The MaCFP Condensed Phase Working Group: A Structured, Global Effort Towards Pyrolysis Model Development

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Abstract
The International Association for Fire Safety Science (IAFSS) Working Group on Measurement and Computation of Fire Phenomena (i.e., the MaCFP Working Group) has been established as a global collaborative effort between experimentalists and modelers in the fire safety science field to make significant and systematic progress in fire modeling, based on a fundamental understanding of fire phenomena. In 2016, the Condensed Phase Phenomena MaCFP Subgroup was formed to maintain an effort focused on improving the predictive capabilities of numerical simulations of thermal decomposition and pyrolysis. Two MaCFP workshops have since been organized as pre-events to recent IAFSS Symposia: the first in Summer 2017, in Lund, Sweden, and the second, in Spring 2021, which was hosted virtually by the University of Waterloo, Canada. This paper details the planning and coordination needed to organize the Condensed Phase Subgroup's contribution to these two events, with special emphasis on the efforts enabling the 2021 Workshop, including: identification, procurement, and distribution of a reference material; development of guidelines for reporting experimental measurements; and development and maintenance of an online repository for experimental measurements and related analysis scripts. Preliminary analysis of the experimental and modeling results submitted to the 2021 Condensed Phase MaCFP Workshop are also briefly discussed.

1 Background

As the fire safety science field matures, building design is moving away from prescriptive approaches and towards performance based design approaches based on predictions of fire development and the resulting structural/system response [1, 2]. Thus, for practicing fire protection engineers (FPEs), fire modeling is probably of most relevance as an engineering design tool. As access to greater computational resources grows, numerical solution schemes evolve, and knowledge and available descriptions of the physical and chemical mechanisms controlling fire behavior matures, the predictive capabilities of numerical solvers designed for fire scenarios continues to advance. Examples of such tools designed specifically for fire scenarios include FireFOAM [4], FDS [5], Gpyro [6, 7], ISIS [8], SIERRA/Fuego [9], and ThermaKin [10, 11]). Thorough reviews of the capabilities of such models are available elsewhere [12, 13, 14].

Although it is widely identified that simulations of the transport of smoke and heat in compartment fires can be accomplished with reasonable accuracy [15, 16, 13], simulating crucial processes such as flame spread and fire growth remains difficult [17, 21]. Advancement of computational models to allow for the quantitative prediction of fire development (i.e., ignition, flame spread, and steady burning behavior) would allow for a significant advance in how FPEs can use these fire modeling tools: no longer would a design fire have to be prescribed as an input to the model (which can often require costly, full-scale experiments or simplifying assumptions to select a suitable, potentially over-conservative, design fire) but this fire growth could be predicted in response to a range of likely ignition conditions based on the properties of the combustible material(s) of interest. Such modeling capability can offer a practical and cost-efficient means for safer design strategies in the built environment.

In a 1994 letter to the editor of the Fire Safety Journal [17], Howard Emmons and colleagues noted that predicting fire growth based on a sound scientific basis is both possible and necessary and to do so requires[1], "international cooperation in resolving the remaining scientific problems so that we harmonize our fire safety objectives, design scenarios, hazard assessment, *methodologies, models and their verification* for eventual incorporation into a common set for fire safety engineering tools. More specifically, we suggest the *formation of a series of technical workshops* having limited attendance to provide the needed *international collaboration*". The Measurement and Computation of Fire Phenomena initative (MaCFP Working Group, https://www.iafss.org/macfp/) represents a significant step towards accomplishing these goals.

The MaCFP Working Group is intended as an open, community-wide, international collaboration between experimentalists and modelers in the fire safety science community. This initiative was started following discussions that took place in February, 2014, at the 11th International Association for Fire Safety Science (IAFSS) Symposium, which led to the production of a white paper [18] that defined the motivation, objectives, and structure of the working group; this white paper received the endorsement of IAFSS in March, 2015. The general objective of the MaCFP Working Group is to establish a structured, collaborative effort to make significant and systematic progress in fire modeling through a fundamental understanding of fire phenomena. 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 Computational Fluid Dynamics (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)

[1] Emphasis in *italics* is that of the authors of this manuscript

- Establish a network between fire researchers and provide a community-wide forum for discussion and exchange of information

Although the MaCFP Working Group initially focused on gas phase phenomena (e.g., buoyancy induced flow, combustion, and flame extinction) [19, 20], in 2016, discussions were started to expand the focus of the initiative to include the modeling of condensed phased phenomena (i.e., pyrolysis). The 2017 MaCFP Workshop (MaCFP-1) thus served as both the first technical meeting for the Gas Phase Subgroup and a planning meeting for the Condensed Phase Subgroup [21]. It is planned that the two subgroups will collaborate in the upcoming 2023 MaCFP Workshop (MaCFP-3) to study the combined condensed- and gas-phase processes that control flame spread.

2 The MaCFP Condensed Phase Subgroup

Surface flame spread has been identified as a key determinant of the rate of fire growth in the early stages of building fires [22]. In simplest terms, flame spread is controlled by positive feedback between heat transfer to the surface of a combustible material (e.g., energy release due to gas-phase combustion in the flame) and the in-depth heating, thermal decomposition, and production of combustible gases by the solid. Thus, a quantitative understanding of the material properties (and their potential dependence on temperature and composition) and the physical and chemical mechanisms that govern ignition and burning of solids is essential for advancing our ability to predict and mitigate fire development. In 2016, the MaCFP Condensed Phase Subgroup was organized to facilitate data sharing and model development to improve computational predictions of thermal decomposition and pyrolysis in fire scenarios.

2.1 MaCFP-1: Lund, Sweden (2017)

At the 2017 MaCFP Condensed Phase Workshop (MaCFP-1) [21], a review was presented of the challenges associated with pyrolysis measurements and modeling for fire applications. Review topics included: identifying experimental apparatus, datasets, and associated analysis tools needed to calibrate the material properties used in computational pyrolysis models (i.e., model inputs); providing accurate descriptions of the condensed- and gas-phase processes occurring at the solid/gas interface, which control ignition and flame spread; discussion of the relevant complexity needed to describe condensed-phase material decomposition and the capabilities of various numerical tools to capture these phenomena; and the need to validate these models to predict material burning behavior across a range of scales. Open discussion between participants of this meeting provided critical input from the fire research community regarding test methods of interest and their respective calibration requirements (and applicability) as well as the need to identify appropriate validation datasets (at small- and large-scale) for relevant test materials that allow for sufficient complexity for real-world application while retaining needed simplicity for modeling purposes. A coordinated effort was thus proposed to develop experimental datasets for pyrolysis model calibration and validation and to develop an open, freely-available digital archive to maintain this information.

The MaCFP-1 program and copies of the presentations can be found at https://iafss.org/3770-2/. At this meeting, specific objectives of the MaCFP condensed phase subgroup were identified as:

- Develop standard data set formats for experimental data on pyrolysis
- Develop requirements for data set quality (and completeness) and establish a data review committee
- Incorporate compliant data into the existing MaCFP data repository
- Catalog state-of-the-art approaches used to parameterize pyrolysis models
- Create a database of pyrolysis property sets
- Assess the impact of the variability of model parameters on fire growth predictions
- Develop minimum requirements for numerical pyrolysis models
- Organize a pyrolysis modeling discussion group

2.2 MaCFP-2: University of Waterloo, Canada (2021)

Organization & Planning

The experimental and modeling effort of the 2021 MaCFP Condensed Phase Workshop (MaCFP-2) has been designed to enable the fire 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. A single reference material - cast black poly(methyl methacrylate), PMMA [2] - was selected for study 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 [23, 24, 25, 26, 27] and computational modeling studies of the flammability response of PMMA exist in the literature [23, 28, 29, 30] this effort represents the first coordinated attempt involving multiple institutions to simultaneously perform a series of pyrolysis experiments across a range of scales, characterize all relevant thermophysical properties of a fully specified material, and to compare the various methodologies for doing so.

A timeline for the preparation leading to MaCFP-2 is provided in Table 1. As seen here, an initial set of guidelines for participation was shared with workshop participants (along with the samples needed for experiments) nearly two full years before final workshop presentations. The 'Guidelines for Participation in MaCFP Condensed Phase Workshop' document was first shared electronically (directly by email to registered participants and publicly posted on the IAFSS website: https://iafss.org/macfp-condensed-phase-phenomena/) and on paper at a series of flammability conferences in Summer, 2019. Later revisions to this document were provided to periodically update participants (e.g., to announce to modelers the availability of experimental datasets or to describe scheduling adjustments due to Covid-19 delays). Workshop participants were updated regularly (at 3 to 4 month intervals) with copies of these new guidelines;

[2]The specific material of interest is a nominally 6 mm (0.236 inch) thick, black, cast PMMA manufactured by Evonik under the tradename: ACRYLITE® cast black 9H01 GT. Note: the identification of any commercial product or trade name does not imply endorsement or recommendation by the National Institute of Standards and Technology, NIST (or any other contributing institution).

with renewed calls for participation and deadline reminders (e.g., submission of experimental or modeling results); and with the announcement of new resources (e.g., availability of experimental datasets and/or tools to analyze these results).

Table 1: MaCFP-2 Workshop Timeline (Condensed Phase Subgroup)

March 2019	Call for participation in MaCFP Condensed Phase Workshop
May 2019	Share 'Guidelines for Participation in MaCFP Condensed Phase Workshop' document. Confirm nature of proposed contribution (experimental and/or modeling work) of workshop participants.
Summer 2019	Coordinate procurement and distribution of material samples. Define formatting requirements for data submission, create online repository (https://github.com/MaCFP/matl-db) to store this data.
Winter 2019/2020	Experimental measurements first available on the MaCFP GitHub Repository. Initial data review and calls to experimentalists to submit new measurements and/or revisions, as needed.
March 2020	Original deadline for submission of modelling results (delayed due to Covid-19)
April 2020	Original workshop date (delayed due to Covid-19)
Early Summer 2020	Share revised 'Guidelines for Participation in MaCFP Condensed Phase Workshop' document with community. Committee members develop (and make available on Github) scripts/tools for analysis, processing, and visualization of experimental results.
Mid-Summer 2020	Committee members prepare 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.
October 2020	Committee shares preliminary summary of experimental measurements. Preliminary Draft Report available online (Oct. 1); overview of results presented in a virtual seminar (Oct. 15). Committee opens virtual discussion forum to enable open scientific and technical communication within the fire modeling community. Call for participants to submit modeling results
Late Fall 2020	Requested deadline for participants to submit revisions to experimental data sets
February 2021	Requested deadline for participants to submit modeling results revisions. Share revised 'Guidelines for Participation in MaCFP Condensed Phase Workshop' document with community.
March 2021	Committee members develop scripts for analysis and visualization of simulations results and prepare summaries of final experimental and modeling results (i.e., pyrolysis model parameter sets, and simulations of material degradation).
April 2021	MaCFP-2 Workshop (hosted virtually by the University of Waterloo, Canada)

No single approach for pyrolysis model parameterization was suggested by the MaCFP Condensed Phase Subgroup Organizing Committee. In fact, a key objective of MaCFP-2 was to catalog the current state-of-the-art approaches used to parameterize pyrolysis models. Participating labs were therefore encouraged to follow their best practices regarding experimental selection and data analysis. However, to reduce uncertainty in measurement results and to enable direct comparison of datasets submitted by each of the participating institutions, the Organizing Committee prepared and provided material samples directly to experimentalists and suggested standard test conditions and reporting formats for likely experiments.

Test samples were made available directly to participating institutions beginning Summer 2019 in the form of 100 mm by 100 mm by 6 mm slabs for bench-scale experiments (e.g., cone calorimeter) and approximately 300 mg vials of powdered[3] PMMA for micro-scale experiments (e.g., thermogravimetric analysis, TGA). Samples were shared directly with participants who attended the 2019 Flammability of Polymeric Materials Conference (FRPM19) in Turku, Finland, and the 15th International Conference and Exhibition on Fire Science and Engineering (Interflam 2019) in London, England. Additionally, participating laboratories could contact MaCFP Condensed Phase Organizing Committee members directly to request that samples be mailed to their institutions (in sufficient quantities for the specific experiments that they could commit to performing). In total, sixteen institutions from ten different countries submitted experimental measurements in time for MaCFP-2. These institutions and their home countries are identified in the Preliminary Summary of Experimental Measurements' document shared by IAFSS [31]; a summary of the initialisms used to identify each participating institution (e.g., in the legends of figures) is provided at the end of this document.

Experimental Results and the MaCFP Repository

Experimental measurements were submitted electronically by participating institutions and were organized and made publicly available in the MaCFP repository, which is hosted on GitHub (https://github.com/MaCFP/matl-db). This database is version controlled, with each addition to (or edit of) measurement data saved with a unique identifier (i.e., commit tag). The repository was created and is managed by members of the MaCFP Organizing Committee. Measurement data can be incorporated or revised by emailing Organizing Committee members or by submitting a pull request directly on GitHub; the latter approach is preferred for efficient long-term maintenance and use of the database by multiple institutions.

As of October, 2021, measurement data from 220 unique experiments (conducted under 35 different test conditions on the same exact PMMA) have been added to the MaCFP respository. All measurement data submitted by each institution is organized in a single folder with the institution's name. A consistent file naming convention is used for all test data (i.e., across all folders). File names indicate the institution name, experimental apparatus, and basic test conditions (e.g., gaseous environment and incident heat flux or heating rate). Measurement data from repeated experiments is saved in separate, ASCII comma-delimited (.csv) files, each numbered sequentially. Participants were also asked to provide a written description of sample preparation, test setup, and test procedure in order to clearly define the conditions associated with the experiments conducted.

[3]Powdered samples were prepared by first pelletizing 6 mm thick slabs using an electric grinder into small (0.5 mm to 5 mm) pieces, which were then ground into a powder using a mechanical grinder with a ceramic burr.

This information is included in each folder as a README.md file; this file is automatically interpreted by GitHub as Markdown (.md) text and provides a brief description of an institution's data.

As seen in Table 1, multiple calls for experimental data were made in the two years leading up to the MaCFP-2 Workshop. A standard data format was requested and templates were provided to experimentalists in both the 'Guidelines for Participation' document and on the GitHub repository. However, during the first months of 2020, a significant effort was required to reformat submitted datasets such that they maintained uniform: naming convention (both filenames and column headers), data reporting order (e.g., for TGA data, only the following three columns of data were provided, in order: Time [s], Temperature [K], and Mass [mg]), starting values and sign conventions (e.g., for TGA data, mass reported at the first time step was equal to initial sample mass; or, for differential scanning calorimetry, DSC, data, positive heat flow indicated endothermic events), and units. To accumulate necessary statistics, a minimum data reporting frequency of 1 Hz (for bench-scale measurements; e.g., cone calorimeter) or 0.5 K^{-1} (for mg-scale measurements; e.g., TGA or DSC) was requested. Higher resolution datasets were accepted and stored as-submitted (though with no higher than 5 times the needed resolution); these results were later post-processed to provide a unified output frequency by the analysis scripts developed for this project.

Although these processing steps are relatively straightforward, performing them was a time-consuming, manual task. This investment was necessary to enable the generation and use of simple scripts for automated processing of final datasets (which was critical to efficiently analyzing the large number of submitted files). In processing submitted datasets, some clear errors were identified: e.g., under-resolved data, measurements that appeared to be conducted under different conditions than reported (i.e., different gaseous environments or heating rates), or calibration issues that led to non-physical measurement data. Experimentalists were contacted directly by email and asked to identify these issues and submit data revisions as needed. With help from the pyrolysis modeling community, once these initial measurements were available, an enhanced standard formatting of the README files was proposed to more thoroughly (and consistently) report sample setup and testing conditions. This information is required to analyze measurement data for the purposes of model calibration (i.e., parameter optimization). README files for each dataset were thus reviewed and revised similarly as submitted measurement data itself, and experimentalists were contacted directly by email when discrepancies or missing information were identified.

On October 1, 2020, a preliminary draft report of measurement results was shared electronically with members of the fire research community. On October 15, 2020, the MaCFP Condensed Phase Organizing Committee presented an overview of these experimental results in a virtual seminar and a virtual discussion forum was opened for all members of the pyrolysis modeling community (both experimentalists and modelers). All scripts needed for the analysis (e.g., data smoothing, averaging, and calculation of statistics, as well as tabulation of key parameters such as onset times or temperatures of decomposition) and plotting of these results were made publicly available on the MaCFP GitHub Repository. To allow for objective review of these preliminary results by the community, in all figures and tables containing experimental measurements, institutions were referred to using a unique, anonymous city name. This allowed for discussion and review of submitted results, based purely on the merit of the data in question.

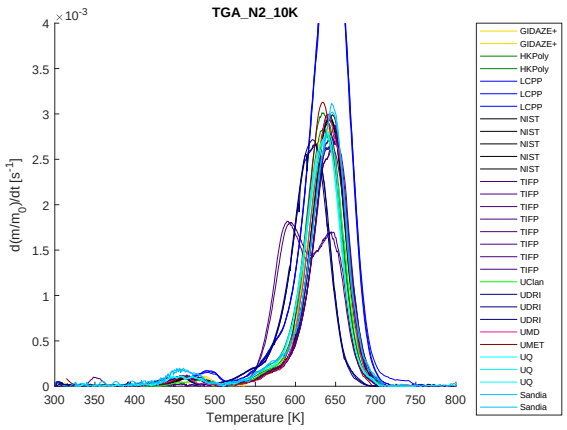
The October 15, 2020 presentation of experimental results included:

- Brief descriptions of all experiments conducted and test conditions used
- A summary of all measurement data, organized by experiment type and test conditions
- Calculations of error for each dataset based on a standard data smoothing methodology and error calculation that was clearly defined and uniformly applied to all measurement data
- Calculations of 'average' curves / datasets (neglecting obvious outliers)
- A preliminary (brief) analysis and comparison of experimental results

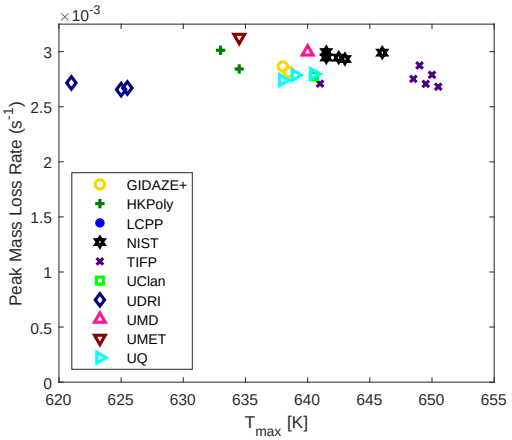
Discussion amongst participants of this virtual seminar indicated a need for an objective rating system to identify data quality or, at a minimum, how to identify which datasets should be excluded as outliers. Additionally, although the repeatability of measurements submitted by each institution was quite good, greater variation was observed between measurement data (obtained under nominally identical test conditions) submitted by different labs. Some of these variations were stochastic; others had identifiable causes (e.g., in bench scale tests, variations in sample backing insulation or heating element type and operating temperature; see Fig. 2b). Understanding the source of these discrepancies is critical. The MaCFP Condensed Phase Organizaing committee thus provided guidance on how to interpret and use measurement data in the MaCFP Github Repository (available: https://iafss.org/macfp-condensed-phase-phenomena/). These guidelines identify key factors influencing material response during mg-scale and g-scale experiments and criteria to identify clearly incorrect behavior in measurement data (e.g., outliers or non-physical measurement signal response).

In the six-month period between this preliminary presentation of experimental results and the MaCFP-2 Workshop, multiple groups of experimentalists provided: further clarity in their respective README documents (e.g., better identifying test setup or boundary conditions), edits and adjustments to their original measurement data (e.g., to improve data resolution), and/or new measurement data. This additional effort by experimentalists helped to quantify some sources of variations among datasets submitted by different institutions and to identify and remove outliers. Final experimental results were presented at the MaCFP-2 Workshop in April 2021; a copy of this presentation is available online:https://github.com/MaCFP/matl-db/releases.

Figures 1 and 2 provide representative examples of mg- and g-scale measurement data submitted to the MaCFP-2 Workshop. Note: although these figures contain measurement data from experiments repeated by multiple institutions under nominally identical conditions, not all institutions that contributed experimental measurements are represented here. A summary of all submitted datasets is provided elsewhere [31].

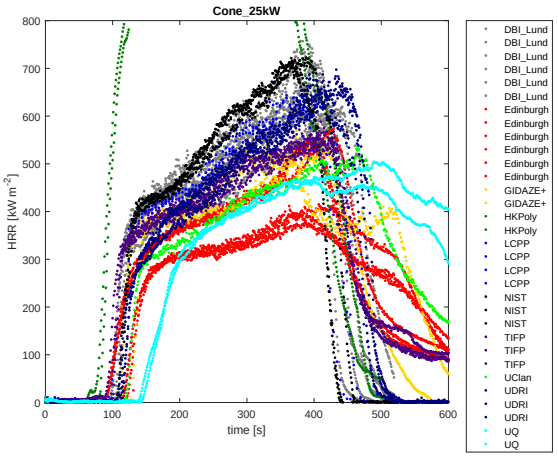


(a) Mass loss rate (normalized by initial sample mass, m_0)

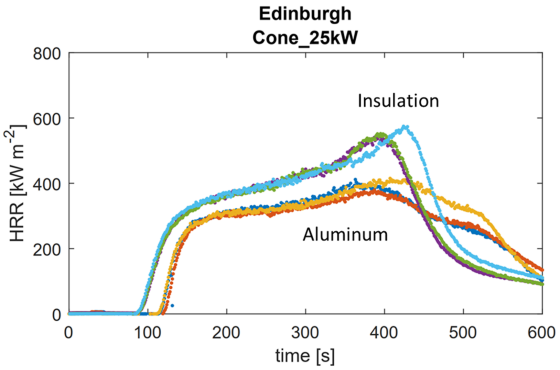


(b) Peak mass loss rate and the temperature at which it was observed

Figure 1: Measurement data from TGA tests conducted in an anaerobic environment at a nominal heating rate of 10 K min^{-1}. Results demonstrate the repeatability and reproducibility of measurements from repeated tests conducted by a single laboratory vs. all contributing institutions.



(a) Measured HRR in cone calorimeter tests performed by all contributing institutions (with this incident heating)



(b) Impact of sample backing material on measured HRR in cone calorimeter tests conducted by the University of Edinburgh

Figure 2: Measured area-normalized heat release rate, HRR, in cone calorimeter tests conducted with an incident heat flux of 25 kW m^{-2}.

Modeling results

The second phase of the MaCFP-2 Condensed Phase Workshop asked modelers to use the experimental measurement data available in the MaCFP Repository to calibrate a full set of pyrolysis model parameters and to use these parameters to provide model predictions for a set of target scenarios (zero- and one-dimensional heating of PMMA in idealized, fire-like environments). At the conclusion of the October 2021, virtual presentation of experimental results (and again, by email,

in December 2021) modelers were encouraged to prepare and submit:

- A description of the process they used to determine (i.e., calibrate) model parameters;
- A formatted table of all model parameters (see Table 2); and
- Predictions of requested target data (simulations of material heating and decomposition in response to well-defined, idealized heating scenarios) using these model parameters.

Although modelers were not provided limitations or suggestions regarding their pyrolysis model parameterization (i.e., calibration) approach, modelers were required to use at least one of the mg-scale data sets (e.g., TGA or DSC) and one g-scale experiment (e.g., cone calorimetery or controlled atmosphere gasification experiments), or at least two of the g-scale experiments available in the MaCFP repository. Modelers could supplement the MaCFP data with any literature data that was deemed necessary. Modelers could *not* use experimental data of the target scenarios (i.e., the idealized zero- and one-dimensional heating scenarios) for model calibration as this would no longer make simulation results true predictions. Table 2 shows the complete set of pyrolysis model parameters that was requested from participants; this standard reporting format, nomenclature, and associated units allowed for direct comparisons of values submitted by contributing institutions.

In total, the MaCFP-2 effort received modeling contributions from nine unique institutions located in six different countries. Collectively, these different contributions used measurement data provided by *all* of the experimental apparatus in the MaCFP repository. Parameter optimization was accomplished using a wide variety of techniques including: automated optimization algorithms, Monte Carlo sampling, manual updating, and direct measurement. Four computational pyrolysis solvers were used for this model calibration (FDS [5], Gpyro [6, 7], SIERRA/Fuego [9], and ThermaKin [10, 11]). Although a large variation was observed in calibrated kinetic parameters (activation energy and pre-exponential constant; i.e., frequency factor), kinetic compensation [32, 33, 34] was clearly observed as illustrated in Fig. 3. For most other properties, calibrated model parameters typically varied within 10 % to 50 % of the average of values submitted to the MaCFP-2 Workshop.

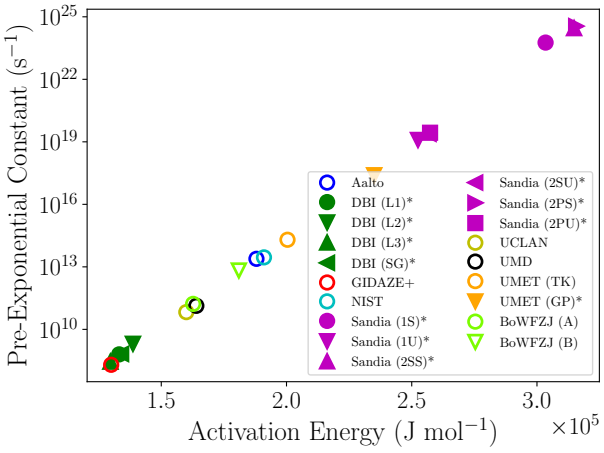


Figure 3: Calibrated kinetic parameters for the main decomposition reaction of PMMA.

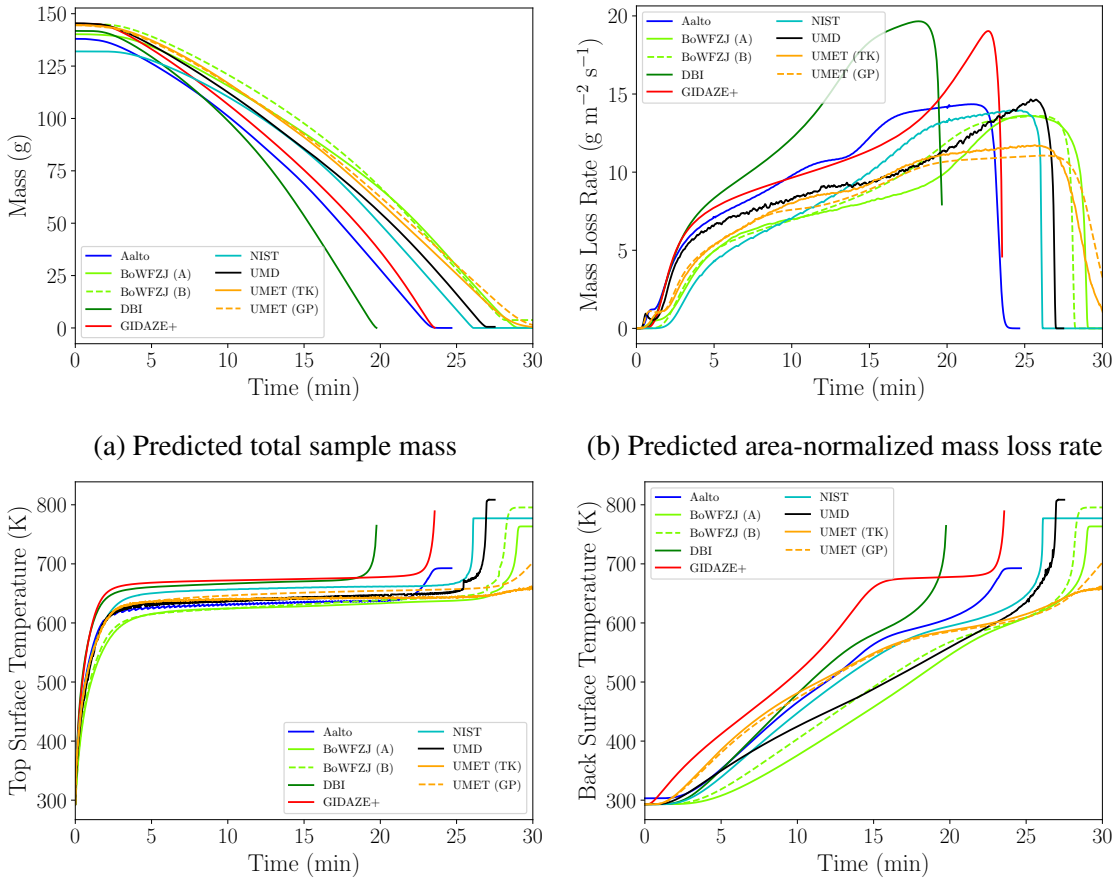
Table 2: Requested Pyrolysis Model Parameters

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

Key questions to consider when analyzing these variations in pyrolysis model parameter sets are: (a) how sensitive (if at all) are model predictions of material flammability response to changes within this variability, (b) what are the most influential properties, and (c) are parameter estimates or simulation results sensitive to the calibration method or the simulation tool used to predict material flammability behavior? To help answer these questions, modelers were asked to use their final parameter sets to simulate zero-dimensional experiments (TGA tests conducted at two heating rates) and one-dimensional gasification scenarios (conducted at three incident radiant heat fluxes and two sample thicknesses). In the case of the TGA simulations, mass loss rate profiles as a function of temperature were reported. In the case of the gasification simulations, mass loss rate and surface temperature profiles as a function of time were reported. Predictions of material behavior in both scenarios were presented and compared at the MaCFP-2 Workshop.

Figure 4 plots predicted sample mass loss and surface temperature in an idealized, one-dimensional gasification scenario (i.e., adiabatic back surface; 25 kW m^{-2} radiant heating at the top surface, with no convection) when using each of the parameter sets submitted to the MaCFP-2 Workshop. As seen here, an order of magnitude variation in predicted onset time of mass loss is observed and, at steady state, predicted top surface temperature varies by up to 50 K between simulations. Model predictions of peak mass loss rate and the time at which it occurs vary by approximately 35 % and 25 %, respectively. At higher heat fluxes (65 kW m^{-2}) peak mass loss rate predictions vary even more (by up to 75 %) and at low heat fluxes (10 kW m^{-2}) predicted time to peak mass loss rate varied by up to 85 % (results not plotted here). These variations in model predictions exceed experimental uncertainty. Further detail regarding parameter optimization, model setup, and final results for each of these simulations is available online:https://github.com/MaCFP/matl-db/releases. Note: the idealized simulations presented at the MaCFP-2 Workshop (including the results shown in Fig. 4) should *not* be considered as verification or validation cases. Rather, they represent well-defined scenarios that can be used to assess the relative similarities or differences in predicted material response (when

heated in fire-like conditions) when extrapolating to a space beyond model calibration conditions. Analysis of these simulations results can potentially provide insight into the underlying reasons for observed differences.



(a) Predicted total sample mass

(b) Predicted area-normalized mass loss rate

(c) Predicted top surface (exposed to incident heat flux) temperature

(d) Predicted back surface (perfectly-insulated) temperature

Figure 4: Simulated response of 12 mm thick PMMA slabs exposed to 25 kW m^{-2} radiant heating at their top surface in an idealized, one-dimensional heating scenario. Each prediction was calculated using parameter sets submitted to the MaCFP-2 Workshop. See note above: these results should *not* be considered as verification or validation cases.

3 Conclusions and Next Steps

The MaCFP Condensed Phase Working Group is a global, collaborative effort between experimentalists and modelers in the pyrolysis modeling community, which is designed to make systematic progress in the simulation of condensed-phase fire phenomena. With the support of the global pyrolysis modeling community, the MaCFP Condensed Phase Working Group successfully organized a multi-year, collaborative effort to systematically study a single reference material in order to assess the current state-of-the-art approaches available to parameterize (i.e., calibrate) pyrolysis

models and to understand the potential impact of variations between these approaches on predictions of material flammability response. Results of this community-led effort were shared in a workshop (MaCFP-2) that preceded the 2021 IAFSS Symposium. Main objectives of the MaCFP-2 Workshop included:

- Cataloging current approaches used to parameterize pyrolysis models
- Quantifying the interlaboratory variability for comparable experimental datasets
- Assessing the impact of the variability of model parameters on predictions of sample decomposition in response to well-defined heating conditions

In total, 16 institutions located in 10 different countries submitted experimental measurements from 220 unique tests to the MaCFP-2 Workshop. This measurement data, which can be used as targets for pyrolysis model calibration and validation, has been uniformly formatted and well-documented (i.e., saved with corresponding metadata describing sample preparation, test setup, and experimental conditions) to allow for efficient, automated analysis. All measurements (and related analysis tools) are maintained in a digital, version-controlled, and freely-available online repository: https://github.com/MaCFP/matl-db. Modelers from 9 different institutions in 6 countries then analyzed these experimental measurements to develop complete parameter sets that could be used to describe the thermal decomposition behavior of the reference behavior of interest. These property sets were then used to predict sample decomposition in response to well-defined zero- and one-dimensional heating scenarios: preliminary results suggest that variations in modeling results exceeds experimental scatter.

With a key focus on determining what the pyrolysis modeling community needs to do to improve predictions of material ignition, burning behavior, and fire growth, ongoing and proposed next steps (both experimental and modeling) in preparation for the MaCFP-3 Workshop in 2023 include:

- Development of requirements for experimental dataset (including metadata) calibration, quality, and completion
- Development of requirements (i.e., completeness/quality and standard format) for material property metadata
- Investigation of sensitivity of model predictions to variations in calibration data, model calibration approach, and the computational pyrolysis models used to simulate material response
- Identification and analysis (experimental and modeling) of combustible solids with more complex degradation behavior and relevance to modern fire safety
- Analysis (experimental and modeling) of flame spread and fire growth over combustible solids at intermediate- and full-scale

With wide international participation, these steps are expected to lead to a substantive improvement in the fire modeling community's capability to predict ignitability, steady burning behavior, and fire growth potential (i.e., due to flame spread over their surface) of combustible solids.

Institutions participating in the Condensed Phase of the MaCFP-2 Workshop

Participating Institution	Legend Entry	Contribution	
		Experimental	Modeling
Aalto University	Aalto	x	x
Dansk Brand og Sikringsteknisk Institut & Lund University	DBI_Lund	x	x
FM Global	FM	x	
Imperial College of London	GIDAZE+	x	x
Hong Kong Polytechnic University	HKPoly	x	
Laboratoire Central de la Préfecture de Police	LCPP	x	
National Institute of Standards and Technology	NIST	x	x
Sandia National Laboratories	Sandia	x	x
Technical Institute of Fire Protection in Prague	TIFP	x	
University of Central Lancashire	UClan	x	x
University of Dayton Research Institute	UDRI	x	
University of Edinburgh	Edinburgh	x	
University of Maryland	UMD	x	x
University of Lille - Unité Matériaux et Transformations	UMET	x	x
University of Wuppertal (Bergische Universität Wuppertal)	BoWFZJ		x
University of Queensland	UQ	x	
Virginia Military Institute	VMI		x

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