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Project title: Experimental and Numerical Investigations for the Development and Validation of Thermo-Chemistry Models and Property Databases for Selected Wall Lining Materials Under Fire Exposure.

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Nomenclature

$\emptyset$	Porosity
${\rho_g}^k$	Mass concentration of the k^{th} gas phase component (kg/m^3)
t	Time (s)
D_{eff}	Effective diffusion coefficient (m^2/s)
${U_g}^D$	Darcy velocity vector (m/s)
${\dot{Q}_m}^{\prime\prime\prime\, k}$	Mass production/consumption rate of the k^{th} gas phase per unit volume (kg/m^3 s)
K	Permeability tensor (m^2)
μ_g	Dynamic viscosity of the gas mixture (Pa s)
P_g	Total pressure of the gas mixture (Pa)
ρ_s	Density of the solid (kg/m^3)
c_s	Specific heat of the solid component (J/ kg K)
N^g	Number of gas phase components
${c_{p,g}}^k$	Constant pressure specific heat of the k^{th} gas phase component (J/ kg K)
T	Temperature (K)
K_{eff}	Effective thermal conductivity (W/m K)
${j_{diff}}^k$	Mass flux vector per unit area of the k^{th} gas phase component due to concentration gradients (kg/s m^2)
${j_{pres}}^k$	Mass flux vector per unit area of the k^{th} gas phase component due to pressure gradients (kg/s m^2)
${\dot{Q}_T}^{\prime\prime\prime}$	Energy production/consumption rate per unit volume (W/m^3)
D_{AB}	Binary diffusion coefficient of water vapor in the air (m^2/s)
τ	Tortuosity factor
∂	Partial derivative operator
∇	Gradient operator

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1. Statement of the Problem

Gypsum plasterboard (also known as Drywall, plasterboard, wallboard, gypsum board, or gypsum panel) is a safe, efficient, easy-to-use, and fire-resistant product that suits the US construction market. The global gypsum production capacity is estimated to be 12.87 billion m^2 per year. The US has some of the largest high-quality gypsum reserves in the world and the US represents around 28% of the world's gypsum wallboard production capacity (www.globalgypsum.com, 2013). Gypsum (Calcium Sulfate Dihydrate) forms naturally when calcium sulfate is hydrated by groundwater and as a by-product of many desulphurization processes. Gypsum is the primary component of gypsum plaster boards. Gypsum undergoes calcination when heated. This endothermic dehydration improves fire safety. The process of gypsum calcination is governed by the coupled heat transfer, rate of dehydration, and the transport of water vapor produced during dehydration (Kozhumal, Hicks, & Sezer, 2019).

Since the beginning of organized fire investigation in the late 1940s, fire investigators have relied on fire patterns as their basis for determining the fire origin (Rethoret, 1945). Fire patterns are defined as the "physical changes, or identifiable shapes, formed by a fire effect or group of fire effects" (NFPA, 2021, p. 12). Absent the testimony of reliable eyewitnesses to the fire's inception, the investigator is required to determine the origin by observation and expert interpretation of the physical evidence (fire patterns) in an attempt to reconstruct the fire. As such, fire origin determination is largely a matter of fire pattern recognition and analysis (NFPA, 2021). Gypsum loses its chemically bound water molecules and undergoes calcination when heated. During exposure to fire or heat flux, gypsum dehydrates leaving a measurable depth of calcination, which is widely used by fire investigators.

Currently, fire investigators identify fire patterns by visible observation or through depth measurements of materials affected by fire. This analysis demands the coupling of the physical laws of fire dynamics with the investigator's inference regarding the damage. The standard of care in the fire investigation profession is the 2021 edition of the National Fire Code NFPA 921 Guide for Fire and Explosion Investigations, as espoused by the National Fire Protection Association (NFPA). Since its inception in 1992, NFPA 921 represents the current "state-of-the-art" and industry "standard of care" for fire and explosion investigations. With the introduction of NFPA 921, the fire investigation profession began a movement toward the implementation of science-based principles in fire investigation. Even though historic and current treatises espouse the use of fire patterns for fire investigations, only limited research has been conducted to study the scientific foundation of fire patterns. The National Institute of Standards and Technology (NIST), National Institute of Justice (NIJ), and the United States Fire Administration (USFA) have completed full-scale fire research specifically to address fire patterns (McGarry & Milke, 1997) (Shanley, Kennedy, & Ward, 1997) (Mealy, Wolfe, & Gottuk, 2013) (Mealy, 2013). Due to the numerous parameters associated with full-scale fire tests and the limited number of studies conducted, there are still many questions unanswered.

The legal and science professions are currently scrutinizing forensic science, which is forcing the nation to question the scientific foundation of all forensics (National Academy of Science, 2009). In this document, the authors outlined the need to improve the scientific foundations of the forensic disciplines, particularly those that are dependent on qualitative analyses and expert interpretation of observed patterns, including fire investigations (National Academy of Science, 2009). Development of a structured methodology used to guide identification and characterization of damage would help in addressing the problem.

The earliest of the investigations about gypsum exposed to fire was reported in the 1960s (Ryan, 1962). Many researchers explored the behavior of gypsum boards exposed to fire using experimental (King, Beretka, & Ridge, 1971), theoretical (Andesson & Jansson, 1987), and numerical methods (Mehaffey, Cuerrier, & Carisse, 1994; Sultan, 1996). These studies focused on testing the behavior of walls made with gypsum board, wood, or steel studs when exposed to fire in order to predict failure. The limited theoretical and numerical studies used many simplifying assumptions on heat transfer, convection, and material properties. Further numerical studies attempted at exploring the process of gypsum calcination (Axenenko & Thorpe, 1996; Ang & Wang, 2004). The thermal behavior of commercially widespread gypsum board exposed to fire was analyzed by Wakili et al. (Wakili, Hugi, Wullschleger, & Frank, 2007). The study resulted in material properties of gypsum board at different temperatures. Following them, heat and mass transfer mechanisms occurring in a gypsum board exposed to fire were analyzed numerically by Kontogeorgos and Founti (Kontogeorgos & Founti, 2010).

Much of the earlier published research for visible identification of changes was focused on examining cross-sections of the wallboard, visibly determining the depth of calcination based on different bands of color within the cross-section (Posey & Posey, 1983). Several researchers supported this analysis but questioned the practical application of such a method (Schroeder, 1999; Kennedy, Hopkins, & Kennedy, 2003). Most investigators in the field do not cut out pieces of the wallboard to visibly identify the damage, nor do they perform depth surveys using a depth tool.

Several studies exist that focus on the baseline characteristics of the varying degree of heat and resulting visible degree of fire damage, which confirms that this progressive visible damage to the surface of gypsum wallboard is repeatable (Schroeder, 1999; Madrzykowski & Fleischmann, 2012; Hicks, et al., 2008; Mann & Putaansuu, 2009)(Mealy et al., 2013). A method for characterizing damage visibly was developed and a reliability study conducted of users with and without a damage scale (Gorbett G. E., Meacham, Wood, & Dembsey, 2015). The study demonstrated that when a scale was used for characterizing damage, the reliability in the analysis amongst users increased significantly.

Numerical models have been developed and tested to reasonably predict fire spread, even though they employ many engineering approximations (McGrattanan, et al., 2012). Simultaneous Thermogravimetric analysis (TGA) and Differential Scanning Calorimetry (DSC) results of gypsum boards available in the literature are significantly different. The mass loss during the gypsum calcination is largely due to the dehydration of gypsum releasing water vapor and a small part is due to the decomposition of calcium carbonate releasing carbon dioxide (Wakili, Hugi, Wullschleger, & Frank, 2007). Recent numerical studies on the gypsum thermo-chemistry with a constant heating rate (Kozhumal, Hicks, & Sezer, 2019) and variable heating rates (Kozhumal & Sezer, 2022) and analysis of the effect of the position of fire on the depth of calcination (Fowlie, Sezer, Gorbett, & Kozhumal, 2020) have quantitatively analyzed depth of calcination when exposed to fire. Thermogravimetry Analysis (TGA) of gypsum boards highlighted the effect of heating rate on calcination (Sezer, et al., 2022). The density and porosity of the gypsum boards were found to be highly sensitive to the prediction of the heating of gypsum boards (Paye, Hancock, Khan, Kozhumal, & Sezer, 2023). A recent 3D analysis of the gypsum calcination found the problem can be reasonably estimated to be one-dimensional (Hasnain, et al., 2023).

A recently concluded study by the authors, funded by NIJ, developed simplified and approximate correlations between the depth of calcination and incident heat flux for a regular gypsum board using experimental measurements and numerical predictions. However, these correlations are limited to regular gypsum boards. Detailed analysis of the gypsum thermo-chemistry for different types of gypsum boards like moisture-resistant gypsum board, mold and mildew-resistant gypsum board, fire-resistant gypsum board, and sound-absorbing gypsum board are required to make such correlations suitable wide practical use. The macroscopic fire experiments are not sufficient to understand the microscale properties of the gypsum board. Detailed microscopic and elemental analyses are required to understand the behavior of different gypsum boards exposed to fire. The effect of local irregularities present in commercial gypsum boards needs to be explored for different gypsum boards. The effect of paint layers on gypsum boards also needs to be investigated. The effect of other elements, like glass fibers and vermiculite components, added to gypsum boards to obtain desired characteristics like moisture resistance and fire resistance, needs to be studied to understand their behavior when exposed to fire. Failure to recognize the differences in the types of gypsum boards and to analyze their effect on fire patterns could mislead fire investigations.

In this context, the proposed project aims to analyze different types of gypsum boards (Drywalls) both macroscopically and microscopically. This would lead to the development and validation of thermo-chemistry models and property databases for different types of drywalls. This will lead to the development of correlations between measurable depth of calcination on the compartment lining and the history of heat flux from the fire. Computational studies will help in understanding the heat and mass transfer mechanisms that govern gypsum calcination and predict the depth of calcination. The experimental measurements can be used to validate and improve the numerical model. The correlations and criteria developed from the study will be tested for real-life fire scenarios.

The following types of drywalls will be analyzed in the study.

Moisture-resistant drywall: This type of drywall is made with a water-resistant gypsum core and a paper facing that is treated to resist moisture. The water-resistant gypsum core is made by adding a small amount of water-resistant material, such as cellulose fiber, to the gypsum powder. The paper facing is treated with a water-resistant coating that helps to protect the drywall from moisture damage. Different types of moisture-resistant drywalls like Green board drywall and Blue board drywall are common types of Moisture-resistant drywall.

Mold and mildew-resistant drywall: This type of drywall is made with a gypsum core that is treated with a mold and mildew inhibitor. The mold and mildew inhibitors are chemicals that help to prevent the growth of mold and mildew on the drywall. The most common mold and mildew inhibitors are copper-based compounds and quaternary ammonium compounds. The fiberglass facing is used on mold-resistant drywalls to avoid organic materials. This is more effective at preventing mold growth due to the lack of any organic materials. These differences could significantly alter how they respond when exposed to fire.

Fire-resistant drywall: This type of drywall is made with a gypsum core that is treated with a fire retardant. Fire retardant is a chemical that helps to slow the spread of fire through the drywall. The most common fire retardants are ammonium phosphate and borates. Both type X and Type C drywall need to be evaluated. Type X drywall is made from gypsum that has noncombustible glass fibers. Type C is a more durable version of type X as it has more glass fibers as well as more vermiculite components, giving it better fire resistance.

Sound-absorbing drywall: This type of drywall is made with a gypsum core that is sandwiched between two layers of sound-absorbing material. The sound-absorbing material is a material that helps to absorb sound waves, which helps to reduce noise levels in the room. The most common sound-absorbing materials are mineral wool, fiberglass, and acoustic foam. Certain fire-resistant drywalls possess sound-absorbing characteristics.

2. Project Design and Implementation

2.1. Summary

Scientific studies with in-depth analysis of the physical and chemical process of gypsum calcination are very limited despite the wide use of gypsum plasterboards and their significance in forensic fire investigations. Based on our preliminary numerical studies and literature review, we identified the areas where significant improvements are required to develop predictive models for gypsum calcination for different types of gypsum boards. The objectives of the proposed project are,

1. Thermogravimetric analysis of the gypsum dehydration with different heating rates to develop reaction rate equations.
2. Characterization of different types of gypsum boards available in the market.
3. Differential Scanning Calorimetry (DSC) of different types of gypsum boards to determine effective heat capacities.
4. Fourier Transform Infrared Spectroscopy (FTIR) of different types of gypsum boards before and after exposure to heat flux to analyze the effect and extend of dehydration.
5. Development of varying heating rate gypsum thermo-chemistry models for the different types of gypsum boards.
6. Experimental analysis of the calcination of different gypsum boards using controlled uniform heat fluxes.
7. Development of computational models for different gypsum boards that consider the endothermic dehydration of chemically bound water in calcium sulfate dihydrate, variable heating rate gypsum thermo-chemistry, variable thermo-physical properties, and heat and mass transfer through the porous material.
8. Validation of the numerical model using experimental measurements of internal temperatures, depth of calcination, and heat flux.
9. Experimental investigation of the effect of paint layers on gypsum calcination with one oil-based and one water-based paint.
10. Development of a three-dimensional computational model that can predict the depth of calcination based on the measured or simulated heat fluxes or temperature of the fire.
11. Numerical analysis of the effect of non-uniform heat flux on different types of gypsum boards.
12. Characterization of the sensitivity of each modeling parameter in the entire practical range.
13. Scanning Electron Microscopy (SEM) of different types of gypsum boards before and after exposure to controlled heat flux and fire.
14. Development and testing of correlations for the depth of calcination.
15. Development of a stand-alone user-friendly executable for the prediction of depth of calcination.
16. Online workshops/webinars engaging fire investigators to understand the requirements of the fire investigators and to explain the prediction and analysis of the depth of calcination using the stand-alone application.

2.2 Preliminary results

Preliminary numerical and experimental studies are conducted to explore the process of gypsum calcination and analyze the feasibility of the proposed study.

2.2.1 Mathematical formulation

2.2.1.1 Gypsum thermo-chemistry

Gypsum ($CaSO_4 \cdot 2H_2O$) contains 21% by mass chemically bound water in addition to a small amount of absorbed free water. The dissociation of chemically bound happens in two stages. In the first stage, the calcium sulfate dihydrate gets converted into calcium sulfate hemihydrate ($CaSO_4 \cdot ½ H_2O$) and releases 75% of the chemically bound water. In the second stage, which requires a high temperature of around 700 ^oC, calcium sulfate hemihydrate dehydrates to form calcium sulfate. The stages in gypsum calcination are shown in Equations 1 and 2.

$$CaSO_4 \cdot 2\ H_2O \rightarrow CaSO_4 \cdot \frac{1}{2} H_2O\ + \frac{3}{2} H_2O \qquad (1)$$

$$CaSO_4 \cdot \frac{1}{2} H_2O\ \rightarrow CaSO_4 + \frac{1}{2} H_2O \qquad (2)$$

2.2.1.2 Species conservation

The mass conservation of the gas phase species in the porous medium is implemented as shown in Equation 3, which considers the diffusion due to the concentration gradients, convection due to the pressure gradient, and the mass generation due to the production of water vapor.

$$\emptyset\ \frac{\partial {\rho_g}^k}{\partial t} = \nabla \cdot \left(D_{eff}\ \nabla {\rho_g}^k\right) - \nabla \cdot \left({U_g}^D\ {\rho_g}^k\right) + \ {\dot{Q}_m}'''^{\,k} \qquad (3)$$

The diffusive mass transfer of water vapor due to the concentration gradients is calculated using Fick’s law. The mass transfer of water vapor due to the pressure gradients, caused by the increased vapor concentration during the evaporation, is calculated using Darcy’s law.

2.2.1.3 Momentum conservation

The gas phase in the porous medium is considered to be a mixture of ideal gases. The pressure is calculated as the sum of the partial pressures of individual gases. The mean filtration velocity vector (Darcy velocity vector) of the gas mixture is obtained from the pressure gradients as shown in Equation (4).

$${U_g}^D = -\frac{K}{\mu_g}\ \nabla P_g \qquad (4)$$

2.2.1.4 Energy conservation

The heat transfer through conduction, heat transfer caused by the mass transfer due to both diffusion and convection, heat absorption or production due to the pressure changes, and the heat absorption due to the endothermic dehydration are calculated to obtain the energy conservation as shown in Equation 5.

$$\left\{\rho_s c_s + \emptyset \sum_{k=1}^{N^g} \left({\rho_g}^k {c_{p,g}}^k\right)\right\} \frac{\partial T}{\partial t} = \nabla \cdot \left(K_{eff}\ \nabla T\right) - \nabla \cdot \left[\sum_{k=1}^{N^g} \left\{{c_{p,g}}^k \left({j_{diff}}^k + {j_{pres}}^k\right)\right\}\right] T + \ \emptyset\ \frac{\partial P_g}{\partial t} + \ {\dot{Q}_T}''' \qquad (5)$$

Here, ${j_{pres}}^k = {\rho_g}^k\ {U_g}^D$, and ${j_{diff}}^k = -D_{eff}\ \nabla {\rho_g}^k$.

2.2.1.5 Water vapor re-condensation

In the early stages of gypsum dehydration, the transport of water vapor released from the side of the gypsum board exposed to fire to the colder ambient side could result in re-condensation of a part of the transported water vapor. In the present model, the effect of water vapor re-condensation is accounted for by adding a negative component to the source terms in the species conservation equation ($\dot{Q}_m{}'''$) for the water vapor and by adding a positive component to the source term in the energy conservation equation ($\dot{Q}_T{}'''$). The source terms are applied in each computational cell during every time step using the saturation vapor pressure and the heat of condensation corresponding to the cell temperature. Therefore, the effect of water vapor condensation diminishes as the temperature inside the gypsum board increases and vanishes as the temperature exceeds the boiling point at the corresponding pressure of the computational cell.

2.2.1.6 Numerical methods

The governing equations are discretized using a finite volume method and the coefficient matrix for the system of differential equations is solved using the TDMA (tridiagonal matrix algorithm). A fully implicit Euler's method is used for the time integration. A 12 mm thick gypsum board with an initial density of 810 kg/m^3 is considered. The decrease in density of the porous material due to the dehydration is considered. A uniform grid spacing of 0.2 mm and a time step of 0.05 s are used. The predictions are ensured to be independent of the grid spacing and time step. Temperature-dependent thermo-physical properties are used for both the solid phase and the gas phase. A central differencing scheme is used for the conductive and diffusive terms along with an upwind scheme, sensitive to the change in velocity direction, for the convection term.

2.2.1.7 Initial and boundary conditions

A gypsum board with a thickness of 12 mm has been considered in the present study. One side of the gypsum board (x = 12 mm) is exposed to the ambient and the other side (x = 0 mm) is exposed to a fire. The total pressure at the outer surfaces of the gypsum board is assumed to be atmospheric pressure. The initial temperature is assumed to be 20 ^{o}C at the ambient side. The initial partial pressure of water vapor at the ambient side is estimated assuming a relative humidity of 40%. The initial partial pressure of water vapor at the 'fire side'- which here means the side of the gypsum board exposed to fire- is estimated assuming stoichiometric combustion products from methane-air mixture. A convection boundary condition is used for the mass and a convection-radiation boundary condition is used for the energy.

2.2.1.8 Properties

A porosity of 0.68 (Craft, Isgor, Hadjisophocleous, & Mehaffey, 2008) and permeability of 10^{-15} m^2 (Bear, 1972) have been used based on the literature. The diffusion coefficient of water vapor in the air is taken as D_{AB} = 2.56 x10^{-5} m^2 (Schwertz & Brow, 1951). The effective diffusion coefficient is calculated as $D_{eff} = \emptyset\, D_{AB}/\tau$. The tortuosity factor, τ, is assumed to be 1.869 (Blondeau, Tiffonnet, Damian, Amiri, & Molina, 2003). A convective heat transfer coefficient of 10 W/m^2 K, a convective mass transfer coefficient of 9.55 x 10^{-3} m/s, and an emissivity of 0.9 are assumed (Ahmed & Hurst, 1997). The endothermic gypsum dehydration significantly absorbs heat and produces water vapor. The present study has used the data from the thermogravimetric analysis (TGA) of Wakili et al. (Wakili, Hugi, Wullschleger, & Frank, 2007) for the mass generation and energy absorption source terms. The effective specific heat of the solid gypsum board (Wakili, Hugi, Wullschleger, & Frank, 2007), water vapor, and air (The Engineering Toolbox, n.d.) are evaluated as a function of temperature and have been updated every time step. The effective thermal conductivity is calculated using the mass-weighted average.

2.2.2 Validation of the one-dimensional model

The numerical predictions are validated with the experimental measurements available in the literature (Wakili, Hugi, Wullschleger, & Frank, 2007). The experimentally measured ‘fire side’ temperature (x = 0 mm) has been used as the temperature boundary condition. The numerical predictions are compared with the experimental measurements as shown in Figure 1. The trends in the temperature evolution are captured well. However, differences are observed between the measured and predicted temperatures, especially in the early stages of gypsum calcination and during the peak rate of dehydration. After around 10 minutes, the predictions match closely with the experimental observations.

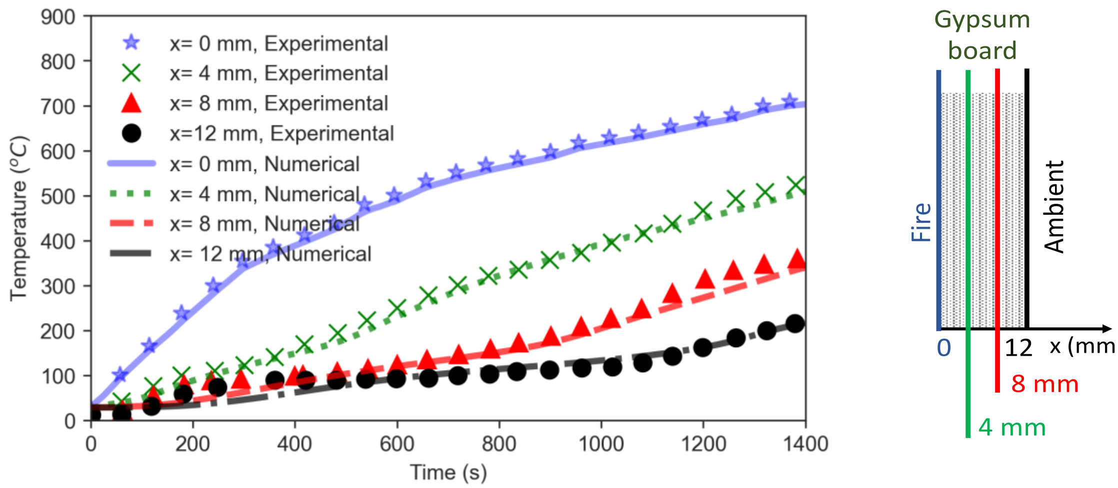


Figure 1: Comparison of the time histories of temperature at different locations inside the gypsum board between the experimental measurements (Wakili, Hugi, Wullschleger, & Frank, 2007) and the present numerical predictions.

2.2.3 Analysis of gypsum calcination

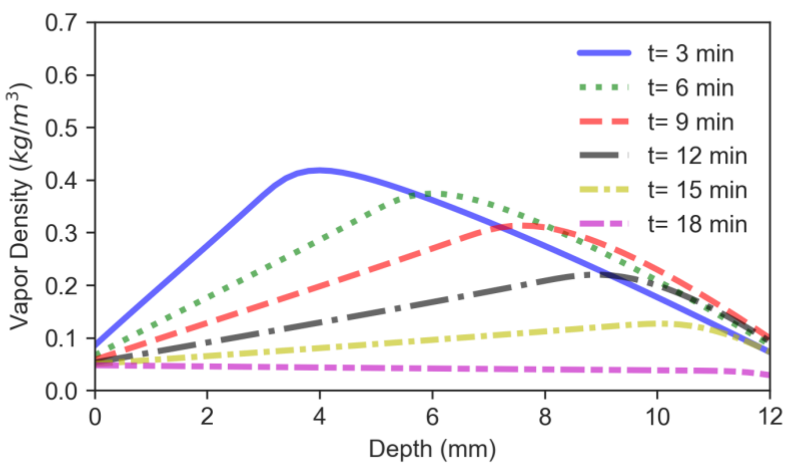


Figure 2: Profiles of vapor density inside the gypsum board at different time instants in the presence of a constant heat flux of 50 kW/m^2. Depth is measured from the side exposed to the heat source.

The process of gypsum calcination has been analyzed by predicting the propagation of the dehydration front, which is extremely difficult to measure. Figure 2 shows the evolution of the dehydration front through the thickness of the gypsum board under a heat flux of 50 kW/m^2 using profiles of the vapor density at different time instants. The location of maximum vapor density gives the location of dehydration front at that instant. As the duration of exposure increases, the dehydration front moves farther inside the porous block. The propagation velocity of the dehydration front varies even with constant heat flux. As the first stage of gypsum calcination nears its completion, the rate of dehydration and the speed of propagation of the dehydration front decrease. This highlights the limitations of the current practice of relying on cumulative heat flux to compare fire damage.

Similar analysis has been performed for a range of heat flux and this resulted in approximate correlations connecting the depth of calcination and exposed incident heat flux. A logarithmic fit is used to display the relationship between the depth of calcination (in mm) and exposed incident heat flux (in kW/m^2) as shown in Figure 3.

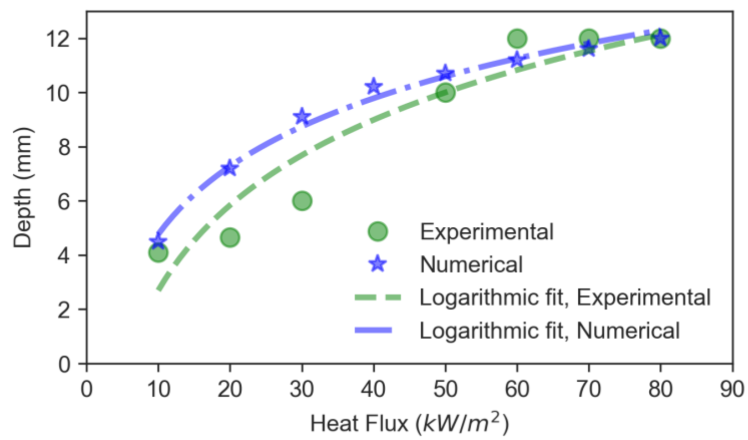


Figure 3: Relationship between depth of calcination and incident heat flux based on numerical predictions and experimental measurements.

Based on numerical predictions, Depth of calcination ~ 3.62 * ln (Heat flux) - 3.57

Based on experimental measurements, Depth of calcination ~ 4.54 * ln (Heat flux) – 7.76

Here, the depth of calcination is in mm and incident heat flux is in kW/m^2. 'ln' represents natural logarithm. The coefficient of determination, denoted R^2, is found to be 0.9886 for the numerical correlation and 0.9011 for the experimental correlation. The proposed project aims to develop similar and improved correlations for different types of gypsum boards.

2.3 Phase 1: Development and validation of gypsum calcination models

During a fire, the fire temperatures, heat release rates, heat fluxes to the walls, wall temperatures, and species concentrations change drastically. The first phase will focus on developing and validating gypsum thermo-chemistry models. This requires TGA to calculate reaction rate coefficients, DSC to calculate effective heat capacities, and experiments with controlled heat flux for validation.

2.3.2 Task 1.A: Thermogravimetry Analysis (TGA)

The TGA Q50 from TA Instruments will be used to perform TGA measurements (Figure 5, left). The mass loss measurements will be performed for the new sample with heating rates ranging from 10 ^{o}C/ min up to 100 ^{o}C/min with a step size of 10 ^{o}C/min. The TGA analysis will also be performed on old samples to analyze its effect on the gypsum board. In both the new and old gypsum board measurements, the temperature will be carried up to approximately 950 ^{o}C where the calcination is expected to be completed. TGA will be performed on different wall lining materials including moisture-resistant drywall, mold, and mildew-resistant drywall, fire-resistant drywall, and sound-absorbing drywall. Each test will be repeated to ensure reproducibility. A total of 80-100 experiments are expected to be required.

Preliminary TGA results for a regular gypsum board with heating rates ranging between 10 ^{o}C/min and 100 ^{o}C/min are shown below in Figure 4. When studied at different heating rates, the temperature derivative of the calcination reaction peaks at the lowest heating rate of 10 ^{o}C/min as this allows a longer time period for the dehydration process. The temperature derivative of the calcination reaction then decreases steadily. The location of the maximum temperature derivative of the calcination also shifts to high temperatures, with the peak for 10 ^{o}C/min appearing at about 150 ^{o}C, and the peak temperature derivative of the calcination reaction shifts to approximately 275^{o}C at high heating rates.

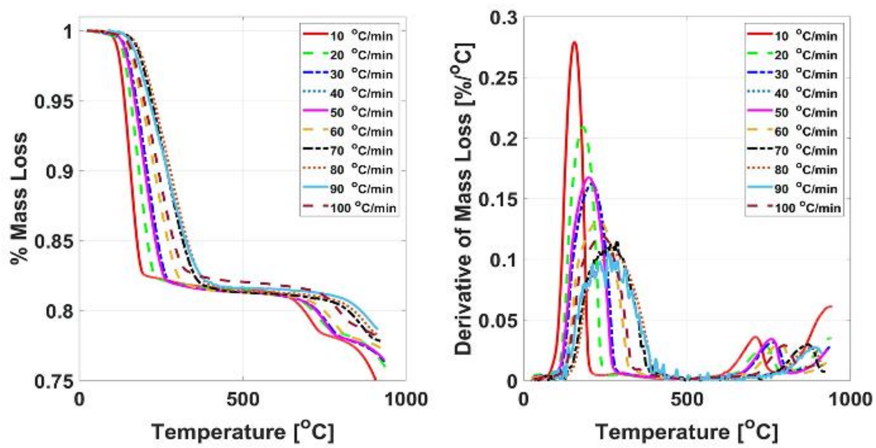


Figure 4: TGA of new gypsum board for heating rates between 10 and 100 ^{o}C/min (left) mass loss from the sample (right) temperature derivative of normalized mass loss.

2.3.2 Task 1.B: Differential Scanning Calorimetry (DSC) and Fourier Transform Infrared Spectroscopy (FTIR)

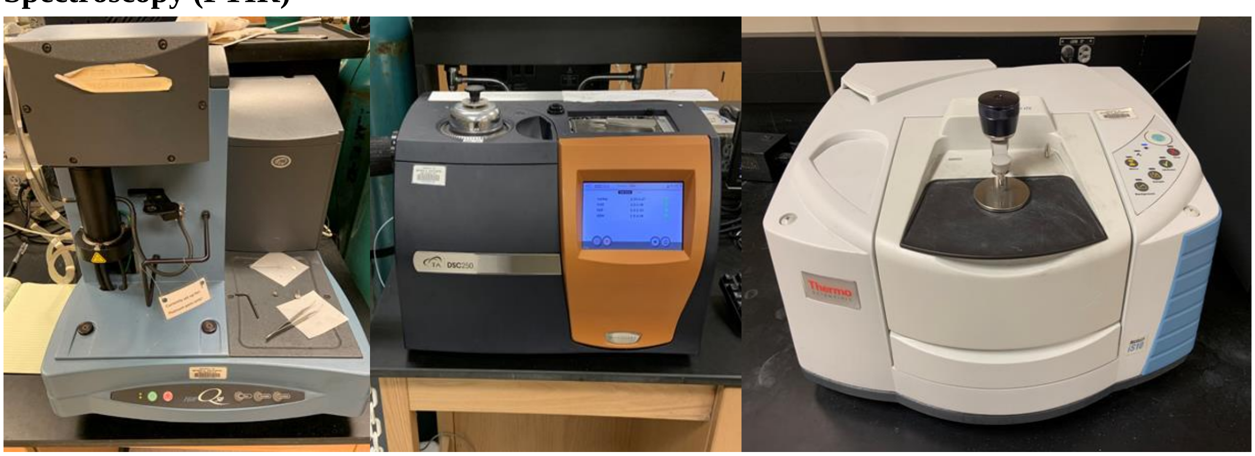


Figure 5: TA Instruments TGA Q50 device utilized to perform TGA (left) TA Instruments DSC250 device to perform DSC (center) and Thermo Scientific Nicolet iS10 FTIR device with Smart iTX accessory to perform FTIR (right).

The DSC analysis will be performed using the TA Instruments DSC250 device (Figure 5, center). The DSC measurements will be performed at different heating rates. DSC measurements will be carried out to ensure coverage of the peak energy absorption. The specific energy absorption of the gypsum board will be examined from the DSC measurements. This will give the effective heat capacity required in the numerical model for the different types of gypsum boards.

To perform FTIR spectroscopy, the Thermofisher Scientific Nicolet iS10 device will be used, with the Smart iTX accessory (Figure 5, right). The FTIR spectroscopy will be performed for wavelengths ranging from 16 μm to 251 μm (corresponding to approximate wavenumbers of 4000 cm^{-1} and 250 cm^{-1}). FTIR data will be collected for different gypsum board samples before and after exposure to heat flux.

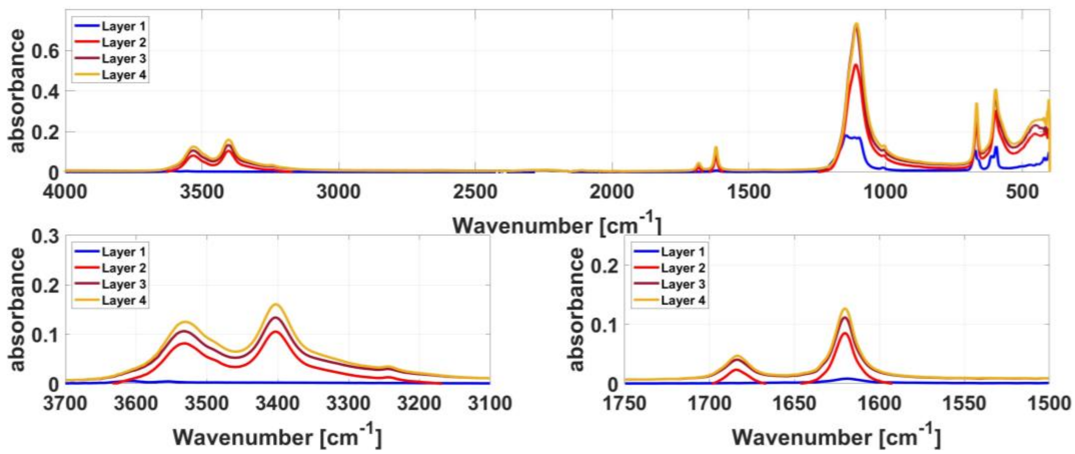


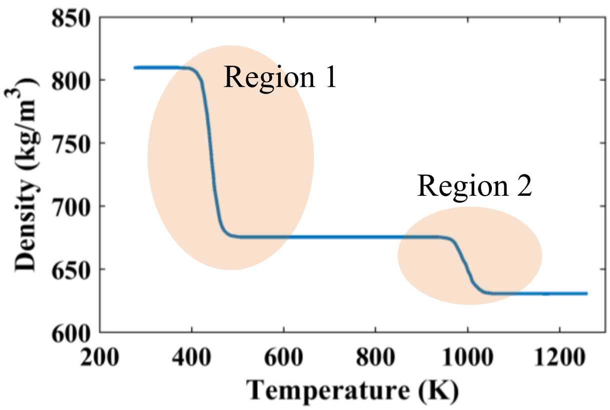
Figure 6: FTIR of gypsum board exposed to heat flux; layer (1) closest to heat source through layer (4) on the ambient side. (a) full FTIR spectrum (b) H_2O stretching spectrum (c) H_2O bending spectrum.

Preliminary FTIR spectroscopy is performed on a regular gypsum board exposed to heat flux with samples taken from different layers along the depth of the gypsum board. The FTIR data shown in Figure 6 displays the effect of layer depth on water concentrations. Figure 6 (b and c) illustrates that the water concentration throughout the gypsum sample increases as the distance from the heat source increases. This is evident by looking at the absorbance data for wavenumbers between 3200 and 3600 cm^{-1}, which corresponds to the H_2O stretching spectrum, as well as for wavenumbers between 1500 and 1750 cm^{-1}, which corresponds to the H_2O bending spectrum. These ranges of the absorbance spectrum illustrate that the concentration of H_2O increases as moving farther from the heat source, with the layer closest to the ambient side having the highest concentration of H_2O.

However, due to the differences in the added elements in the gypsum board, further FTIR studies are required for different wall lining materials including moisture-resistant drywall, mold, and mildew-resistant drywall, fire-resistant drywall, and sound-absorbing drywall. These will be performed, and the results will be analyzed to understand the change of composition of different types of gypsum boards when exposed to fire. Around 10 DSC experiments and around 10 FTIR experiments are expected to be required for the study.

2.3.2 Task 1.C: Development of gypsum thermo-chemistry models

For the numerical model, the rate of dehydration ($\dot{Q}_m{}'''$) needs to be calculated and applied as a source term in the species transport equation for water vapor. The rate of dehydration will be calculated based on total water content, time integration of the rate of water production, the temperature, and two coefficient values as in the equation given in Figure 7. From the TGA data, the derivative of mass loss of the gypsum with respect to temperature will be calculated. This value will be multiplied by the density and the heating rate to find the mass loss rate per unit volume of gypsum. The rate of dehydration ($\dot{Q}_m'''$), estimated for the numerical model will then be compared to the calculated rate of dehydration (mass loss rate) from the experimental measurement for the two stages of the gypsum calcination process. The coefficients for the reaction rate equations for each heating rate will then be estimated. The reaction rates are calculated from these reaction rate equations. The reaction rate coefficients depend on the temperature range and the heating rate.



Experimental

$$\dot{Q}_m'''(T) = -\frac{d\rho}{dT}\frac{\Delta T}{\Delta t}$$

Heating rate,

$$\frac{\Delta T}{\Delta t} = 10 - 100\ K/min$$

Numerical

$$\dot{Q}_m'''(T, t, x) = A\, e^{(-B/T)} \left[H_2O_{max} - \int_0^{t-dt} \dot{Q}_m'''\, dt \right]$$

Figure 7: Modeling of rate mass loss rate. The mass loss curve produced from the TGA data and the method to calculate the mass loss rate (or vapor production rate numerically.

The numerical and experimental mass loss rates from the preliminary studies for a regular gypsum board are compared in Figure 8. The rate of dehydration ($\dot{Q}_m'''$) is calculated numerically as in the equation given in Figure 7. The rate of dehydration ($\dot{Q}_m'''$), estimated for the numerical model is then compared to the calculated rate of dehydration from the experimental measurement for the two stages of the gypsum calcination process as shown in Figure 8. Thus, converting the TGA results into just two sets of coefficients, A and B. The sets of coefficients need to be verified for different types of gypsum boards and a wide range of heating rates. These coefficients are expected to be significantly different for different types of gypsum boards. Moisture-resistant and fire-resistant gypsum boards are expected to deviate the most from the regular gypsum board due to the materials added to them to get the desired characteristics. However, such a study has hitherto not been reported in the literature. Hence, this will be performed in Task 1.C and the results will be used to improve the chemistry models.

The results are in very good agreement at low temperatures and heating rates. The agreement with the exponential relationship is acceptable, despite the complex dehydration process involved during the release of chemically bound water. The first range (the low-temperature range) represents purely vapor production. At higher temperatures, reactions other than dehydration can occur including decomposition of calcium carbonate (Sanders & Gallagher, 2002). Also, higher heating rates could result in more experimental noise. These need to be further analyzed for different types of gypsum boards. Despite all these factors, the developed chemistry model is capable of closely predicting the reaction rates and mass loss rates over the wide range of heating rates.

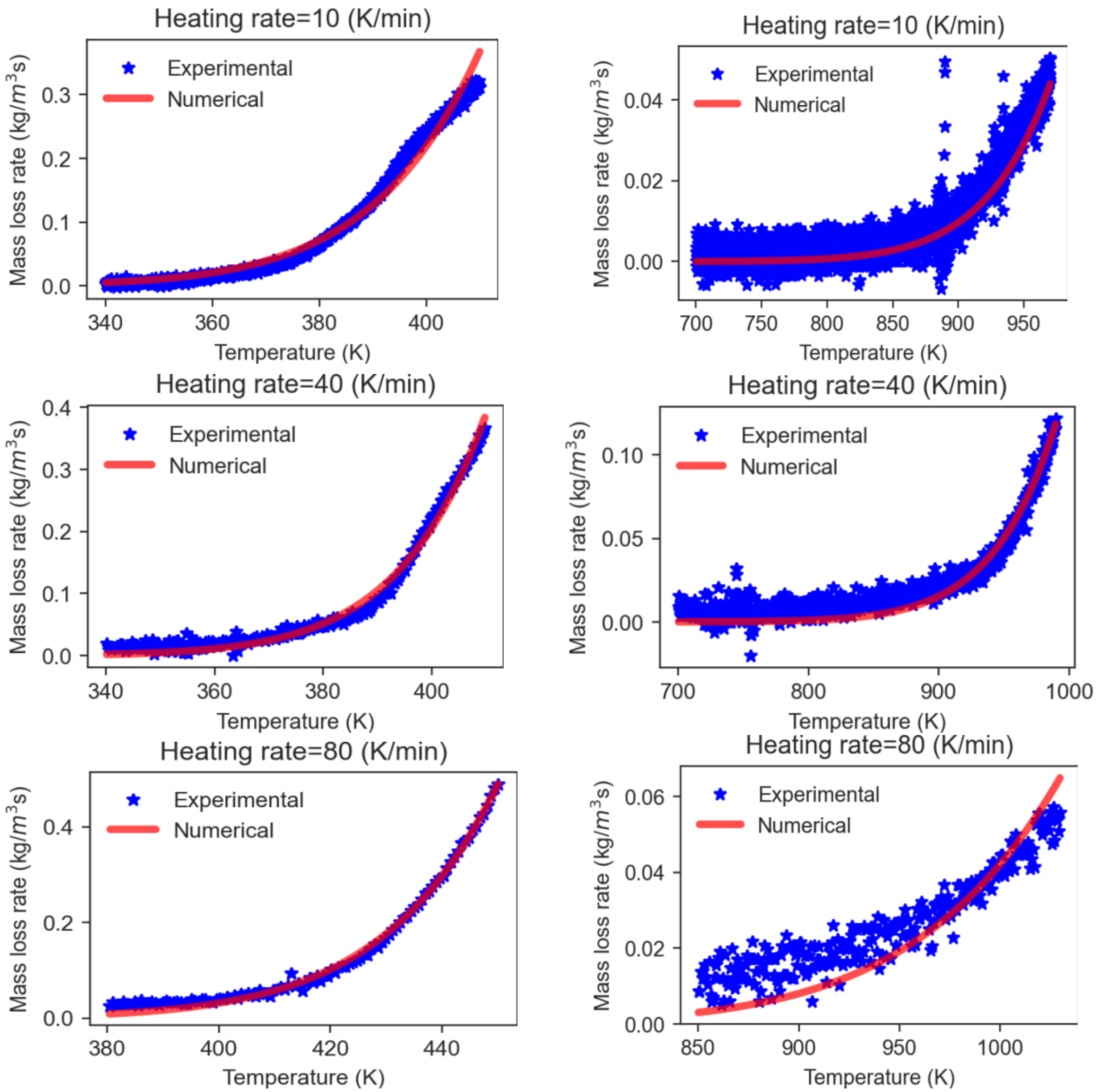


Figure 8: The mass loss rate per unit volume from the experimental TGA data and comparison of numerical predictions from the developed reaction rate equations in two regions- the low-temperature region (left) and the high-temperature region (right)- during the gypsum dehydration under heating rates, 10 K/min, 40 K/min, and 80 K/min.

2.3.4 Task 1.D: Experiments with controlled heat flux and duration of exposure

As there are too many variables due to unsteady fire dynamics, varying temperatures, heat fluxes, and species concentrations, a repeatable and reproducible characterization of the gypsum calcination requires simplification of the number of uncontrolled variables. Experiments will be conducted with controlled uniform heat flux from a radiant burner. Preliminary studies showed that experiments with turbulent flames result in significant uncertainties. Radiant burner can offer more uniform heat flux which dictated the rate of calcination. The temperature inside the gypsum board will be measured along with the depth of calcination. A premixed burner will be used to achieve higher heat fluxes. An array of twelve thermocouples with four heat flux gauges will be used to check and ensure that the heat flux is uniform in the entire experimental region. Gypsum boards with dimensions 0.6 m x 0.6 m will be used for the experiments to avoid boundary effects on lateral heat and mass transfer and ensure one-dimensionality. Experiments will be conducted by varying the heat flux in the range of 0-100 kW/m^2 and duration of exposure from 0-30 minutes or until the board is entirely calcinated. Even though the heat fluxes can exceed 100 kW during compartment fires, sustained exposure to such extreme heat fluxes result in the calcination of the entire gypsum board. Hence further quantification of the death of calcination under such extreme heat fluxes is not expected to yield additional information worth the additional equipment and caution needed for the experiment. Systematic reproducibility and uncertainty analyses will be conducted to verify the reliability of experimental measurements. A series of 5 to 7 experiments will be conducted with uniform heat flux. The depth of calcination and temperature profile in the gypsum board will be measured until a statistically reliable standard error is obtained. A total of 40-45 sets of experiments are estimated to be required for the different types of gypsum boards considered

2.3.1 Task 1.E: Development and validation of a comprehensive 1D model

A one-dimensional model will be developed based on the methodology described in preliminary results with improved variable heating rate gypsum-thermochemistry models from Task 1.C. In the model, the heating rate, reaction rates, and mass loss rates will be calculated for each computational cell, for every iteration. Hence the model will be capable of analyzing situations when different parts of the gypsum boards are undergoing different heating rates which is very common when exposed to fire. Density, porosity and other key material properties of different types of gypsum board will be verified and tabulated.

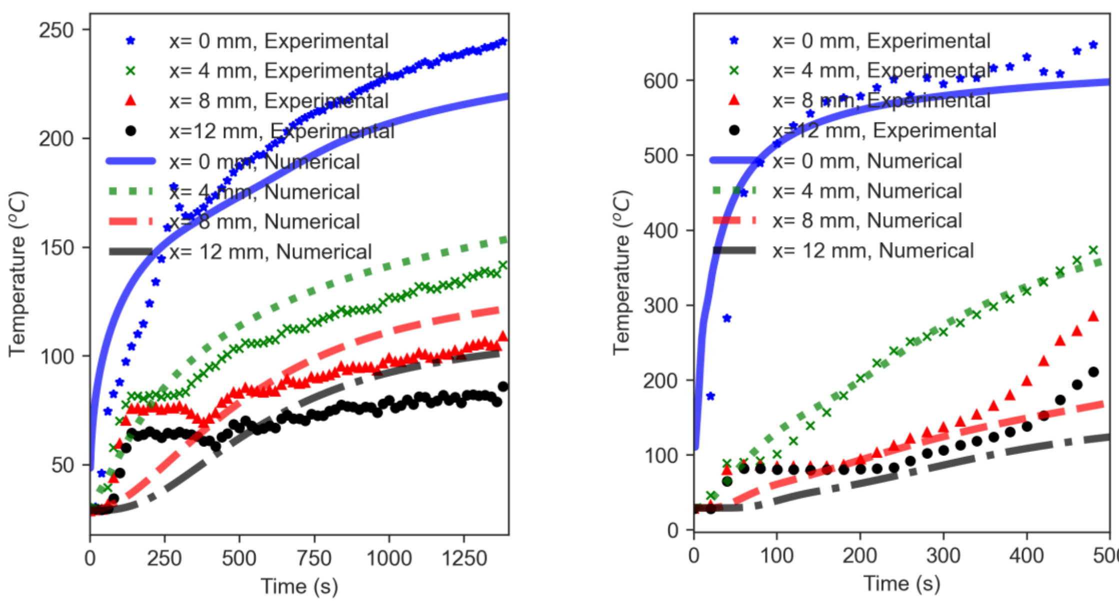


Figure 9: Comparison of time histories of temperature at different depths inside the gypsum board between the experimental measurements and the numerical predictions when exposed to heat fluxes of 10 kW/m^2 (left) and 50 kW/m^2 (right). Depth is measured from the side exposed to the heat source.

The preliminary one-dimensional model for the regular gypsum board has been validated by comparing the numerical predictions of the internal temperature with the experimental measurements for a wide range of heat fluxes Figure 9. Experimental uncertainties at higher heat fluxes are found to be significant. Numerical predictions are found to be within or close to experimental uncertainties. Computational models for different wall lining materials including moisture-resistant drywall, mold, and mildew-resistant drywall, fire-resistant drywall, and sound-absorbing drywall will be validated against their experimental measurements from Task 1.D.

2.3.6 Expected outcomes from Phase 1:

1. A validated gypsum thermo-chemistry model for different gypsum boards that consider variable heating rate gypsum thermo-chemistry.
2. Characterization of different gypsum boards available in the market from different manufacturers.
3. A computational model with variable heating rate gypsum thermo-chemistry, variable thermo-physical properties, and heat and mass transfer through the porous material.
4. Validation of the 1D numerical model and characterization of the sensitivity of each modeling parameter in the entire practical range
5. Analysis of depth of calcination with varying heat flux, and duration of exposure.

2.4 Phase 2: Analysis of different wall lining materials under fire exposure

2.4.1 Task 2.A: Experiments with painted drywalls

The effect of painted drywall exposed to fire also needs to be analyzed. Painted drywall can act as an insulator in the early stages but can ignite and burn more easily than unpainted drywall. This is because the paint provides a fuel source for the fire, especially in the initial stage, affecting the heat and mass transfer mechanisms. Oil-based paints are more flammable than water-based paints. Experiments will be conducted with five different heat fluxes for one oil-based and one water-based paint on a regular gypsum board. The effect of paint layer thickness will be analyzed for a selected heat flux. A series of 5 to 7 experiments will be conducted for a selected heat flux to verify the reproducibility of the experiments. A total of 18 to 22 experiments are expected to be required.

2.4.2 Task 2.B: Development of a 3D model and analysis of non-uniform heat flux

A three-dimensional computational model will be developed following the mathematical formulation used in Phase 1, however, considering lateral heat and mass transfer. The model will solve for the species transport equations and momentum equations in all three directions. The special gradients in heat flux and surface temperature will be considered. The model will be able to predict the depth of calcination in the entire compartment envelope even with the unsteady non-uniform heat flux from the fire. In addition to the source terms in the species transport equations, and energy equation as described in Phase 1, the gravity will be accounted for using a source term in the y-momentum equation. Due to the turbulent combustion, irregularities in the fuel, mixing, and reaction rates, most fires possess significant gradients in the temperature and local heat release rate. This leads to non-uniform heat flux to the wall or gypsum board exposed to fire. Earlier experimental studies show the effect of three-dimensionality is minimal and often less than the experimental uncertainties making it challenging to study experimentally. However, the effect of lateral gradients in heat flux can be effectively and accurately analyzed numerically.

2.4.3 Task 2.C: Sensitivity analysis

2.3.4.1 Sensitivity analysis

As there are significant differences in the material properties between different gypsum boards available in the market. This leads to differences in the density, moisture content, porosity, emissivity, mass convection coefficient, thermal convection coefficient, specific heat, unbound and bound water fraction. A systematic sensitivity study is required to quantify the impact of these variations on the gypsum calcination and the prediction of internal temperatures. If the fire behavior is highly sensitive to even small changes in these properties, the reliability of the methods can only be established after analyzing the impact of possible variations in these properties. If the effect of the variations in any material property of the gypsum board is insignificant or within the already established margin of uncertainty, those effects can be neglected to simplify the methods of investigation. The proposed study will perform global sensitivity analysis through the Sobol method (Sobol, 1993; Sobel, 2001), in order to determine the effects of differences between estimated and real material properties. A Monte Carlo integration scheme with around 100,000 trials is expected to be required to approximate the variances caused by changes in the input parameters for each type of gypsum board with significantly different properties. Local sensitivity analysis will also be performed as a benchmark for the sensitivity of the model with a 1% change in the transport parameters and gypsum material properties. The simulations will be automated with a prescribed range for ease of analysis.

2.4.4 Task 2.D: Scanning Electron Microscopy

Scanning Electron Microscopy (SEM) with Energy Dispersive X-ray Spectroscopy (SEM–EDX) analysis will be carried out using a Hitachi FlexSEM 1000 II scanning electron microscope fitted with a Bruker ESPIRIT Compact energy dispersive X-ray spectrometer. The elemental composition will also be determined. Backscatter electron (BSE) mode will be used with an accelerating voltage of 5 kV for visualization and 20 kV for elemental analysis. Preliminary studies with regular gypsum boards exposed to heat show significant local irregularities and the presence of elements like fiberglass used for support. Figure 10 (left) shows a location with fiberglass and Figure 10 (center) shows a location without it. Figure 10 (right) shows a further magnified view. Different types of gypsum boards will be analyzed using SEM to understand the difference in the composition of different types of gypsum boards and how they respond to exposed heat and fire.

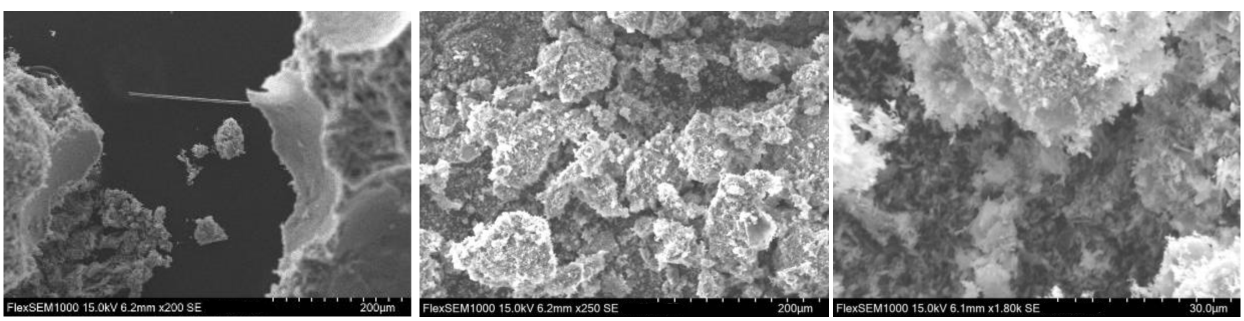


Figure 10: SEM images with different levels of magnification at different locations of a regular gypsum board exposed to heat

2.4.5 Task 2.E: Development of correlations and a stand-alone application

Verification of the developed correlations will begin through re-evaluating previous experiments conducted at EKU. A user-friendly application will be developed that would help the fire investigators predict the depth of calcination based on either the heat fluxes to the gypsum board or the temperatures. Correlations for different types of gypsum boards and correction factors for the paint layers will be developed. Preliminary correlations developed for regular gypsum boards are reported are shown section 2.2.3. of preliminary studies. The proposed project aims to develop similar and improved correlations for different types of gypsum boards. A database of material properties, thermo-physical properties, and thermo-chemical properties of different wall lining materials including moisture-resistant drywall, mold, and mildew-resistant drywall, fire-resistant drywall, and sound-absorbing drywall will be developed.

2.4.6 Expected outcomes from Phase 2:

1. Characterization of the effect of paint layers on gypsum calcination for both oil-based and water-based paints.
2. Development of a three-dimensional computational model and analysis of the effect of non-uniform heat flux on the calcination of different types of gypsum boards.
3. Characterization of the sensitivity of each modeling parameter in the entire practical range.
4. Microscopic characterization of the effect of heat flux and fire on different gypsum boards.
5. Development and verification of a stand-alone user-friendly application for the prediction of depth of calcination based on the heat flux from fire dynamics solvers.

2.5 Timeline of the proposed study

The general time frame for the proposed investigations is illustrated in Figure 11. Both phases of the proposed project will be completed in 24 months from the start of contract. Experimental and numerical investigations will be carried out in parallel to ensure active feedback between them. Meticulous recording of the observations and documentation of the information and findings will be done as a continuous process throughout the project. Evaluation of the satisfactory completion of the interim objectives will be carried out by comparing the project outputs wilt the expected outcomes from each phase. All aspects of the project will be managed by the PI. We will have weekly project meetings to ensure that the proposal deadline will be met. Regular meetings will be arranged between the PI, Co-PIs, and student workers. Additional personnel will be included based on the specific needs of Phases I and II of the project.

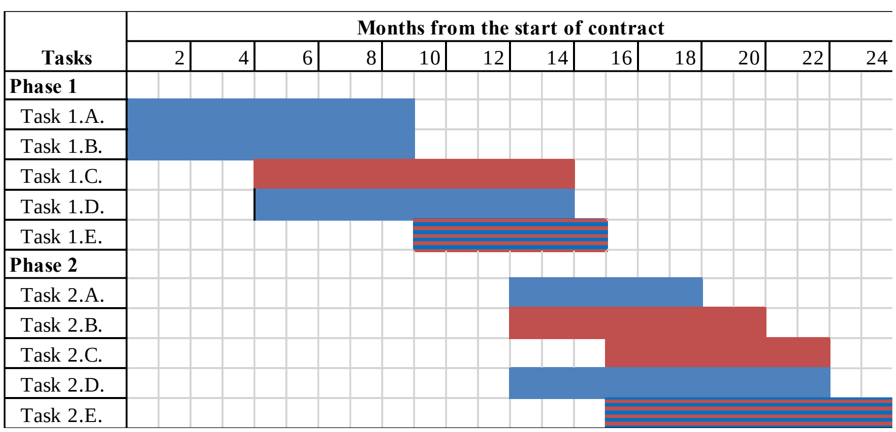


Figure 11: Timeline of the proposed project. Experimental tasks (1.A., 1.B., 1.D., 2.A., and 2.D.), Numerical tasks (1.C., 2B., and 2.C.), and combined tasks (1.E. and 2.E.) are colored differently.

3. Potential Impact

3.1. Direct benefits to the fire investigator

Currently, there is no guidance in any authoritative treatise on how to address the uncertainty and reliability related to comparing depth of calcination with fire characteristics. A recently completed study by EKU, resulted in correlations between the depth of calcination and incident heat flux for a regular gypsum board using experimental measurements and numerical predictions. However, these correlations are limited to regular gypsum boards. Different types of wall lining materials like moisture-resistant drywall, mold and mildew-resistant drywall, fire-resistant drywall, and sound-absorbing drywall are commonly used. These gypsum boards have different elements- like glass fibers, cellulose fiber, mineral wool, copper-based compounds, ammonium phosphate, and borates- added to them to get the desired characteristics. This could significantly change their behavior when exposed to fire. Failure to recognize the differences in the types of gypsum boards and their effect on fire patterns could mislead fire investigations. The proposed project aims to analyze different types of gypsum boards both macroscopically and microscopically to address this concern. Developing new correlations between fire history and depth of calcination will standardize fire investigations. It is expected that the correlations and criteria developed from this study will provide the fire investigator with an easy roadmap on interpreting the measured depth of calcination and determining the origin for a given fire. Detailed analysis of the gypsum thermo-chemistry and development of a database of material, thermo-physical, and thermo-chemical properties of different wall lining materials will make fire investigations more scientific and reliable.

3.2. Dissemination

Research outcomes from the proposed project will be presented at professional conferences and workshops and will be published in peer-reviewed journals. The PI and Co-PIs plan to present the outcomes of the proposed project at annual meetings such as Fire Department Instructors Conference, International Association of Arson Investigators' and the International Symposium on Fire Investigations since they are the most influential scholastic meetings for the forensic fire investigation and research community. The PI and Co-PIs will actively participate in workshops in fire dynamics, forensic fire investigation, and combustion to disseminate the project outcomes about the forensic investigation methods, developed correlations, and the criteria on whether certain fire pattern is reliable for identifying the origin and cause. The research materials will be published in peer-reviewed journals in fire and fire forensics such as Fire technology, Journal of Fire Sciences, Fire Arson Investigator Journal of IAAI, and the Journal of Forensic Sciences.

Two online workshop/webinar will be conducted by engaging the fire investigators. The first webinar will be conducted in the early stage of the project to understand the requirements of the fire investigators. The second one will be conducted towards the end of the project to explain the methods and research outcomes and introduce the stand-alone application developed along with the requirements and limitations of the model.

Graduate and undergraduate students involved in the project will play critical roles in presenting the research outcomes at professional conferences, workshops, and peer-reviewed journal articles. The PI and co-PI will prepare them to be capable of presenting materials and writing manuscripts in a professional manner. The research outcomes will be presented at various outreach programs and undergraduate/graduate students will be educated and trained through the projects.

4. Capabilities and Competencies

4.1. Resources available at Eastern Kentucky University (EKU)

Eastern Kentucky University is a regional comprehensive university in Richmond, Kentucky, established in 1906. The College of Justice and Safety is Eastern Kentucky University's first and only Program of Distinction. The College offers unique degree programs and has a reputation for being on the frontline of learning and research in the fields of justice and safety. Eastern Kentucky University also houses a full-scale test burn building, located on the Richmond, Kentucky campus. This structure is a specially constructed, single-story building with overall dimensions of approximately 62' X 32'. It incorporates six interconnected burn rooms and two hallways with 8" reinforced concrete walls and roof. There are also 12 pre-fab buildings that can be constructed in a variety of scenarios for fire testing, experimentation, and demonstrations. The facilities at EKU are already constructed for the purposes of fire investigation education, which lessens the time and cost associated with running these experiments. EKU also has a Hitachi FlexSEM 1000 II Scanning Electron Microscope (SEM) fitted with a Bruker ESPIRIT Compact energy dispersive X-ray spectrometer suitable for Energy Dispersive X-ray Spectroscopy (SEM–EDX) analysis and elemental analysis.

4.2. Resources available at Georgia Southern University (GSU)

Georgia Southern University (GSU) is a public research University in US state of Georgia. At Georgia Southern facilities, DSC, TGA, and FTIR are readily available tools.

4.3. Key personnel and responsibilities

i. **PI: Shijin Kozhumal, Ph.D.** – planning and numerical approach. Primary responsibility will be designing the numerical models, repeatability studies, and laboratory experimental design. Dr. Kozhumal will also oversee the progress of the studies and numerical methods and verify the numerical design. Dr. Shijin Kozhumal has expertise in modeling and analyzing unsteady reactive flows with complex physics, developing novel grid refinement approaches (Kozhumal, Sundaram, Raghavan, & Babu, 2014) (Kozhumal, Raghavan, & Babu, 2016) (Kozhumal, Aravindh, & Raghavan, 2016), developing and verifying specific numerical models for wildland fire spread, gas phase radiation, flame-flow interaction, fire growth, and control of in-situ burning (Kozhumal, et al., 2017) (Worcester Polytechnic Institute, 2017), and artificial intelligence (Gorbett & Kozhumal, 2022). Dr. Kozhumal has over ten years of experience in numerical and experimental research including the development of new computational models and algorithms. Dr. Kozhumal served as the project director of an NIJ-funded study on gypsum plasterboards under fire exposure during 2021-2022.

ii. **Co-PI: Gregory E. Gorbett, Ph.D.** – operations and planning. Dr. Gorbett will also verify the laboratory experimental design and results and make recommendations and adjustments for the planned tests along the project time span. Dr. Gregory Gorbett has twenty years of experience as a fire and explosion investigator. He has in-depth knowledge in the field, evident from the comprehensive review of all experimental work conducted on the topic of fire patterns (Gorbett G. , Meacham, Wood, & Dembsey, 2015). He has conducted experimental research on the production of fire patterns [(Gorbett G. E., Hicks, Kennedy, & Hopkins, 2006), (Gorbett, Hicks, & Tinsley, 2010) (Gorbett, Hicks, & Tinsley, 2013), and on the reliability and validity in the use of fire patterns (Gorbett, Morris, Meacham, & Wood, 2015), (Gorbett G. E., Meacham, Wood, & Dembsey, 2015). Dr. Gorbett serves as a principal member on the technical committee that serve as the standards of care for the fire investigation profession, NFPA 1033.

iii. **Co-PI: Hayri Sezer, Ph.D.** – developing computational models and material characterization. A three-dimensional computational model that solves for species, momentum and heat transfer in gypsum board will be developed based on the previously developed one-dimensional model. Dr. Sezer has expertise in computational fluid dynamics, heat and mass transfer. He has developed numerical models based on heat, mass and momentum transfer for fire-related problems, fuel cells, batteries, and wildland fire. (Sezer, Arsava, Kozhumal, & Rangwala, 2017; Sezer, H. and Celik, I.B, 2015; Sezer, H., Arsava, K.S. and Rangwala, A.S., 2017)

iv. Student workers will be charged with the construction of the experiments. Student workers will assist with experiments and clean up from the experiments. In addition, Forensic Fire Analysis Institute has expressed support for the proposed project. The letter of support is attached as appendix. Resumes of Key Personnel are attached as appendix.

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