Cover Page Final Research Report

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Project Title: Development of an Interactive Database of Contemporary Material Properties for Computer Fire Modeling

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Summary of the Project:

Motivation:

For the past several years, the NIJ Technology Working Group's Operational Requirements for Fire and Arson Investigation have included several scientific research needs that require improved knowledge of properties of materials that are common in the built environment, and therefore likely to be involved in a fire scene. The specific areas of research include adequate materials data inputs for accurate computer models, understanding the effect of materials properties on the development and interpretation of fire patterns, and evaluation of incident heat flux profiles to walls and neighboring items in support of fire model validation. Each of the three aforementioned research topics rely, in part, on accurate knowledge of the physical conditions of a material prior to the fire, how the material will respond to the exposure of heat, and how it will perform once it has ignited. The project described herein has made advancements in terms of collecting experimental data and property information on a multitude of materials commonly encountered in the built environment for the purpose of making the data publicly available and easily accessible to fire investigators, fire protection engineers, and fire researchers.

Major Goals and Objectives:

With the Fire and Arson Investigation Technology Working Group Operational Requirements in mind, the goal was to improve fire modelling capabilities for fire investigations by improving the quality, quantity, and accessibility of materials input data available to a fire model user. The approach is to develop stakeholder consensus on the data needed, generate the data, and then develop an interactive, web-based repository that the fire investigation and fire modeling communities can easily access for information. The goals for the project included:

- Develop material properties and fire test data on a combination of at least 70 construction materials, interior finishes, and furnishings for use as fire model input.
- Transfer the experimental results through NFPA 921 and peer reviewed reports, onsite trainings and seminars, and interactive online content (transferring data gained from the lab into forensic standard operating practices).
- Demonstrate and test the use of the database for hypothesis testing.

Research Design, Methods, Analytical, and Data Analysis Techniques:

This study was designed and conducted in 5 major tasks:

- Conduct a literature review.
- Hold a workshop to develop initial materials list and measurement methods.
- Perform experiments.
- Compile and analyze data.
- Build experimental data repository and interactive database.

Literature Review

A comprehensive search and review of the literature on property requirements for fire models and empirical correlations, existing databases and repositories for material properties, and the state-of-the-art in experimental techniques and analytical procedures to determine material properties was conducted and synthesized into a report. The report was disseminated to the project technical panel, which consisted of public and private sector fire investigators, fire protection engineering consultants, and fire researchers. The technical panel reviewed the report prior to the first meeting with the technical panel, which occurred during the workshop to develop an initial materials list and measurement methods.

Materials list and measurement methods workshop

The project technical panel convened a virtual meeting to discuss the literature review, provide guidance and input on the initial list of target materials, and to provide feedback on the list of proposed experimental methods and analytical techniques. The technical panel of experts also provided recommendations for uncertainty analysis, validation, and the scope of the database during this period of performance. A major outcome of the workshop was a finalized initial list of materials of which the properties were measured.

Perform Experiments

A NETZSCH STA 449 Jupiter F3 Simultaneous Thermal Analyzer (STA) was used to simultaneously conduct TGA to determine the kinetics of thermal degradation as well as DSC to determine specific heat capacities, the heat of reaction, and the heat of gasification for materials. Tests were conducted on powdered samples of the material with a mass of 4.0 ± 0.1 mg at heating rates of 3, 10, and 30 °C/min with an initial temperature of 50 °C and a maximum temperature chosen to ensure decomposition was completed (typically approximately 650 °C). The tests at heating rates of 10 and 30 °C/min were tested in triplicate and a single test was conducted at a heating rate of 3 °C/min. All experiments for this period of performance were conducted in nitrogen.

A Fire Testing Technology microscale-combustion calorimeter (MCC) was used to measure the heat release rate of the pyrolyzate evolved during pyrolysis of the sample material with respect to temperature and the heat of complete combustion for the gas mixture evolved during pyrolysis in general accordance with ASTM D7309. Tests were conducted on powdered samples of the material with a masses of 4.0±0.1 mg. Tests were conducted with a heating rate of 30 °C/min with an initial temperature of 50 °C and a maximum temperature that was typically approximately 750 °C in a nitrogen atmosphere. Tests were conducted with samples in ceramic crucibles with no lids to ensure there was no added resistance to flow of pyrolyzate gases and vapors from the sample to the combustion chamber.

A TA instruments FOX 200 HFM, shown in Figure 2.5 was used to measure the thermal conductivity and specific heat capacity of the materials in the database. Tests were conducted on 8 in x 8 in samples in dried and unconditioned preparations in general accordance with ASTM C518 to measure the thermal conductivity and a modified version of ASTM C1784 to measure the specific heat capacity. The temperatures at which thermal conductivity was measured were initially 15 °C and 45 °C, but the higher temperature value was shifted upward during the project due to procurement and adoption of an additional standard reference material. The temperature range at which specific heat capacity was measured was 10 °C to 40 °C.

A Bruker A562-G gold-coated integrating sphere was used in conjunction with a liquid nitrogen-cooled Mercury Cadmium Telluride (MCT) detector in a Bruker Invenio-R Fourier Transform Infrared (FTIR) Spectrometer to measure diffuse reflection and transmission for the materials in the database. Spectral reflection measurements ranging from 1.3 to 16.0 microns were collected for all materials and spectral transmission was measured for materials that were non-opaque to visible light. When spectral transmission was measured, the test was conducted on several thicknesses of the material to allow for calculation of the absorption coefficient.

A Deatak Cone Calorimeter was used to measure the HRRPUA of a sample material subjected to a well-defined external heat flux and under flaming conditions. The cone calorimeter features a truncated conical heater with the bottom surface parallel to and 25 mm above the surface of a 0.1 m square sample. The standard test features a spark igniter that ignites gaseous pyrolyzate when the concentration of gases 13 mm from the surface of the sample exceeds the lower flammability limit. During the test, the mass of the sample is measured, and the gaseous effluent is pulled into a ventilation system at a well-defined flow rate. A gas sampling system measures the reduction in oxygen and increase in carbon dioxide and carbon monoxide from baseline conditions. A laser system also measures the optical density of the effluent throughout the duration of the test, which can be directly related to the specific extinction area and smoke yield per mass of sample lost. Sample were conditioned at 23 °C and 50% RH until equilibrium was achieved. Tests were conducted in triplicate at heat fluxes of 25, 50, and 75 kW/m^2.

Data Compilation and Analysis

The data collected in the experiments were analyzed according to consensus standard methods or recently published and technically defensible analytical methods to determine input parameters that model practitioners must use in models of various complexities. The quantities provided in the database and the expected user groups that will use each quantity are provided in Table 1.

Table 1. Properties provided in the FSRI MaP Database and Expected User Groups that will Need Each Property (X indicates the property will be used directly, and V denotes a dataset or property that will likely be used for model validation)

User Group	HRR	Time to Ignition	Ignition Temperature	Soot Yield	CO Yield	Reaction Kinetics	Melting Temperature	Heat of Reaction	Heat of Gasification	Heat of Combustion	Density	Thermal Conductivity	Specific Heat Capacity	Emissivity	Absorption Coefficient
Fire Investigators	X	X	X	X			X			X	X	X	X		
Fire Protection Engineers	X	X	X	X	X	X			X	X	X	X	X		
Fire Researchers	V	V	V	V	X	X	X	X	X	X	X	X	X	X	X

Experimental Data Repository and Interactive Database

Although partial data sets have been collected on over 100 materials, the materials that are currently characterized and available in the FSRI MaP Database website (https://materials.fsri.org) are listed in Table 2.

As part of the approach to transparency, all the raw experimental data may be found in a public, version controlled repository: https://github.com/ulfsri/fsri_materials_database. The database includes the experimental data, processing scripts, and documentation. The experimental data is organized by material name and further broken down within that directory by the respective testing apparatus with which the the materials were tested. Python scripts are also included to allow users to generate the full set of interactive graphs and tables found on the website, local to their computers. Identical versions are included that produce pdf files for inclusion in reports. To help keep users in sync with the website, each graph (whether built locally or on the website) is tagged with the git version of the repository. A technical reference guide and user guide are also included in the repository to provide direct access to the analysis performed on the experimental data and to help users maximize the value of their interactions on the website and repository.

Further, by included the raw data and base processing scripts, other researchers can leverage this unique data set to help develop new analysis methods. These edits can then be incorporated back into the database infrastructure for use by the larger fire modeling and investigation communities.

Table 2. List of Fully Characterized Materials Currently Available in the FSRI MaP Database

Number	Category	Material
1	Roofing	EPDM Membrane
2	Roofing	Roof Felt Underlayment
3	Roofing	Cedar Shingle
4	Roofing	Fiberglass Asphalt Shingle
5	Exterior Finish	Composite Decking
6	Exterior Finish	Vinyl siding
7	Exterior Finish	Pine siding
8	Exterior Finish	Window Screen Material (Vinyl-Laminated)
9	Exterior Finish	Fiber Cement siding
10	Structural	Exterior Plywood
11	Structural	Oriented Strand Board
12	Structural	SPF Wood Joist/Stud
13	Structural	Particle Board
14	Structural	Medium Density Fiberboard
15	Insulation	Extruded Polystyrene Rigid Foam (XPS)
16	Insulation	House Wrap
17	Insulation	Polyisocyanurate Rigid Foam
18	Insulation	Cellulose
19-21	Insulation	Paper-faced R30 Fiberglass Insulation
22	Insulation	Homasote
23	Insulation	Mineral Wool
24	Interior Finish	Rebond foam carpet padding
25	Interior Finish	Memory foam padding with moisture barrier
26	Interior Finish	Wool Rug
27	Interior Finish	Low-pile Polyolefin Carpet
28	Interior Finish	Fiber Reinforced plastic panel
29	Interior Finish	Laminate flooring
30	Interior Finish	Vinyl plank flooring
31	Interior Finish	Vinyl tile
32	Interior Finish	Cotton Rug
33-35	Interior Finish	Bamboo Rug
36	Interior Finish	Rubber rug pad
37	Interior Finish	Luan Paneling
38	Interior Finish	Solid Oak Hardwood flooring
39	Interior Finish	Basswood panel
40	Interior Finish	Engineered hardwood flooring
41	Interior Finish	Eucalyptus Hardboard paneling
42-45	Interior Finish	Ultralite Gypsum Board (2 Coats of Latex Paint)
46-48	Interior Finish	Standard Gypsum
49	Plumbing	Polyethylene Foam insulation
50	Plumbing	Rubber Foam Pipe Insulation
51	Plumbing	Cross linked polyethylene (PEX)
52-54	Engineered Wood	Counter top, Plastic Laminate over particle board
55	Upholstered Furniture	Cotton Batting
56-59	Upholstered Furniture	Polyester Microfiber/Polyester batting/PUF (Overstuffed Chair)
60	Sleeping Products	Polyester Sheets
61	Sleeping Products	Microfiber Sheets
62	Sleeping Products	Cotton sheets
63	Sleeping Products	Bamboo Sheets
64	Sleeping Products	Hemp Sheets
65	General Polymers	High-Density Polyethylene (HDPE)
66	General Polymers	Low-Density Polyethylene (LDPE)
67	General Polymers	Polypropylene (PP)
68	General Polymers	Polyethylene Terephthalate (PET)
69	General Polymers	Polyethylene Terephthalate Glycol (PET-G)
70	General Polymers	Polycarbonate (PC)
71	General Polymers	Polyamide (PA) (Nylon)
72	General Polymers	Poly(methyl methacrylate) (PMMA)
73	General Polymers	Black Cast Acrylic (Black PMMA)
74	General Polymers	Polyvinyl chloride (PVC)

Expected Applicability of the Research

This study provides standard fire test data, thermo-physical properties, and model inputs for over 70 materials that are commonly encountered in the built environment. The database website provides complete transparency on the procedures used to prepare materials for testing as well as the experimental protocol used to test the material samples. In addition, the current industry best practices and recommendations on analysis of the raw data and guidance on how the data may be used to effectively simulate burning of materials with common computational models and heuristics is provided. With these data and the provided guidance, fire investigators and fire model practitioners may represent solid materials into fire models and analyses that they previously could not include while also enjoying higher confidence in the simulations and results of these analyses than prior to publication of this research and database.

The website was designed to allow investigators and practitioners with any level of education and understanding of heat transfer, thermodynamics, and data structures to easily access and understand the data and properties.

Participants and Other Collaborating Organizations

The Fire Safety Research Institute was the only organization which participated during this period of performance. Discussions have commenced for potential future collaborations with the University of Maryland and the National Institute of Standards and Technology.

Outcomes:

Results and Findings

A dataset of this size and with the breadth of data that has been collected provides users of the database with an unprecedented opportunity to improve understanding of fire behavior and causality in fire spread and fire growth scenarios. Analysis of the data collected for the database and a comparison of material properties for different classes of materials and products has the potential to elucidate fundamental differences between materials that result in better fire performance.

Additional analysis of this dataset will allow for the discovery and development of new correlations between properties and fire behavior and improvement of existing correlations. These correlations are the simplest form of fire models and may be used by fire investigators and engineers in the field to propose and test hypotheses.

Limitations

There are no limitations to access of the data by the public. One current limitation of the FSRI MaP Database is the relatively low maximum temperature of the thermal conductivity data that has been measured. This is an area of active research by FSRI and the pyrolysis modeling community and, when an appropriate method to measure elevated temperature thermal conductivity is identified, it will be conducted and the data will be added to the database.

Another limitation of the database at present is the relative lack of validation data for large-scale and full-scale fire phenomena. FSRI has a large cache of data from full-scale experiments that may be used to validate fire models and parameter sets, but they are not included in the database in its current form. There is also no way for outside organizations to contribute or request to upload data to the database.

Future work will work to address these current limitations and will include improvement of the user experience for the website, integration with common fire models and heuristics, identification and quantitation of gaseous effluents released during pyrolysis and burning, and additional validation experiments (larger scales and more complicated geometries).

Artifacts:

List of Products

Literature Review to Support the Development of a Database of Contemporary Material Properties for Fire Investigation Analysis, by Mark McKinnon, Daniel Madrzykowski and Craig Weinschenk https://dx.doi.org/10.54206/102376/WMAH2173

Development of a Database of Contemporary Material Properties for Fire Investigation Analysis – Methods and Materials, by Mark McKinnon, Daniel Madrzykowski and Craig Weinschenk https://dx.doi.org/10.54206/102376/ZMPA6638

Evaluation of Uncertainty in Direct Measurement of Thermo-Physical Properties for Pyrolysis Models. Mark B. McKinnon, Matthew J. DiDomizio, and Conor McCoy, UL Firefighter Safety Research Institute, Columbia, Maryland, USA. https://www.astm.org/stp164220210109.html

Impact of STA Specimen Preparation on Derived Kinetic Parameters and Pyrolysis Model Predictions. Matthew J. DiDomizio and Mark B. McKinnon, UL Firefighter Safety Research Institute, Columbia, Maryland, USA. https://www.astm.org/stp164220210106.html

The Effect of Uncertainty in Calibration Data on Burning Rate Predictions, Mark B. McKinnon and Holli Knight, UL's Fire Safety Research Institute, Columbia, MD, USA. Submitted for the proceedings of the 14th International Symposium on Fire Safety Science, Oct 22-27, 2023.

Materials and Products Database - Technical Reference Guide, Mark McKinnon, Craig Weinschenk Daniel Madrzykowski and UL's Fire Safety Research Institute, 6200 Old Dobbin Ln., Columbia, MD, USA. https://dx.doi.org/10.54206/102376/RNNP3809.

Reports and links to journal articles as they are published will be found at https://fsri.org/.

The FSRI Materials and Products (MaP) Database may be accessed at https://materials.fsri.org/.

Dissemination Activities

Standards and Guides

Information from this study will be shared with the NFPA Technical Committee on Fire Investigations. Information and findings from this study have been shared with the ASTM E05 Committee for the purpose of working toward a standard on determination of material properties and inputs for fire models. The data in the database will be shared with the IAFSS community and FSRI will work directly with the Working Group on Measurement and Computation of Fire Phenomena (MaCFP) to develop guidance on fire modeling best practices.

Presentations

Completed presentations:

Two presentations at the ASTM International Symposium on Obtaining Data for Fire Growth Models, Dec 14-15, 2021.

Evaluation of Uncertainty in Direct Measurement of Thermo-Physical Properties for Pyrolysis Models, Mark B. McKinnon and Matthew J. DiDomizio, UL Firefighter Safety Research Institute, Columbia, Maryland, USA

Impact of STA specimen Preparation on Derived Kinetic Parameters and Pyrolysis Model Predictions, Matthew J. DiDomizio and Mark B. McKinnon, UL Firefighter Safety Research Institute, Columbia, Maryland, USA

Development and Validation of a Material Property Database for Fire Models, Mark McKinnon, UL's Fire Safety Research Institute, Columbia, MD, USA. Society of Fire Protection Engineers Annual Conference, October 12-14,2022.

Development of an Interactive Database of Contemporary Material Properties for Computer Fire Modeling, Mark McKinnon, UL's Fire Safety Research Institute, Columbia, MD, USA. 2023 NIJ Forensic Science R&D Symposium, February 14, 2023. (Poster)

Planned Presentations:

Development of a Material Property Database for Fire Models, Mark McKinnon, UL's Fire Safety Research Institute, Columbia, MD, USA. FM Global Open Source Fire Modeling Workshop, April 4, 5, 2023

FSRI Fire Investigation Research Program, Daniel Madrzykowski, UL's Fire Safety Research Institute, Columbia, MD, USA . IAAI 74th International Training Conference, Cherokee, NC., April 23-28, 2023.

Fire Model Validation and Insights with the FSRI Materials and Products Database, Mark McKinnon, UL's Fire Safety Research Institute, Columbia, MD, USA. Society of Fire Protection Engineers Annual Conference, October 8-13, 2023.

The Effect of Uncertainty in Calibration Data on Burning Rate Predictions, Mark B. McKinnon and Holli Knight, UL's Fire Safety Research Institute, Columbia, MD, USA 14th International Symposium on Fire Safety Science, Tsukuba, Japan, Oct 22-27, 2023.