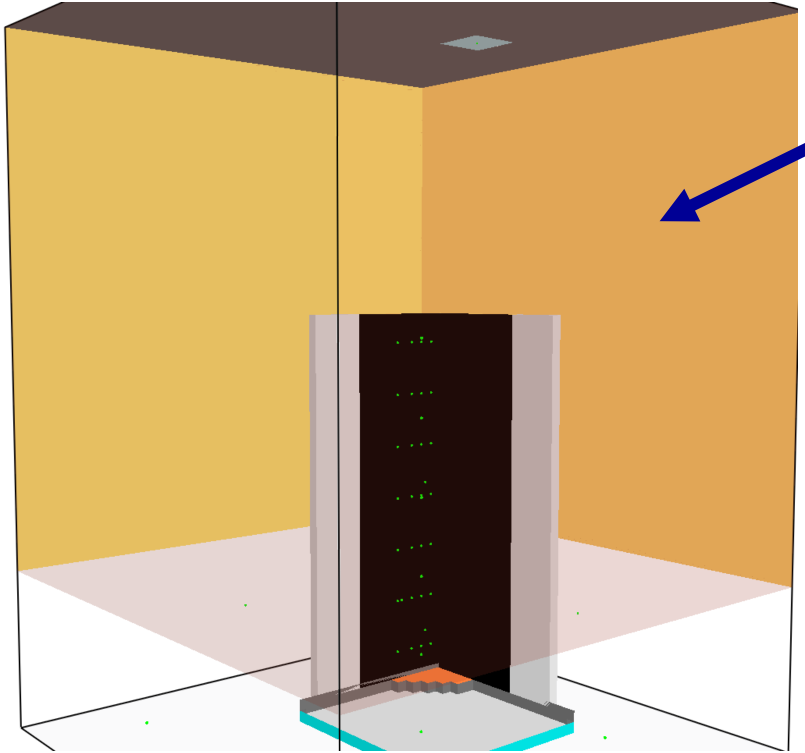
PMMA

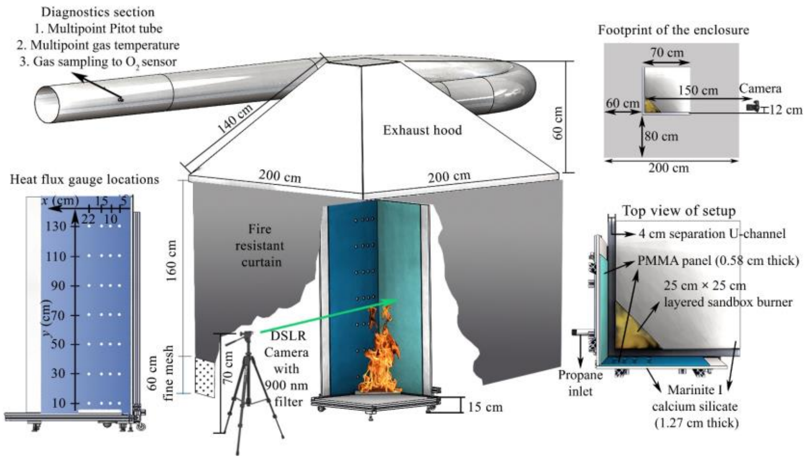
OSB



How does including gas-phase calculations affect flame spread predictions?

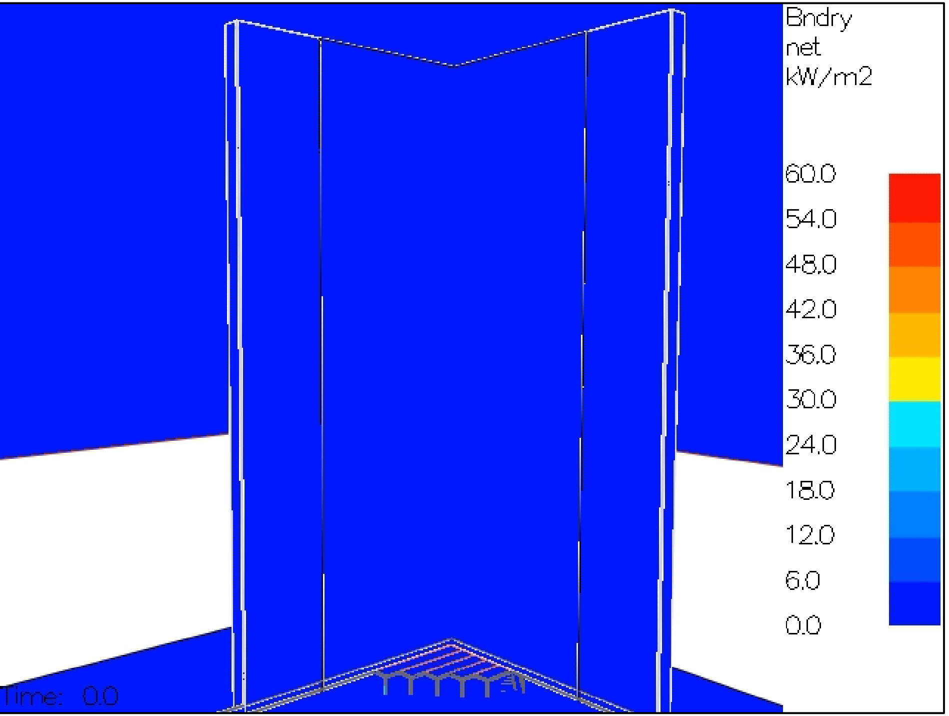
FDS Simulations – PMMA

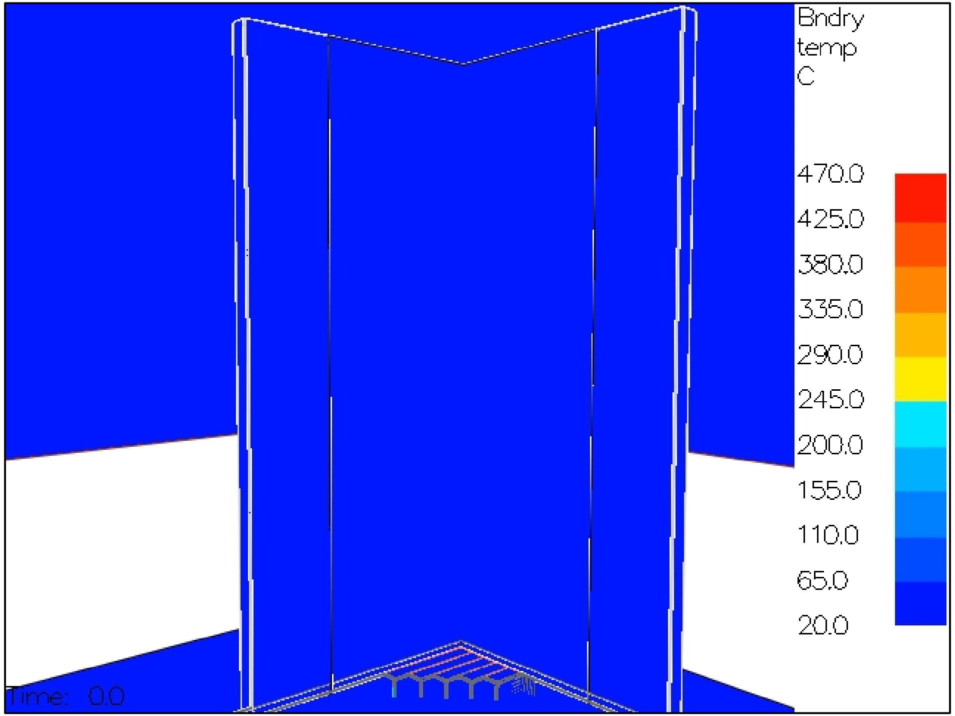




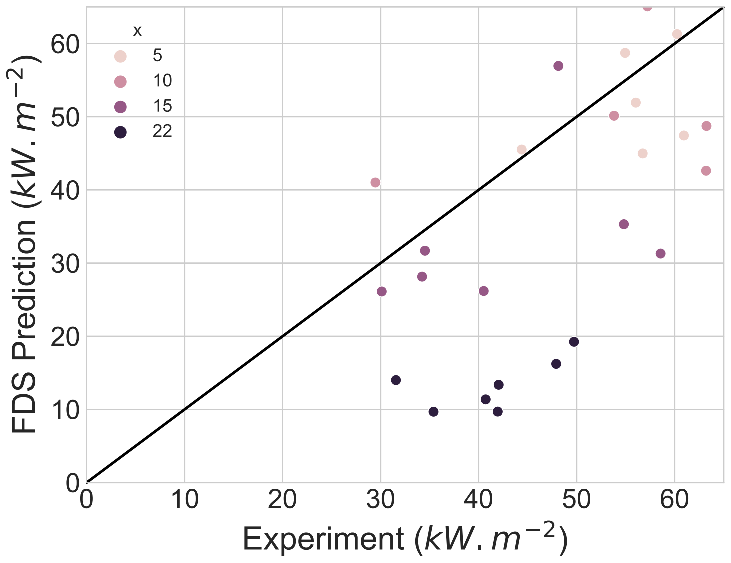
- 4cm mesh for the region around the fire
- Pyrolysis model implemented in FDS validated to reproduce TGA, CAPA II, and Cone calorimeter tests
- Two detailed chemistry reactions implemented
    - Propane with 1.5% soot yield and 47.5 kJ/g heat of combustion
    - PMMA pyrolyzates with 2.2% soot yield with 24.1 kJ/g heat of combustion
- Exhaust flow rate at 0.56 m^3/s

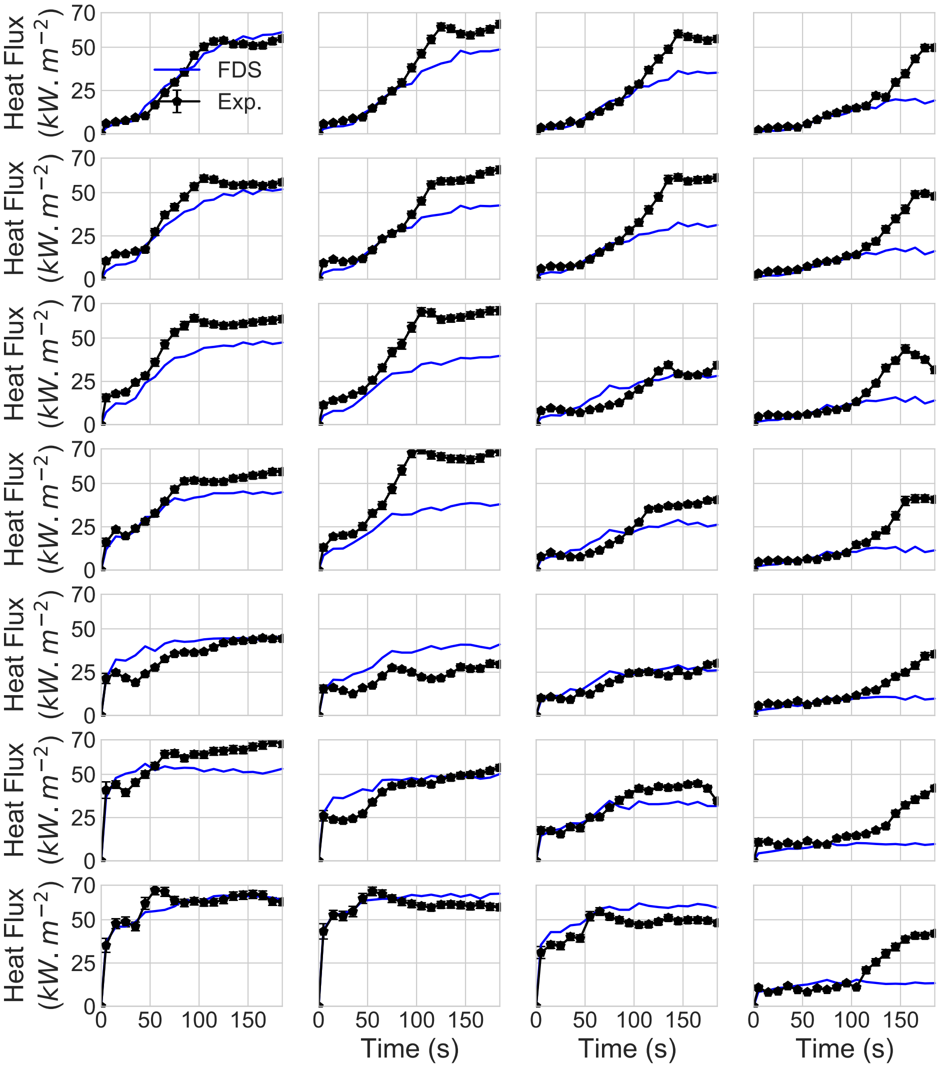
FDS results – PMMA – Total flame heat flux and wall temperature





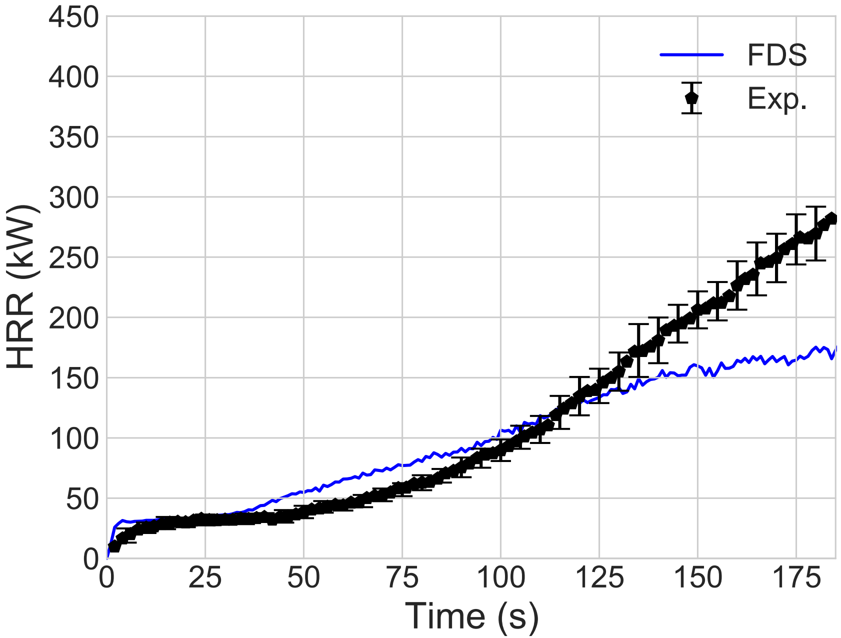
FDS results – PMMA Flame Heat Flux



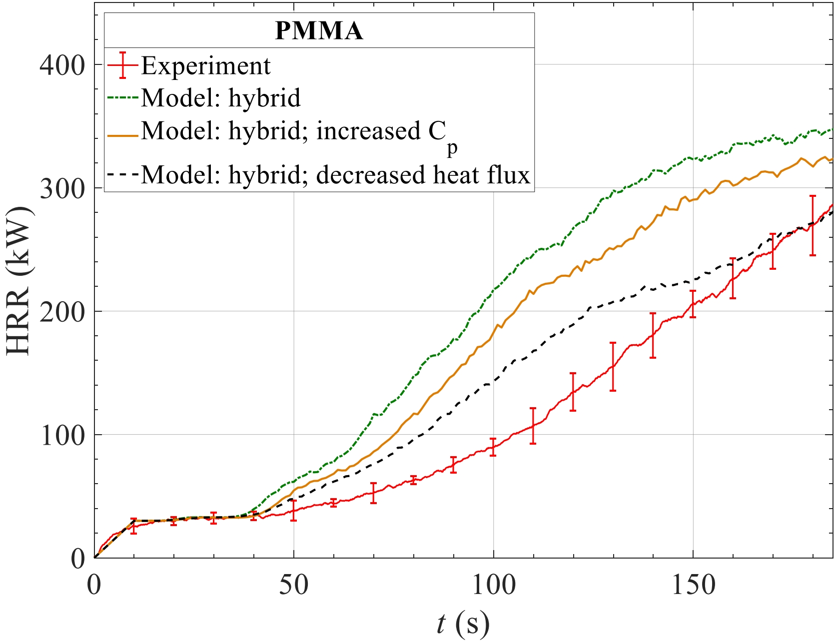


FDS results – PMMA
Heat Release Rate

FDS



Empirical Flame Spread Model



Conclusion

- Previously developed flame spread model framework applied to three materials
  - Contribution of convection and radiation affected the modeling results
  - Sensitivity of the model prediction increase for materials supporting significant flame growth
  - Underprediction for OSB attributed to the limitation of the flame heat feedback model which was calibrated on PMMA data
  - This limitation could be overcome by calibrating the flame heat feedback model for materials with different radiative fractions
- Preliminary FDS simulations indicate that FDS can predict flame spread over PMMA
  - Further refinement of mesh and sensitivity to other model parameters is part of the future work

Acknowledgements

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Thank you for your attention!

Contact: dushyant.chaudhari@ul.org for questions/comments/discussion