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DETERMINATION OF MATERIAL PROPERTY INPUT DATA FOR FIRE MODELING

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1. BACKGROUND

This research effort provided a demonstrated methodology to determine thermal, physical, and combustion property data for use in predicting the burning behavior of materials in fire dynamics simulations. Through the research, the project has addressed a need in the forensic discipline of Fire and Arson Investigation to have accurate material properties for input into the material pyrolysis models included in the simulations. The methodology developed in the research used controlled, standard experiments to generate data on the material response and used an optimization routine to quantify the material properties. In the new approach, the method was developed to both minimize the number of experiments while maximizing the accuracy of the properties.

This research study investigated whether more realistic (and hence more accurate) properties can be achieved through limiting the number of properties determined through optimization techniques based on well-designed experiments. The decision on which properties to measure versus determine through optimization was based on the sensitivity of the model to the property as well as ease of measuring properties. Therefore, a model sensitivity analysis was performed on three different types of pyrolysis models that have a range of sophistication to identify the level of accuracy each property needs to be quantified. Based on the difficulty and time required to measure properties as well as the accuracy at which properties must be measured, a methodology was developed to identify which properties should be measured versus determined through optimization. For properties determined through optimization, necessary tests were identified in this research to accurately determine properties by limiting the physics that are occurring in the experiments. In addition, benchmarking and validation tests were performed to provide data for optimization and validation processes. This newly developed methodology was used to determine the properties of seven different materials. As a result, this research provides and validates a methodology that practitioners can follow to determine material properties for use in their material pyrolysis models as well as a benchmark data set for future reference. It is expected that the results of this research

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will not only provide a more standardized approach for material property determination for forensic applications but also for the general fire protection engineering community.

2. PURPOSE AND TASKS

The project determined a complete set of properties of a material for use in a fire simulation through a combination of property measurement and multi-objective optimization. The goal of this research is to develop a methodology where properties are either measured or determined through optimization based on test data, all within three-man days. The decision on which properties to measure using a previously described approach versus develop through multi-objective optimization was determined by considering the difficulty of the measured property testing and well as the sensitivity of the model to the property. Experiments to support the optimization were designed to limit the complexity of phenomena occurring and generate conditions favorable for accurate property determination. The project primary objectives include the followings:

1. Measuring all of the fire-related properties for a select number of materials (PMMA, MDF, wood, *etc.*) with accurate methods so that the cost and difficulty of measurement would be evaluated;
2. Performing sensitivity analyses on three different pyrolysis models to identify properties that most strongly affect simulation results and use this to identify properties that should be measured through experiments versus directly determined through optimization;
3. Developing a property determination methodology including formulating tests to quantify properties through optimization, generate properties for select materials;
4. Designing benchmark tests to evaluate the predictive capabilities of the models;
5. Conducting pyrolysis model benchmarking using properties developed with the new methodology as well as using measured properties.

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An overview of the project tasks and the initial proposed timeline is provided in **Error! Reference source not found.**. The project was conducted through a collaborative research effort between Virginia Tech (VT) and JENSEN HUGHES (JH). The tasks that were performed by each are highlighted in **Error! Reference source not found.** below. The project was completed ahead of schedule.

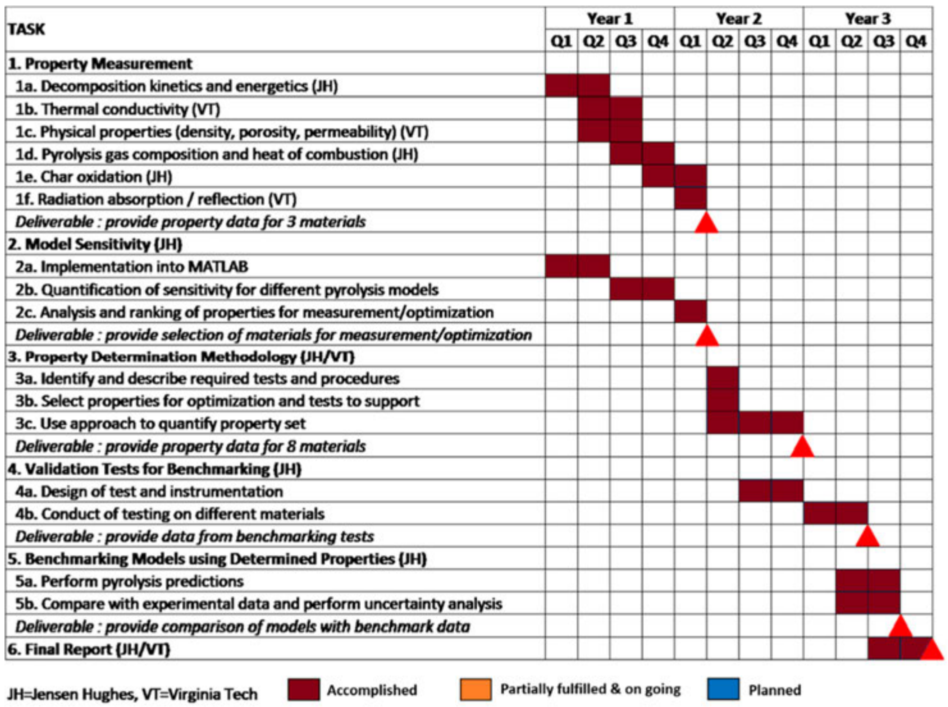

Figure 1. Project tasks and timeline.

3. PROJECT DESIGN AND METHODS

During the funded period, the researchers from both JH and VT have accomplished the goals and tasks that were set at the beginning of this project. In summary, the project was designed following the goals and general purpose. The detailed methods and approaches of this project are listed below:

1. Measured most of the fire-related properties of PMMA, white pine, MDF and cardboard by carefully designed experiments to understand the difficulty and accuracy of measurements;
    - Measured porosity of materials using helium gas pycnometry and controlled atmosphere furnace

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- Measured permeability of materials using the test set-up generalized from the ASTM standards
- Measured thermal expansion coefficient of materials using the TMA Q400 equipment
- Measured thermal diffusivity of materials using laser flash and hot disk method

2. Performed sensitivity analysis on the three commonly used pyrolysis models to identify properties that most strongly influence simulation results;
3. Developed a methodology for determining material properties through the rational design of experiments and optimization;
4. Designed and performed corresponding tests, which serve as input and validation tests for the newly developed methodology;
   - Performed thermal gravimetric analysis with three different heating rates on selected materials to estimate the kinetic parameters
   - Performed cone calorimeter tests on selected materials to generate optimization inputs and benchmarking data
5. Validated the properties estimated by the new methodology against the validation test and prove the effectiveness of the new methodology.

4. DATA ANALYSIS AND FINDINGS

To develop the methodology, a rational analysis was performed to rank the parameters based on a sensitivity analysis of the pyrolysis model as well as the effort and cost of performing tests to measure parameters. Through this analysis, it was determined that the kinetic parameters should be determined from TGA tests and other parameters should be optimized based on cone calorimeter test data. Based on the results of analyses, the recommended methodology for determining input parameters to predict material pyrolysis using FDS is

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- Conduct TGA experiments at three heating rates (e.g., 5, 10, 20 C/min) and determine kinetic parameters,
- Conduct three cone calorimeter tests each at a different exposure (e.g., 25, 50 and 75 kW/m^2),
- Determine kinetic parameters using the SCE optimization algorithm with the TGA data,
- Use the SCE optimization algorithm with kinetic parameters as known input, and use mass loss from two cone calorimeter tests at different exposure levels to determine remaining properties, and
- Validate the predictive capability of determine the properties against the third cone calorimeter test data set.

Using this approach, determined properties were determined to be within 20% of actual values.

To prove the effectiveness of the developed methodology on predicting material response in fire, the TGA and three cone calorimeter tests were performed for all materials, i.e., PMMA, fiberglass reinforced plastic (FRP), Medium-density fibreboard (MDF), white pine, white spruce, cardboard, oriented strand board (OSB). The results of these TGA and cone calorimeter tests were used with the methodology mentioned above to demonstrate the methodology. Specifically, this included the following analysis steps: (1) The TGA results were used to obtain the kinetic parameters of the pyrolysis reactions with SCE optimization method; (2) The results from standard cone calorimeter tests at exposures of 25 kW/m^2 and 70 kW/m^2 with ignition were used to along with the FDS pyrolysis model and SCE optimization method to determine material properties; (3) The material properties along with the kinetic parameters were implemented into the FDS pyrolysis model to predict the mass loss and mass loss rate of the sample at 50 kW/m^2 exposure for validation against experimental data; (4) The properties were also input into a gas phase FDS simulation with material pyrolysis (the typical end-use model) that includes heat feedback from

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the environment to the material surface to further demonstrate the predictive capability of the properties. If needed, the flame heat flux was changed in the property determination step to further refine properties.

The heat release rate per unit area (HRRPUA) from the gas phase FDS simulations with material pyrolysis including heat feedback to the surface was benchmarked against standard cone calorimeter experimental data. Figure 2 and Figure 3 include plots of HRRPUA predicted from the simulations and measured in experiments with an exposure of 50 kW/m^2 for all seven materials. Note that these simulations predict both the time to material ignition as well as the HRRPUA with time.

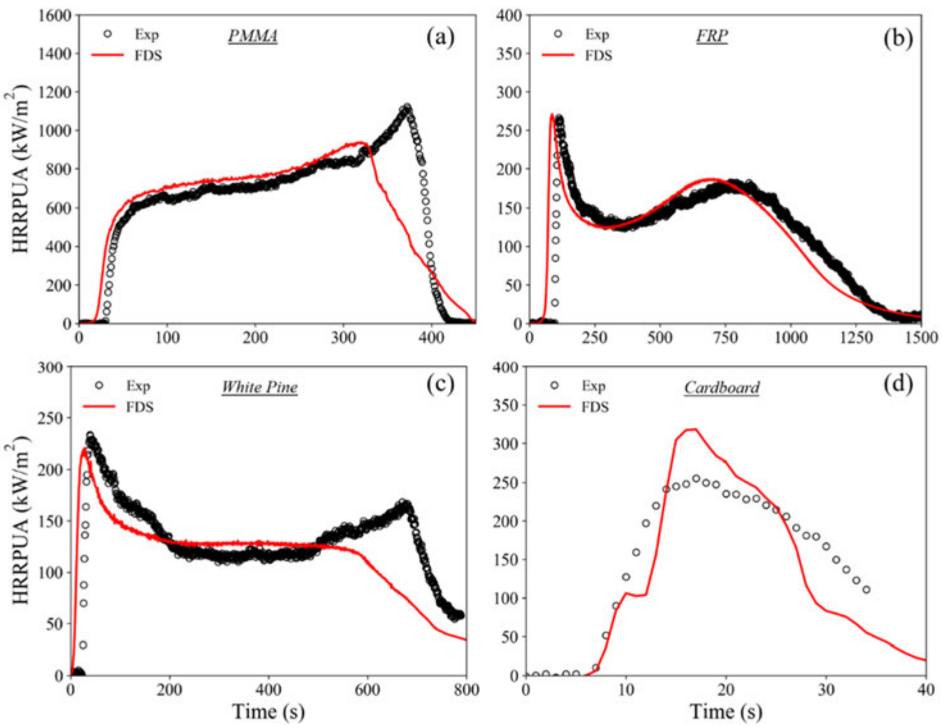

Figure 2. Validation of HRRPUA as a function of time obtained by using optimized fuel properties against cone calorimeter experiments at 50 kW/m^2 for PMMA, FRP, white pine and cardboard fuel samples.

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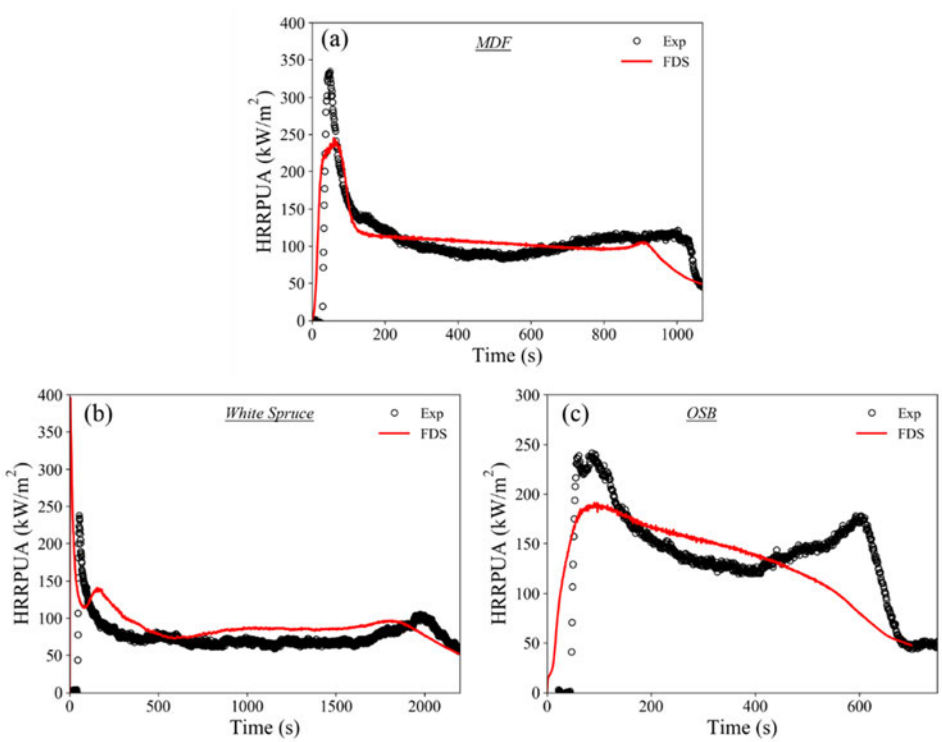

Figure 3. Validation of HRRPUA as a function of time obtained by using optimized fuel properties against cone calorimeter experiments at 50 kW/m^2 for MDF, white spruce and OSB fuel samples.

Overall, it was found that the HRRPUAs obtained from cone calorimeter simulations using optimized material properties were within 30% of the data except near the end of the simulation near burnout. This was attributed to differences in char fraction between TGA and cone calorimeter data. The predicted and measured ignition times were within 30s of actual times with the model providing a conservative prediction of the time of ignition. This is in part due to the FDS gas phase ignition model which assumes that if gaseous fuel and oxygen are present the gas with ignite and produce heat.

Overall, the properties determined using the proposed methodology provide results that well represent the experimental data. In addition, the overall effort to determine the properties has been dramatically reduced. To measure all of the properties would require 3-4 weeks of time with some experiments being very difficult, non-standard test methods. Using the new methodology, there is approximately 1 day of experimental time to run TGA and cone calorimeter experiments and approximately 2 days for optimization and validation making for a total of 3 days effort.

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5. IMPLICATIONS

This research project provided a methodology that practitioners can follow to determine material properties for use in their material pyrolysis models as well as a benchmark data set for future reference. The results of this project address the need for the forensic discipline of Fire and Arson Investigation for more adequate materials property data inputs for accurate computer fire models. In addition, this research project also benefits the fire protection field for a cost effective, validated approach to determine properties for material pyrolysis modeling. It is expected that this new method will improve the accuracy of fire modeling when predictions need to include material burning and its feedback with the predicted environment.

In addition, this new method developed by this funded project has been successfully applied in both government and commercial projects related to fire and safety. Jensen Hughes has applied this method to estimate the material properties used in railcars for the US Department of Transportation. In addition, multiple commercial projects have directly used this new methodology to determine material properties to include in FDS fire modeling. The research is currently being published in a series of journal articles and conference papers. This includes one journal article that is under final consideration and two other journal articles that are in final preparation. In addition, one paper is being published and presented at the upcoming international conference Interflam 2019. These references are provided below.

1. Yang, F., Hodges, J.L., Rippe, C.L., and Lattimer, B.Y., "Methodology for Material Property Determination," *Fire and Materials*, https://doi.org/10.1002/fam.2721, 2019.
2. Yang, F., Hodges, J.L., and Lattimer, B.Y., "Material Burning Property Estimation Methodology and Validation," Interflam 2019, London, UK, 2019.

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