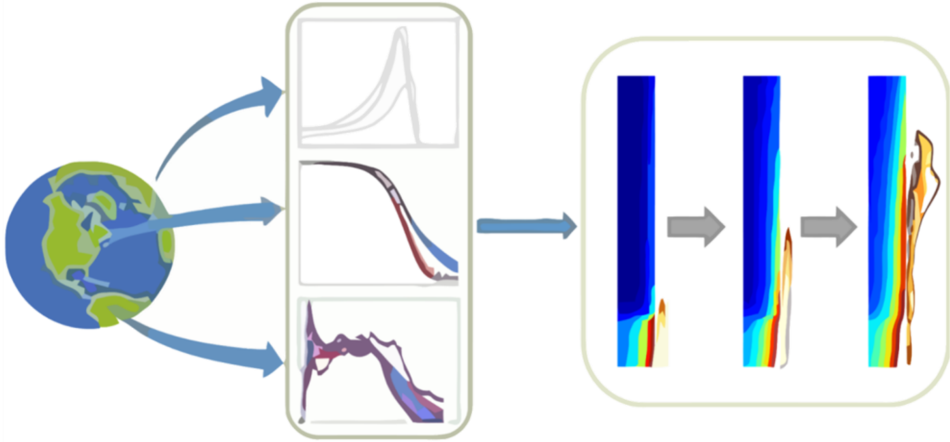
Presentation of Pyrolysis Models for use in the MaCFP-3 Workshop

<u>NIST-Gasification Session Chairs:</u>
Morgan Bruns (St. Mary's University, USA)
Jason Floyd (UL-FSRI, USA)
Bjarne Husted (DBI, Denmark)
Isaac Leventon (NIST, USA)

<u>Condensed Phase Organizing Committee:</u>
Benjamin Batiot (University of Poitiers, France)
Morgan Bruns (St. Mary's University, USA)
Simo Hostikka (Aalto University, Finland)
Isaac Leventon (NIST, USA)
Yuji Nakamura (Toyohashi Univ. of Technology, Japan)
Pedro Reszka (Universidad Adolfo Ibáñez, Chile)
Thomas Rogaume (University of Poitiers, France)
Stanislav Stoliarov (University of Maryland, USA)



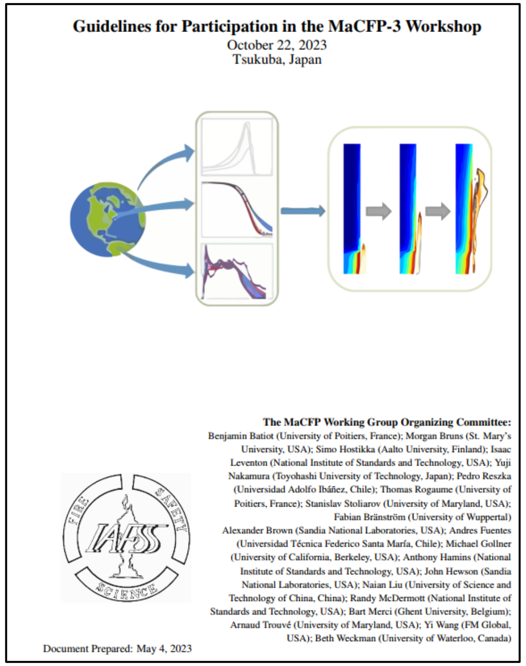
This meeting will be recorded

Virtual Meeting Agenda (June 20, 2023)

- Timeline of Events in Preparation for the MaCFP-3 Workshop
- Pyrolysis Model Development
  - Material Selection (MaCFP-PMMA)
  - MaCFP-2
    - Experiments & Model Calibration Techniques
    - Model-to-Model Comparison (ideal gasification scenario)
  - MaCFP-3
    - Experimental measurements (NIST-Gasification dataset)
    - Model (Re)Calibration
    - Model Validation (Simulation Results)
    - Identification of recommended material property sets
- Next Steps
  - Simulation of flame spread over MaCFP-PMMA: 1.46 m tall corner wall, 2.44 m tall parallel panels
  - MaCFP-3 Target Cases and Timeline
- Open Discussion
  - What are the MaCFP Community's wants/needs?
  - How can the MaCFP Organizing committee help to facilitate/coordinate these efforts?

Workshop Timeline

Date	Objective
December 20, 2022	Share call for participation in MaCFP-3 Experimental Measurements (fire growth) added to repo
March 14, 2023	Share 'Guidelines for Participation in MaCFP-3' document Modeling results from MaCFP-2 organized and added to Github Repo (simulations data + PMMA pyrolysis model parameters) Pyrolysis modeling validation dataset added to repo
March 23, 2023 12:30 PM (EST)	Virtual meeting (all participants welcome) Share new experimental data (NIST gasification apparatus); condensed-phase modelers are asked to perform: (a) Blind validation: Predict these new results based on their original pyrolysis model properties. (b) Recalibration: Adjust pyrolysis model parameters *as needed* to provide better predictions (modelers must describe any changes made) Introduce MaCFP-3 gas-phase and coupled condensed- and gas-phase target cases
June 1, 2023	Condensed-phase modelers asked to prepare and submit final parameter sets and model predictions of: (1) New experimental data (NIST Gasification Apparatus) (2) Ideal gasification tests (Incident heat flux, $\dot{q}''$ =10, 25, 65 kW m^{-2}; Sample thickness, 6 mm and 12 mm)
June 20, 2023	Virtual Meeting (all participants welcome): Present validation of pyrolysis model parameter sets based on new gasification data Preliminary analysis - relative impact on variability in final model predictions
June 30, 2023	Poster abstract submission deadline (abstract of modeling submissions for the MaCFP-3 Workshop).
August 31, 2023	Deadline to share flame spread modeling results
October 22, 2023	MaCFP-3 Workshop: Tsukuba, Japan


Guidelines for Participation in the MaCFP-3 Workshop
October 22, 2023
Tsukuba, Japan

The MaCFP Working Group Organizing Committee:
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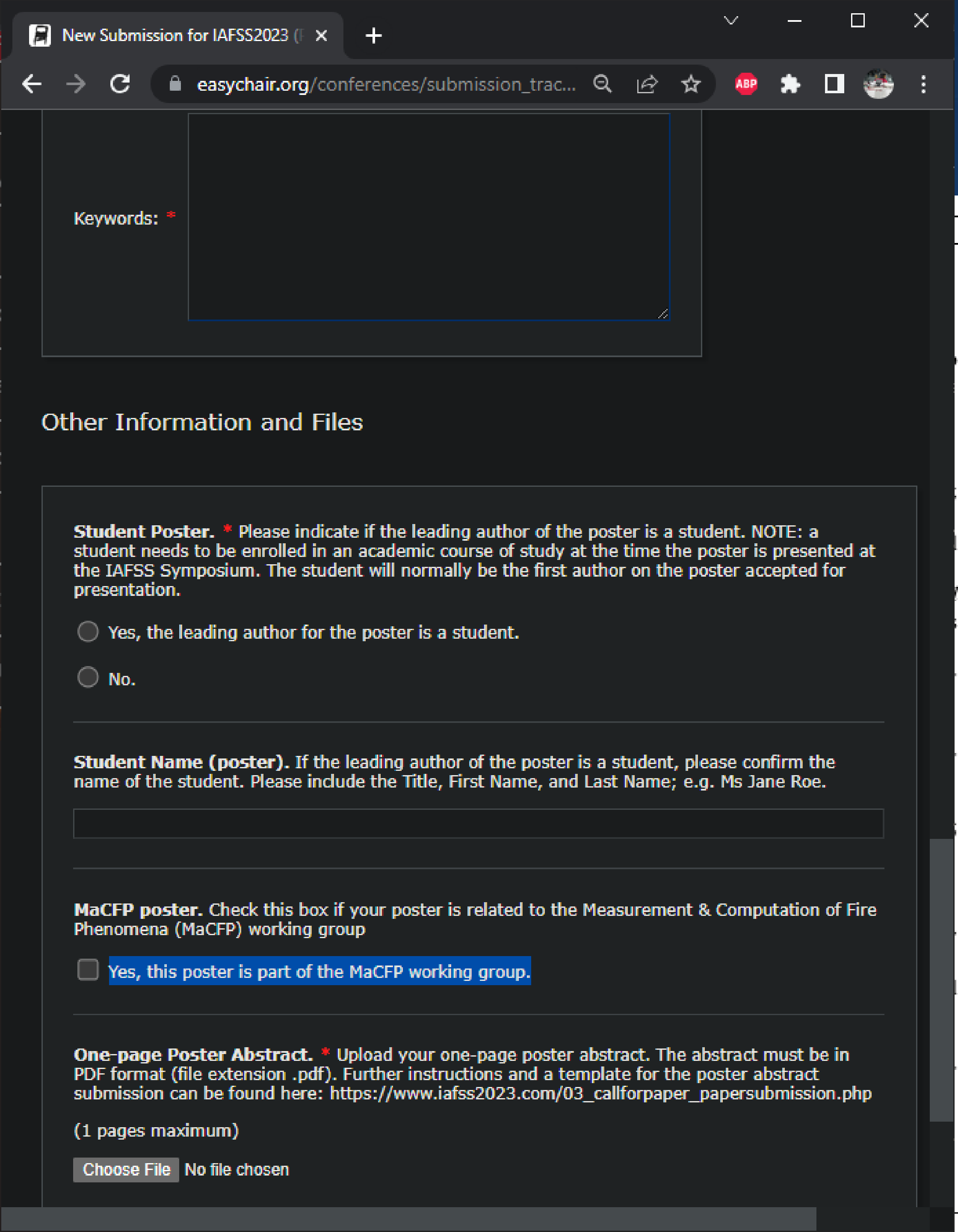
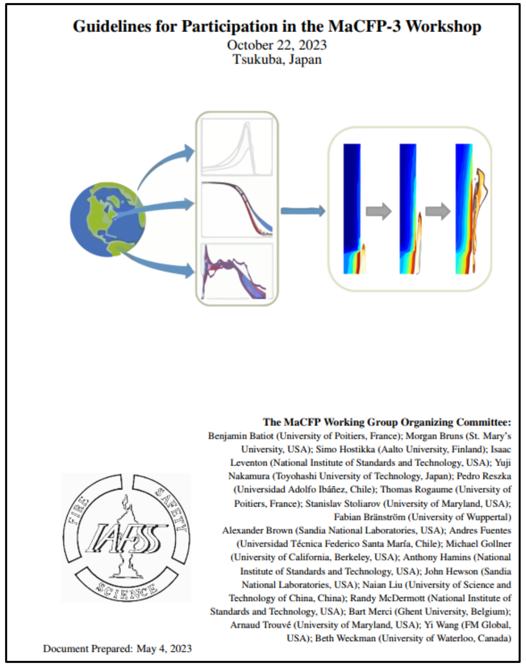
Document Prepared: May 4, 2023

A video recording of this presentation, session slides, and a .pdf copy of the Guidelines Document that summarizes all five target experiments and describes how to participate in this workshop by submitting modeling results is available as a MaCFP Github Repository Release.

All participants who wish to participate in MaCFP-3 by submitting modeling results are asked to prepare a poster summarizing their work for display at the Workshop.

One-page poster abstracts should be electronically submitted by **June 30, 2023:** Submit MaCFP Poster Abstract.





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MaCFP-2 Material Selection

- Cast black poly(methyl methacrylate) (PMMA)
  - Evonik ACRYLITE® cast black 9H01 GT
  - Distributed in summer 2019
    - 100 mm by 100 mm by 6 mm slabs
    - 300 mg vials of powdered PMMA

- Suitable first reference material
  - Maintains density/shape while burning
  - Simple decomposition kinetics
  - Low transparency to infrared radiation

The identification of any commercial product or trade name does not imply endorsement or recommendation by NIST (or any other contributing institution).

Summary of MaCFP-2 Results: Experimental Data & Pyrolysis Models (Property Sets) Submitted

- Three objectives:
  1. Develop repository of experimental data for model calibration
  2. Derive material property sets from experimental data
  3. Use material property sets to predict TGA & ideal gasification
- Experimental Measurements prepared by 16 institutions:

Aalto	FM Global	NIST	UCLAN	UMET
DBI-Lund	GIHAZE+	Sandia	UDRI	UQueensland
Edinburgh	LCPP	TIFP	UMD	VMI

Additional data later received from USDA, Ulster, UL-FSRI

- Property sets and predictions from 9 institutions: Aalto, BUW-FZJ, DBI, GIDAZE+, NIST, SANDIA, UCLAN, UMD, UMET
  - 12 complete property sets
  - 7 pure kinetics property sets
- Property sets stored on Github Repo in JSON
  - JSON is Parseable (Python) + Readable (Human)
  - Data organized as “Material”, “Lab”, “Calibration” (metadata on property determination), “Kinetics”, “Thermodynamics”, and “Transport”
  - Available at: https://github.com/MaCFP/matl-db/tree/master/PMMA/Material_Properties

Calibration Method Summary

Data	Models	Methods
• TGA at many heating rates • Gasification/CAPA • STA (TGA/DSC) • Heat flow meter • Hot disk • UV-Vis and FTIR • Literature data and values	• FDS, Gpyro, ThermaKin, Sierra Thermal/Fluids • One-step, two-step (series and parallel) reaction mechanism • 1st order and nth order kinetics	• PROPTI, Gpyro, MatCal+Dakota tools • Shuffled complex evolution • Other optimization • Algebraic • Monte Carlo sampling • Manual updating • Direct measurment

```
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    "Lab": "Aalto",

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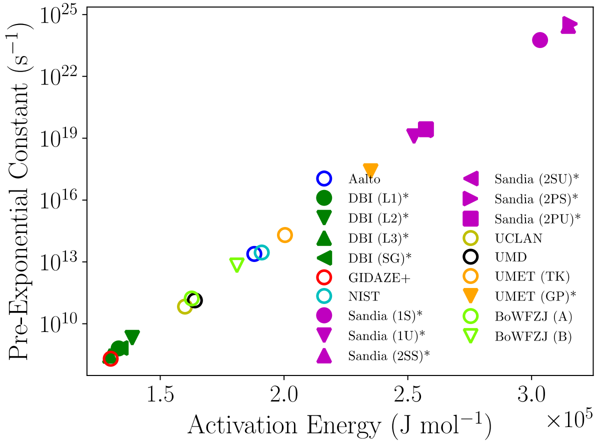
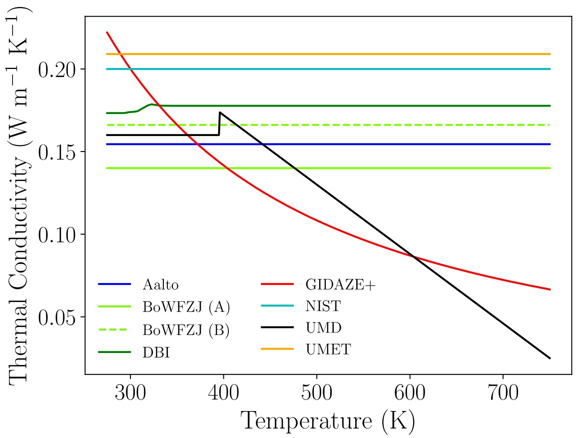
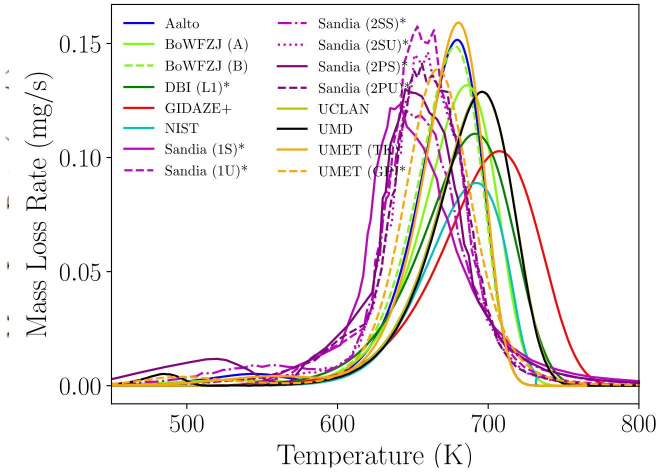
Summary of MaCFP-2 Results: Pyrolysis Model Variability

- Variation in Material Properties:
  - Typical variability within 10 % to 50 % of averages
  - No order of magnitude differences
- Predicted TGA behavior
  - At 10 K/min:
    - Scatter is about twice that seen in experimental
    - 30K range in Tpeak
  - At 100 K/min:
    - 80K range in Tpeak
- Key Questions
  - What are the most influential properties?
  - Are predictions sensitive to changes within this variability?
- Consider impact of these variations in idealized gasification scenario (model to model comparison)







Predicted TGA at 100 K min^{-1}

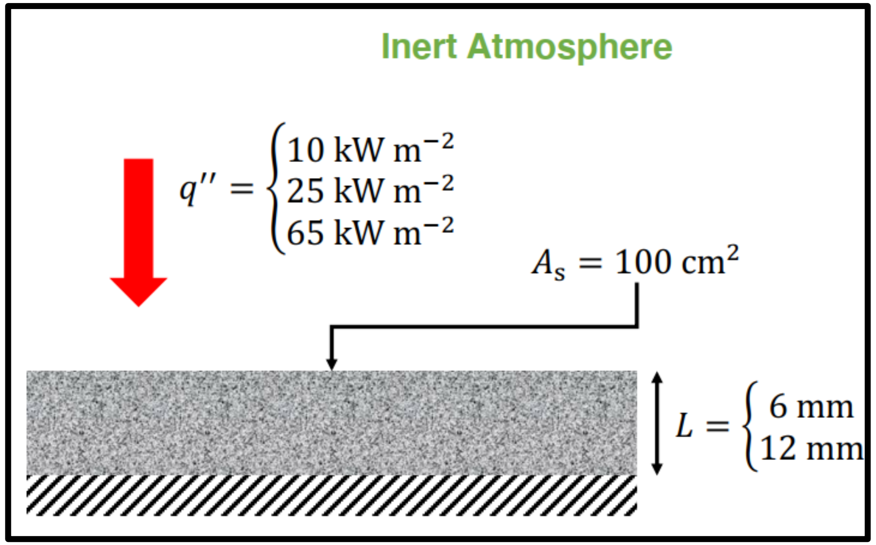
Summary of MaCFP-2 Results:
Sensitivity Analysis: Impact of Model Variability

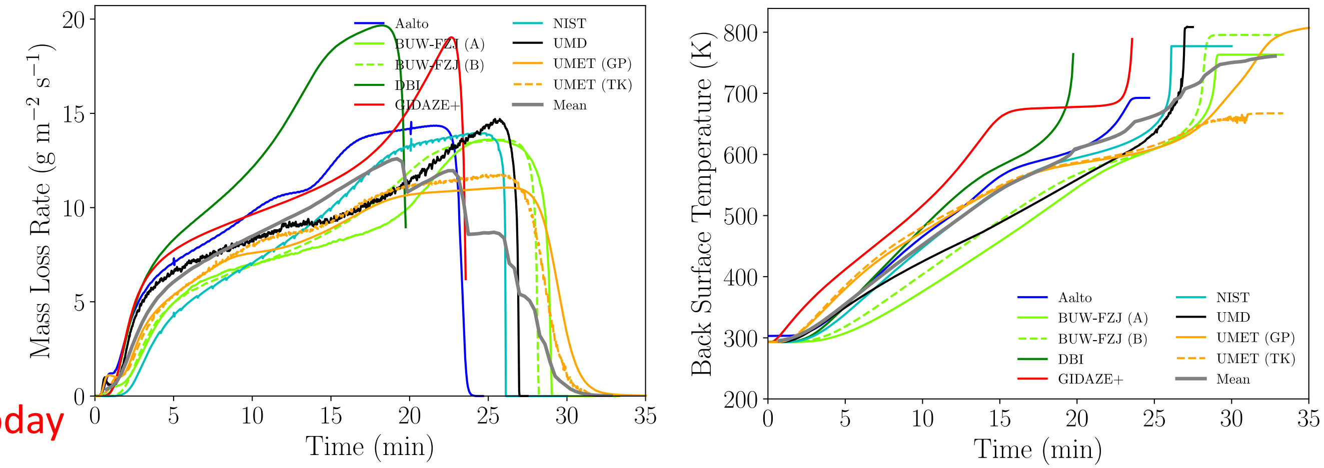
- Variation in Material Properties:
  - Typical variability within 10 % to 50 % of averages
  - No order of magnitude differences

- Predictions of [Idealized Slab Gasification]using MaCFP-2 property sets:
  - Peak Mass Loss Rate:
    - High heat fluxes, Peak MLR varies by up to ~75 %
    - Low heat fluxes: time to peak MLR varies by up to ~85 %
  - Time to onset of gasification
    - Order of magnitude variations at all heat fluxes

- Which property set to use for flame spread modeling?
  - March 2023: "Most central" property set: [UMD]
    - Property set with predictions closest (sum of square errors) to mean gasification predictions
    - NOT implied to be the most accurate property set
  - June 2023: "Most representative" property set: defined today
    - Define Property set that most closely reproduces validation experiments of the [NIST-Gasification dataset]

Idealized gasification scenario



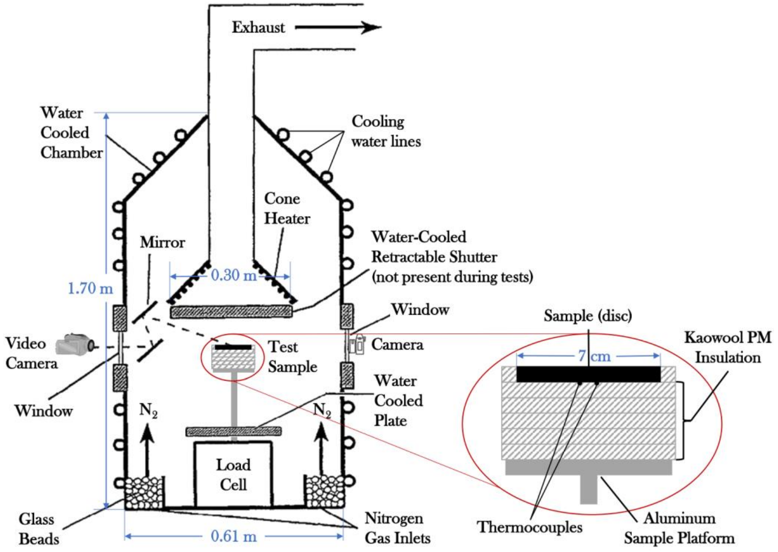


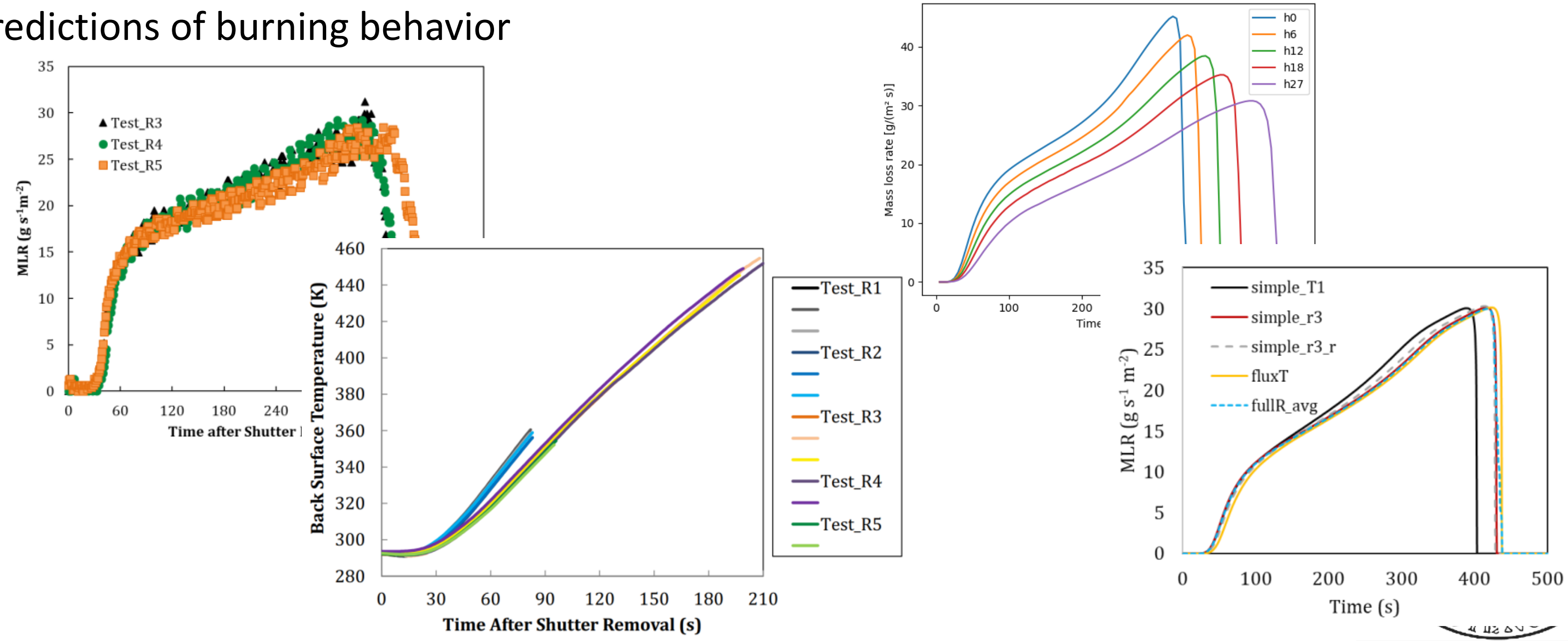
Gasification at q''=25 kW m^{-2}, L = 12 mm

MaCFP-3 Pyrolysis Model Validation Exercise

- Experimental
  - Develop a carefully characterized experimental dataset for pyrolysis model validation
- Model Validation
  - Compare experimental measurements and model predictions of validation dataset
  - Recalibrate models (material property sets) if/as needed
  - Identify a recommended material property set for use in MaCFP-3 flame spread cases
- Model Sensitivity
  - Relative impact of variability in material properties on model predictions of burning behavior
  - Impact of model parameterization on predictions of burning behavior

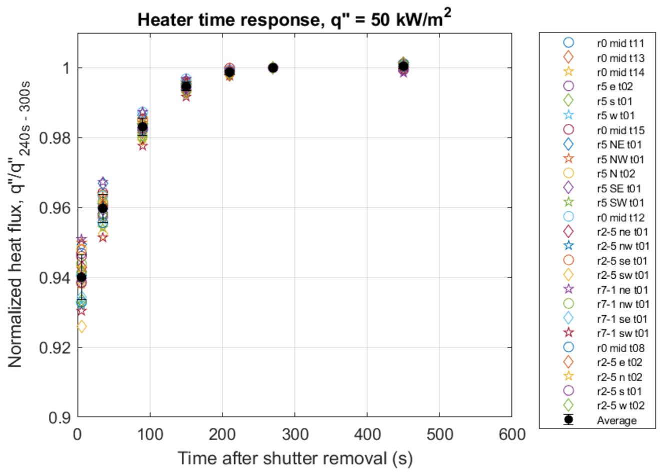
Symbol	Units	Name
	Degradation Kinetics	
A	s^{-1}	Pre-exponential constant
E	$J\ mol^{-1}$	Activation energy
n	[-]	Reaction order
ν	[-]	Stoichiometric coefficient
	Thermodynamic Properties	
c_p	$J\ kg^{-1}\ K^{-1}$	Heat capacity
h_r	$J\ kg^{-1}$	Heat of reaction
ρ	$kg\ m^{-3}$	Density
	Transport Properties	
k	$W\ m^{-1}\ K^{-1}$	Thermal conductivity
D	$m^2\ s^{-1}$	Mass diffusivity
α	m^{-1} or $m^2\ kg^{-1}$	Absorption coefficient
ε	[-]	Emissivity

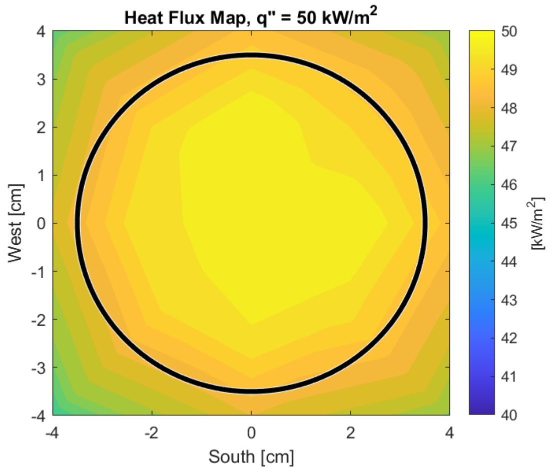


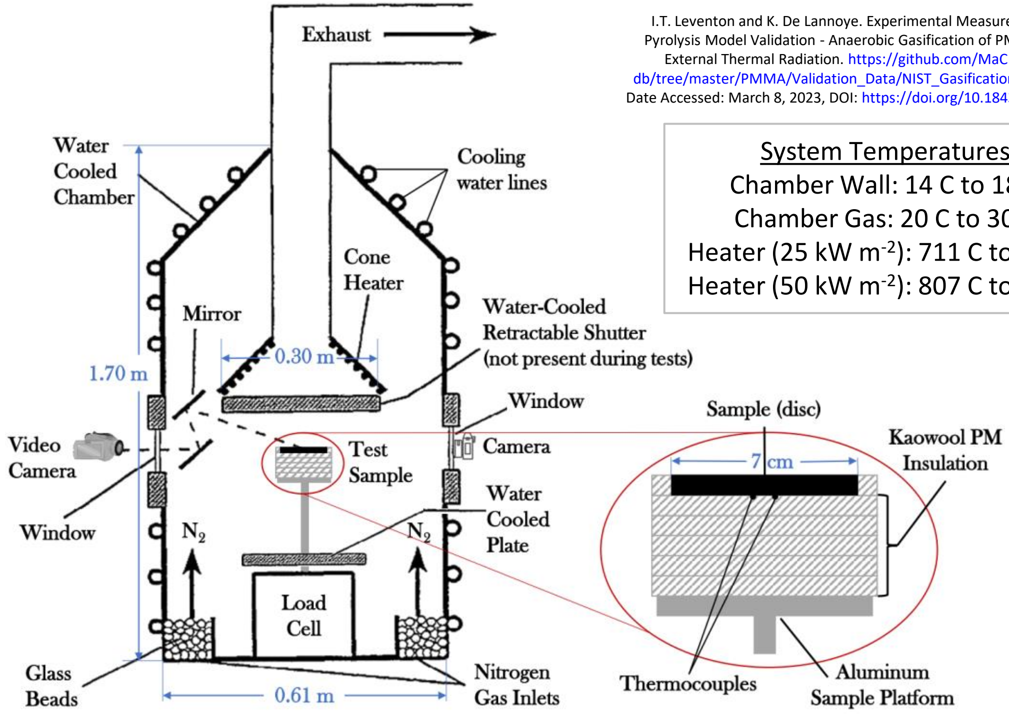


NIST-Gasification-Apparatus: Experimental Setup

- Anaerobic environment (N_2); 30 cm cone heater; water-cooled chamber
- Boundary conditions carefully characterized: time- and spatially-resolved measurements of incident radiant heat flux [25 or 50 kW m^{-2}]; chamber wall temperatures; chamber gas temperature).
- Samples: PMMA discs (7 cm diameter, ~5.8 mm thickness), mounted to rigid ceramic insulation (Kaowool PM)
- Store sample/insulation in desiccator >24 hours, confirm incident heat flux, load sample, purge chamber (N_2), expose sample to radiant heat flux







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System Temperatures

Chamber Wall: 14 C to 18 C
Chamber Gas: 20 C to 30 C
Heater (25 kW m^{-2}): 711 C to 713 C
Heater (50 kW m^{-2}): 807 C to 808 C

Measurement data includes:

- Time-resolved measurements of PMMA sample mass [g]
- Time-resolved measurements of PMMA back surface temperature [K]
- Photographs & video of PMMA decomposition behavior
- Additional Validation tests: Time-resolved measurements of temperature rise of inert materials (copper and Kaowool PM insulation)

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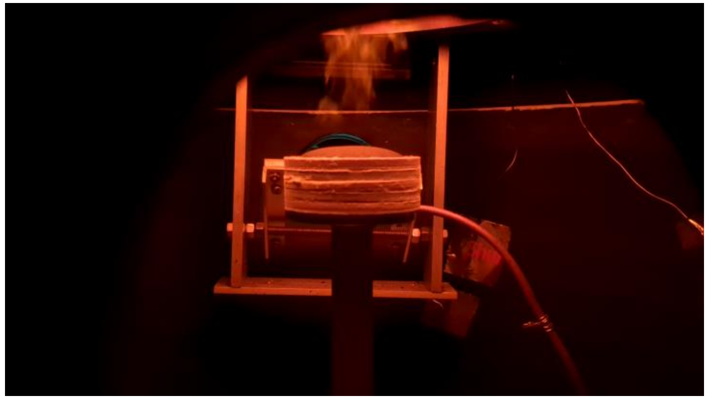
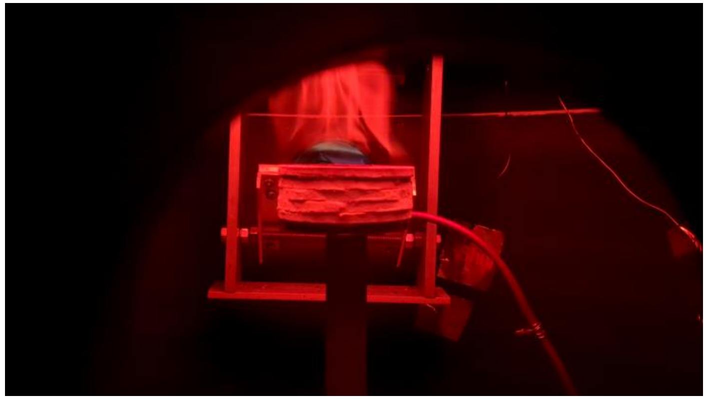
NIST-Gasification-Apparatus: Experimental Measurements / Modeling Targets

- Validation Exercise:
  - Predict material response to these test conditions using <u>original</u> MaCFP-2 pyrolysis models; recalibrate if needed



Sample Deformation Not Controlled



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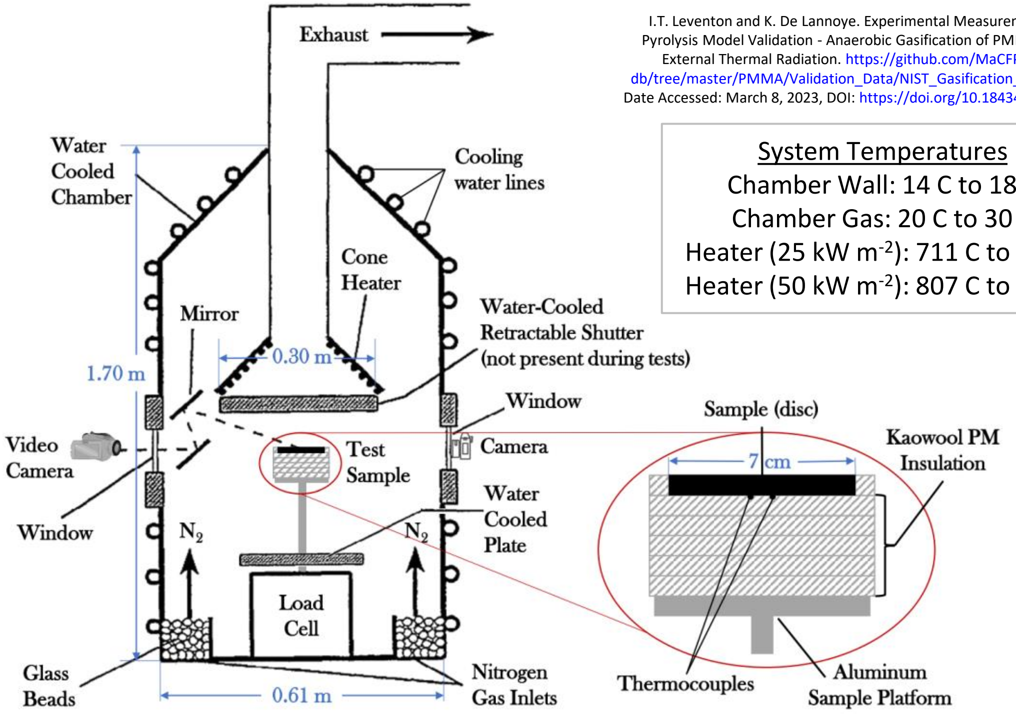

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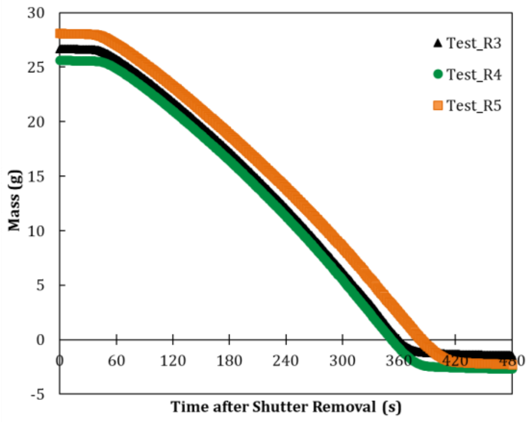
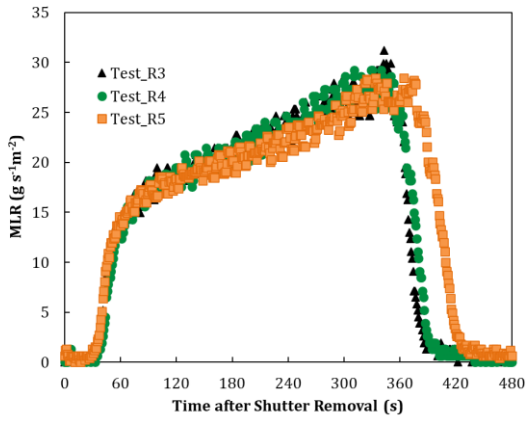
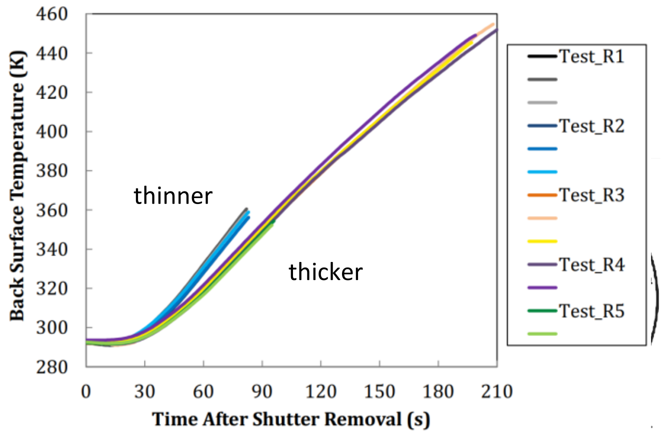
Measured mass loss and back surface temperature rise at $\dot{q}''_{ext} = 50$ kW m^{-2} →







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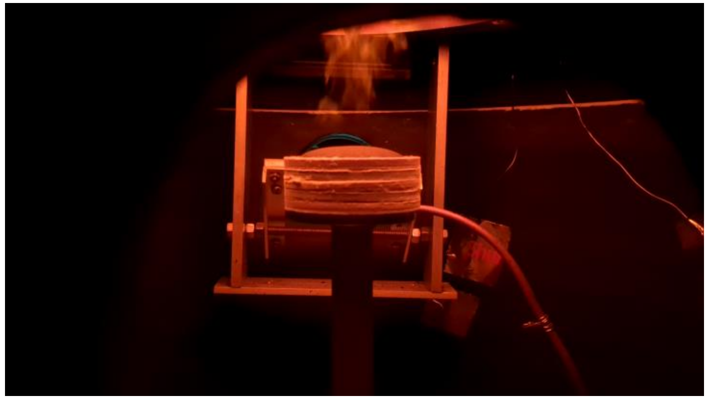

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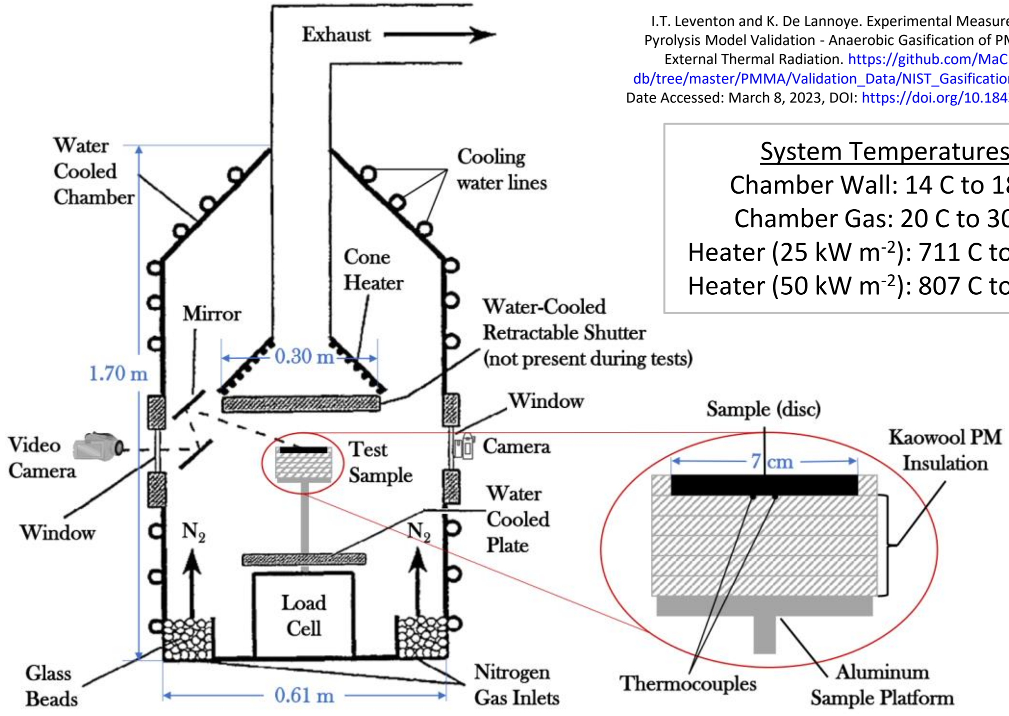

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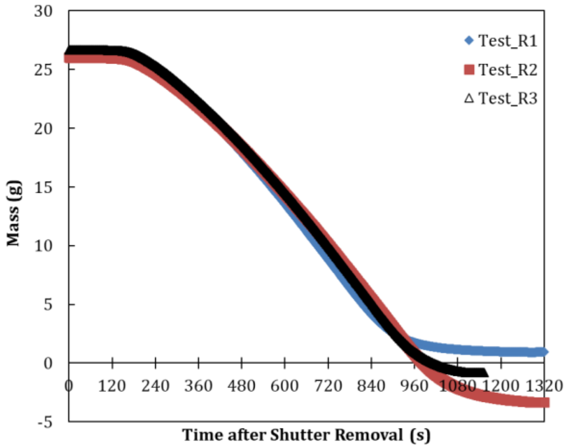
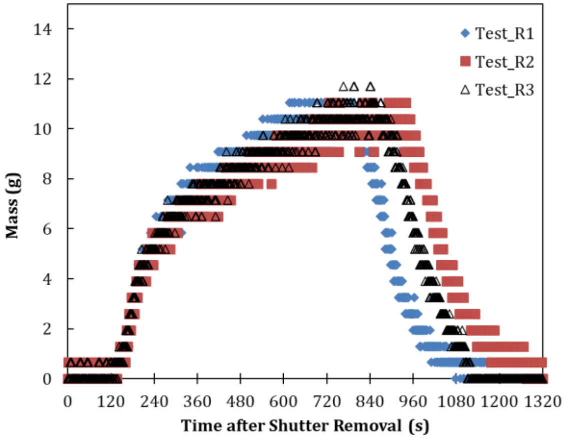
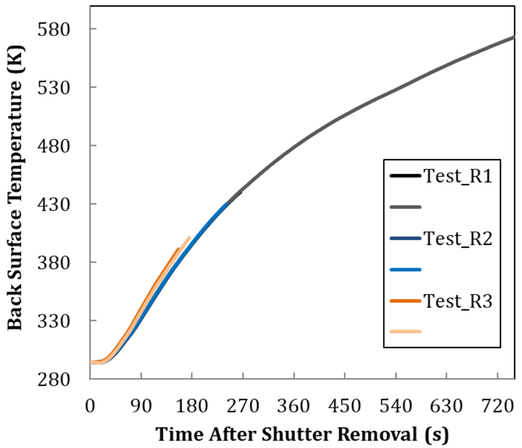
Measured mass loss and back surface temperature rise at $\dot{q}''_{ext} = 25$ kW m^{-2}







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NIST-Gasification-Apparatus: Model Validation

- Complete pyrolysis models (material property sets) considered:
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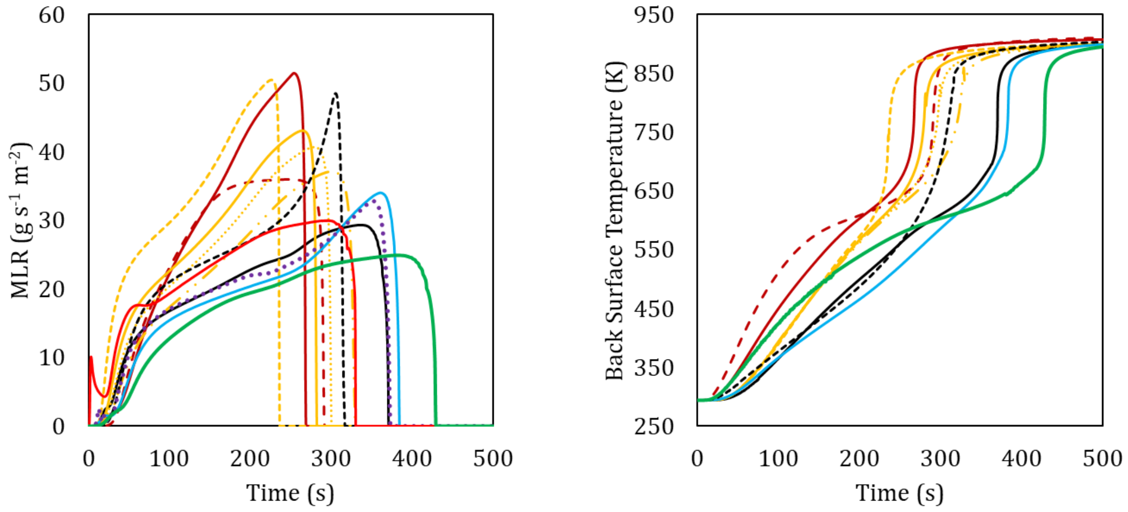
MaCFP-2

$$q''_{ext} = 50 \text{ kW m}^{-2}$$



Acknowledge: Jason Floyd

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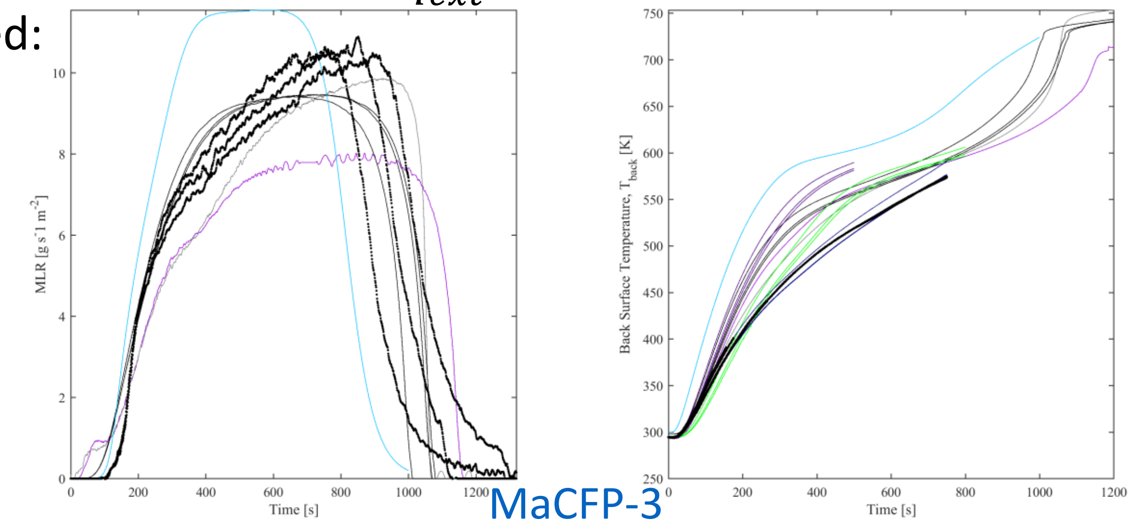
  - MaCFP-3 (New/Recalibrated): Aalto, BUW-FZJ, DBI, EDF, NIST-StMU

$\dot{q}''_{ext} = 25$ kW m^{-2}



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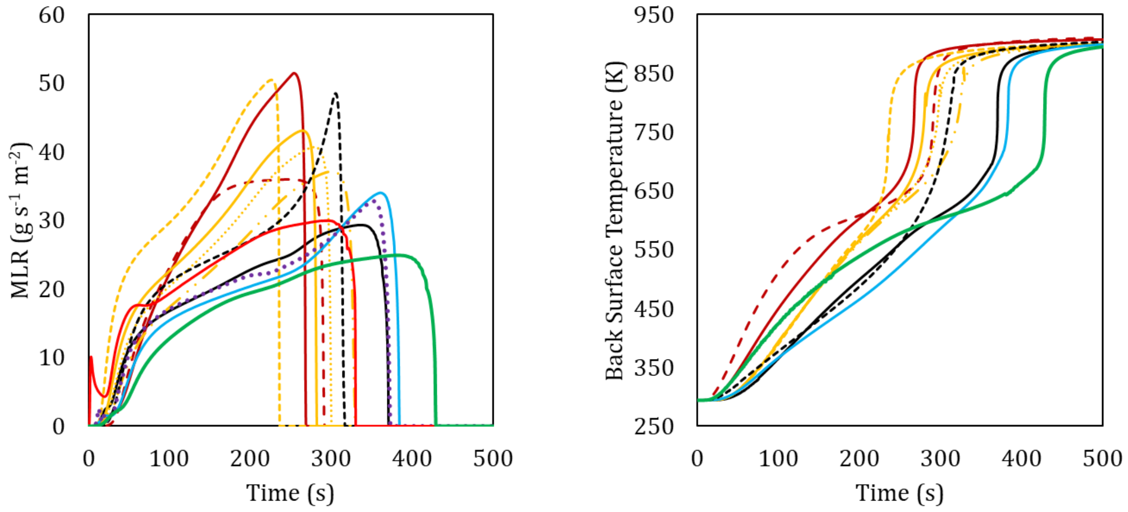
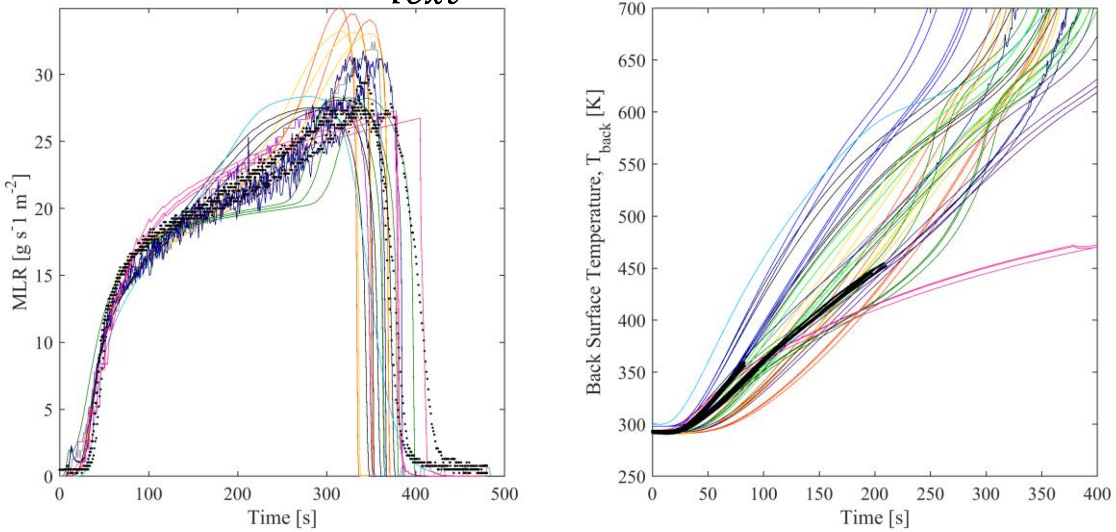


MaCFP-3

$\dot{q}''_{ext} = 50$ kW m^{-2}



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  - MaCFP-3 (New/Recalibrated): Aalto, BUW-FZJ, DBI, NIST-StMU, UMET
- Recalibrated Property sets:
  - DBI: peak MLR too high, identified low heat of decomposition, recalibrate vs. new DSC data
  - BUW-FZJ: include additional datasets during model calibration (PROPTI)
  - NIST: Recalibrate using suite of automated calibration tools
  - Aalto: Additional model with [hi-fidelity treatment of radiation absorption/emission]
  - UMET: New property set based on literature values

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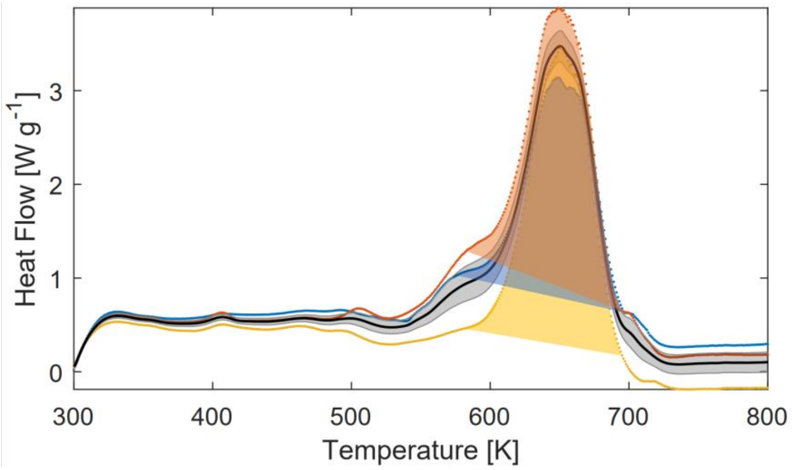
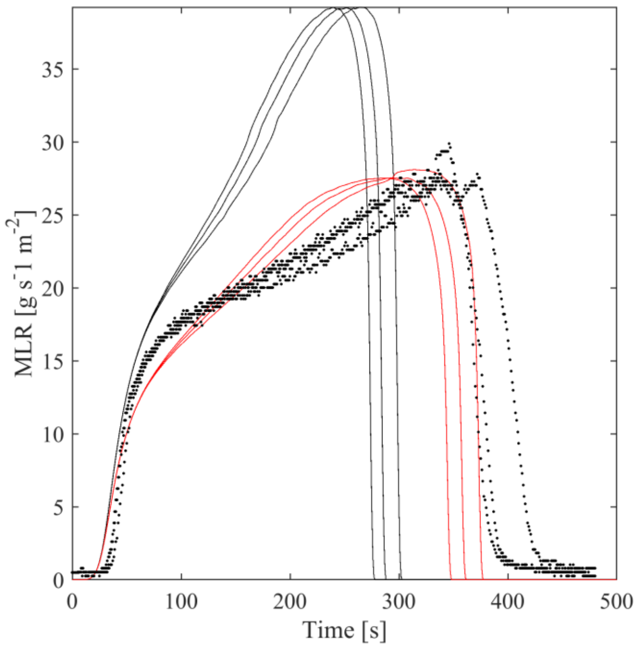
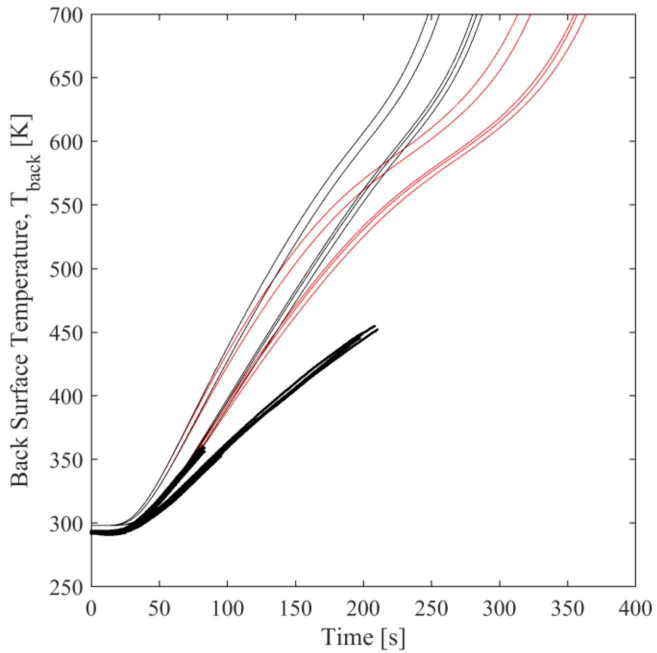






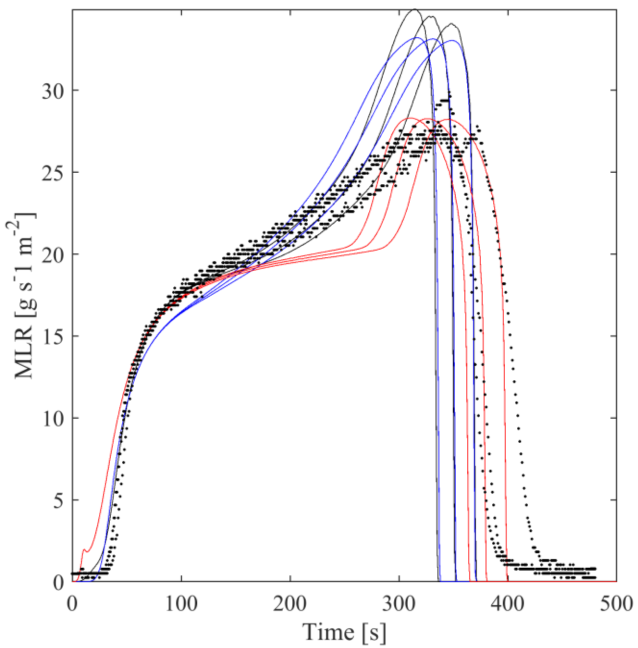
$q''_{ext} = 50 \text{ kW m}^{-2}$

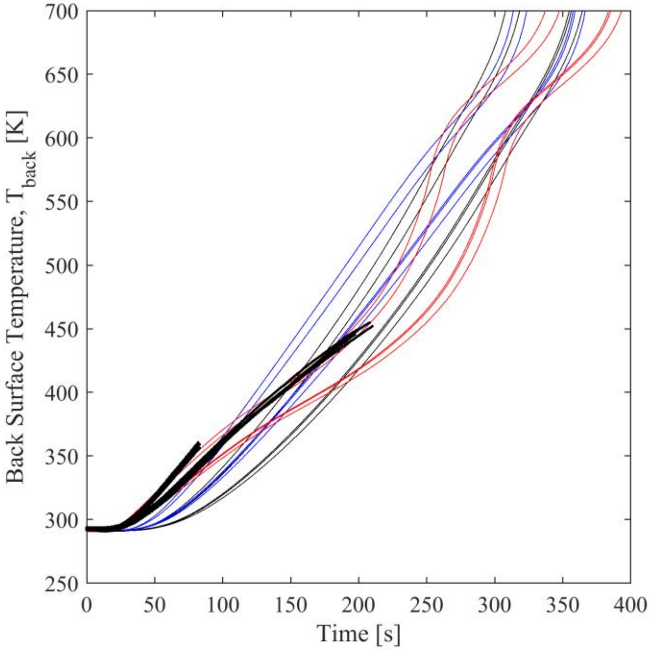
NIST-Gasification-Apparatus: Model Validation

- Complete pyrolysis models (material property sets) considered:
  - MaCFP-2: Aalto, BUW-FZJ, DBI, GIDAZE+, NIST, UMD, UMET
  - MaCFP-3 (New/Recalibrated): Aalto, BUW-FZJ, DBI, NIST-StMU, UMET
- Recalibrated Property sets:
  - BUW-FZJ: include additional datasets during model calibration (PROPTI)

<u>Calibration by inverse analysis</u>
Shuffled Complex Evolution (SCE)

<u>Differences in calibration target datasets:</u>
Model A (MaCFP-2): TGA, kinetics; Gasification, all others
Model B (MaCFP-2): Gasification, all properties
Model C (MaCFP-2): MCC, TGA, DSC, Cone





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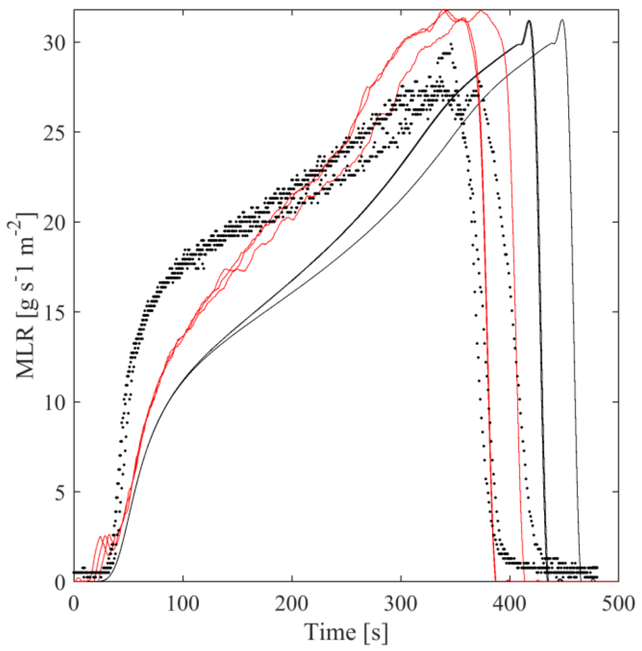
  - MaCFP-3 (New/Recalibrated): Aalto, BUW-FZJ, DBI, NIST-StMU, UMET
- Recalibrated Property sets:
  - NIST: Recalibrate using suite of automated calibration tools

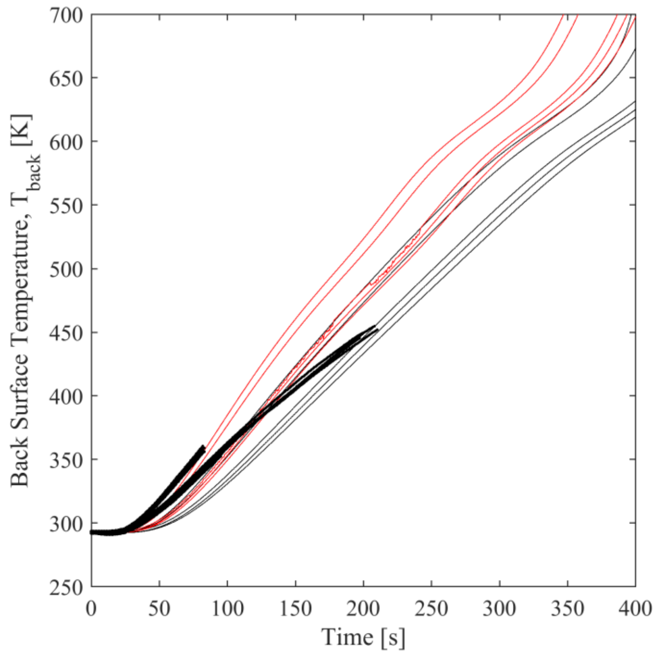
Bruns, M.C. and Leventon, I.T., "**Automated Fitting of Thermogravimetric Data**," *Fire and Materials*, 2021

Bruns, M.C. and Leventon, I.T., "**Automated Characterization of Pyrolysis Kinetics And Heats of Combustion Of Flammable Materials**," Ninth Triennial International Fire & Cabin Safety Research Conference, Atlantic City, New Jersey, October, 2019

Bruns, M.C. and Leventon , I. - **"Automated Characterization of Heat Capacities and Heats of Pyrolysis of Flammable Materials"**, Tenth Triennial International Fire & Cabin Safety Research Conference, Atlantic City, New Jersey, October, 2022

Leventon, I. and Bruns, M. - **"The NIST Material Flammability Database: Experimental Measurements for Fire Model Calibration and Validation"**, ACS Fire and Polymers, Napa, CA, June, 2022.





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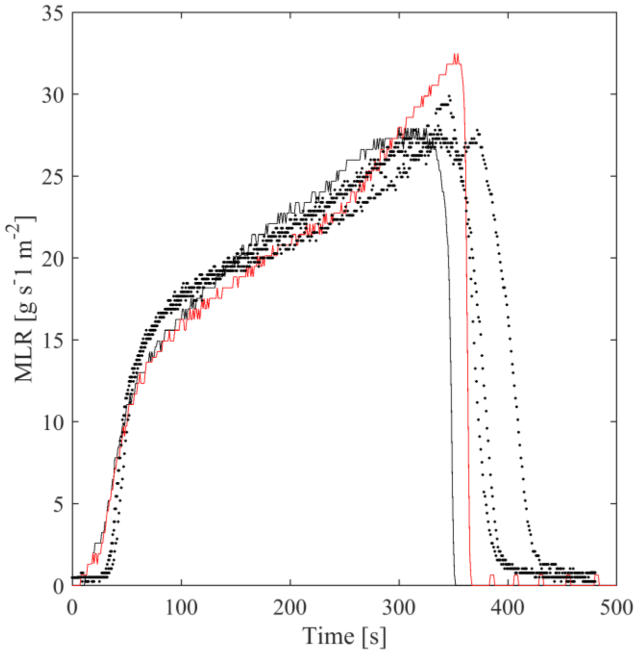
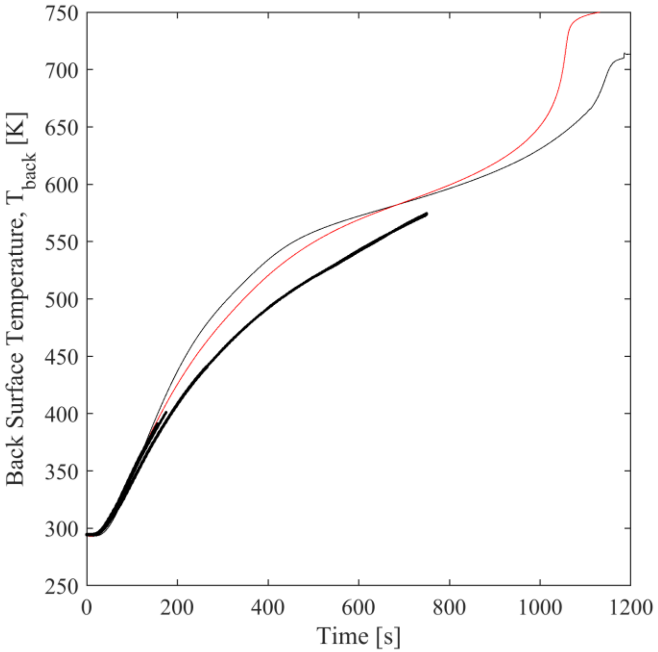
  - MaCFP-3 (New/Recalibrated): Aalto, BUW-FZJ, DBI, NIST-StMU, UMET
- Recalibrated Property sets:
  - Aalto: Additional model with [hi-fidelity treatment of radiation absorption/emission]

Aalto I (MaCFP-2): Radiation with constant kappa. Public FDS features.
Aalto II (MaCFP-3): Radiation with depth- and source temperature -dependent kappa [1]. The two-parameter fit was obtained by first measuring black PMMA spectral properties [3,4], and fitting an effective kappa to the averaged data of spectrally accurate calculation [4].
→ Reproduces the effect of wavelength -dependent absorption with low computational cost. Method is implemented in Farid Alinejad's FDS fork [5]



$q''_{ext} = 50$ kW m^{-2}



$q''_{ext} = 25$ kW m^{-2}

NIST-Gasification-Apparatus: Model Validation

- Complete pyrolysis models (material property sets) considered:
  - MaCFP-2: Aalto, BUW-FZJ, DBI, GIDAZE+, NIST, UMD, UMET
  - MaCFP-3 (New/Recalibrated): Aalto, BUW-FZJ, DBI, NIST-StMU, UMET
- Recalibrated Property sets:
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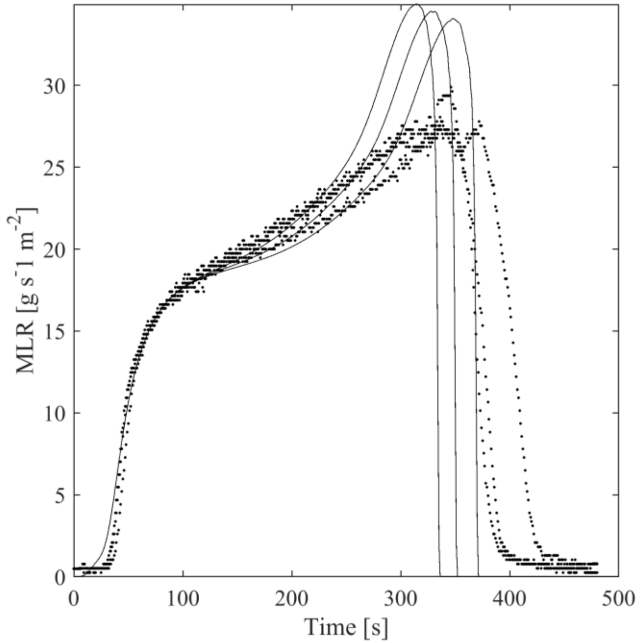


$q''_{ext} = 50$ kW m^{-2}

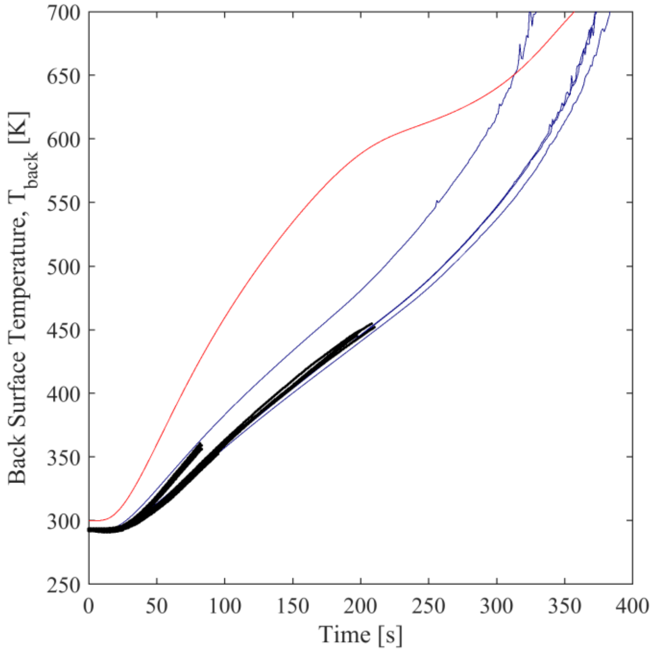
1. Alinejad, F., Bordbar, H., & Hostikka, S. (2023). On the importance and modeling of in-depth spectral radiation absorption in the pyrolysis of black PMMA. *Fire Safety Journal*, *135*, 103706. https://doi.org/10.1016/j.firesaf.2022.103706
2. Alinejad F., Bordbar H., Makowska M., Hostikka S. A dataset for spectral radiative properties of black poly (methyl methacrylate) Data Brief, 42 (2022), Article 108097
3. Alinejad F., Bordbar H., Makowska M., Hostikka S. Spectroscopic determination of the optical constants and radiative properties of black PMMA for pyrolysis modelling. Int. J. Therm. Sci., 176 (2022), Article 107501
4. Alinejad, F. (2023). *Modeling in-depth transfer of thermal radiation in non-gray condensed materials*. [Doctoral Thesis, Aalto-yliopisto]. Aalto University. http://urn.fi/URN:ISBN:978-952-64-1249-8
5. https://github.com/FaridAlinejad/fds/tree/aaltofds

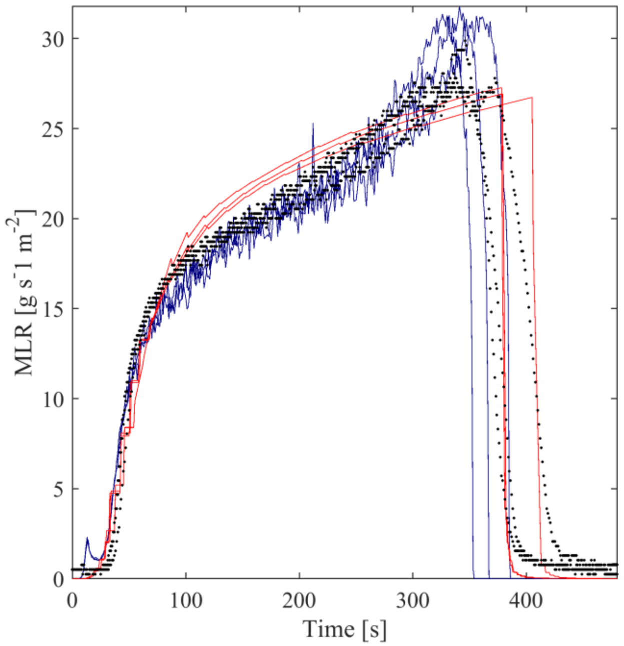
NIST-Gasification-Apparatus: Model Validation

- Complete pyrolysis models (material property sets) considered:
  - MaCFP-2: Aalto, BUW-FZJ, DBI, GIDAZE+, NIST, UMD, UMET
  - MaCFP-3 (New/Recalibrated): Aalto, BUW-FZJ, DBI, NIST-StMU, UMET

Same material property calibration approach;
Difference Material
Unique model validation simulation setup

- Recalibrated Property sets:
  - UMET: New property set based on literature values
    - Same model calibration approach as other property set, potentially demonstrates impact of material variability (Clear PMMA, 2013) OR model setup

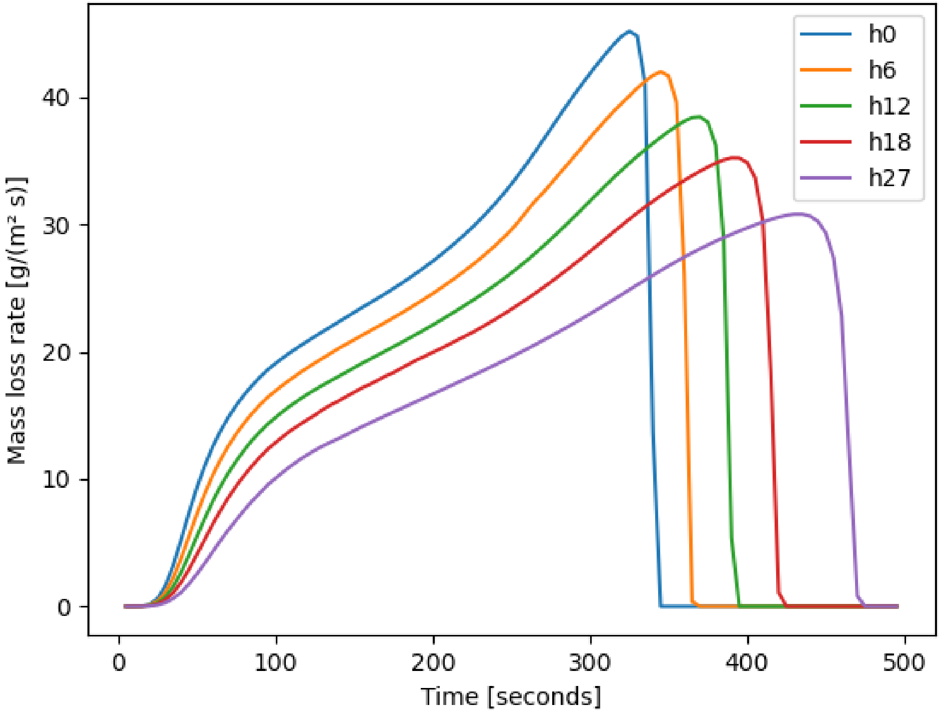




$\dot{q}''_{ext} = 50\ \mathrm{kW\ m^{-2}}$

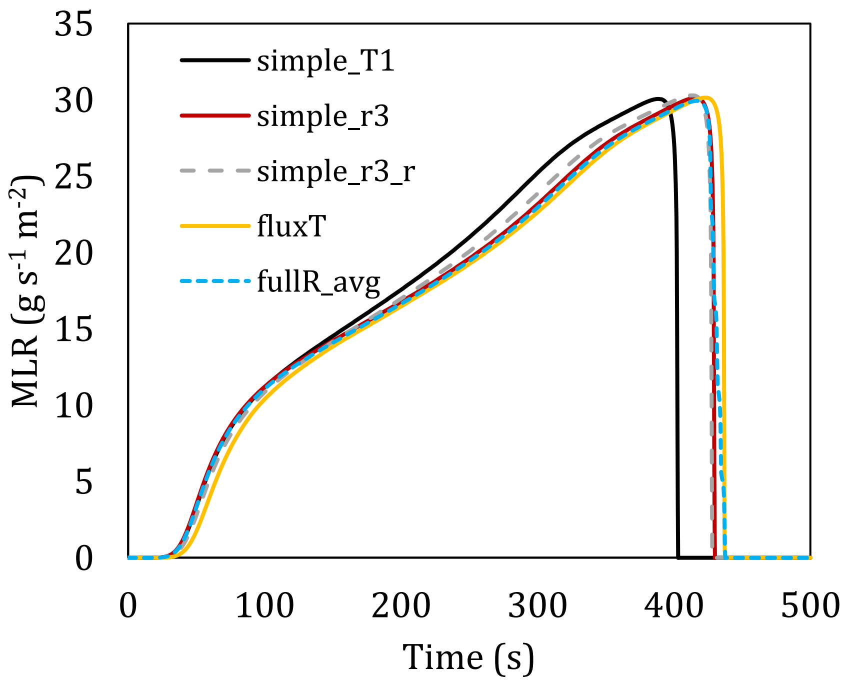
NIST-Gasification-Apparatus: Model Sensitivity to Boundary Conditions

- Complete pyrolysis models (material property sets) considered :
  - MaCFP-2: Aalto, BUW-FZJ, DBI, GIDAZE+, NIST, UMD, UMET
  - MaCFP-3 (New/Recalibrated): Aalto, BUW-FZJ, DBI, EDF, NIST
- Impact of Boundary Conditions on Model Calibration
  - DBI – Convection Heat Transfer at the Sample's Front surface



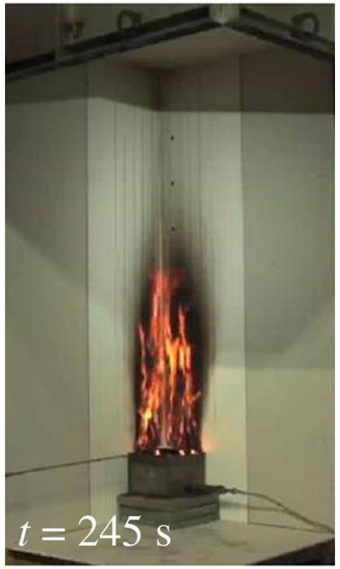
NIST-Gasification-Apparatus: Model Sensitivity to Boundary Conditions

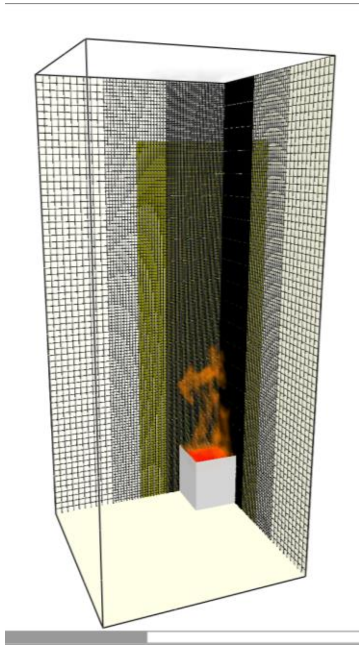
- Complete pyrolysis models (material property sets) considered :
  - MaCFP-2: Aalto, BUW-FZJ, DBI, GIDAZE+, NIST, UMD, UMET
  - MaCFP-3 (New/Recalibrated): Aalto, BUW-FZJ, DBI, EDF, NIST
- Impact of Boundary Conditions on Model Calibration
  - UL-FSRI – Constant vs. temporally- or spatially-dependent incident heating



Representative Fire Growth case: Model Sensitivity to Boundary Conditions

- 36 meshes, cubic grid cells; finer resolution (2 cm) near wall
- Turbulence model:
    - Deardorff model (Sc_t=0.5 and Pr_t=0.5)
- Combustion model:
    - Mixing controlled (EDC);
    - Two fuels (burner, C_3H_8; wall flame, $C_{5.2}H_{9.1}O_{1.8}$);
    - 'Extinction Model 1' (combustion when T>600 C, unless $Y_{O_2}^{local} = 0$)
- Radiation model
    - $N_{solid\ angles}$ = 104
    - Optically thick, gray gas model, specified radiant fraction (χ_r = 0.35)
    - Soot yields for each fuel ($Y_{soot}^{C_3H_8} = 0.01$ and $Y_{soot}^{C_{5.2}H_{9.1}O_{1.8}} = 0.075$)
    - RadCal species 'PROPANE' and 'MMA' (for burner, combustible solid)
- Sensitivity study:
    - Soot yield, $0 \leq Y_{soot}^{C_3H_8} \leq 0.02$ and $0.01 \leq Y_{soot}^{C_{5.2}H_{9.1}O_{1.8}} \leq 0.20$ [57,58]
    - Radiation Path Length, 0.05 m < $L_{rad} = 0.30$ m
    - Grid resolution, 1 cm < Δx < 4 cm near wall

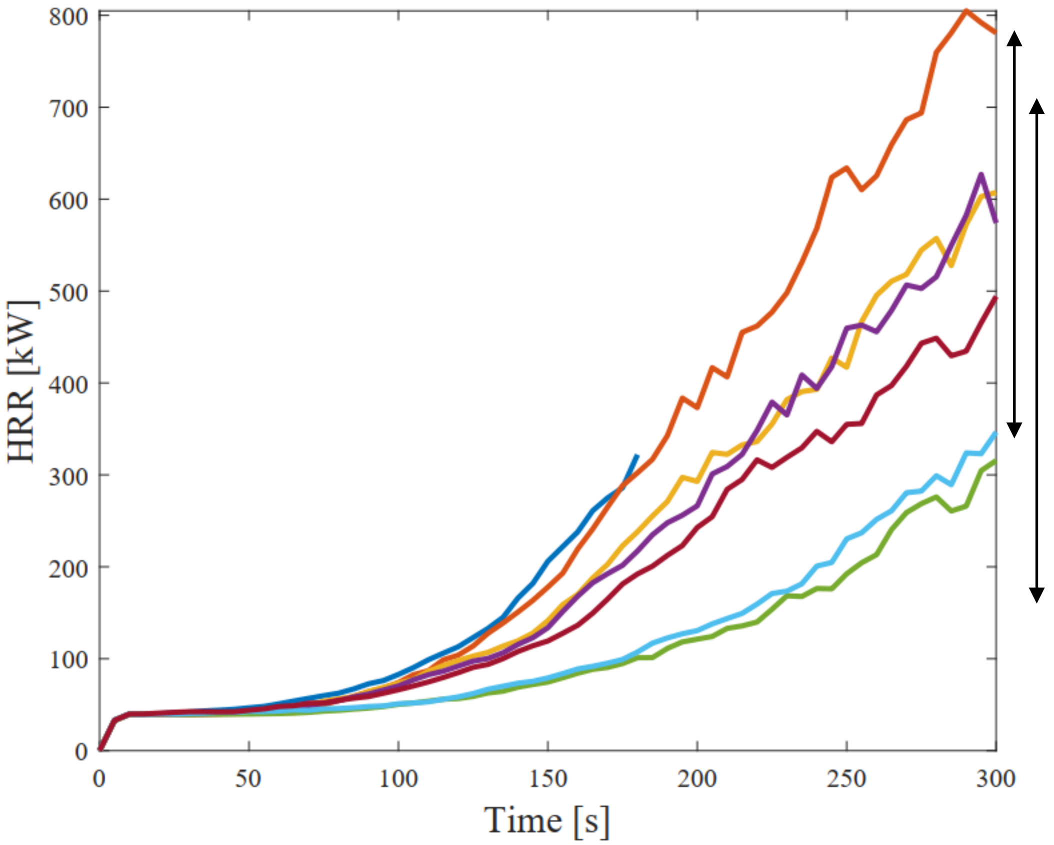


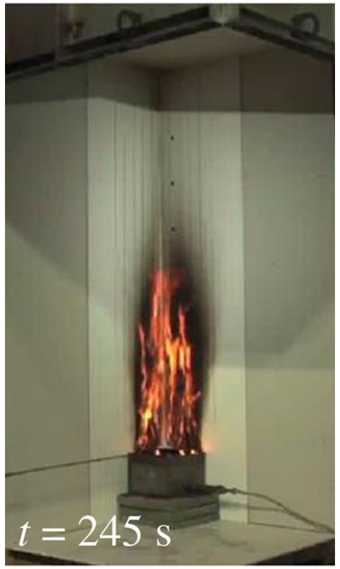


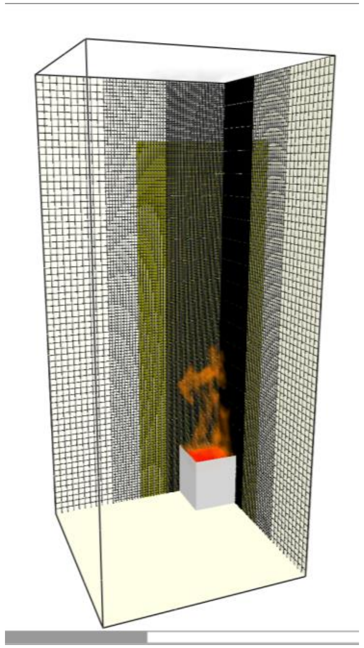
https://doi.org/10.1016/j.polymdegradstab.2023.110405

Representative Fire Growth case: Model Sensitivity to Boundary Conditions

- Complete pyrolysis models (material property sets) considered :
  - MaCFP-2: Aalto, BUW-FZJ, DBI, GIDAZE+, NIST, UMD, UMET
  - MaCFP-3 (Recalibrated): DBI, NIST-StMU







At 300s:

Heat Release Rate: Factor of ~2.5x difference

Mass Loss Rate: Factor of ~4x to 6x difference

Representative Fire Growth case: Model Sensitivity to Boundary Conditions

- Complete pyrolysis models (material property sets) considered :
  - MaCFP-2: Aalto, BUW-FZJ, DBI, GIDAZE+, NIST, UMD, UMET
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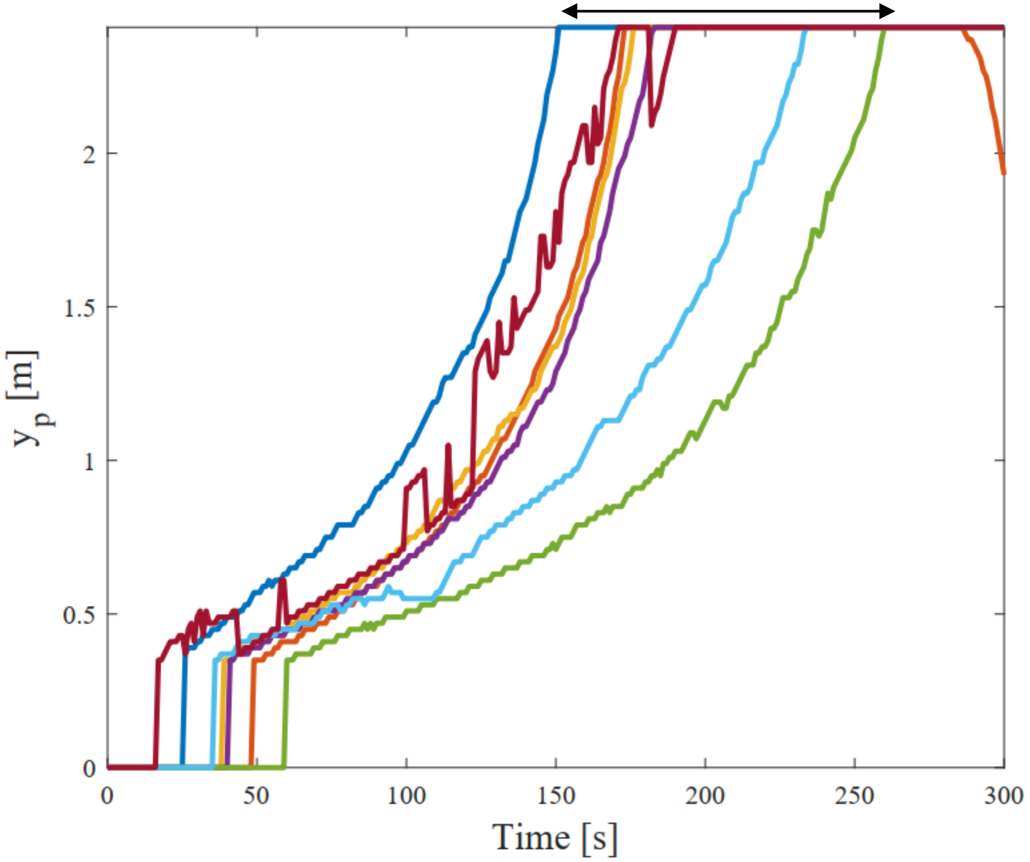
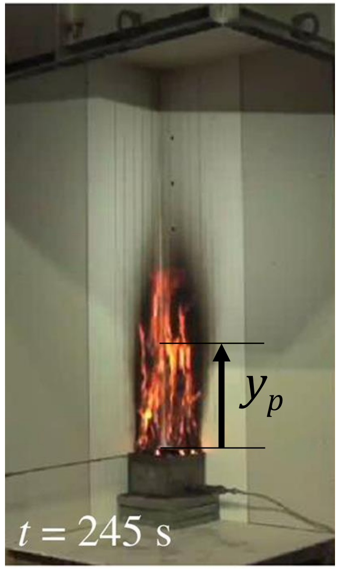
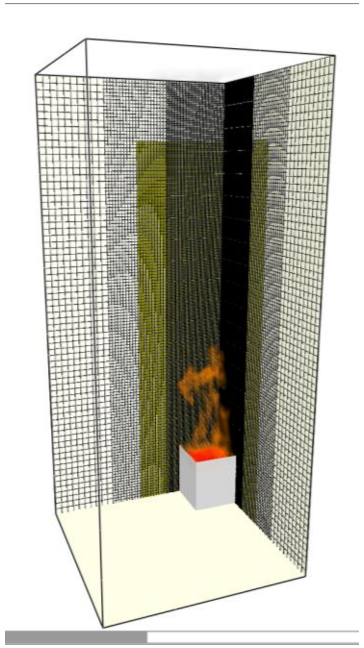




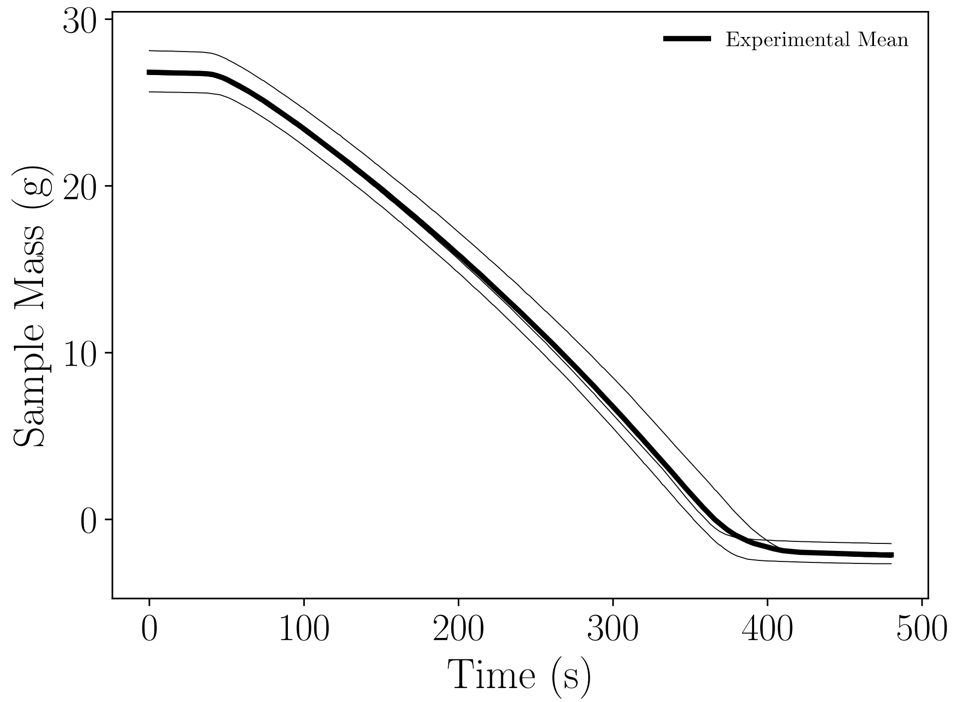


Flame Spread Rate (pyrolysis front location, y_p)
Time to top of wall: 150 s to 260 s

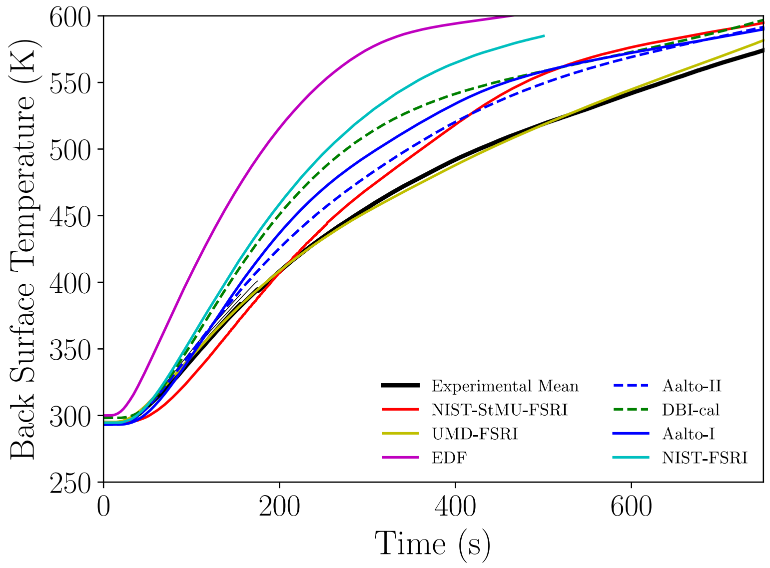
NIST-Gasification-Apparatus: Quantifying Model Similarity to Experimental Measurements

- Questions
  - **How good are our predictions?**
  - **Which material property set best predicts NIST gasification data?**
  - Which model assumptions work best?
  - Which calibration approaches work best?
  - …many more for October meeting.
- Compare model **average** predictions to experimental **average** data
- Four measurements
  1. Back surface temperatures at 25 kW/m²
  2. Back surface temperatures at 50 kW/m²
  3. Sample mass at 50 kW/m²
  4. Sample mass loss rate (MLR) at 50 kW/m²

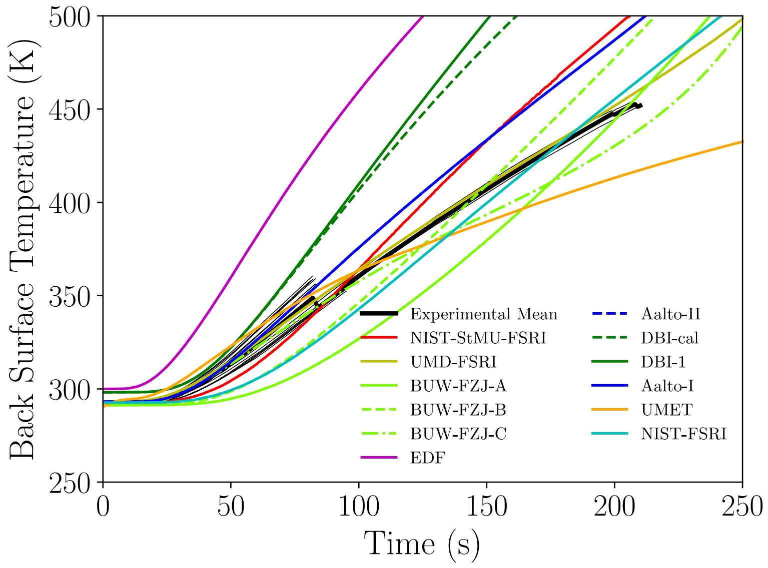
Experimental Sample Masses at 50 kW/m²



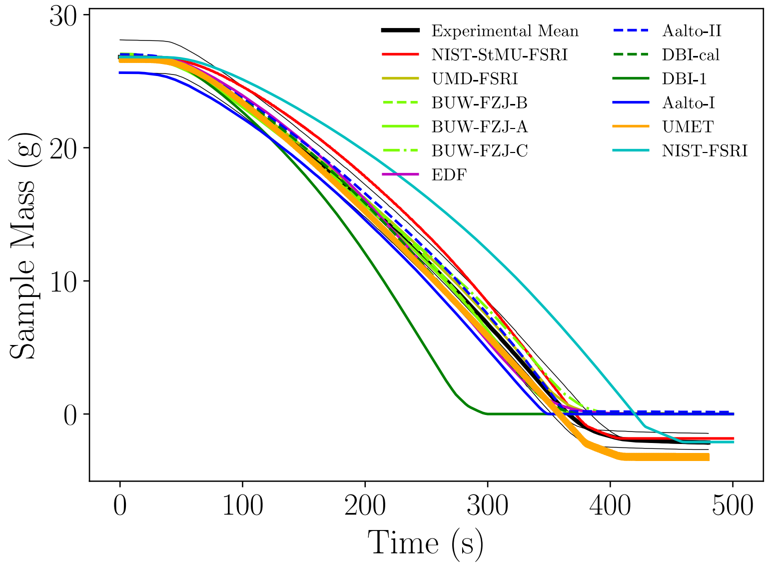
Back Temperature at 25 kW/m²



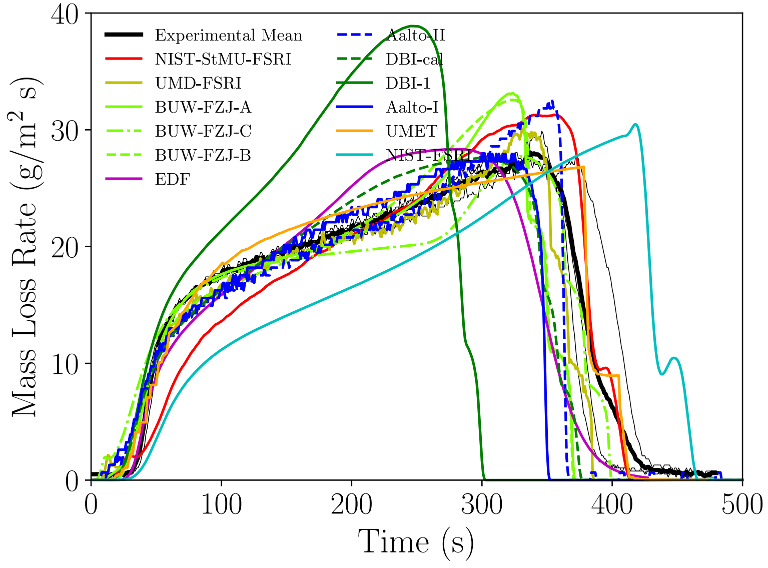
Back Temperature at 50 kW/m²



Sample Masses at 50 kW/m²

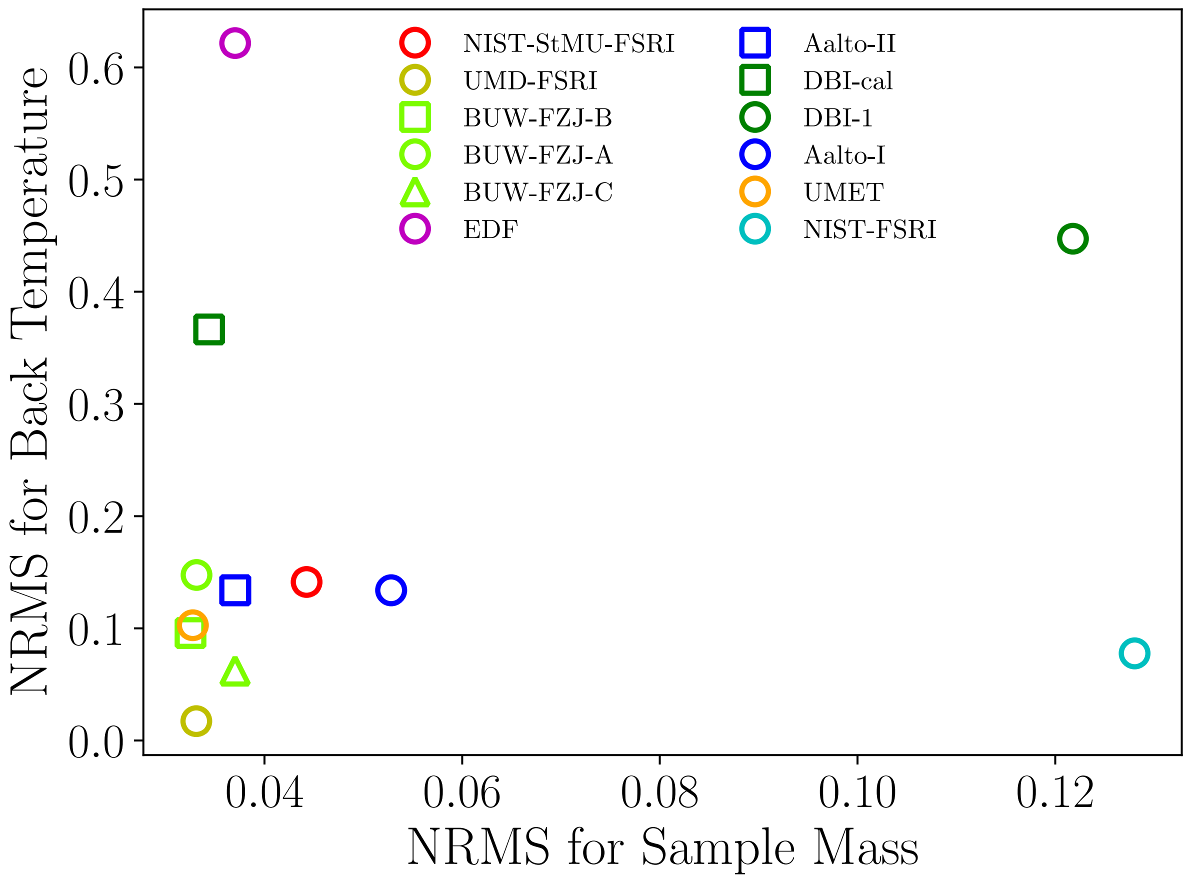


Mass Loss Rate at 50 kW/m²



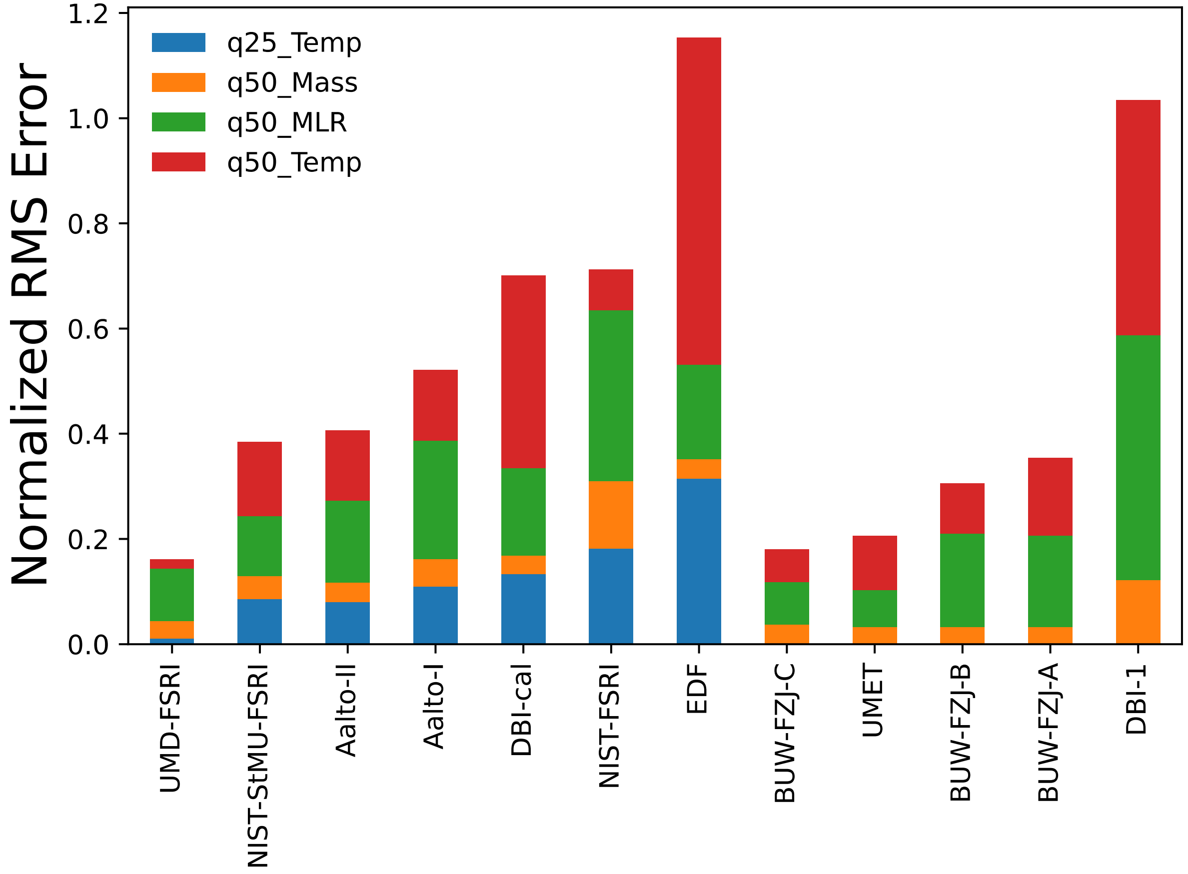
NIST-Gasification-Apparatus: Quantifying Model Similarity to Experimental Measurements

Prediction Errors for 50 kW/m²



- Measure of error: normalized root mean square error (NRMS) of four measurements
- Other possible comparisons
  - Onset time of decomposition ("ignition")
  - Peak mass loss rate
  - Average mass loss rate ("burning rate")
  - Time to critical temperature at back surface ("heat transfer through material")
  - Others?

NIST-Gasification-Apparatus: Quantifying Model Similarity to Experimental Measurements



Normalized Root Mean Squared Errors

	q25_Temp	q50_Mass	q50_MLR	q50_Temp
UMD-FSRI	0.010841	0.033107	0.099934	0.017163
NIST-StMU-FSRI	0.085370	0.044262	0.113250	0.141264
Aalto-II	0.080108	0.037044	0.155704	0.133875
Aalto-I	0.109076	0.052818	0.225658	0.133875
DBI-cal	0.133706	0.034404	0.166840	0.366397
NIST-FSRI	0.181980	0.128032	0.324935	0.077635
EDF	0.314577	0.037035	0.179658	0.621618
BUW-FZJ-C	NaN	0.037024	0.080598	0.062255
UMET	NaN	0.032755	0.069805	0.102685
BUW-FZJ-B	NaN	0.032522	0.177435	0.095763
BUW-FZJ-A	NaN	0.033131	0.173106	0.147482
DBI-1	NaN	0.121789	0.465453	0.447314

NIST-Gasification-Apparatus:
Quantifying Model Similarity to Experimental Measurements

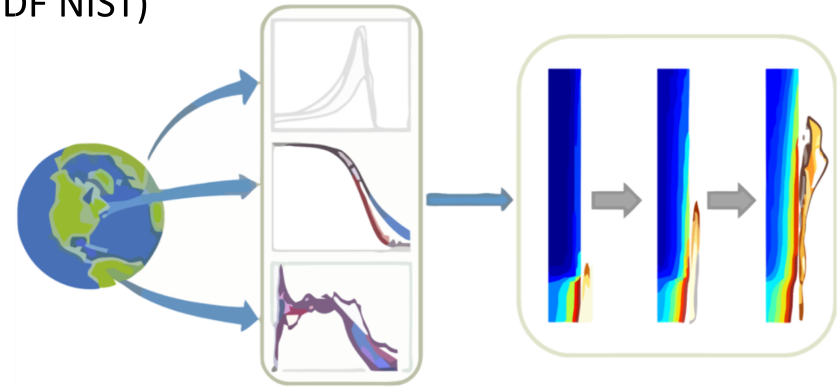
- Recommended property set
  - UMD, matl-db/PMMA/Material_Properties/2021/MaCFP_PMMA_UMD.json
- Python script for analyzing and plotting validation data and predictions
  - matl-db/Scripts/NIST_Gasification_Validation.py
- Please feel free to
  - Submit additional material property data sets
  - Submit additional NIST gasification predictions
  - Suggest additional measures of fit for validation
  - Improve validation analysis scripts
  - Play with the data

Summary of Pyrolysis Model Validation Exercise

- Experimental measurements provided for pyrolysis model validation(NIST-Gasification dataset)
  - Apparatus boundary conditions carefully characterized at q”ext = 25 kW m^{-2} and 50 kW m^{-2}
  - Mass loss rate and back surface temperature rise of MaCFP-PMMA measured

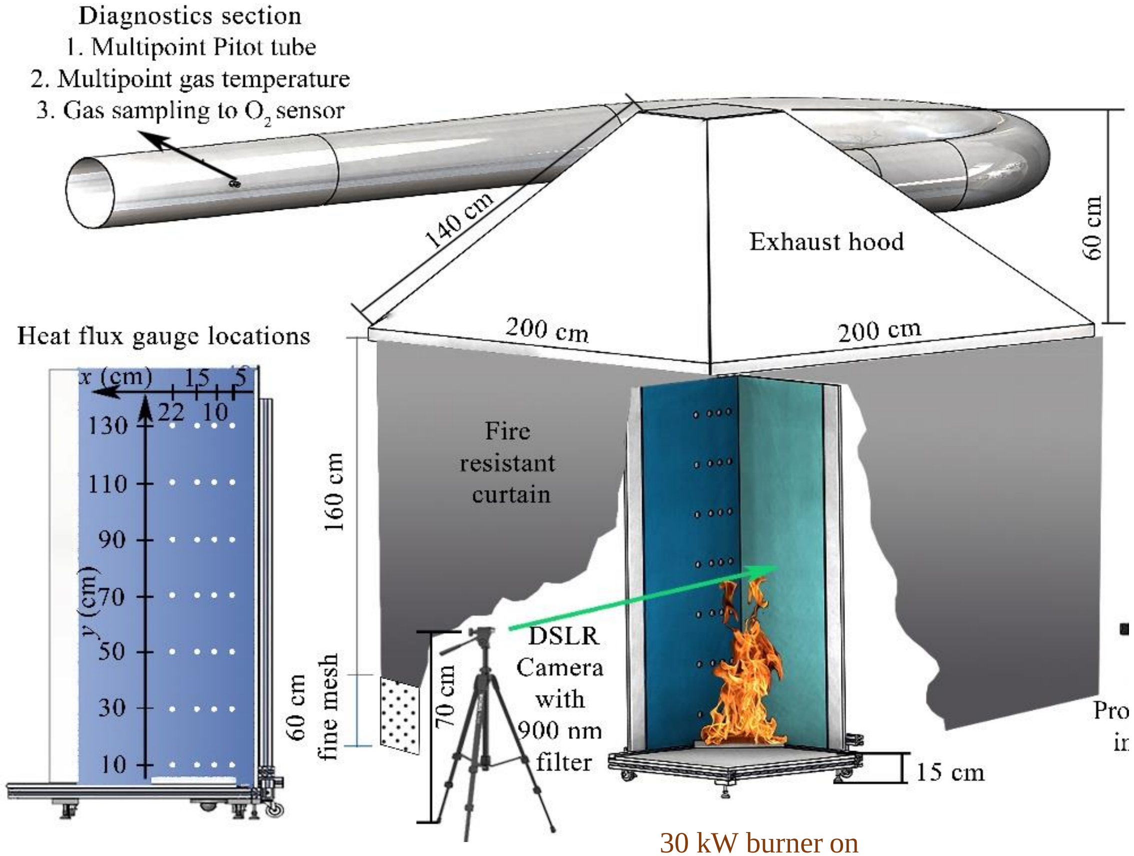
- Model (Re)Calibration
  - Five new / recalibrated material property sets submitted (BUW-FZJ, Aalto, DBI, EDF NIST)

- Model Validation (Simulation Results)
  - Compare model average predictions to experimental average data
    - Back surface temperatures at 25 kW/m^2
    - Back surface temperatures at 50 kW/m^2
    - Sample mass at 50 kW/m^2
    - Sample mass loss rate (MLR) at 50 kW/m^2
  - Identification of recommended material property
    - Most Average (compared to all pyrolysis models): UMD
    - Closest agreement to validation dataset: UMD

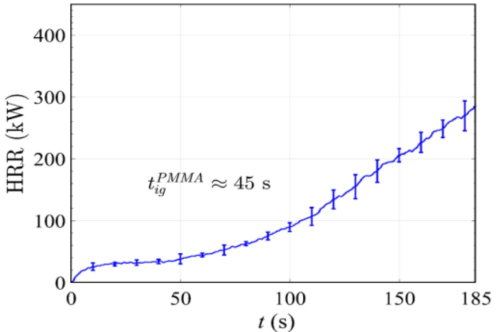


- Preliminary Sensitivity Analysis

UMD-SBI:
Flame Spread on PMMA in Corner-wall Configuration



30 kW burner on throughout experiment



Description of setup & experimental procedure available online:
https://doi.org/10.1016/j.polymdegradstab.2020.109433

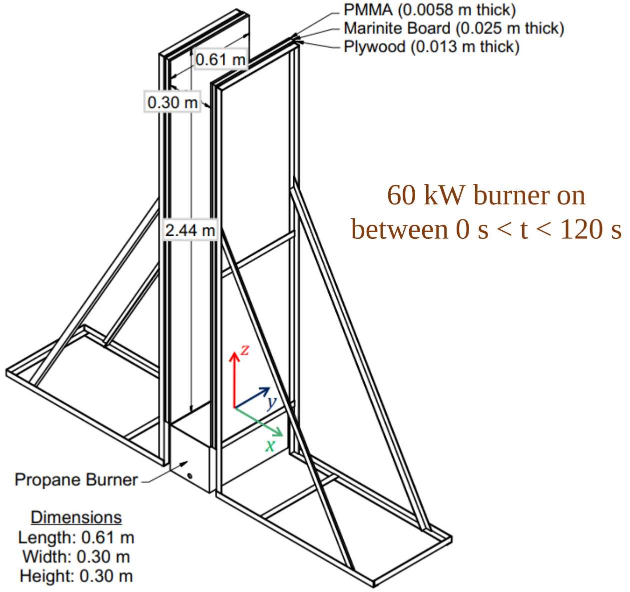
Simulated data required for comparison with experiments:

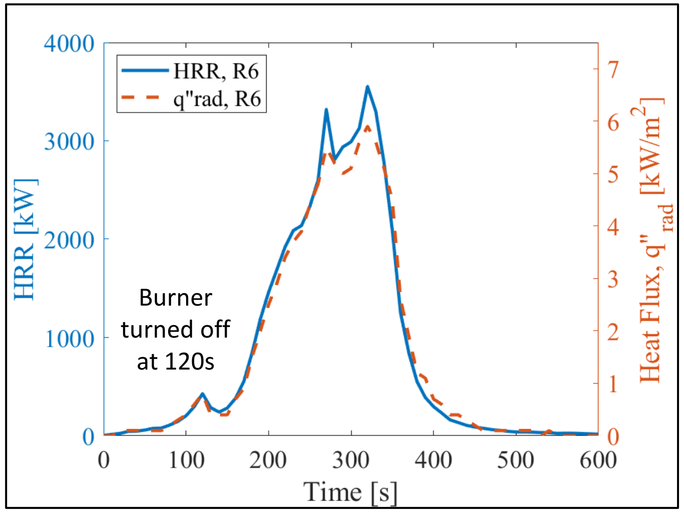
- HRR with time (*t*)
- Instantaneous flame shapes (define as the 200 kW m^{-3} iso-contour of volumetric HRR)
- PMMA surface heat fluxes to total cold gauges
- Radiative heat fluxes at a distance from the corner wall

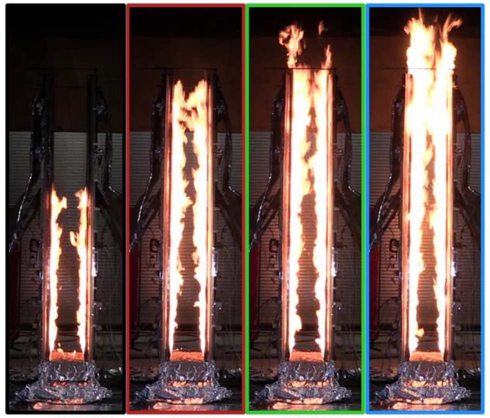
Additional simulated data for comparison between simulations:

- Vertical variations of the fuel mass loss rate, surface temperature, net surface heat flux, and the convective and radiative components of the net surface heat flux at specified horizontal distances and times
- Variations of the mean and rms gas temperature along the direction normal to one of the two PMMA surfaces at specified positions and times
- Variations of the mean and rms vertical flow velocity

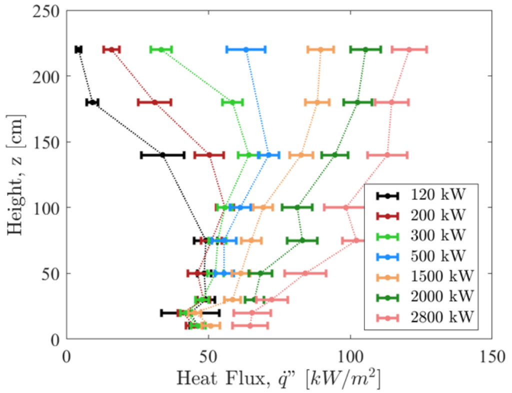
NIST-Parallel-Panel: Flame Spread on PMMA in Parallel Panel Configuration







120 kW 200 kW 300 kW 500 kW



1500 kW 2010 kW 2800 kW

- Collaboration with Nuclear Regulatory Commission (NRC); NIST/NFRL Support; apparatus design based on FM 4910

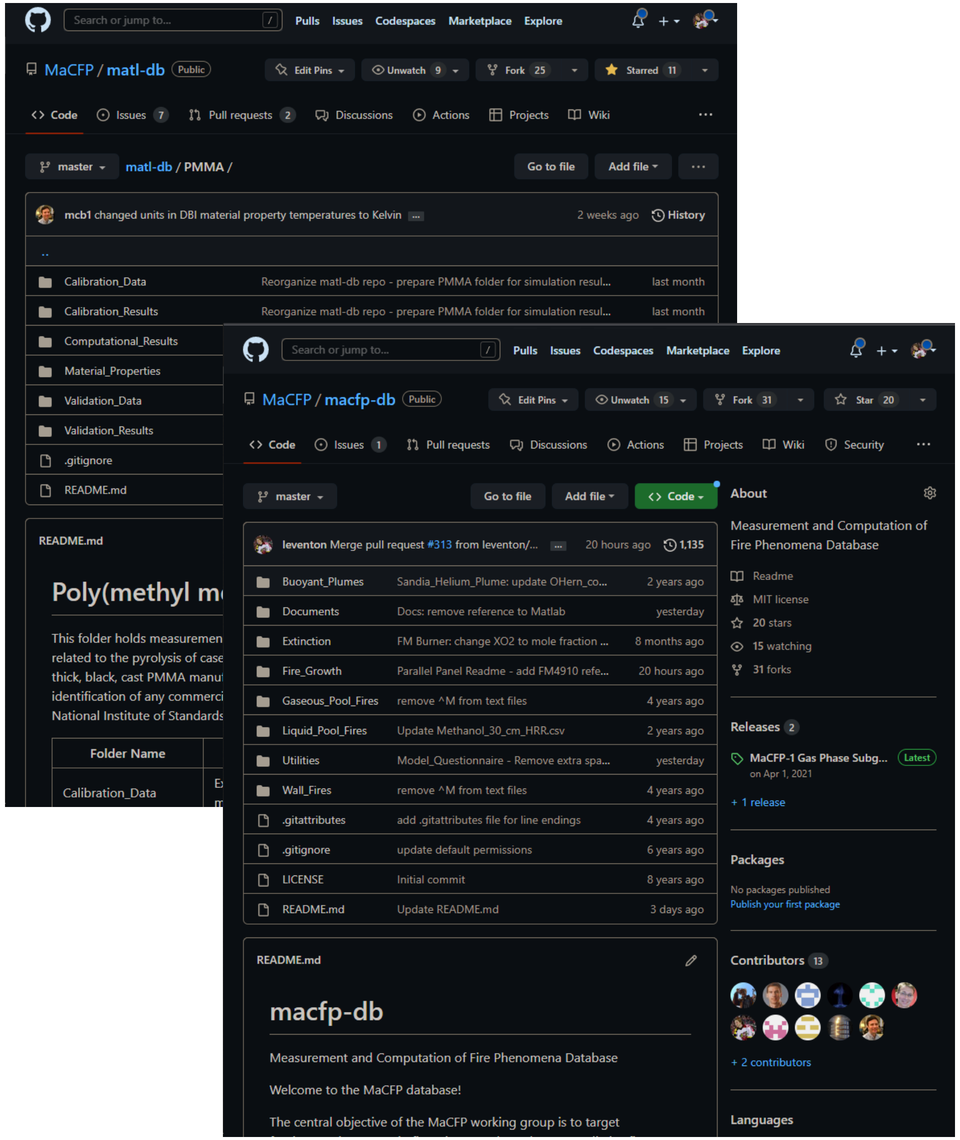
Target data highlighted in red represents simulated data for comparison between simulations (NOT measured experimentally)

- Propane Burner
  - Heat Release Rate, HRR
  - Flame shape (200 kW m^{-3} iso-contours)
  - Total flame heat flux:
    - Centerline values (time resolved), steady state (spatially-resolved)
- PMMA Panels
  - Heat Release Rate, HRR
  - Flame shape (200 kW m^{-3} iso-contours)
  - Radiative heat flux at a distance (q''_{rad})
  - On wall: Centerline fuel MLR, surface temperature, flame heat flux (total, radiative, convection)
  - Mid-panel (x,y = 0): mean, RMS gas temperature and vertical velocity

NIST NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY U.S. DEPARTMENT OF COMMERCE

U.S.NRC United States Nuclear Regulatory Commission Protecting People and the Environment

Next Steps:
Working with the MaCFP Repository (Github)



- https://github.com/MaCFP/
  - [//matl-db](https://github.com/MaCFP/matl-db) – experimental measurements for material property calibration and validation; material property sets
  - [//macfp-db](https://github.com/MaCFP/macfp-db) – experimental measurements for fire model validation
- Encourage participants to navigate GitHub to:
  - Access & compile most current datasets, reports
  - Review README files (descriptions of the test setup, conditions, and procedure)
  - Submit modeling predictions (by pull request)
  - Star/Watch/Follow for regular updates

Next Steps:
Contact Information

Further details on how to participate in the MaCFP-3 Workshop available:

Guidelines for Participation Document (.pdf) & MaCFP 2023 Modeling Guidelines (Github Wiki)

Video recording + presentation slides introducing MaCFP-3 Target Cases

Additional Points of Contact:

For general MaCFP questions, please contact Bart Merci (bart.merci@ugent.be) and Arnaud Trouve (atrouve@umd.edu)

For questions on the GitHub MaCFP repository, please contact Randy McDermott (randall.mcdermott@nist.gov)

For questions on specific target experiments, please use the following points of contact:

MaCFP-3 Session/Case	Session Co-Chairs; Technical Point of Contact
NIST-Waterloo-Pool-Fires	Tarek Beji, Ryan Falkenstein-Smith; Anthony Hamins, Beth Weckman
FM-Burner	Ning Ren, Gang Xiong; Yi Wang
NIST-Gasification	Jason Floyd, Bjarne Husted; Isaac Leventon
UMD-SBI	Dushyant Chaudari, Alexander Snegirev; Stanislav Stoliarov
NIST-Parallel-Panel	Lukas Arnold, Kevin McGrattan; Isaac Leventon

Next Steps: Upcoming Deadlines

June 20 – August 31, 2023

Modelers are asked to simulate the following target cases:

- Gas-Phase Modeling: Pool Fires, Gaseous Burner flames
- Condensed-Phase Modeling: NIST-Gasification
- Coupled Modeling (Fire growth): 1.46 m tall corner wall, 2.44 m tall parallel panels
    - Modelers Encouraged to Repeat simulations with **two** material property sets:
        - 'Most Central': UMD
        - Closest to NIST-Gasification: UMD

June 30, 2023

Deadline to submit poster abstract (abstract of modeling submissions for the MaCFP-3 Workshop)

August 31, 2023

Deadline to submit modeling results (pool fires, gaseous burners, fire growth cases)

October 22, 2023

MaCFP-3 Workshop, Tsukuba Japan

Discussion

- Discussion topics may include:
  - Experimental Measurements
    - Questions on existing data
    - Guidelines for experimental calibration/description needs
    - Future needs: Minimum requirements for dataset quality (calibration, number of repetitions, types of data)
  - Uncertainty analysis, propagation of error from:
    - Experimental uncertainty
    - Model calibration approach
      - Optimization target
      - Optimization techniques

    Impact on: Burning behavior & Fire growth
  - Minimum requirements for numerical pyrolysis models

What are the MaCFP Community's wants/needs?
Do we have the time/resources to address these next steps?
How can the MaCFP Organizing committee help to facilitate/coordinate these efforts?

Discussion

- Additional discussion topics for October may include:
  - Guidelines, needs, and/or knowledge gaps in pyrolysis/fire model verification and validation
  - Understanding fire model sensitivity to variability in pyrolysis model parameters
  - Pyrolysis model *verification* exercise for MaCFP-4
  - Identification of a new material of interest for MaCFP-4?
  - Frequency and locations of future MaCFP meetings and workshops (virtual + in person)

Discussion Forum: https://groups.google.com/g/macfp-discussions/

Discussion

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Summary of Pyrolysis Model Validation Exercise

MaCFP-3 target cases include:

• NIST-Waterloo-Pool-Fires: 30 cm, 37 cm, and 100 cm diameter liquid pool and gaseous burners studied at NIST and Waterloo featuring multiple fuels;

• FM-Burner: 13.7 cm inner diameter (15.2 cm outer diameter) ethylene diffusion flames studied at FM Global and featuring a controlled co-flow oxygen-nitrogen oxidizer;

• NIST-Gasification-Apparatus: bench-scale thermal degradation experiments conducted in the NIST gasification apparatus, providing validation data for PMMA pyrolysis models;

• UMD-SBI: Flame spread experiments in a 1.46 m corner wall configuration studied at the University of Maryland with MaCFP PMMA (based on the Single Burning Item (SBI) Test, EN13823);

• NIST-Parallel-Panel: Flame spread experiments in a 2.44 m parallel panel configuration studied at NIST with MaCFP PMMA (based on the FM4910 Parallel Test)

Workshop Schedule (Oct. 22, 2023)

- Morning session: Focus on gas-phase-only or condensed-phase-only target experiments (e.g., pool fires, gas burners; determination of solid-phase material properties) Introduce new radiation heat transfer subgroup

- Mid-day session: Focus on coupled solid/gas phase experiments (fire growth/flame spread)

- Afternoon session: Organized for experimentalists and modelers to discuss current results and possible future Target Experiments / MaCFP Exercises

- The workshop will be organized to allow substantial time for open discussion and interaction among participants. Discussion topics may include:
  - Guidelines for experimental calibration/description needs
  - Guidelines, needs, and/or knowledge gaps in pyrolysis/fire model verification and validation
  - Understanding fire model sensitivity to variability in pyrolysis model parameters
  - Pyrolysis model verification exercise for MaCFP-4
  - Identification of a new material of interest for MaCFP-4
  - Proposed new target cases for radiation heat transfer and gas-phase model validation
  - Frequency and locations of future MaCFP meetings and workshops (virtual + in person)

MaCFP Specific Objectives

https://github.com/MaCFP/macfp-db/blob/master/Documents/FIRE_PHENOMENA.md

Condensed Phase Phenomena

Priority	Condensed Phase Phenomena	Benchmark Experiment
Primary	Thermal decomposition of solid fuels	6, 7
	Ignition	6
	Gasification of condensed phase fuels	7 (see matl-db repo)
Secondary	In-depth radiative absorption	
	Charring	
	Condensed phase heat transfer in complex materials	
	Liquid phase transport effects	

Gas Phase Phenomena

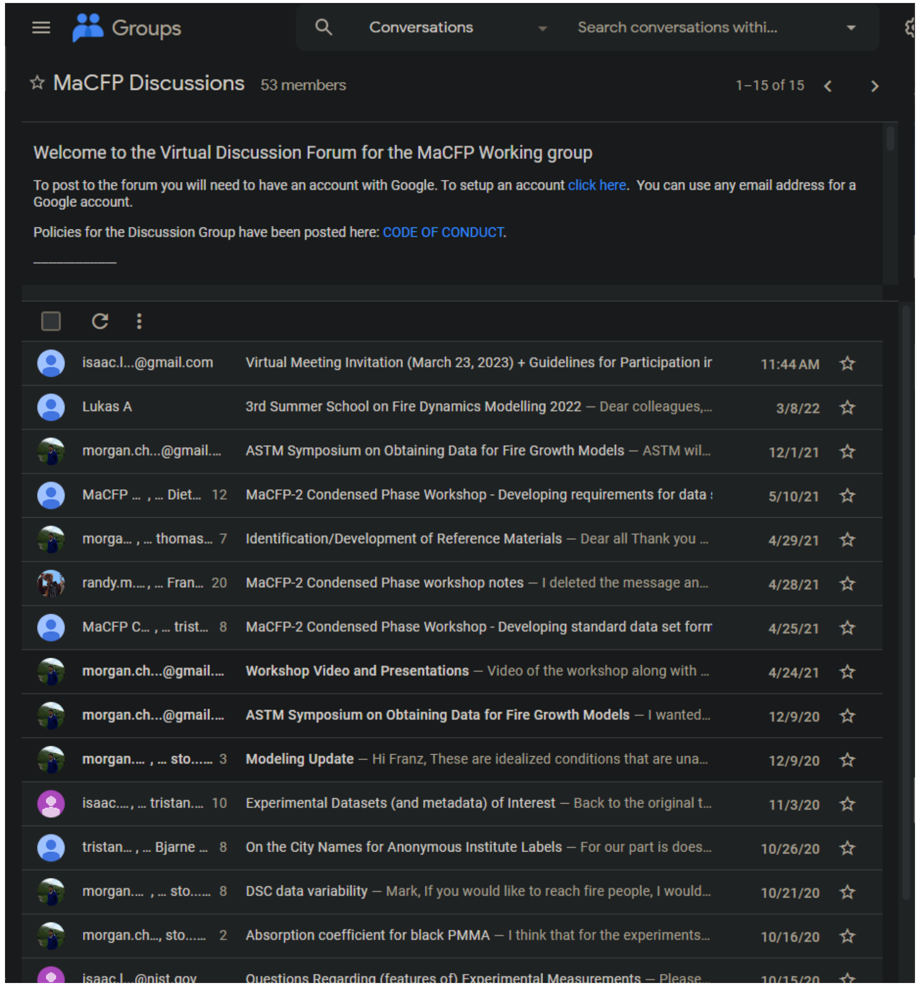
Priority	Gas Phase Phenomena	Benchmark Experiment
Primary	Buoyant plumes	1
	Convective heat transfer	3b, 6a,b
	Radiative heat transfer	3b, 6a,b
	Turbulent flow	3a
	Turbulent mixing	3a
	Species transport and composition	3b
Secondary	Soot formation and oxidation (aerosol species)	3b
	Toxicity (yields of particles and toxic gases)	3b
	Scale effects	3b
	Compartment fire effects including ventilation	
	Visibility	
	Local extinction and re-ignition	5
	Suppression	5
	Fire growth	6a,b
	Instabilities (large-scale puffing/small-scale phenomena)	3a,3b

Coupled Condensed- and Gas-Phase Phenomena

Priority	Condensed- and Gas-Phase Phenomena	Benchmark Experiment
Primary	Fire spread	6a, 6b
	Fire growth	
Secondary	Wall-flame interactions	

- Develop a digital archive of well-documented **fire experiments** that can be used as targets for CFD model validation;
- Develop a digital archive of well-documented CFD-based **numerical simulations** corresponding to the selected target experiments;
- Develop **protocols for detailed comparisons** between computational results and experimental measurements;
- Identify key **research topics and knowledge gaps** in computational and experimental fire research;
- Develop **best practices** in both computational and experimental fire research (including quality control and quantification of uncertainties);
- Establish a **network between fire researchers** and provide a community-wide forum for discussion and exchange of information.

Virtual Discussion Forum



- https://groups.google.com/g/macfp-discussions/

- Encourage participants to visit Forum to:
  - Continue discussions started during MaCFP Events
  - Ask questions regarding measurements on Github Repository, related metadata, analysis of those results
  - Review measurement data/modeling approaches
  - Propose current/future measurement data of interest
    - What's needed (different scales, more detail at same scale)
    - What can you/your lab offer (measurement data, analysis, scripting, database management)