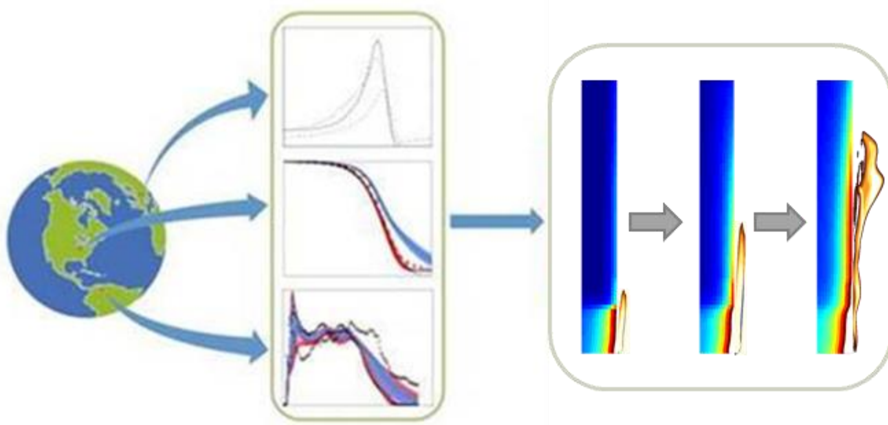
Guidelines for Participation in the
2021 MaCFP Condensed Phase Workshop

April 24-25, 2021
Waterloo, Canada



The MaCFP Condensed Phase Working Group Organizing Committee:
Benjamin Batiot (University of Poitiers, France)
Morgan Bruns (Virginia Military Institute, 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)

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Background

MaCFP Working Group Motivation

The general objective of the MaCFP Working Group is to establish a structured effort in the fire research community to make significant and systematic progress in fire modeling, based on a fundamental understanding of fire phenomena. This is to be achieved as a joint effort between experimentalists and modelers, identifying key research topics of interest as well as knowledge gaps, and thereby establishing a common framework for fire modeling research. The MaCFP Working Group is intended as an open, community-wide, international collaboration between fire scientists. It is also intended to be a regular series of workshops.

The specific objectives of the MaCFP Working Group are to:

- 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.

Condensed Phase Subgroup Objectives

Historically, the fire modeling community has self-organized into two distinct groups: a first group that studies combustion and heat transfer in the gas phase, and a second group that studies thermal degradation and pyrolysis in the condensed phase. The early discussions of the MaCFP Working Group have focused on gas phase phenomena, but with the understanding that quantitatively predicting flame spread and fire growth requires modeling of coupled gas phase and condensed phase processes. Following discussions that took place in April 2016, it was proposed that the MaCFP Working Group be expanded to include a subgroup dedicated to the predictive modeling of condensed phase phenomena. A committee was formed to produce a white paper and organize a planning meeting during the first MaCFP workshop conducted in Lund, SE at the 2017 IAFSS meeting [1].

The purpose of the Condensed Phase Phenomena subgroup is to facilitate data sharing and model development to improve computational predictions of thermal degradation and pyrolysis in fire scenarios.

The specific objectives of the subgroup are to:

- Develop standard data set formats for experimental data on pyrolysis;
- Develop requirements for data set quality and establishing a data review committee;
- Incorporate compliant data into the existing MaCFP data repository;
- Create a database of pyrolysis property sets;
- Develop minimum requirements for numerical pyrolysis models;
- Organize a pyrolysis modeling discussion group.

MaCFP Repository

The MaCFP repository is hosted on GitHub (https://github.com/MaCFP). The repository was created and is managed by Dr. Randy McDermott (National Institute of Standards and Technology, NIST). It contains:

- A description of each selected target experiment, including a description of the experimental configuration and a description of measured quantities and measurement uncertainties (if known);
- An electronic copy of experimental data organized in simple comma-delimited ASCII files;
- An electronic copy of computational results submitted by the different modeling groups that participated in the first MaCFP workshop, also organized in simple comma delimited ASCII files;
- Protocols to perform comparisons between experimental data and simulation results based on (provided) MATLAB-based post-processing tools.

The 2021 MaCFP Condensed Phase Workshop

Workshop Objectives

The experimental and modeling effort proposed for the 2021 MaCFP Condensed Phase Workshop has been designed to enable our research community to make significant progress towards establishing a common framework for the selection of experiments and the methodologies used to analyze these experiments when developing pyrolysis models. Ultimately, such a framework will support reliable computational predictions of how materials burn, how flames spread, and how fires grow in realistic fire scenarios.

The four main objectives of this workshop are listed as follows:

- To catalogue current approaches used to parameterize pyrolysis models;
- To quantify the interlaboratory variability for comparable experimental datasets;
- To assess the impact of the variability of model parameters on predictions of sample burning rate; and
- To present a rigorous analysis of these results in the *Fire Safety Journal*.

Workshop Presentation Topics

The four workshop objectives above will be addressed systematically at the workshop in the context of the following presentation topics:

- Direct comparisons of experimental data;
- Descriptions of various methods for determination of pyrolysis model parameters from the experimental data;
- Comparisons of derived pyrolysis parameters and parameter sets; and
- Comparisons of pyrolysis model predictions of zero-dimensional TGA at several heating rates and one-dimensional gasification scenarios at several incident radiant heat fluxes.

Workshop Timeline

March 2019	Call for participation in MaCFP Condensed Phase Workshop
May 2019	Guidelines for Participation in MaCFP Condensed Phase Workshop Confirm nature of participation (experimental and/or modeling work) of workshop participants
Summer 2019	Coordinate procurement of material samples Define formatting requirements for data submission, open/create repository to store this data
Spring 2020	Experimental measurements first available on the MaCFP GitHub Repository
April 2020	Original submission deadline of modelling results Original workshop date
Early Summer 2020	Committee members develop (and make available on Github) scripts/tools for analysis, processing, and visualization of experimental results
Mid-Summer 2020	Committee members prepare (and share with Participants) a draft report summarizing experimental results; this report will provide the framework of Part I of a rigorous analysis of the results of this workshop to be published in the *Fire Safety Journal* Open discussion forum (online) for experimental results
September 2020	Deadline for participants to submit modeling results
October 2020	Final deadline for participants to submit experimental data revisions
Late Fall 2020	Committee members develop (and make available on Github) scripts/tools for analysis and visualization of simulations results. Committee members prepare a draft report summarizing modeling results for presentation at the 2021 Workshop: this report will provide the framework of Part II of a rigorous analysis of the results of this workshop to be published in the *Fire Safety Journal* Open discussion forum (online) for modeling results
February 2021	Final deadline for participants to submit modeling results revisions
March 2021	Committee prepares final presentations for workshop based on final experimental and modeling results (i.e., pyrolysis model parameter sets, and simulations of material degradation)
April 2021	MaCFP Workshop

Experimental

Material Information

The 2021 MaCFP Condensed Phase Workshop will focus on cast black poly(methyl methacrylate), PMMA. This material was selected because of its tendency to maintain its density while burning, insignificant melt flow, simple decomposition kinetics, and low transparency to infrared radiation. Although multiple experimental and computational modeling studies of the flammability response of PMMA exist in the literature, this effort represents the first coordinated attempt involving multiple labs to simultaneously characterize all relevant thermophysical properties of a fully specified material and to compare various methods for accomplishing this characterization.

The specific material of interest is a 6 mm (0.236 inch) thick, black, cast PMMA manufactured by Evonik under the tradename: ACRYLITE® cast black 9H01 GT. This material can be ordered, cut to size, directly from the manufacturer at: https://www.acrylite.co/cast-black-9h01-gt.html.

Limited quantities of the test material can also be made available directly to participants conducting experiments by contacting the organizing committee, as needed. To request samples, members of the fire research community participating in the experimental component of the 2021 MaCFP Condensed Phase Workshop are invited to contact Dr. Isaac Leventon [National Institute of Standards and Technology (NIST), USA] at Isaac.Leventon@NIST.gov. Please indicate the number and type (e.g., mg-scale thermal analysis and/or bench scale gasification experiments) of tests that you can commit to performing.

Measurements

No single approach for pyrolysis model parameterization is suggested by this committee. In fact, a key objective of this workshop is to catalogue current approaches used to parameterize pyrolysis models. Thus, we encourage participating labs to follow their best practices so that we may meet in April 2021 to discuss only the similarities and differences of our approaches and their results (i.e., final parameterization) without explicitly requiring a final validation versus a given test. We expect that each lab will present data from experiments such as: thermogravimetric analysis (TGA), differential scanning calorimetry (DSC), the Cone Calorimeter, slab gasification experiments, and the Fire Propagation Apparatus (FPA).

Although participants may conduct any experiments they deem necessary to provide calibration data for pyrolysis model development, a key objective of this effort is to quantify the interlaboratory variability for comparable experimental datasets. With that in mind, the following test conditions are recommended for standard experiments that are often performed for material property characterization in flammability laboratories. The tests and test conditions written below are not required from all participants (and additional experiments not listed here or tests performed outside of these conditions are acceptable). However, if you conduct any of the experiments described below as part of your pyrolysis model development, please consider repeating experiments using the guidelines below, to allow for direct comparison of results between laboratories.

When submitting measurement data, participants are asked to clearly define the following conditions associated with the experiments conducted; recommended values for some of these test conditions are included in parentheses. Details of the testing and calibration conditions of all experiments conducted should be provided in a separate document along with measurement results.

Thermogravimetric Analysis (TGA) and Differential Scanning Calorimetry (DSC)

Test Conditions

- Heating Rate (10 K min^{-1})
- Temperature Program: initial temperature, conditioning isotherm (if used), and maximum temperature
- Sample mass (2 mg to 6 mg)
- Sample geometry (powdered)
- Calibration type, materials used, and frequency
- Carrier gas and associated flow rate
- Crucible type and volume

Test Outputs

- Initial and Final Sample Mass [mg]
- Time-resolved Sample Mass [mg]
- Time-resolved Sample Temperature [K]

Cone Calorimeter, Fire Propagation Apparatus (FPA), and Gasification Experiments

Test Conditions

- Radiant heat flux (25 and 65 kW m^{-2})
- Heater Temperature
- Extracting flow rate of the gas
- Initial and Final Sample Mass
- Sample holder geometry and characteristics
- Thermal properties of backing insulation, if used

Test Outputs

- Sample Surface Area [m^2]
- Initial and Final Sample Mass [mg]
- Time-resolved Sample Mass [mg]
- Time-resolved Sample Back-Surface Temperature [K]

Communicating Results

How to Submit Your Results

Experimental and Modeling Results will eventually be submitted, stored, and made publicly available on the MaCFP GitHub Repository. Details on how to contribute are available on the MaCFP-db wiki. For the time being, all results should be emailed directly to Dr. Morgan Bruns [brunsmc@vmi.edu].

For simplicity, please collect your files in a single folder with your INSTITUTE name and ZIP the folder to create a single attachment named "INSTITUTE.zip". Please save measurement results with a name indicating your INSTITUTE and the experimental apparatus used, for example: "INSITUTE_TGA.csv" or "Institute_ConeCalorimeter.csv". Measurement data from repeated experiments should be saved and submitted as separate files, numbered sequentially (e.g., "INSITUTE_TGA1.csv" and "INSITUTE_TGA2.csv").

Please also include two separate files (.txt or .docx) that provide:

1) A description of the test conditions of *all* experiments conducted and submitted (see the 'Measurements' section of this document for details on what information should be included in this file). [INSITUTE_ExpSetup.txt OR .docx]
2) A description (written and corresponding governing equations) of the participant's proposed reaction mechanism as well as the method of determination of associated kinetic parameters and material properties. [INSITUTE_ModelDescription.txt OR .docx]

Note, some iteration on formatting may be required before the results can be merged into the MaCFP database.

File Format

Experimental and Model results should be organized in simple ASCII comma-delimited files (*.csv files) with clear header names. Note: For all submitted measurement data, please ensure that results are obtained with a data acquisition rate between 1 and 10 Hz. Examples of how to format data submissions (for experimentally-measured or model-predicted results) are included below.

Examples of these simple files, which may be used as templates, are also available on the MaCFP GitHub Repository for(1) TGA, (2) DSC, and (3) slab gasification experiments.

Thermogravimetric Analysis (TGA)

Time	Temperature	Mass
[s]	[K]	[mg]
0	300	4.321
0.1	300.1	4.321
0.2	300.2	4.320
0.3	300.3	4.318

Differential Scanning Calorimetry (DSC)

Time	Temperature	Heat Flow
[s]	[K]	[W g^{-1}]
0	300.0	0.005
0.1	300.1	0.008
0.2	300.2	0.006
0.3	300.3	0.007

Cone Calorimeter, Fire Propagation Apparatus, or Slab Gasification Experiments

Time	Mass	HRR$^{\psi}$	Back Surface Temperature 1	Back Surface Temperature 2*	Back Surface Temperature 3*
[s]	[g]	[kW/m2]	[K]	[K]	[K]
0	40.00	0.0	300.0	300.0	300.0
0.1	40.00	0.0	300.0	300.0	300.0
0.2	39.99	0.2	300.0	300.0	300.0
0.3	39.98	0.3	300.0	300.0	300.0

$^{\psi}$ If measured

*At a minimum, sample back surface temperature must be measured at one location; however, if temperature measurements are obtained at multiple locations (at the sample's back surface) during the *same* experiment, please submit those measurements in separate columns, as indicated above. If providing temperature data from multiple locations, please provide a clear description of these locations in your INSITUTE_ExpSetup.txt (or .docx) file.

<u>Units</u>

This may seem like a minor issue, but we must compare the results from all groups in the same units. The units we will use are provided in the Pyrolysis Modeling section of this document. If there is ambiguity in the units or you otherwise have questions along these lines, please let us know.

Pyrolysis Modeling

Standard Data Set: Model Parameters of Interest

Table 1 lists all pyrolysis model parameters of interest for this study. Note: degradation kinetics and thermodynamic parameters can be component- or reaction-step-specific. If your model includes multiple reaction steps and/or components, please include all relevant parameters below for each one. Participants should provide a detailed description of the method of determination of each of these parameters as well as a description (written and mathematical) of their proposed decomposition reaction mechanism.

Table 1. Pyrolysis Model Parameters.

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
$\mathcal{D}$	$m^2\ s^{-1}$	Mass diffusivity
α	m^{-1} or $m^2\ kg^{-1}$	Absorption coefficient
ε	[-]	Emissivity

Target Simulations

Comparisons of pyrolysis model predictions of zero-dimensional Thermogravimetric Analysis (TGA) experiments conducted at two heating rates and one-dimensional gasification scenarios conducted at three incident radiant heat fluxes and two sample thicknesses will be presented and compared at the 2021 MaCFP Condensed Phase Workshop. These simulations will be repeated using all complete pyrolysis model parameter sets submitted by workshop participants. These simulations will be employed to compare performance of different models. In the case of the TGA simulations, mass loss rate profiles as a function of temperature will be used for comparison. In the case of the gasification simulations, mass loss rate and surface temperature profiles will be used for comparison.

<u>Thermogravimetric Analysis (TGA) Experiments</u> [*Two simulations*]

Temperature Range:	300 K to 1000 K
Heating Rates:	10 K min^{-1} and 100 K min^{-1}
Initial Sample Mass	5 mg
Output:	time [s] Time-resolved Sample Temperature [K] Time-resolved Sample Mass [mg]
Test Description:	Simulations of idealized TGA experiments in which sample temperature must remain spatially uniform.

<u>Gasification Experiments</u> [*Six simulations*]

Simulations should be performed using a computational pyrolysis solver.

Initial Temperature	Initial ambient and sample temperatures should be 293K.
Top Surface Boundary Conditions:	Sample surface exposed to 10, 25, and 65 kW m^{-2} of incident radiant heat flux; no convection
Bottom Surface Boundary Conditions:	Sample back surface should be perfectly insulated. (i.e., no convection or radiation)
Sample Dimensions:	Simulations should be repeated at each incident heat flux using sample thicknesses of 6 mm and 12 mm. Simulation outputs should be scaled such that samples are initial 10 cm x 10 cm, squares.
Output:	Time [s] Time-resolved Sample Mass [g] Time-resolved Sample Back-Surface Temperature [K] Time-resolved Sample Top-Surface* Temperature [K], (*reported as the average value of temperatures calculated across a 1-mm-thick layer at the top of the sample)

File Format (Model Simulations)

Please email your simulation results as individual .csv files directly to Dr. Morgan Bruns at (brunsmc@vmi.edu) using the following naming convention: "INSTITUTE_TGA_10K.csv" or "INSTITUTE_Gasification_25kW_6mm.csv". Examples of how to format simulation data submissions are included below.

Thermogravimetric Analysis (TGA) Simulations

Time	Temperature	Mass
[s]	[K]	[mg]
0	300	4.321
1	300.17	4.321
2	300.33	4.320
3	300.50	4.318

Gasification Simulations

Time	Mass	Back Surface Temperature	Top Surface Temperature
[s]	[g]	[K]	[K]
0	40.00	300.0	300.0
1	40.00	300.0	300.2
2	39.99	300.0	300.4
3	39.98	300.0	300.6

Contact Information

Benjamin Batiot
University of Poitiers, France
benjamin.batiot@univ-poitiers.fr

Morgan Bruns
Virginia Military Institute, USA
brunsmc@vmi.edu
+1 540-464-7523

Simo Hostikka
Aalto University, Finland
simo.hostikka@aalto.fi
+358504471582

Isaac Leventon
National Institute of Standards and Technology (NIST), USA
Isaac.Leventon@NIST.gov
+1 301-975-6887

Yuji Nakamura
Toyohashi University of Technology, Japan
yuji@me.tut.ac.jp

Pedro Reszka
Universidad Adolfo Ibáñez, Chile
pedro.reszka@uai.cl

Thomas Rogaume
University of Poitiers, France
thomas.rogaume@univ-poitiers.fr

Stanislav Stoliarov
University of Maryland, USA
stolia@umd.edu
+1 301-405-0928

References

[1] A. Brown, M. Bruns, M. Gollner, J. Hewson, G. Maragkos, A. Marshall, R. McDermott, B. Merci, T. Rogaume, S. Stoliarov, J. Torero, A. Trouvé, Y. Wang, E. Weckman. Proceedings of the first workshop organized by the IAFSS Working Group on Measurement and Computation of Fire Phenomena (MaCFP). Fire Safety Journal, vol. 101, pp. 1-17, 2018.