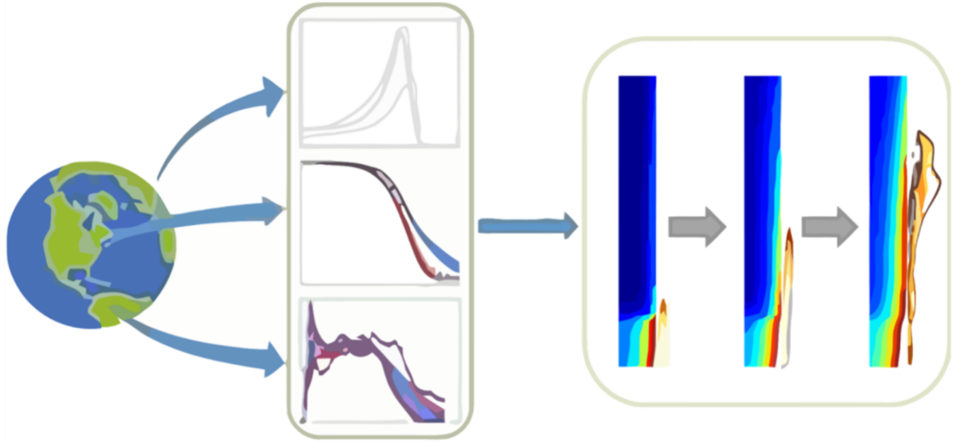
MaCFP-3 Target Experiments and Modeling Guidelines



This meeting will be recorded

Condensed Phase Organizing Committee:
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)

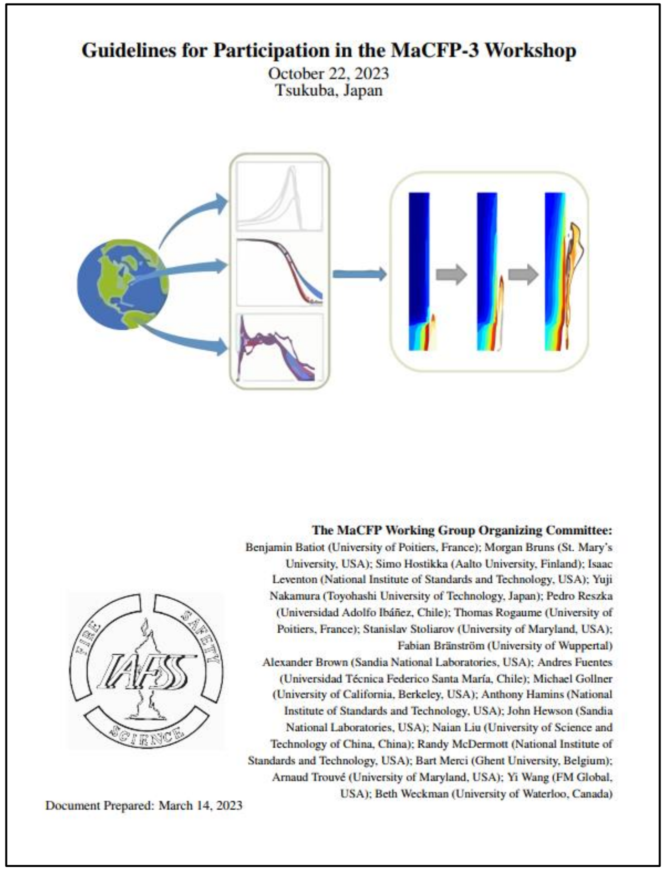
Gas Phase Organizing Committee :
Alexander Brown (Sandia National Laboratories, USA)
Andres Fuentes (Univ. Técnica Federico Santa Maria, Chile)
Michael Gollner (Univ. of California, Berkeley, USA)
Anthony Hamins (NIST, USA)
John Hewson (Sandia National Laboratories, USA)
Naian Liu (Univ. of Science and Technology of China, China)
Randy McDermott (NIST, USA)
Bart Merci (Ghent University, Belgium)

Gas Phase (continued):
Arnaud Trouvé (University of Maryland, USA)
Yi Wang (FM Global, USA)
Beth Weckman (University of Waterloo, Canada)

Radiation Heat Transfer Organizing Committee :
Fabian Brännström (University of Wuppertal)
Simo Hostikka (Aalto University, Finland)

Virtual Meeting Agenda (March 23, 2023)

- Overview of the Measurement and Computation of Fire Phenomena (MaCFP) Working Group
- Timeline of Events in Preparation for the MaCFP-3 Workshop
- Target Cases
  - Gas-Phase Modeling
    Pool Fires, Gaseous Burner flames
  - Condensed-Phase Modeling
    Material property set validation exercise
  - Coupled Modeling (Gas- and Condensed-Phase)
    Fire growth: 1.46 m tall corner wall, 2.44 m tall parallel panels
- Open Discussion



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

The MaCFP Working Group Organizing Committee:
Benjamin Batiot (University of Poitiers, France); Morgan Bruns (St. Mary's University, USA); Simo Hostikka (Aalto University, Finland); Isaac Leventon (National Institute of Standards and Technology, USA); Yuji Nakamura (Toyohashi University of Technology, Japan); Pedro Reszka (Universidad Adolfo Ibáñez, Chile); Thomas Rogaume (University of Poitiers, France); Stanislav Stoliarov (University of Maryland, USA); Fabian Bränström (University of Wuppertal)
Alexander Brown (Sandia National Laboratories, USA); Andres Fuentes (Universidad Técnica Federico Santa María, Chile); Michael Gollner (University of California, Berkeley, USA); Anthony Hamins (National Institute of Standards and Technology, USA); John Hewson (Sandia National Laboratories, USA); Naian Liu (University of Science and Technology of China, China); Randy McDermott (National Institute of Standards and Technology, USA); Bart Merci (Ghent University, Belgium); Arnaud Trouvé (University of Maryland, USA); Yi Wang (FM Global, USA); Beth Weckman (University of Waterloo, Canada)

Document Prepared: March 14, 2023

This meeting will be recorded for future viewing by MaCFP Participants. The recording will be made available on the MaCFP Github Repository. This recording could be released to the public through a Freedom of Information Act (FOIA) request. Do not discuss or visually present any sensitive (CUI) material. Ensure that no inappropriate material or any minors are contained within the background of any recording.

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

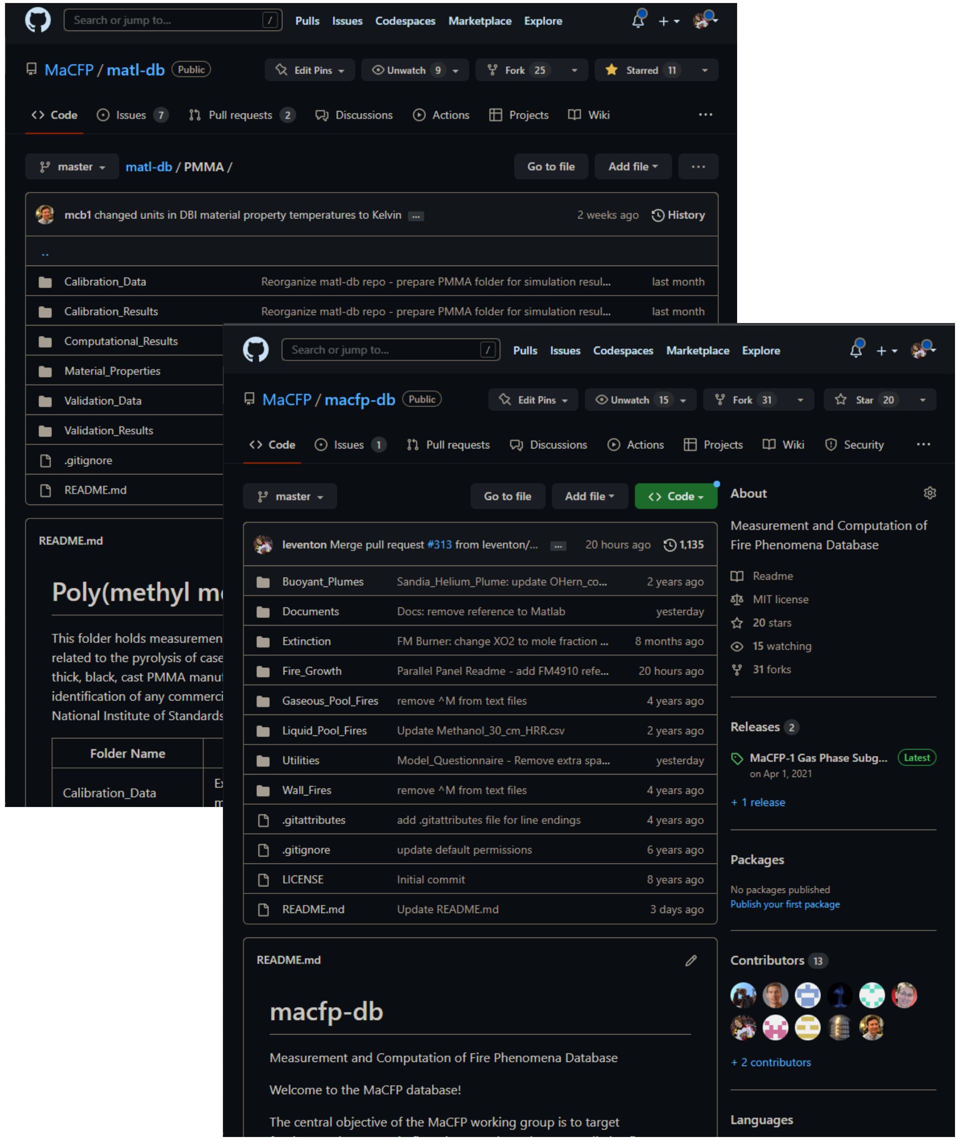
Priority	Gas Phase Phenomena	Benchmark Experiment
Primary	Buoyant plumes	1
	Convective heat transfer	3b, 6a,b
	Radiative heat transfer	3b, 6a,b
	Turbulent flow	3a
	Turbulent mixing	3a
	Species transport and composition	3b
Secondary	Soot formation and oxidation (aerosol species)	3b
	Toxicity (yields of 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.

The MaCFP Repository (Github)

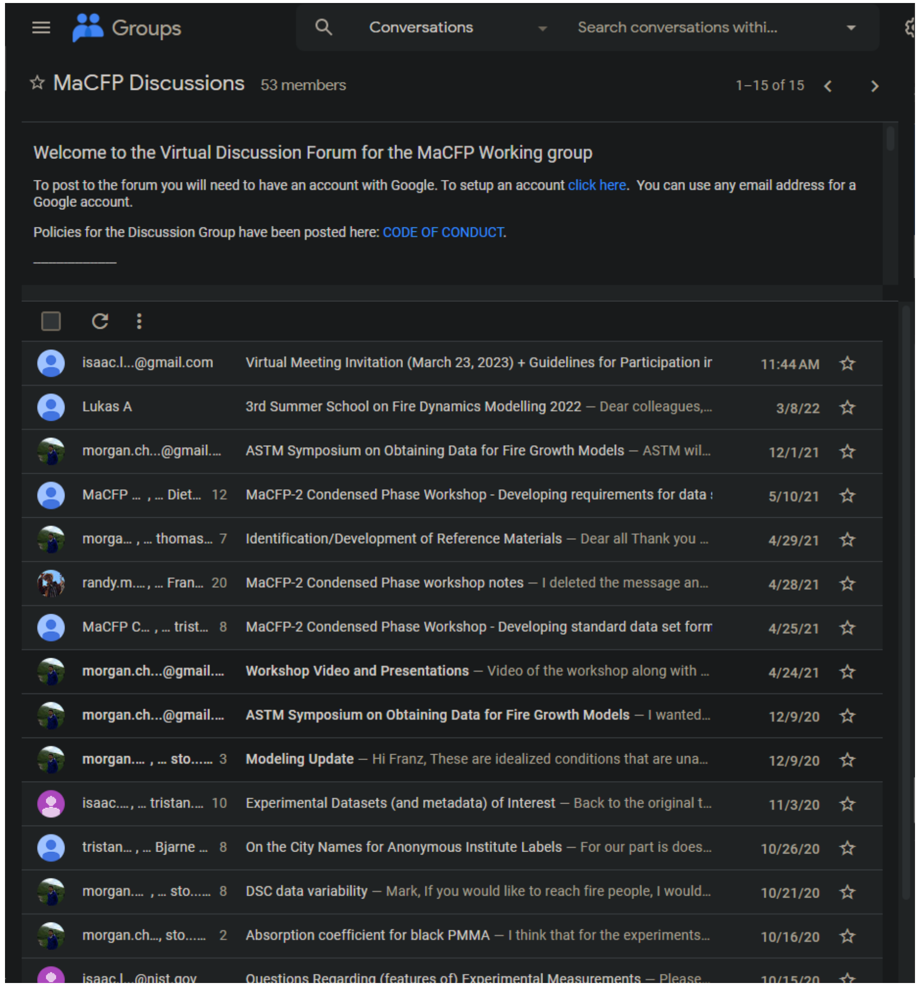


- https://github.com/MaCFP/
  - //matl-db – experimental measurements for material property calibration and validation; material property sets
  - //macfp-db – experimental measurements for fire model validation

- 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)

- Some lessons from previous databases
  - Metadata is critical
  - Maintenance is necessary but not cheap
  - Must connect to applications

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)

Workshop Schedule (Oct. 22, 2023)

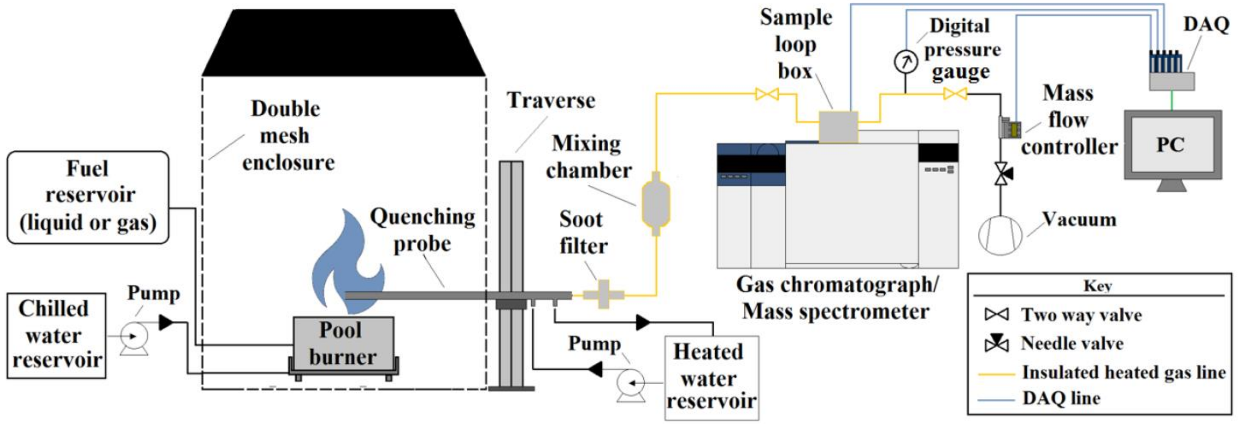
- Morning session: Focus on gas-phase-only or condensed-phase-only target experiments (e.g., pool fires, gas burners; determination of solid-phase material properties)
  Introduce new radiation heat transfer subgroup
- Afternoon session: Focus on coupled solid/gas phase experiments (fire growth/flame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

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)
Summer 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
August 31, 2023	Deadline to share flame spread modeling results
October 22, 2023	MaCFP-3 Workshop: Tsukuba, Japan

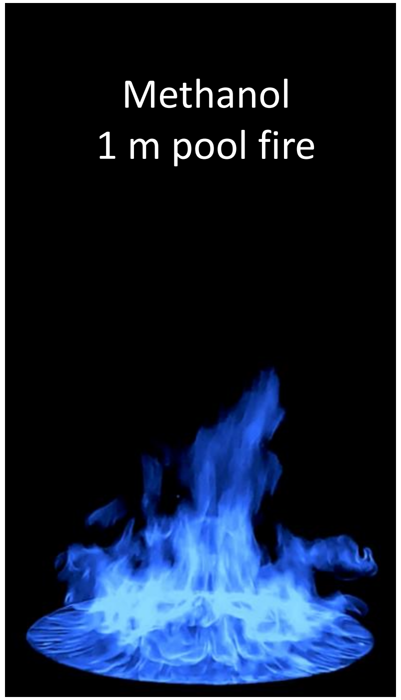
NIST-Waterloo Pool Fires: Overview



NIST gas species and soot analysis setup with extractive sampling and GC/MS

Fire Characteristics							
Fuel	D (cm)	$\dot{Q}$ (kW)	$\dot{Q}^*$	freq (Hz)	height H/D	χ_{rad}	Ys_max (g/g)
1. Methanol	30	19	0.34	2.6	1.4	0.22	0
2. Acetone	30	35	0.64	2.6	3.1	0.31	$5{\cdot}10^{-3}$
3. Methanol	100	254	0.21	1.4	1.1	0.22	0
4. Methane	37	35	0.37	2.3	1.7	0.15	$8{\cdot}10^{-4}$
5. Propane	37	35	0.37	2.3	1.4	0.30	$6{\cdot}10^{-3}$

	Measurements
Global	Mean flame height
	Pulsation frequency
	Mass burning rate
	Heat release rate
	Radiative fraction
	Soot and CO yields
Local	Gas-phase temperature
	Gas-phase velocity
	Radiative flux to surroundings
	Gas species & soot
	Vertical temperature in liquid fuel
	Heat flux onto fuel surface



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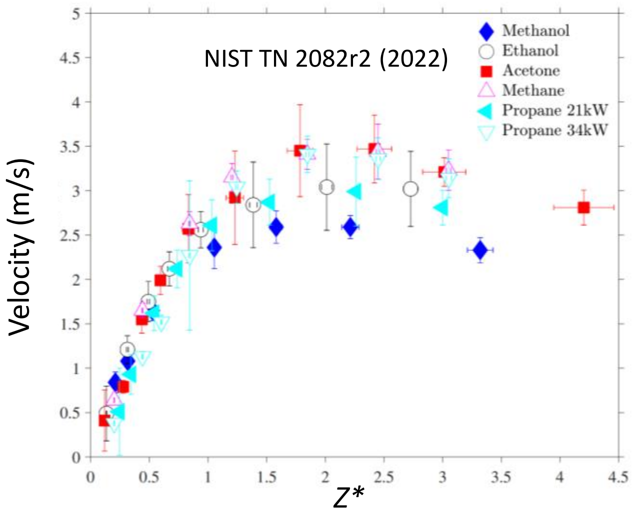
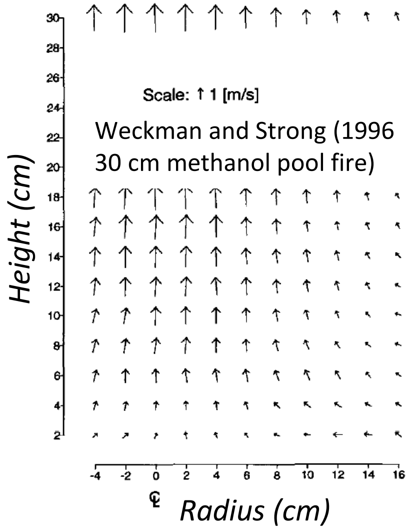
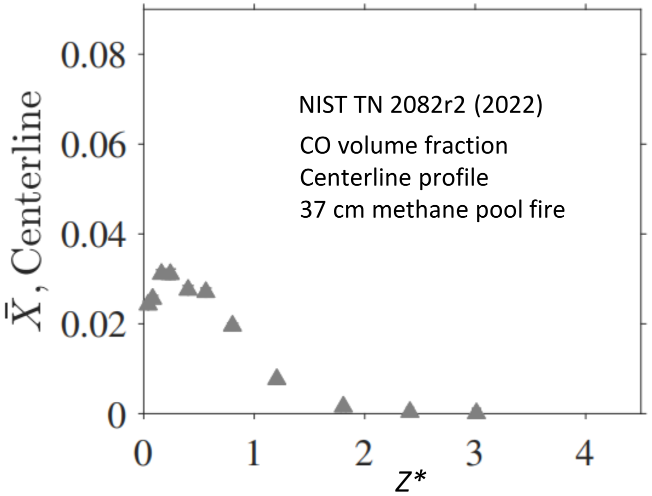
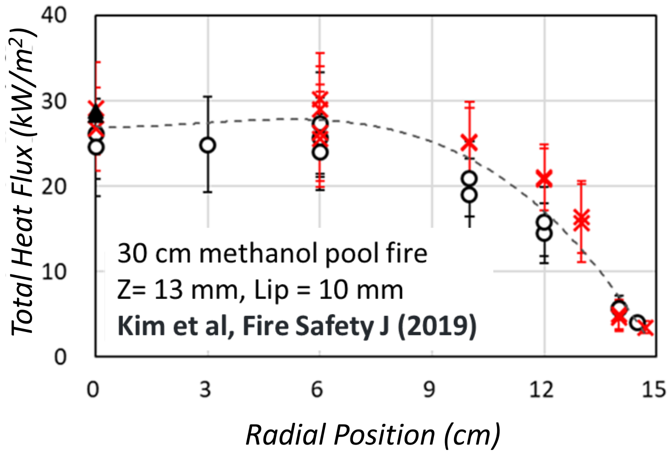
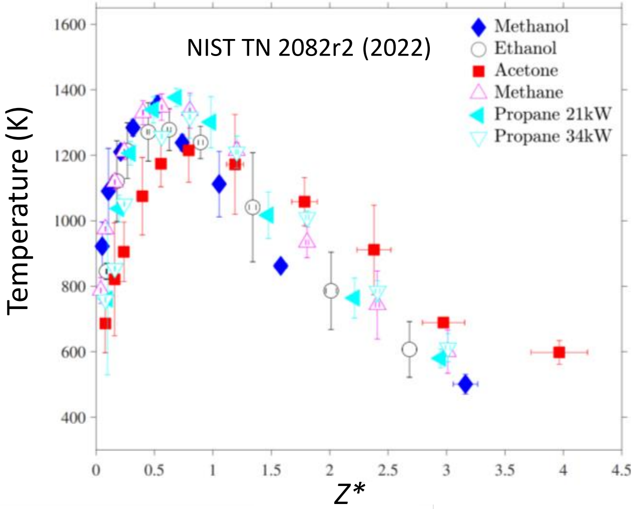
NIST-Waterloo Pool Fires: Typical Results

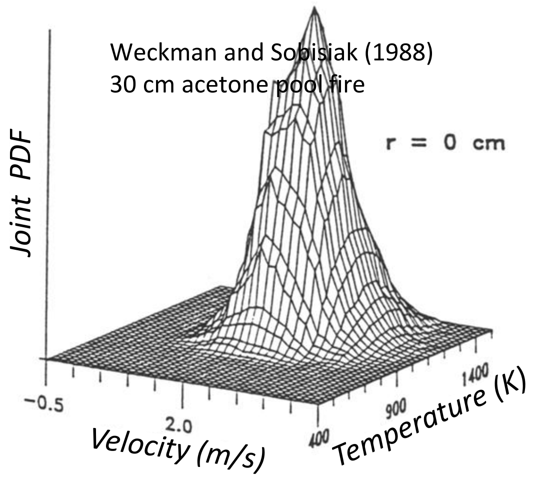


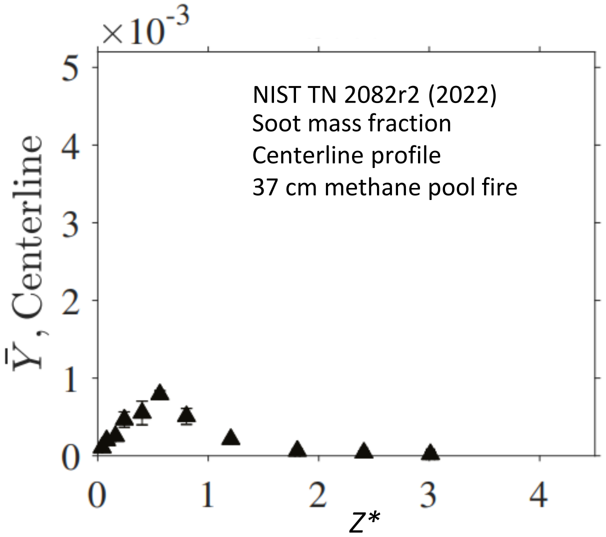


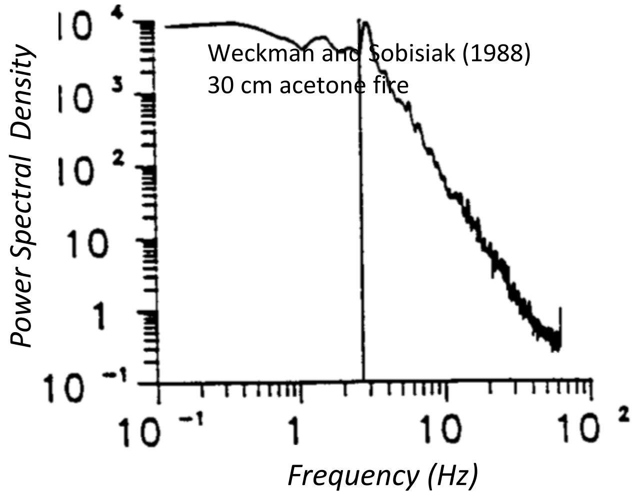








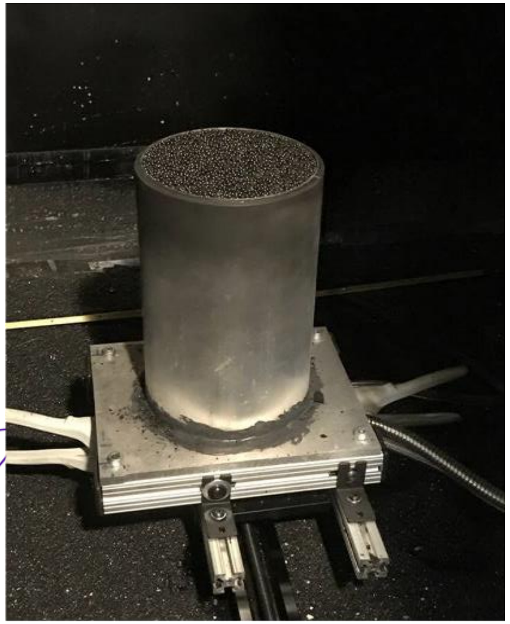


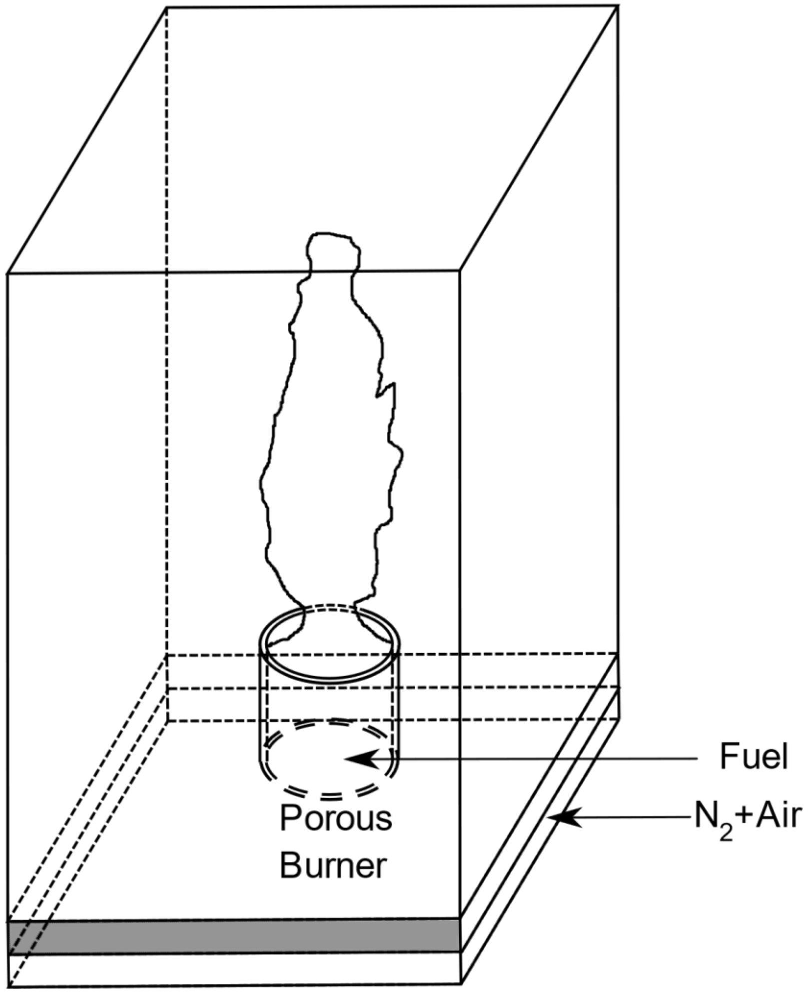


For experimental details, see references in MaCFP GitHub README files:
https://github.com/MaCFP/macfp-db/tree/master/Liquid_Pool_Fires

FM-Burner: Experimental Setup

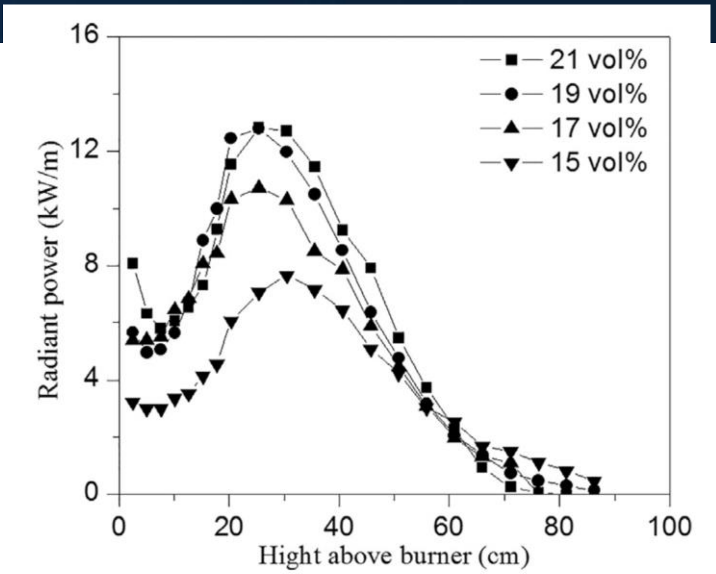
- Porous burner: ID 13.7 cm, OD 15.2 cm
- Enclosure: 122 × 122 × 183 cm
- Ethylene 15 kW flame
- X_{O_2}: 20.9 %– 15.2%

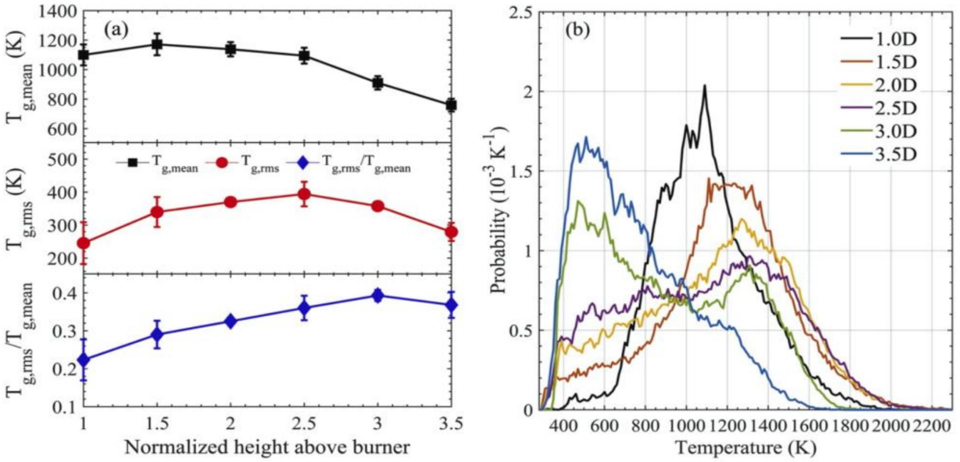


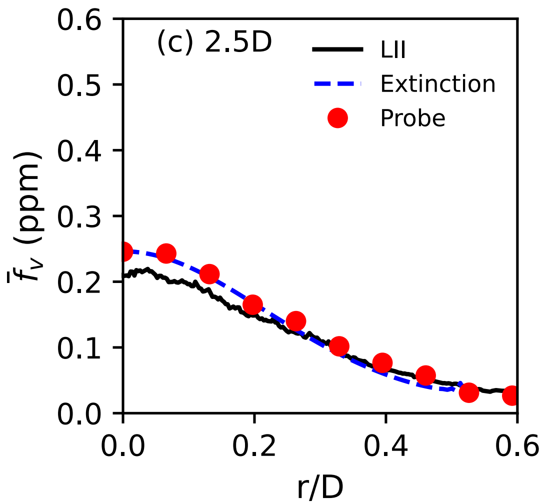


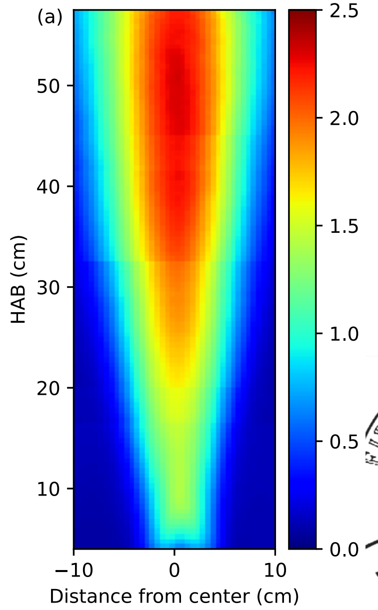
FM-Burner: Measurement results

- Global measurement:
  - Radiant fraction; Radiant power distribution; Combustion efficiency
- Local measurements (at 0.5 OD to 3.5 OD heights):
  - Soot volume fraction (by laser induced incandescence)
  - Temperature (by thermocouple, air case only)
  - Radiation intensity, soot temperature and volume fraction (by two-color radiation probe)
  - Velocity (by particle imaging velocimetry)









FM Global

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FM-Burner: Modeling Targets

Plots of interest include (for ethylene only):

- Plots showing the **mean and rms temperature** as a function of radial position r, for different elevations z;
- Plots showing the probability density function **(PDF) of temperature** for different radial positions r and elevations z;
- Plots showing the **mean and rms soot volume fraction** as a function of radial position r, for different elevations z (for comparisons, use the experimental soot data corresponding to Laser Induced Incandescence – LII – measurements);
- Plots showing the probability density function **(PDF) of soot volume fraction** for different radial positions r and elevations z (for comparisons, use the experimental soot data corresponding to Laser Induced Incandescence – LII – measurements);
- A plot showing the time variations of the **heat release rate**;
- Representative plots showing the instantaneous **flame shape** (e.g., identified as the 200 kW/m3 iso-contour of the volumetric heat release rate, or using some other method to be specified);
- A plot showing the variations of the **predicted global radiant fraction** with the coflow oxygen mole fraction;
- Plots showing the **vertical variations of the radiative emission power** per unit height of the fire (kW/m) (in numerical simulations, this quantity can be estimated by calculating the average of the radiation source term that appears in the energy equation integrated over each horizontal plane and over time).

Plots of interest include (for all fuels):

- A plot of **combustion efficiency** as a function of coflow oxygen mole fraction

MaCFP-2 Material Selection

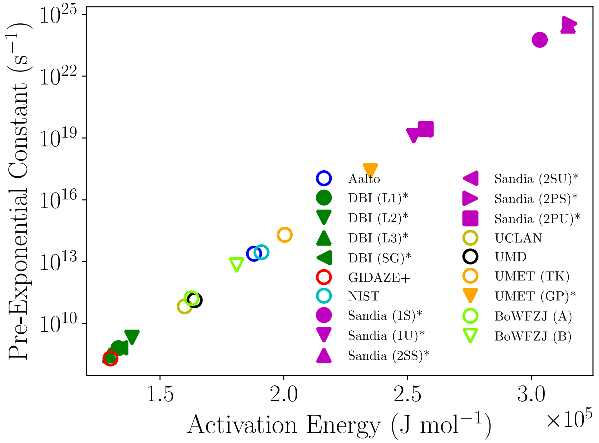
- Cast Black Poly(methyl methacrylate) (PMMA)
  - Evonik ACRYLITE® cast black 9H01 GT
  - Distributed in summer 2019
    - 100 mm by 100 mm by 6 mm slabs
    - 300 mg vials of powdered PMMA

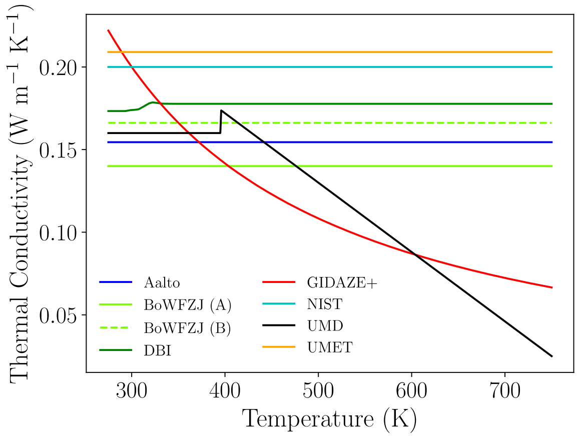
- Suitable first reference material
  - Maintains density/shape while burning
  - Simple decomposition kinetics
  - Low transparency to infrared radiation

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 (Condensed Phase)

- Two objectives:
  1. Derive material property sets from experimental data for MaCFP-PMMA
  2. Use material property sets to predict TGA and gasification
- 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 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



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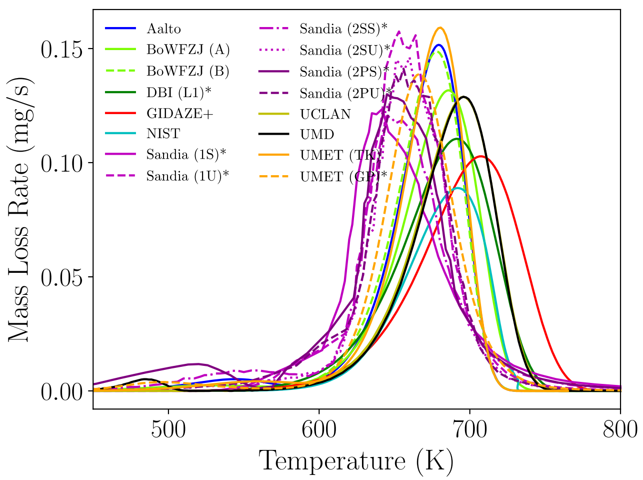
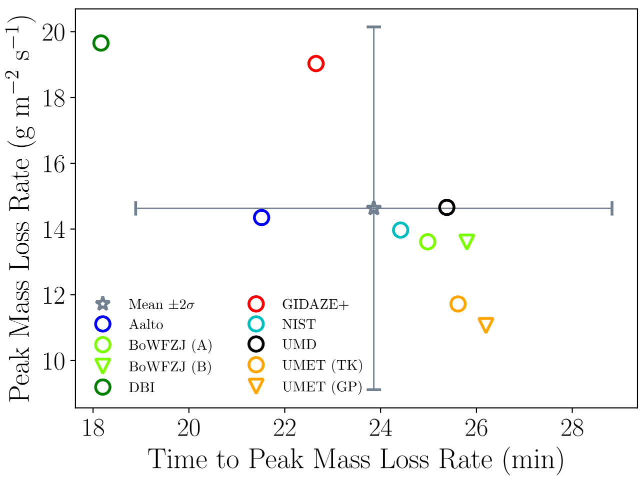
Summary of MaCFP-2 Results (Condensed Phase)

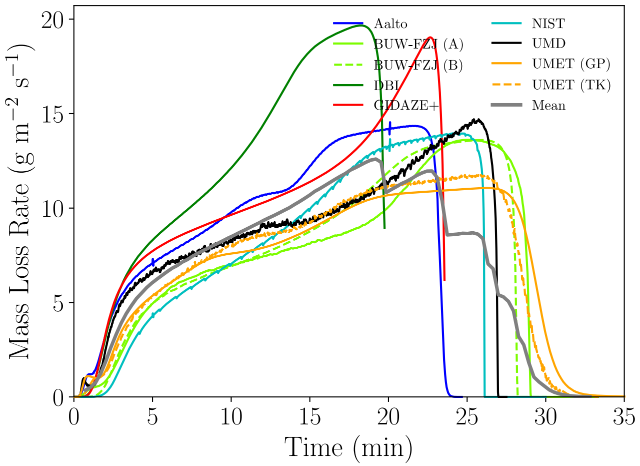
- Predictions using property sets
  - TGA: Heating rates of 10 K min^{-1} and 100 K min^{-1}
  - Slab Gasification: Heat fluxes of 10 kW m^{-2}, 25 kW m^{-2}, and 65 kW m^{-2} and thickness of 6 mm and 12 mm
- "Most average" property set: UMD
  - Property set with predictions closest (sum of square errors) to mean gasification predictions
  - Common parameters for MaCFP PMMA suggested for modelers
  - NOT implied to be the most accurate property set

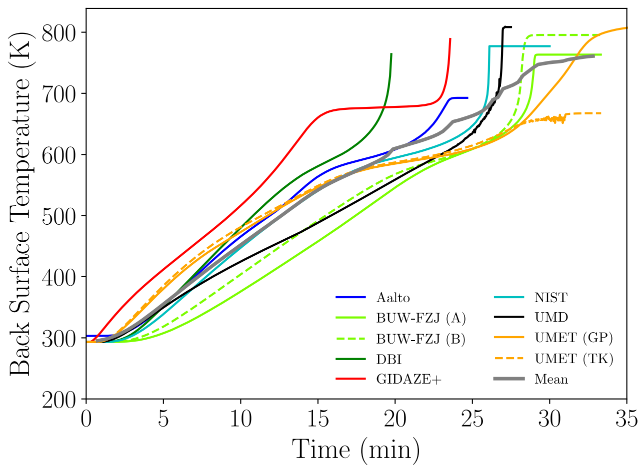


TGA at 100 K min^{-1}



Gasification at 25 kW m^{-2}, 12 mm

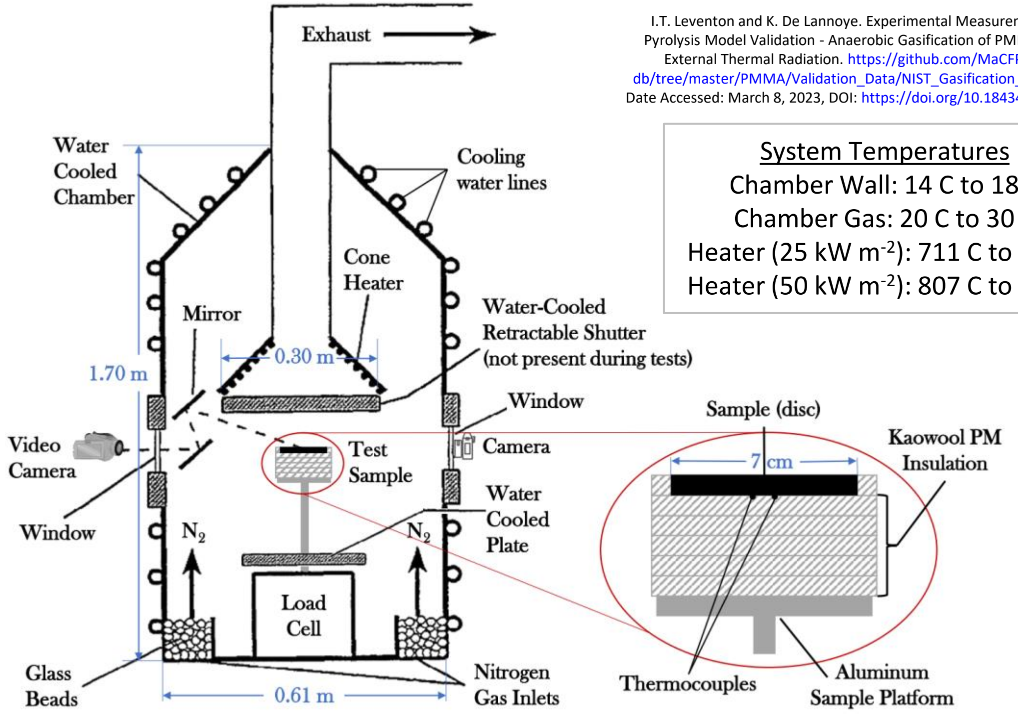




Gasification at 25 kW m^{-2}, 12 mm

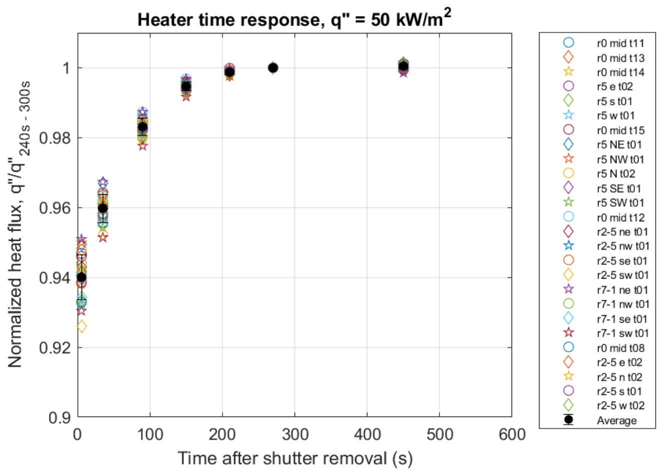
NIST-Gasification-Apparatus: Experimental Setup

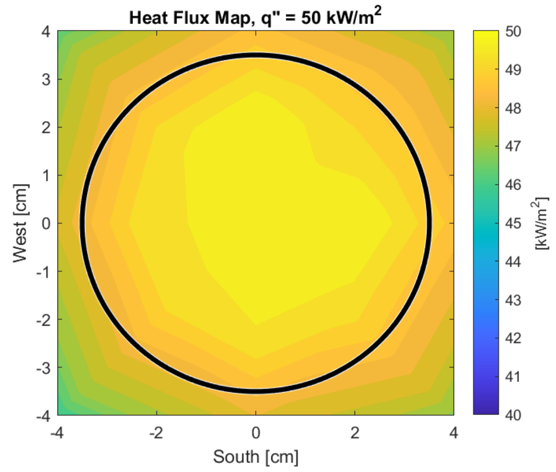
- Anaerobic environment (N_2); 30 cm cone heater; water-cooled chamber
- Boundary conditions carefully characterized: time- and spatially-resolved measurements of incident radiant heat flux [25 or 50 kW m^{-2}]; chamber wall temperatures; chamber gas temperature).
- Samples: PMMA discs (7 cm diameter, ~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



I.T. Leventon and K. De Lannoye. Experimental Measurements for Pyrolysis Model Validation - Anaerobic Gasification of PMMA Under External Thermal Radiation. https://github.com/MaCFP/matl-db/tree/master/PMMA/Validation_Data/NIST_Gasification_Apparatus, Date Accessed: March 8, 2023, DOI: https://doi.org/10.18434/mds2-2940

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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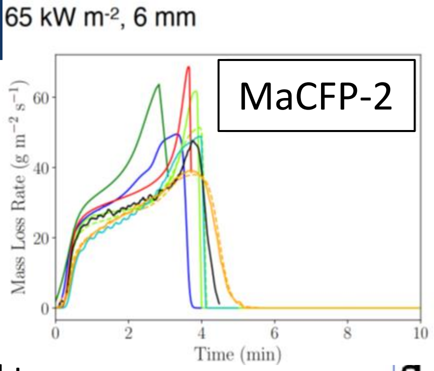
NIST-Gasification-Apparatus: Modeling Targets



- Validation Exercise:
  - Submit new predictions of material response to these test conditions using your <u>original</u> MaCFP-2 pyrolysis models
- (Re)Calibration Exercise:
  - If sufficient agreement is not observed, modelers are asked to recalibrate their property sets (new models are also welcomed)
  - Need to use independent model calibration and model validation datasets: pyrolysis models should <u>not</u> be directly calibrated to new validation data
- Submission deadline: June 1, 2023
  - Simulations of validation experiments using MaCFP-2 property sets
  - Updated material property datasets + simulations of gasification tests
  - Results shared with the community in a virtual meeting (Summer, 2023)

I.T. Leventon and K. De Lannoye. Experimental Measurements for Pyrolysis Model Validation - Anaerobic Gasification of PMMA Under External Thermal Radiation. https://github.com/MaCFP/matl-db/tree/master/PMMA/Validation_Data/NIST_Gasification_Apparatus, Date Accessed: March 8, 2023, DOI: https://doi.org/10.18434/mds2-2940

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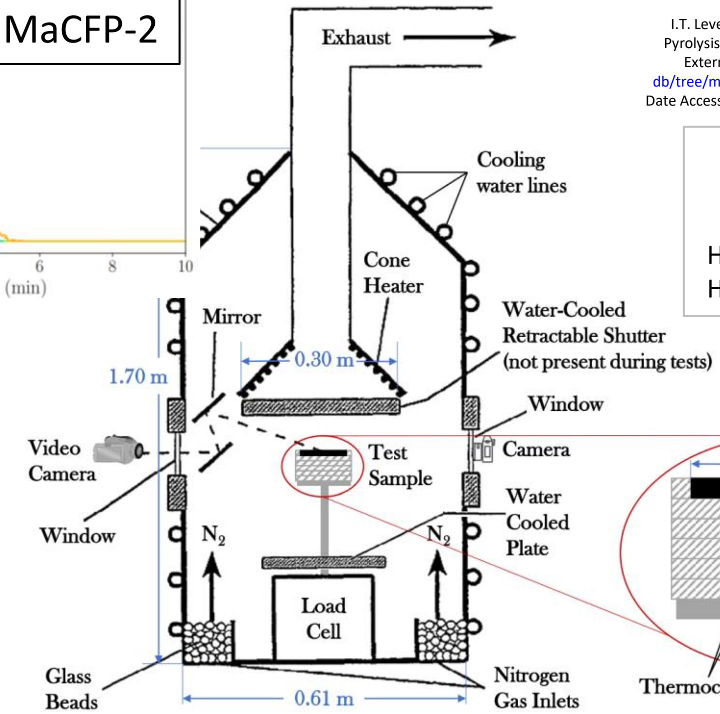
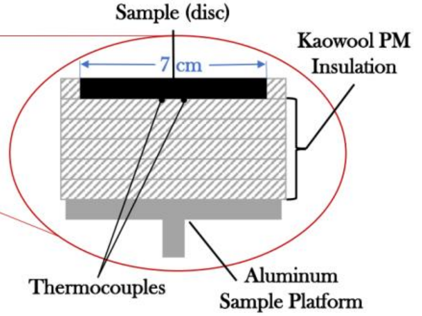
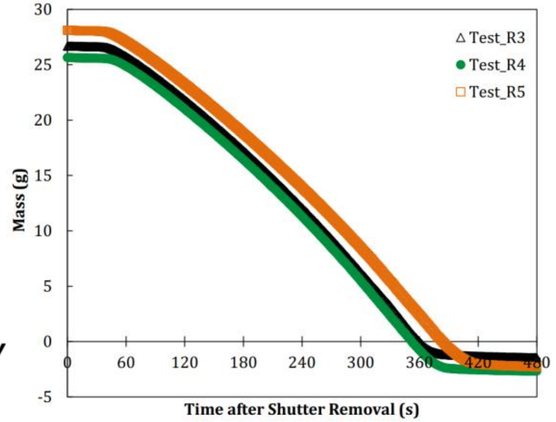
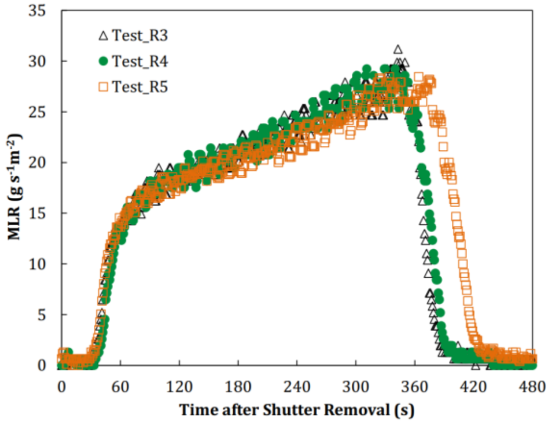
Heater (50 kW m^{-2}): 807 C to 808 C

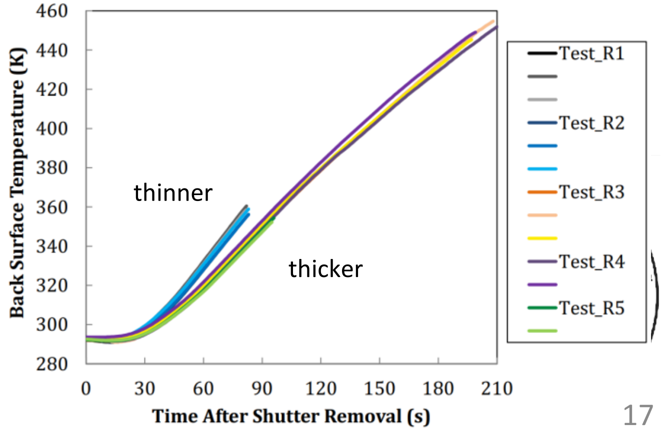




Measured mass loss and back surface temperature rise at $\dot{q}''_{ext} = 50$ kW m^{-2}







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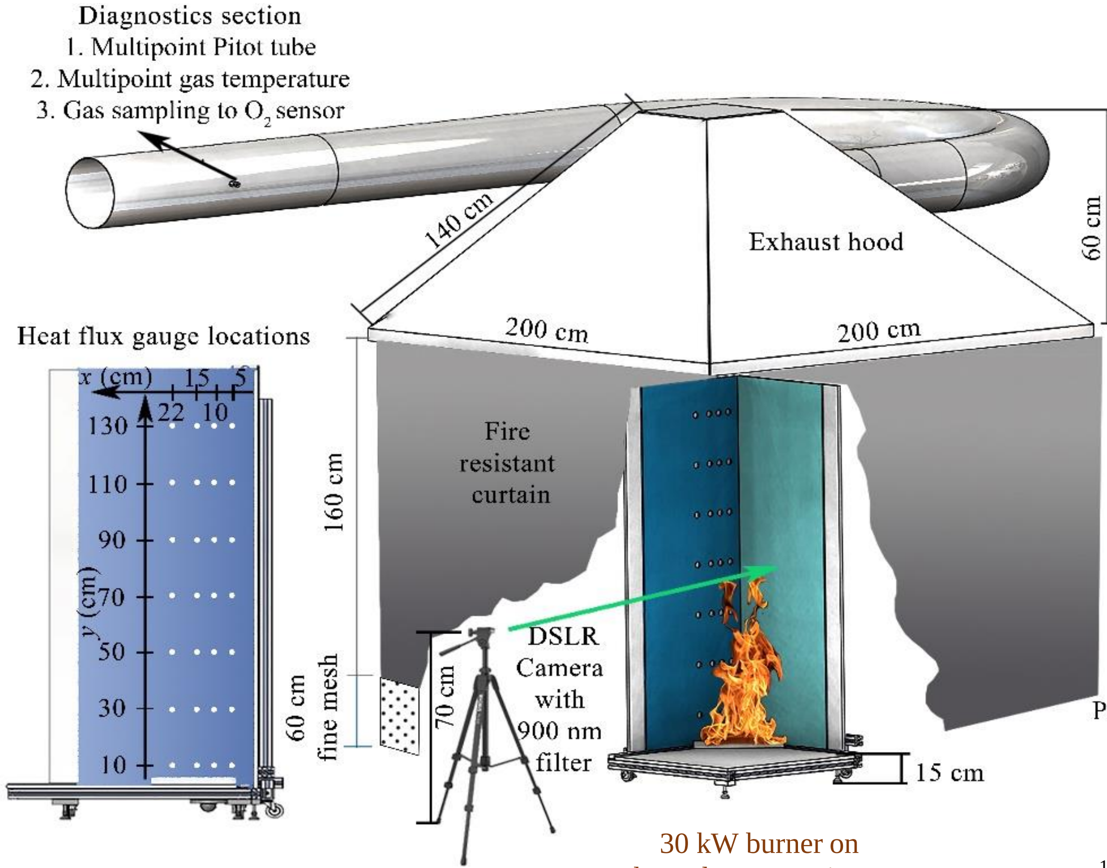
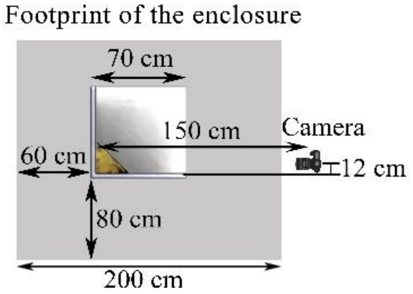
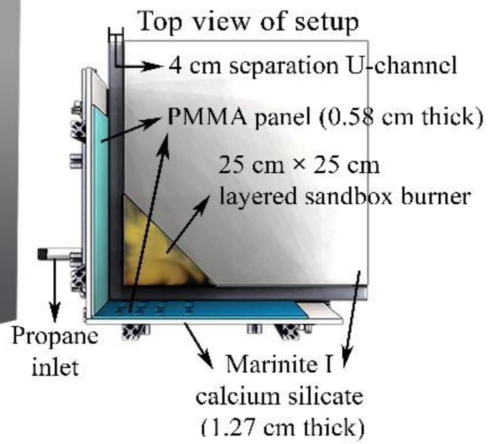
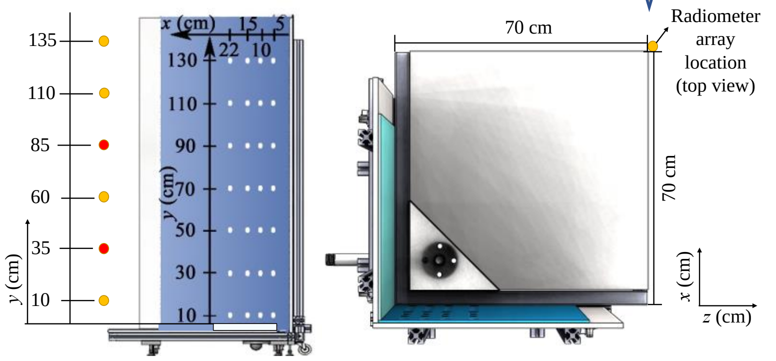
UMD-SBI: Flame Spread on PMMA in Corner-wall Configuration



30 kW burner on throughout experiment







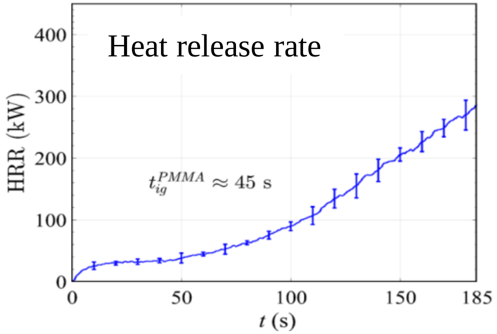
Measurements:

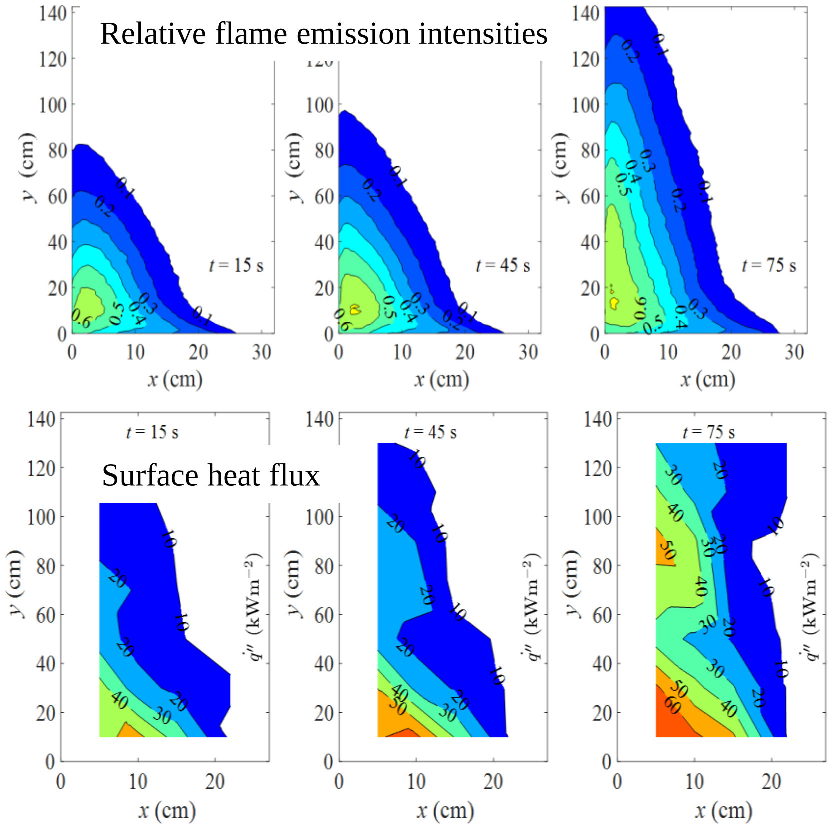
1. Fast-response (13 s) heat release rate (HRR)
2. Flame heat flux with water-cooled gauges positioned in 28 locations distributed over the PMMA surface
3. Radiative heat flux collected at a distance from the corner wall
4. Monochromatic, 900 nm, video of the spreading flame using DSLR camera with a linear sensor response

A description of the setup and experimental procedure can also be found in https://doi.org/10.1016/j.polymdegradstab.2020.109433

UMD-SBI: Simulated Data Required for Submission

<u>Representative experimental results:</u>





<u>Simulated data required for comparison with experiments:</u>

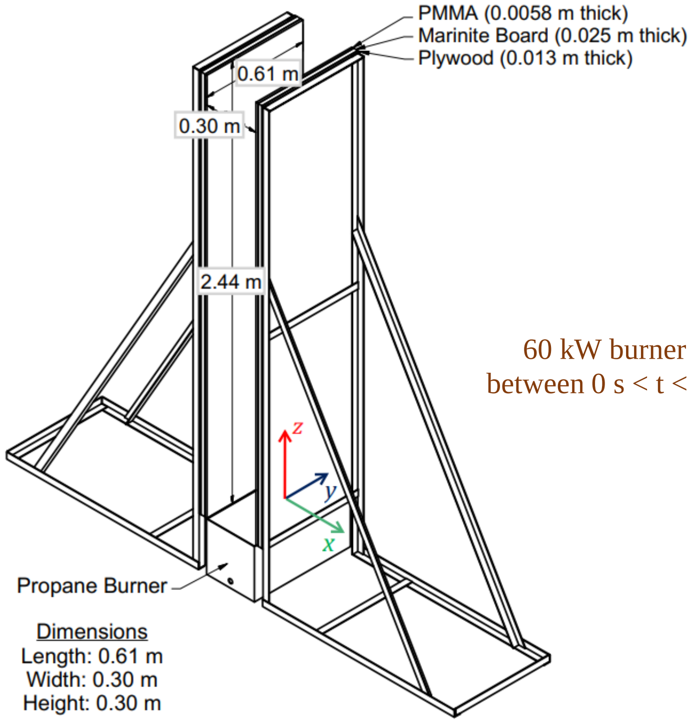
- HRR with time (t)
- Instantaneous flame shapes (identified as the 200 kW m^{-3} iso-contour of volumetric HRR
- PMMA surface heat fluxes to total cold gauges
- Radiative heat fluxes at a distance from the corner wall

<u>Additional simulated data for comparison between simulations:</u>

- 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 along the direction normal to one of the two PMMA surfaces at specified positions and times

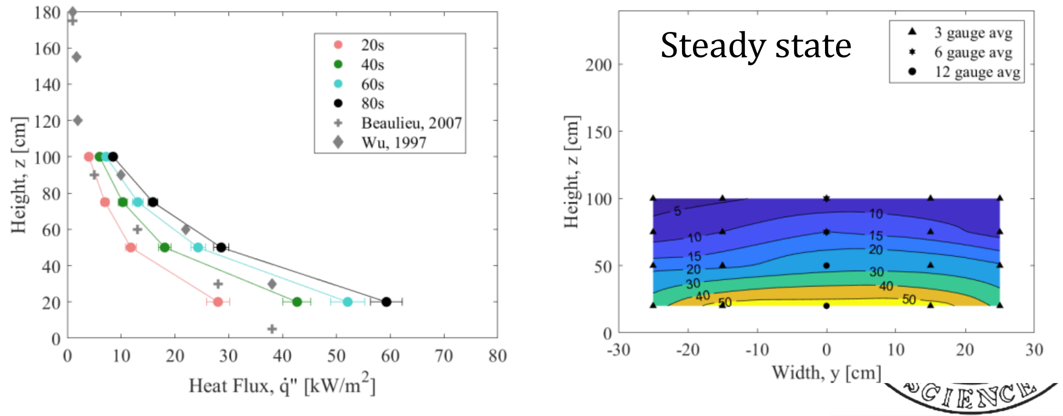
NIST-Parallel-Panel: Experimental Setup

- Collaboration with Nuclear Regulatory Commission (NRC); NIST/NFRL Support; apparatus design based on FM 4910
- Sample size: 2.44 m tall, 0.61 m wide
- Measurement data includes:
  - Time-resolved measurements of fire size (kW), soot generation, and gaseous species production (CO and CO_2)
  - Spatially resolved measurements of flame to wall heat transfer [kW m^{-2}]
  - Radiative heat flux at a distance [kW m^{-2}]
  - Initial and final sample mass
  - Photographs and video of material ignition and fire growth behavior



60 kW burner on between $0 \text{ s} < t < 120 \text{ s}$

Total burner flame heat flux to wall



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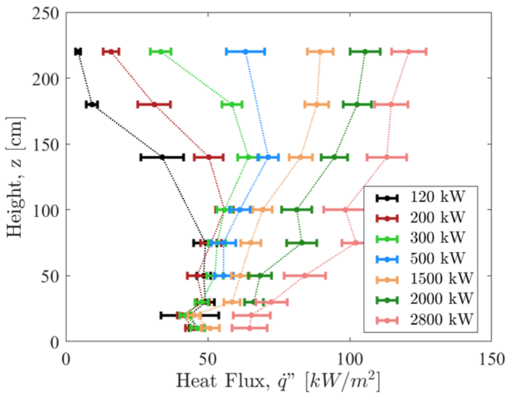
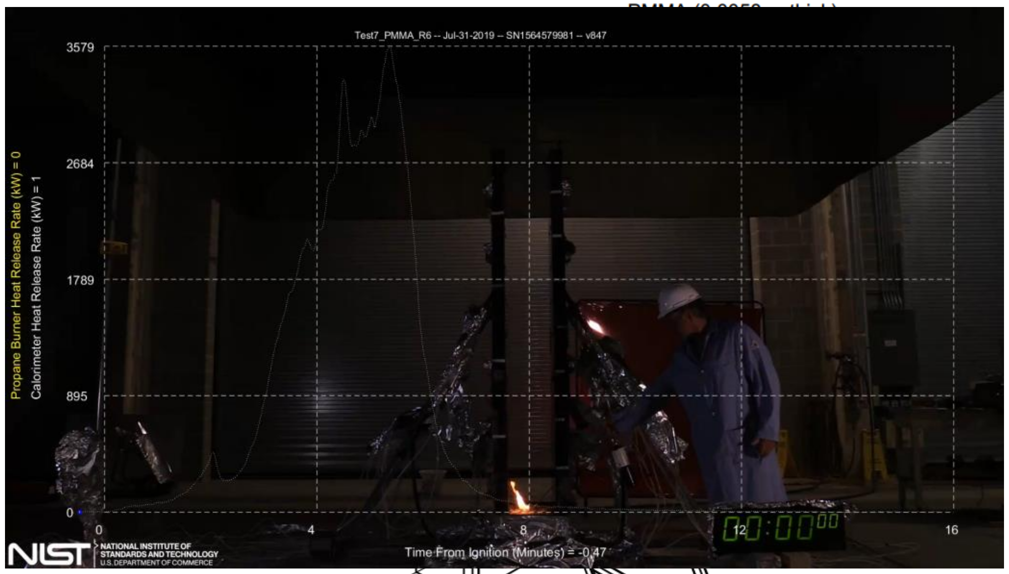
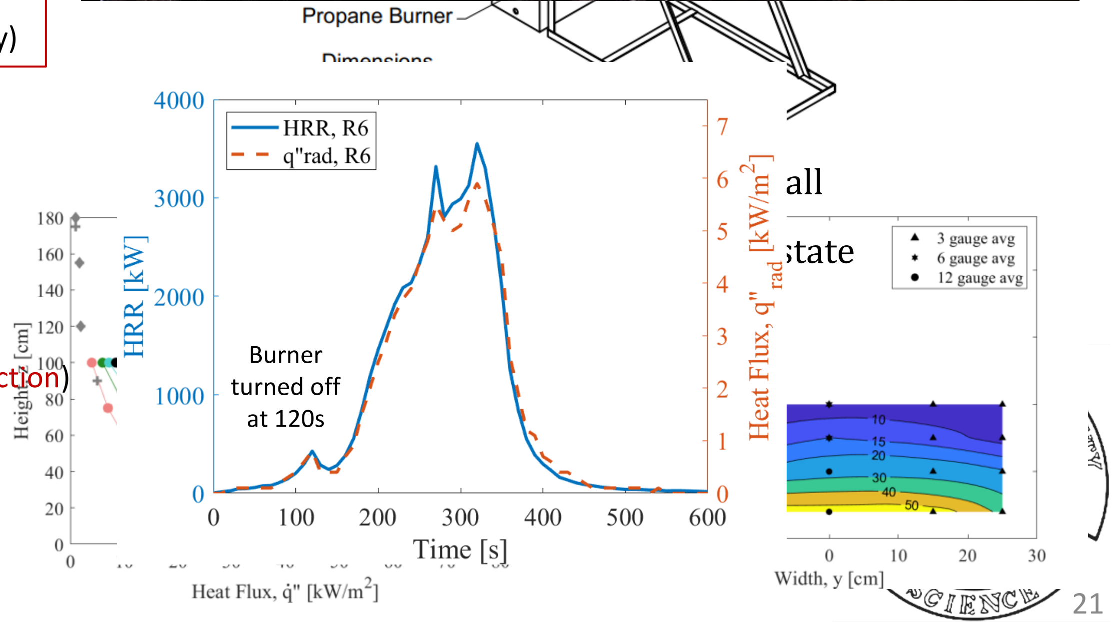
NIST-Parallel-Panel: Modeling Targets





- 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

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



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Summary

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)

Summary

Further details on how to participate in the MaCFP-3 Workshop available:
Guidelines for Participation Document (.pdf) & MaCFP 2023 Modeling Guidelines (Github Wiki)

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:

NIST-Waterloo-Pool-Fires (Liquid pool fires and gaseous burner experiments)	Anthony Hamins anthony.hamins@nist.gov
FM-Burner (Controlled co-flow round diffusion flame experiments)	Yi Wang yi.wang@fmglobal.com
NIST-Gasification-Apparatus (Benchmark gasification experiments of MaCFP-PMMA)	Isaac Leventon isaac.leventon@nist.gov
UMD-SBI (Flame spread experiments in a 1.46-m tall corner wall configuration; based on EN13823)	Stanislav Stoliarov stolia@umd.edu
NIST-Parallel-Panel (Flame spread experiments in a 2.44-m tall parallel panel configuration; based on FM4910)	Isaac Leventon isaac.leventon@nist.gov

Next Steps

March 23 - June 1, 2023

Condensed-phase modelers are asked to perform:

(a) Blind validation: Predict these new results based on their original (MaCFP-2) pyrolysis model properties.

(b) Recalibration: Adjust pyrolysis model parameters *as needed* (or submit new property sets) to provide better predictions (modelers must describe any changes made)

June 1, 2023

Condensed-phase modelers asked to submit final parameter sets and model predictions of:

(1) New experimental data	(NIST Gasification Apparatus)
(2) Ideal gasification tests	Incident heat flux, $\dot{q}''_{inc}$=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

August 31, 2023

Deadline to share pool fire, gaseous burner, and flame spread modeling results

Discussion

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