The NIST Material Flammability Database

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

Leventon, I.T.*[A], Bruns, M.C.[B], Heck, M.V.[A] | *Technical Point of Contact: Isaac.Leventon@NIST.gov
[A] National Institute of Standards and Technology
[B] St. Mary's University, San Antonio

Material Property Measurements

Experimental Tools

Trusted Measurement Data
- Traceable calibrations and measurement data
- Digitally archived, version controlled
- Comprehensive, freely available dataset: multiple instruments allow for property calibration to unique datasets
- Detailed metadata: manufacturer, distributor, trade name, common name, sample images, and material description (e.g., thermoset, thermoplastic, or vegetative fuel)

Multi-Step Data Review
- Automated and manual data quality review (repeatability statistics, outlier identification uncertainty quantification)

Current Suite of Experimental Tools

Milligram-scale tools
- Thermogravimetric Analysis (TGA)
- Differential Scanning Calorimetry (DSC)
- Microscale Combustion Calorimetry (MCC)

Bench-scale tools
- Cone Calorimeter
- NIST Gasification Apparatus
- Gier Dunkle reflectometer

Composition/Evolved Gas Analysis**
- Gas Chromatography Mass Spectrometry (GC-MS)
- Fourier Transform Infrared Spectroscopy (FTIR)
- Gel Permeation Chromatography
- Organic Elemental Analysis (CHNS/O)

**See Future Applications at Bottom Right

Automated Analysis Tools[3-6,8]

Open source, freely available tools developed for property calibration

Accurate: Parameters predict data
Realistic: Values agree with physics
Efficient: Fast parameter evaluation (property determination in seconds)
Robust: Can handle complex behavior (e.g., multi-step decomposition)
Stable: Values do not vary

Archived, version-controlled property sets; demonstrated accuracy:

Verification | Validation

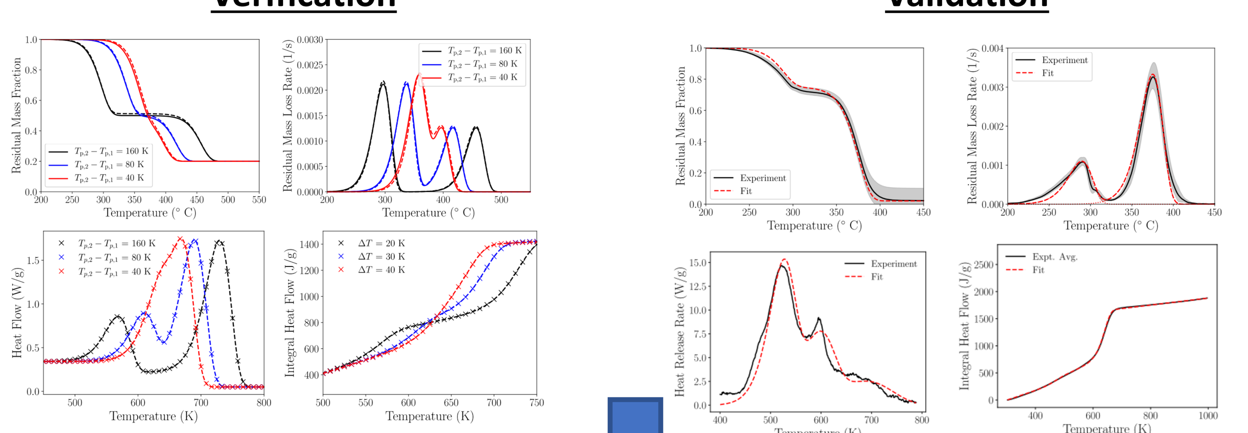


Figure 1. Calibrated model fits vs. simulated data of known kinetics, thermodynamics

Figure 2. Model fits vs. experimental data (top) TGA; (bottom) MCC and DSC

Material Property Values

Comprehensive Pyrolysis Modeling

- Reaction mechanism and kinetics (A, E, ν, n)
- Heat capacities and heats of reaction (c_p, h_{rxn})
- Heat(s) of combustion ($\Delta H_{c,tot}$ & $\Delta H_{c,i}$)

Heat transfer:
- Conductivity (k)
- Radiation absorption (α)
- Emissivity (ε)

Engineering Calculations (burning response to known heating)
- Ignition time (t_{ign})
- Ignition temperature (T_{ign})
- Time-resolved, steady, or peak mass loss rate and heat release rate (MLRPUA, HRRPUA)

Fire Model Validation

Intermediate Scale Flame Spread[9]

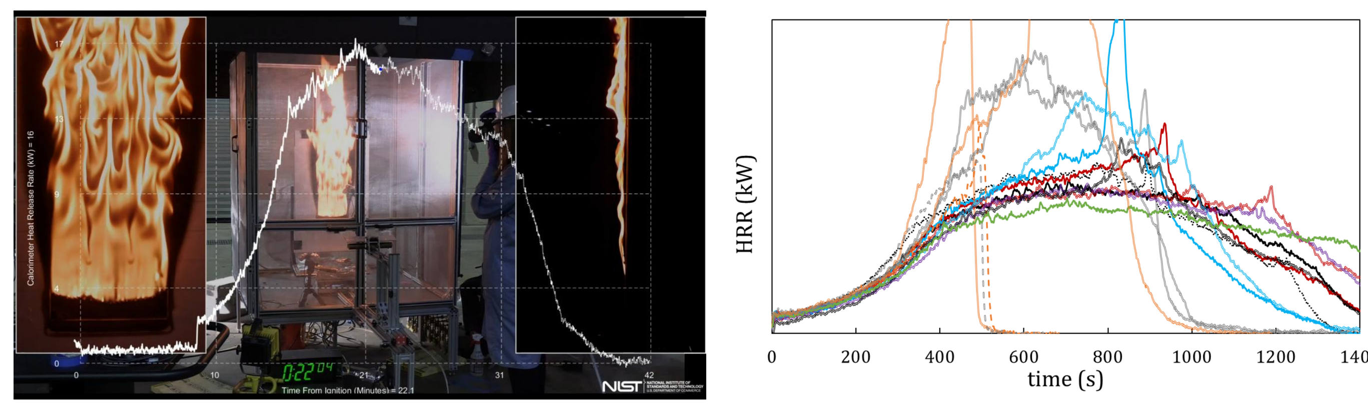
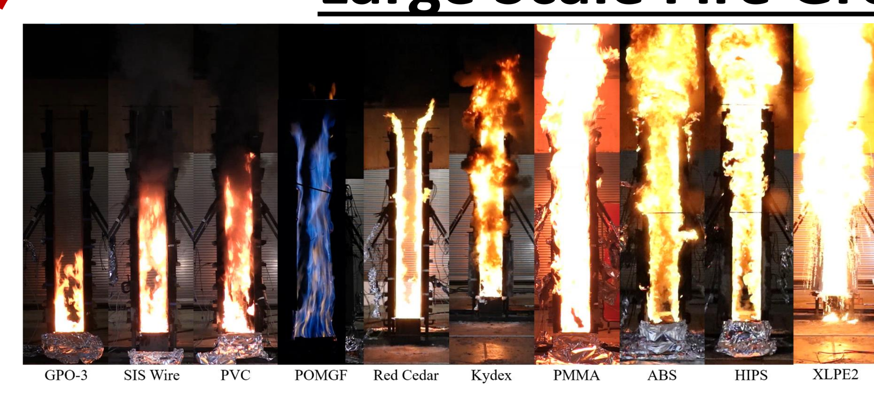
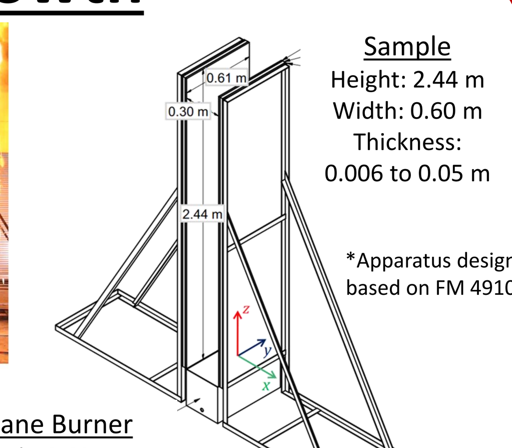


Figure 4.
Top Left: Peak fire size during burning of 0.5 m tall, 0.2 m wide samples; enclosure dimensions 1.2 m wide, 1.8 m tall
Bottom Left: Well-characterized ignition source; repeatable between upward (+90°), downward (-90°), and horizontal (0°) flame spread
Top Right: Impact of sample variability, deformation, and melt pool formation (and pool burning) on measured fire development

Large Scale Fire Growth[7]





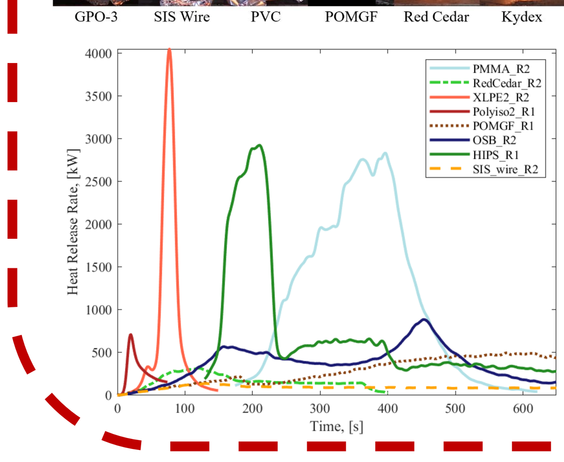


Figure 5.
Top Left: Representative flame structure of selected materials at their respective peak heat release rates (peak HRR)
Top Right: Schematic of Parallel Panel test apparatus showing propane burner (ignition source, 65 kW) at base of assembly
Bottom Left: Representative Heat Release Rate (HRR) curves of selected materials

Fire Modeling

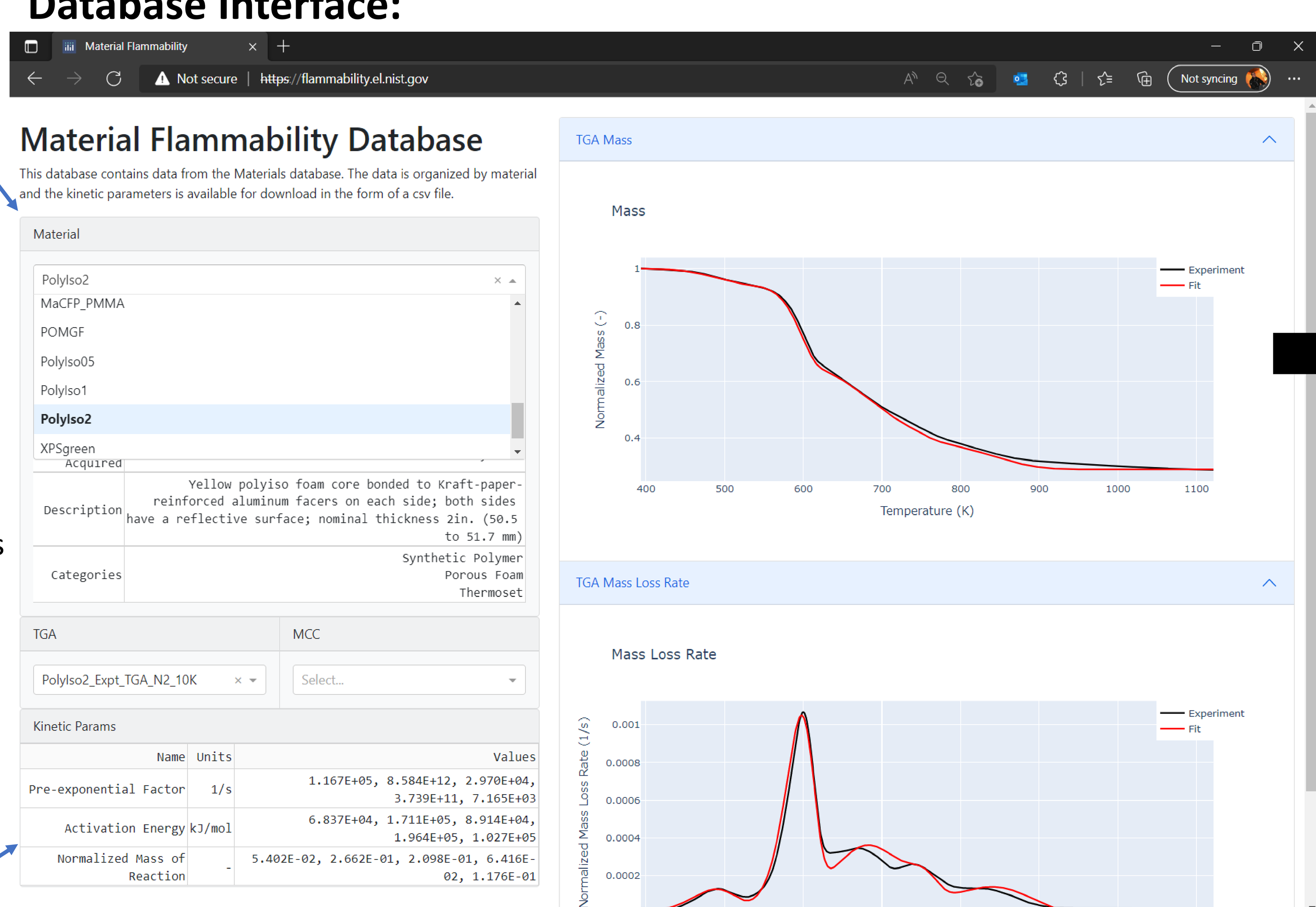
Select Material from Archive:

Varied Chemical Compositions
- Synthetic Polymers
- Natural (Wood-based) Materials
- Copolymers and Composites
- Electrical Cable
- Porous Polymer Foams
- Vegetative Fuels

Wide Range of Burning Behaviors
- Varied Ignitability
- Charring/Non-charring
- Varied Sooting Propensity
- Deformation (i.e., melt flow)

Available Properties

Database Interface:



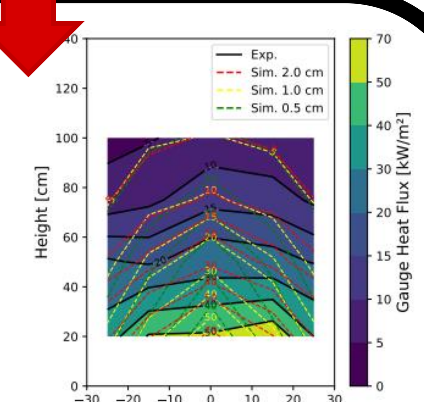
Demonstrated calibration accuracy

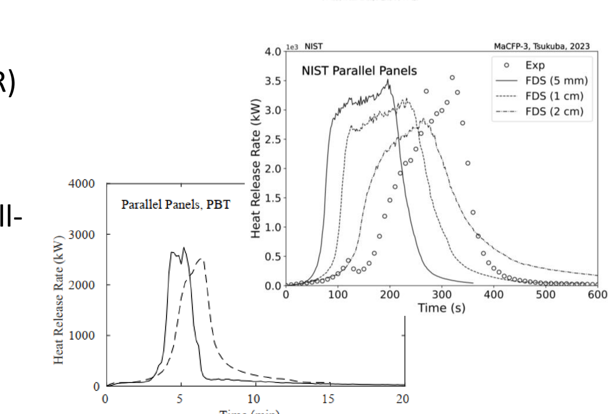
Experiments are conducted (and are ongoing) to provide a comprehensive set of validation data for computational fluid dynamics (CFD) simulations of fire growth due to flame spread over the surface of combustible solids. Final datasets are archived[12] in the comprehensive, searchable, and freely-available database NIST Fire Calorimetry Database:

https://www.nist.gov/el/fcd

Controlling mechanisms of fire growth and global quantities characterizing fire behavior & development are measured:

- Time-resolved measurements of:
  - Sample mass loss rate (MLR) and heat release rate (HRR)
  - Soot and gaseous species production (CO and CO_2)
  - Total flame to wall heat flux (kW/m²)
- Ignition time (s) and fire growth rate, in response to well-characterized ignition sources
- Flame heat transfer mechanism (radiation vs. total)
- Peak heat release rate (kW), total heat released (MJ)
- Radiative heat flux at a distance (kW/m²)
- Heat of combustion (kJ/g); Species yields (g/g)





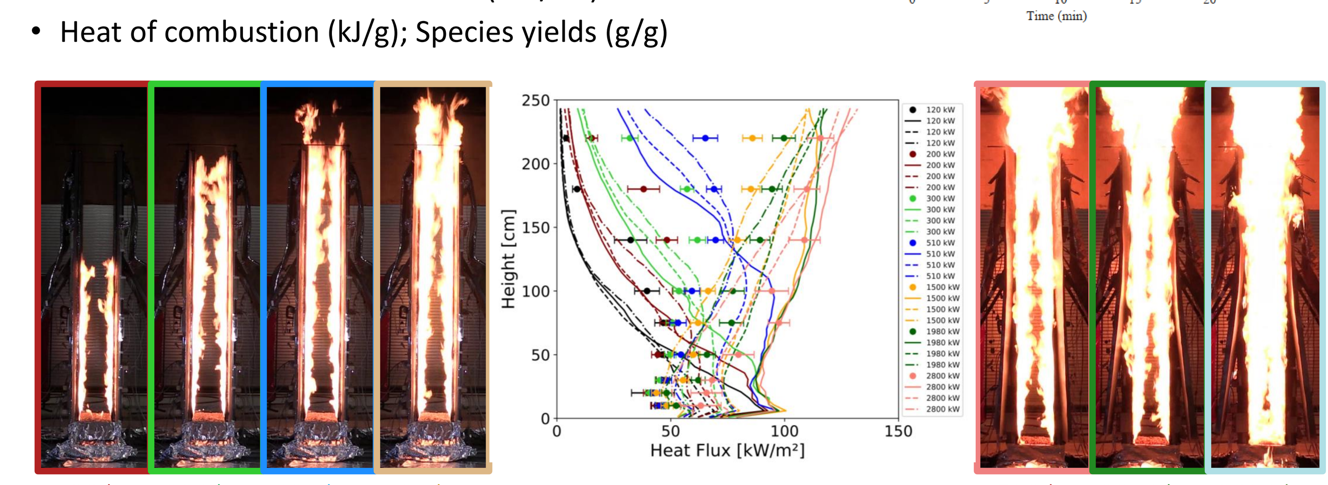


Figure 6. (top) spatially-resolved flame heat flux [steady flaming]; (middle) time-resolved fire growth rate (HRR); and (bottom) centerline flame heat flux during upward flame spread.

Database Origins

Initially proposed at ACS in 2016[1], the NIST Fire Research Division is developing a database to maintain the tools (experimental and analytical) needed to enable quantitative prediction of material flammability behavior (e.g., ignition, steady burning, and fire growth). This framework offers:

- Experimental measurements for a large variety of materials collected across a range of length scales (multiple test apparatus).
- Material properties relevant to fire modeling are determined (i.e., calibrated) through automated analysis of these mg-scale and g-scale measurements.
- Calibrated properties can be used as model inputs in simulations of fire behavior conducted in the Fire Dynamics Simulator (FDS).
- FDS predictions of burning behavior are then validated versus measurement data collected from a unique series of bench- and full-scale experiments (burning rate, flame spread, fire growth).

The NIST Material Flammability Database has evolved to include new classes of measurement data, a growing library of automated tools for property calibration, and an ever-increasing set of target materials[2-6].

Ongoing Development

The tools developed here have been applied in a range of applications including quantifying the impact of material composition on ignitability and fire growth (materials found in nuclear power plants)[7] and quantifying how differences in vegetative fuel decomposition affect CFD simulations of wildfire spread[8]. Current applications include:

1. Calibration[9] and validation[10,11] data provided to support the Measurement and Computation of Fire Phenomena Working Group (MaCFP, a global effort to advance fire modeling)
2. Development of automated scripts for thermal transport property determination from gasification data
3. Standardization of experimental data sets & property formatting
4. Continuous production of pyrolysis property sets (maintaining a living, growing database): apply tools to characterize additional fuels (e.g., vegetation) and fire behaviors (e.g., smoldering)
5. Quantify and validate model sensitivity (fire growth rate) to measured variations in material properties and their respective measurement uncertainties

Future Applications

1. Guided Uncertainty Reduction Utilities (GURU)
   a) Informed collaboration between experimentalists and modelers: feedback to enable measurement *and* model improvement
   b) Compute probability distributions for model parameters
   c) Propagate this uncertainty through fire models in multiple scenarios and perform sensitivity analyses of model predictions
   d) Compare model prediction probability distributions to validation data
   e) Compute statistically informed model selection criteria
   f) Develop requirements for data set quality and completeness
   g) Develop minimum requirements for numerical pyrolysis models
2. Incorporate additional NIST Fire Research Division tools into the Material Flammability Database**
3. Incorporate new contributors and users of data

Fire Protection Engineers | Researchers | Materials Companies
Product Designers | Fire Modelers | Fire Investigators

References

1. Bruns, M.C. and Leventon, I.T., Design of a Material Flammability Property Database," ACS, 2016
2. Leventon, I.T. et al., "Experimental Measurement of Material Flammability at the Micro-, Bench-, and Full-Scales for Fire Model Development" ASTM Symposium on Obtaining Data for Fire Models, 2021
3. Bruns, M.C. and Leventon, I.T., "Automated fitting of thermogravimetric analysis data," Fire and Materials 2021
4. Bruns, M.C. and Leventon, I.T., "Automated Characterization of Pyrolysis Kinetics and Heats of Combustion of Flammable Materials," FAA Fire & Cabin Safety Research Conference, 2019
5. Bruns, M.C. and Leventon, I.T., "Automated Characterization of Heat Capacities and Heats of Gasification of Combustion of Flammable Materials," FAA Fire & Cabin Safety Research Conference, 2022
6. Bruns, M.C. and Leventon, I.T., "Automated Characterization of Thermal Conductivity of Flammable Materials," ACS, 2024
7. Leventon, I.T., Heck, M. V., McGrattan, K.B., Bundy, M.F., and Davis, R.D., 'The Impact of Material Composition on Ignitability and Fire Growth. Volume 1: Full-Scale Burning Behavior of Combustible Solids' NIST Technical Note 2282, 2024
8. Leventon, I.T., Yang, J., Bruns, M.C., ''Thermal Decomposition of vegetative fuels…', Fire Safety Journal, 2023
9. https://github.com/MaCFP/matl-db/tree/master/PMMA/Calibration_Data/ (DOI: https://doi.org/10.18434/mds2-2586)
10. https://doi.org/10.18434/mds2-2940
11. https://doi.org/10.18434/mds2-2812
12. NIST Fire Calorimetry Database | https://doi.org/10.18434/mds2-2314

Acknowledgements: Parts of this work were supported by the Office of Nuclear Regulatory Research of the US Nuclear Regulatory Commission (US NRC). This program was directed by Mark Henry Salley with support from K. Hamburger, N. Melly, G. Taylor, and D. Stroup