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Development of CFAST Based Fire Simulation Toolkit

for Fire Investigators

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ABSTRACT

The primary goal of the work summarized in this report was to make compartment fire modeling more accessible to fire investigators by developing a fire investigator-friendly electronic fire simulation toolkit based on the computer zone fire model CFAST and by facilitating its use in support of fire origin and cause determination through the development of a short course.

The electronic toolkit consists of two databases and a pre- and post-processor. The first database is a collection of CFAST input data for more than 200 different combustible items.

The second database contains thermal property data for interior surface materials and various target materials. The pre-processor facilitates the creation of CFAST input files for a base case and variations in which one or several input parameters are changed from the base case.

Post-processing involves the calculation of specific quantities of interest to the fire investigator and a comparison of output data from different runs.

Materials were developed for a short course to train fire investigators in the use of CFAST. The materials consist of two PowerPoint presentations, an instructor's manual and CFAST input files for six case studies. The course runs over two days, followed by a half day of 'train the trainer'.

Three studies were conducted to quantify errors in the CFAST predictions that are a result of the assumption that surface materials have constant thermal properties and consist of a single layer backed by an air gap. A fourth study was conducted to examine the effect of variations in density and composition of gypsum board on calcinations depth for a given thermal exposure.

TABLE OF CONTENTS

	Page
ABSTRACT.....	ii
FIGURES.....	v
TABLES.....	v
1.0 SUMMARY OF THE PROJECT.....	1
1.1 Major Goals and Objectives.....	1
1.2 Research Questions.....	2
1.3 Research Design and Methodology.....	3
1.4 Expected Applicability of the Research.....	4
2.0 PARTICIPANTS AND OTHER COLLABORATING ORGANIZATIONS.....	5
3.0 CHANGES IN APPROACH FROM ORIGINAL DESIGN.....	5
4.0 OUTCOMES.....	7
4.1 Activities and Accomplishments.....	7
4.1.1 Fire object database.....	7
4.1.2 Material database.....	9
4.1.3 Pre- and post-processing.....	11
4.1.4 Short course materials.....	11
4.1.5 Case studies.....	12
4.2 Results and Findings.....	14
4.2.1 Thermal properties of gypsum board at ambient temperature.....	14
4.2.2 Calcination study.....	18
4.2.3 Effect of temperature dependency of surface material thermal properties.....	27

4.2.4 Effect of substrates30

4.3 Limitations31

5.0 ARTIFACTS32

5.1 List of Products32

5.1.1 Short Course Materials32

5.1.2 Conference papers and journal articles32

5.2 Data Sets Generated33

5.3 Dissemination Activities34

6.0 REFERENCES34

FIGURES

	Page
Figure 1. Time-squared heat release rate profile proposed by Kim and Lilley [14].....	9
Figure 2. Effect of density on thermal conductivity of gypsum board at ambient temperature...	16
Figure 3. Relative thermal conductivity of gypsum board as a function of temperature.....	23
Figure 4. Effect of temperature-dependent wallboard properties on T _{UL} predictions for Fire 1 ..	28
Figure 5. Effect of temperature-dependent wallboard properties on T _{UL} predictions for Fire 2 ..	29
Figure 6. Effect of temperature-dependent wallboard properties on T _{UL} predictions for Fire 3 ..	29
Figure 7. Proposed correction to constant wallboard properties to improve T _{UL} predictions.....	30
Figure 8. Effect of the substrate on T _{UL} predictions for a post-flashover fire	31

TABLES

	Page
Table 1. Initially proposed short course schedule.....	13
Table 2. Average thermal property values of gypsum board at ambient temperature	16
Table 3. Summary of CFAST simulation results for Fire 1	19
Table 4. Summary of CFAST simulation results for Fire 2.....	19
Table 5. Summary of CFAST simulation results for Fire 3.....	20
Table 6. Kinetic parameters and heat of reaction for thermal decomposition reactions	24
Table 7. Summary of results of the first set of FDS simulations.....	26
Table 8. Summary of results of the second set of FDS simulations.....	26
Table 9. Summary of results of the third set of FDS simulations.....	27

1.0 SUMMARY OF THE PROJECT

1.1 Major Goals and Objectives

Computer fire model simulations can greatly facilitate the process of determining the origin and cause of a fire. However, computer fire models are currently underutilized by fire investigators because of difficulties in obtaining the necessary input data, complexities in the setup of the simulations, and challenges with interpretation of the results of the calculations. The primary goal of the work was to alleviate these difficulties, complexities, and challenges by developing a fire investigator-friendly electronic fire simulation toolkit based on the computer zone fire model CFAST (Consolidated model of Fire and Smoke Transport) developed at and maintained by the National Institute of Standards and Technology (NIST) in Gaithersburg, Maryland, and by facilitating its use in support of fire origin and cause determination through the development of a short course.

The primary objectives of the work were as follows:

- Create a comprehensive database of complete sets of CFAST input data for a wide variety of fire objects.
- Create a comprehensive database of thermal and pertinent flammability properties for specific floor, wall, ceiling, and ignition or damage target materials.
- Create a pre-processor to facilitate input data collection and model setup, and to manage tasks that require multiple simulations.
- Develop a post-processor of CFAST output to calculate and report specific quantities of interest to the fire investigator.

- Create educational materials for a 2–3 day short course on the use of CFAST and the toolkit in support of fire investigation.
- Identify experimental and actual fires that can serve as illustrative examples and can be used as case studies for the short course.

1.2 Research Questions

Despite its favorable features, CFAST has significant limitations and its use in support of fire investigation and reconstruction faces several challenges that required additional research:

1. Existing collections of ignition and burning rate data for fire objects are incomplete, in that they do not include a full set of input parameters that are needed for a CFAST simulation. Moreover, the data are not available in a format that is suitable for import into CFAST.
2. Heat release rates of fire objects are generally obtained from furniture calorimeter experiments. However, the burning rate of an object can increase in response to thermal radiation from the hot gas layer (HGL), flames, and heated walls and ceiling in a compartment. CFAST has no mechanism to account for this thermal feedback effect.
3. CFAST assumes that the floor, walls, and ceiling of the compartment consist of a single layer of a homogeneous material with constant thermal properties. In reality, thermal properties are temperature-dependent, and the backing material may have a significant effect on the heat losses through a wall or ceiling.
4. CFAST calculates the generation rates of smoke and carbon monoxide (CO) based on user-specified CO, soot yields, and elemental fuel composition. However, the yields

vary as a function of time due to changes in fire temperature and ventilation conditions, which are not *a priori* known.

5. CFAST does not calculate the generation rate of important toxic gases such as hydrogen bromide (HBr), hydrogen fluoride (HF), and sulfur dioxide (SO₂), while the version available at the start of the project typically overestimated the generation rate of hydrogen cyanide (HCN) by an order of magnitude compared to experimental data.
6. The smoke detector actuation algorithms in CFAST “are very crude and the uncertainty in predictions are substantial”, as stated in the CFAST Technical Reference Guide [1].
7. Propagating input parameter uncertainties through the simulation to quantify the resulting uncertainty in the CFAST predictions is a tedious process. Automating this process would be greatly beneficial to investigators.

The project involved research to specifically address these limitations and challenges.

1.3 Research Design and Methodology

The toolkit includes two databases. The first database contains CFAST input data for more than 200 fire objects. The data for each object are compiled in an individual Excel workbook. The workbook is used to create a fire object file that can be imported directly into the CFAST graphical user interface (GUI), CEdit. The second database consists of a compilation of thermo-physical property data for common compartment interior surface materials, and for different types of target materials in another Excel workbook. The material database includes macros to calculate the properties for wood products (based on type of product, density and moisture content), ignition targets (based on surface temperature at ignition and thermal inertia derived from a series of ignition tests at different heat fluxes) and melting targets (averages between ambient and melting temperatures). The data in the workbook for materials that are

pertinent to the analysis are used to create a fire object file that can be imported directly into the CFAST GUI, CEdit.

The pre-processor is an Excel app that allows the user to first set up a base case. The base case is then used to create variations in which one or several input parameters are changed. After running the base case and pertinent variations, post-processing is performed to calculate specific quantities of interest to the fire investigator (e.g., time to untenable conditions in the compartment, calcination depth at specified target locations, etc.) and compare output data from different runs.

Materials were developed for a short course to train fire investigators in the use of CFAST and the toolkit. The materials consist of two PowerPoint presentations, an instructor's manual and CFAST input files and results for six case studies. The course is scheduled to run over 2 days. It is followed by an optional half a day of 'train the trainer' for new instructors.

1.4 Expected Applicability of the Research

Several research studies were conducted as part of this work (see Section 4.2) that are not only of interest to fire investigators who are using fire modeling in their work but to the fire science community more generally. The results of these studies will be disseminated through scholarly publications (see Section 5.1.2).

The short course will serve as the primary mechanism for dissemination of the results of this research to the target audience. It is expected to significantly expand the use of fire modeling in general and CFAST by arson and fire investigators. Moreover, the toolkit will also be useful to fire scientists and engineers who use CFAST for other purposes.

2.0 PARTICIPANTS AND OTHER COLLABORATING ORGANIZATIONS

The SwRI team consisted of Dr. Marc Janssens (PI), Mr. Jason Huczek, Ms. Alexandra Schluneker and Mr. George Adams.

The short course materials were developed by Prof. David Icove and Mr. Fred Martin at the University of Tennessee, Knoxville.

3.0 CHANGES IN APPROACH FROM ORIGINAL DESIGN

The CFAST software package consists of two parts, an executable of the CFAST model code and a user-friendly GUI (CEdit) for input data entry. From the start, the plan was not to change the CFAST source code for the following reasons:

- The CFAST source code is complex and modifications to the code may have unintended consequences, causing the program to behave in an unexpected or erratic manner.
- Substantive changes to the source code would require additional verification and validation of the executable.
- Future CFAST bug fixes and upgrades would need to be implemented to maintain consistency with the versions released by NIST, which is nearly impossible to do.

To make the toolkit easier to use by fire investigators who are already familiar with CFAST, the initial plan was to develop a modified version of CEdit as the GUI for the pre-processor. We acquired the proprietary software that is needed to modify CEdit and started making the necessary changes. However, over the past 2 years, NIST has released eight revisions of the CFAST software (see release notes: <<https://github.com/firemodels/cfast/wiki/Release-Notes>>). In the summer of 2020, NIST announced the release of the next major update to Revision 7.6

(exact date still to be determined). Many of these revisions have resulted in significant changes to CEdit. More than halfway through the first year of the project it became apparent that it would be very difficult to maintain consistency between our version and the NIST version of CEdit. To address this issue, we changed our approach and decided to develop the pre-processor as a Microsoft Excel[®] app, which allows the user to create and run the base case and variations to the base case directly from the GUI of the installed revision of CFAST.

Research questions two and six could not be addressed as originally intended due to limitations in CFAST. Therefore, an alternative approach is proposed for use by fire investigators as they use the toolkit in its current configuration:

- To evaluate the effect of thermal radiation from heated walls and ceiling, the hot gas layer and flames from other burning fire objects on the burning rate of a fire object, it is proposed that the fire investigator perform a sensitivity analysis in which the peak heat release rate of the fire object is increased by up to 32 percent. The upper limit is the maximum increase expected for upholstered furniture with a peak heat release rate of 400 kW or higher in a small room [2]. The fire object database is not capable of making this adjustment at the present time.
- Smoke detector response depends on the concentration of particulates in the vicinity of the detector. As a result of the two-zone assumption, CFAST instantaneously and uniformly distributes particulate matter in the hot gas layer, which covers the entire ceiling. Consequently, the particulate concentration at the detector is under-estimated and CFAST predicts a much longer time to actuation. To estimate the time to actuation of a smoke detector mounted on a flat ceiling, the fire investigator can use the Excel workbook that performs the calculations described in Chapter 11 of NUREG 1805 [3]. For more complex situations, such as a smoke detector mounted on a sloped ceiling or

on a flat ceiling between two beams, the field fire model Fire Dynamics Simulator (FDS) developed at NIST can be used to estimate the actuation time [4, 5].

The uncertainties in the input parameters are significantly greater for CFAST simulations performed in support of a fire investigation compared to simulations of a compartment fire experiment (as in the CFAST validation guide [6]) and a comprehensive uncertainty analysis is likely to result in an excessive amount of information that is hard to interpret. The fire investigator is better served by focusing on the principal unknowns and conducting a sensitivity analysis. The toolkit is designed to facilitate such an analysis.

Finally, several studies were conducted on gypsum board because it is the most common room interior surface material and calcines when exposed to heat in a fire. A depth of calcination survey may help the fire investigator “locate areas of greater or lesser heat damage and recognized lines of demarcation defining patterns” [7].

4.0 OUTCOMES

4.1 Activities and Accomplishments

This section provides an overview of the elements of the toolkit and the short course materials that were developed.

4.1.1 Fire object database

A common misconception is that compartment fire models predict how a fire develops. With a few exceptions, however, compartment fire models predict the effects in terms of gas temperatures, heat fluxes, visibility through and toxic potency of smoke, etc. of a user-specified fire. CFAST is not one of the exceptions. A fire typically involves multiple combustible items. For example, a living room fire may start with the ignition of an upholstered chair and may

subsequently involve a sofa and other contents and furnishings in the room. To fully characterize a combustible item or fire object, CFAST needs the following information:

- Heat release rate as a function of time.
- Average value of the heat of combustion.
- Radiative fraction (i.e., the fraction of the heat release rate that is lost by the flame in the form of thermal radiation).
- Chemical composition of the fuel.
- Yields of soot, CO, HCN and other toxic gases.
- Area and height of the fire base.

Experimental heat release rate data were collected for more than 200 items from 14 reports and data collections [8-21]. For some tests, the data were available in electronic form but for others the electronic data had to be generated by digitizing plots in the report. The heat release rate curves were parametrized by fitting a time-squared fire growth and decay profile through the data points as proposed by Kim and Lilley [14] and shown in Figure 1. The five parameters that uniquely define the curve are the ignition time (t_0), the time at which the heat release rate levels off (t_{lo}), the maximum heat release rate (HRR_{max}), the time when the heat release rate starts to decay (t_d) and the burnout time (t_{end}).

Some of the remaining CFAST input parameters are provided in the report but most are based on generic values in the literature [22-33]. Data for the radiative fraction and the yield of soot and toxic products of combustion are particularly hard to find and may have large uncertainties. A sensitivity analysis can be performed to determine up to what extent the results of the CFAST simulation are sensitive to variations in the values for these input parameters.

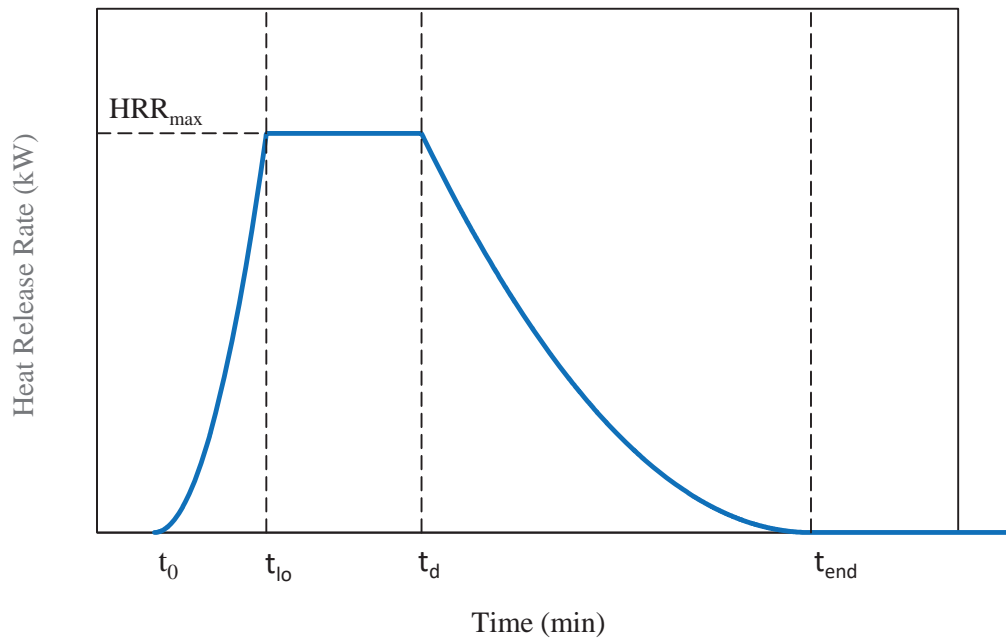


Figure 1. Time-squared heat release rate profile proposed by Kim and Lilley [14]

4.1.2 Material database

The materials database includes thermal properties (i.e., density ρ , thermal conductivity k and specific heat capacity, c) for six different categories of materials.

- *Interior Surface Materials*—This category consists of common materials that are used to cover the floor, walls and ceiling of a compartment such as gypsum board, different types of concrete, carpet, etc. The database also includes properties for common insulation materials. The thermal property values for materials in this category are based on ambient temperature data in the literature.
- *Wood Products*—This category consists of solid sawn wood and various wood panel products such as plywood, particleboard, oriented strand board, and medium density fiberboard. Wood products are treated differently from other interior surface materials because their properties depend on density and moisture content, which vary widely as

a function of wood species and environmental conditions. Correlations developed by Ten Wolde et al. [34] are used to calculate ρ , k , and c based on oven dry density and moisture content specified by the user.

- *Ignition Target Materials*—Ignition targets are used to determine when the second and subsequent items ignite. The thermal properties for the materials in this category are apparent values (i.e., constant values that are averages over the temperature range between ambient and ignition) that are estimated based on the surface temperature at ignition (T_{ig}) and the effective thermal inertia ($k\rho c$) derived from an analysis of ignition data (i.e., time to ignition measured over a range of radiant heat fluxes in the Cone Calorimeter or similar device) [35, 36]. For all materials in this category, properties were estimated from piloted ignition data but for some materials the database includes a second set that was derived from auto-ignition data.
- *Metal Target Materials*—Metals with a low melting point such as aluminum, lead, magnesium, tin, and zinc can be useful as temperature indicators. The thermal properties for materials in this category are average values between 20 °C and the melting point based on temperature-dependent data and correlations in the literature [37, 38].
- *Plastic Target Materials*—Thermoplastics also can be used as temperature indicators. As for metal targets, the properties for materials in this category are average values calculated from temperature-dependent data and correlations in the literature [39].
- *Damage Target Materials*—This category consists of materials that do not fit into one of the other categories. An example of a material in this category is human skin.

For each material, the database includes a default value for the thickness and surface emissivity. The user can adjust these values so that they are consistent with the in-use thickness and actual surface conditions of the material (e.g., painted versus bare surface, polished versus oxidized metal surface, etc.), respectively.

4.1.3 Pre- and post-processing

Pre-processing for a new case first involves the creation of a material property file and one or several fire object files for the materials and fire objects that are pertinent to the case. The user then creates a base case directly in CEdit. The material properties and fire object data needed for the simulation are imported from the files that were created earlier. After data entry for the base case is completed, the user can create variations to the base case in which one or several input parameters are changed. These variations can be used to explore the sensitivity of results to uncertainties in contributing parameters. For example, variations can be used to explore the effect of varying the time when a door was opened or closed, if that time is not exactly known.

In addition to generating comparison plots of results from the CFAST runs, post-processing allows the user to perform calculations of calcination depth and tenability of occupants at specified locations in the room. The former is discussed in detail in Section 4.2.2. The latter requires some post-processing if fractional effective dose (FED) is affected by exposure to toxic gases other than CO and HCN, for which CFAST does not calculate the time to untenable conditions due to toxic gas exposure.

4.1.4 Short course materials

The educational materials for the short course were developed by Dr. David Icove and Mr. Fred Martin at the University of Tennessee, Knoxville. The materials consist of two PowerPoint presentations (144 slides for day one and 129 slides for day two), a 107-page

instructor's manual and CFAST input files and results for six case studies (see Section 4.1.5). The course materials were evaluated in the spring of 2020 as an assignment for Dr. Icove's students in the Forensic Fire Analysis (ENFP 661) class, which is a mandatory course in the online graduate program in Fire Protection Engineering at the University of Maryland, College Park, Maryland.

The course is scheduled to run over two days. It is followed by an optional half a day of 'train the trainer' for new instructors. The initially proposed CFAST short course schedule is provided in Table 1. The course schedule will be adjusted to meet specific needs and the materials will be updated periodically in response to student feedback and changes in the CFAST software. The course is now "Certified" in Tennessee for fire and arson investigators and has been incorporated into the University's Graduate Certificate Course, ECE 564 – Enclosure Fire Dynamics, which is offered via distance education both on-campus and remotely.

4.1.5 Case studies

In addition to the three examples that were used in the studies that are discussed in Section 4.2, the following case studies were developed for the short course:

- March 6, 1982 Westchase Hilton hotel fire in Houston, Texas.
- March 28, 1994 Watts Street fire in lower Manhattan, New York.
- HAZARD I ranch house fires.
- HAZARD I town house fires.
- HAZARD I two-story house fires.
- Living room fire test in single story house conducted by Underwriters Laboratories (UL).

Table 1. Initially proposed short course schedule

Time	Section	Day 1 Student Course
8:00 AM - 8:30 AM	Kickoff	Preliminaries, Introductions, Previews
8:30 AM - 9:30 AM	1	CFAST Introduction and Installation
9:30 AM - 10:00 AM	2	Hazard Assessments
10:00 AM - 10:30 AM	3	CFAST Application: 8-Compartment CFAST Model Actual Fire: 62 Watts Street
10:30 AM - 12:00 PM	4	Constructing a 2-Room Model from 62 Watts Street 8-Compartment CFAST Model
12:00 PM - 1:00 PM		Lunch
1:00 PM - 1:30 PM	5	CFAST Model Review
1:30 PM - 3:30 PM	6	Ranch House Model Fires 8 Scenarios
3:30 PM - 4:00 PM	7	Townhouse Model Fires
4:00 PM - 4:30 PM	8	Two-story House Model Fires
4:30 PM - 5:00 PM	9	General Discussion
Time	Section	Day 2 Student Course
8:00 AM - 8:30 AM	1	Advanced Enclosure Fire Dynamics Introduction
8:30 AM - 9:00 AM	2	Advanced Enclosure Fire Dynamics Lexicon, Units, Material Properties, Objects, Heat Release Rate
9:00 AM - 9:45 AM	3	Heat Transfer
9:45 AM - 10:30 AM	4	The Science of Fire
10:30 AM - 12:00 PM	5	Enclosure Fires
12:00 PM - 1:00 PM		Lunch

Table 1. Initially proposed short course schedule (continued)

Time	Section	Day 2 Student Course (continued)
1:00 PM - 3:00 PM	6	UL Tests: Various Examples Featuring Single Story Small House Lab Burn
3:00 PM - 4:00 PM	7	Overview of the Toolkit and How it Affects Using CFAST
4:00 PM -5:00 PM	8	Final Assignment
Time	Section	Day 3 Train the Trainer
8:00 AM - 10:00 AM	1	Training Packages: Computers/Software Pre-course Manuals
10:00 AM - 11:00 AM	2	References: Materials, Objects, Heat Release Rates
11:00 AM - 12:00 PM	3	Software References: GITHUB Problems Certifications and Submission

HAZARD I is a fire hazard assessment software package that was developed at NIST in 1989 and updated in 1991 [40-42]. The single story house fire test was conducted by UL as part of a project funded by the National Institute of Justice (NIJ) under award 2015-DN-BX-K052 [43].

4.2 Results and Findings

Several studies were conducted in support of the development of the toolkit. These studies, which mostly focus on gypsum board, are summarized in the subsections that follow.

4.2.1 Thermal properties of gypsum board at ambient temperature

4.2.1.1 Types of gypsum board

The term 'gypsum board' refers to a family of sheet products consisting of a noncombustible core, primarily of gypsum with paper surfacing on both sides. Gypsum is a mineral consisting mainly of fully hydrated calcium sulfate (i.e., $\text{CaSO}_4 \cdot 2\text{H}_2\text{O}$ or calcium sulfate dihydrate). It is

very likely that the walls and ceiling of the compartment(s) in the fire investigator's CFAST model are finished with gypsum board, at least in North America.

Gypsum has excellent fire-resistant properties due to the large amount of energy required for complete dehydration to anhydrate (i.e., CaSO_4 or calcium sulfate). This dehydration process is referred to as calcination and occurs between 80°C and 220°C. The performance in a fire depends on the type of gypsum board. The 60-90 percent gypsum in regular gypsum board loses about 21 percent of its mass during calcination, which results in shrinkage and crack formation that adversely affects fire performance. The core of Type X gypsum board contains glass fibers, which reduce the shrinkage and result in improved fire performance. The core of Type C gypsum board has additional components such as vermiculite, which further improve fire performance. Regular and Type X must meet standard specifications while Type C is proprietary; consequently, its fire performance varies between manufacturers.

4.2.1.2 Survey of fire research studies

The most common type of interior finish material in residential occupancies in the United States (U.S.) is 12.7-mm ($\frac{1}{2}$ -inch) thick regular gypsum board. The density of regular gypsum board significantly declined from more than 800 kg/m³ in 1950 to about 600 kg/m³ in 2000, but has remained relatively steady since then [44]. To determine the effect of density on the thermal conductivity of gypsum board, a survey was conducted of thermal property values at ambient temperature used in fire research studies involving testing or numerical modeling of the performance of gypsum board wall and ceiling assemblies in fire [45-63]. The results of the survey are summarized in Table 2, which indicates that the average thermal property values for the three types of gypsum board are similar. Moreover, there is no correlation between density and thermal conductivity at ambient temperature, as shown in Figure 2.

Table 2. Average thermal property values of gypsum board at ambient temperature

Gypsum Board Type	# of Data Points	ρ_0 (kg/m ³)	k_0 (W/m·K)	c_0 (kJ/kg·K)
Regular	19	726	0.25	972
Type X	12	720	0.23	1024
Type C	6	766	0.22	984
Overall Mean		730	0.24	990
Standard Deviation		82	0.06	131

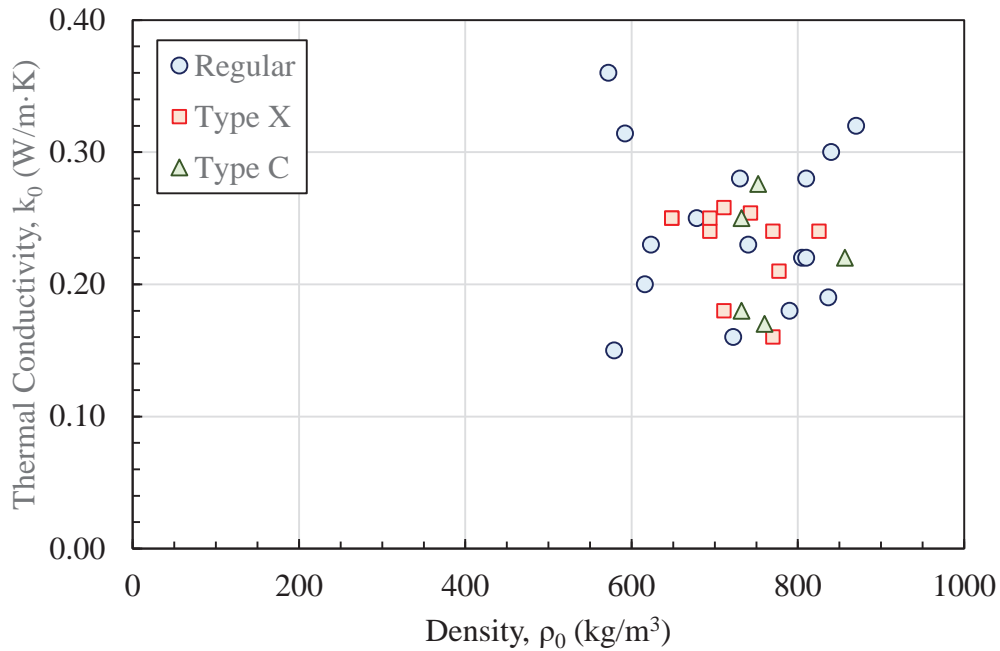


Figure 2. Effect of density on thermal conductivity of gypsum board at ambient temperature

4.2.1.3 *Effect of variations in the thermal properties on CFAST predictions*

Table 2 also shows that there is some uncertainty in the thermal property values. To quantify the uncertainty of the CFAST predictions resulting from variations in the thermal properties of the gypsum board, a sensitivity analysis was performed for the following three compartment fires that are briefly described here and discussed in more detail in [64].

- Fire 1 is a demonstration test in a simulated living room of mass timber construction with interior surfaces protected with gypsum board. The test room was approximately 4.1-m wide, 3.6-m deep, and 2.4 m high. The front narrow wall of the compartment was provided with an open doorway, approximately 1.9-m wide by 2.1-m high. The test was started by igniting a sofa seat cushion with a small flame (British Standard BS 5852 Source 2). Flashover occurred in approximately 4 minutes. The contents were largely consumed in less than 15 minutes.
- Fire 2 is a test on an upholstered chair that was conducted as part of a research program for the NIJ [13]. The test was conducted in a 3.4-m wide, 4.7-m deep, 2.4-m high compartment of light wood-frame construction covered with gypsum board on the inside. A 0.74-m wide by 2-m high open doorway was located in the center of one of the short walls of the room. The chair was ignited with a small flame (British Standard BS 5852 Source 2). It took nearly 10 minutes to reach a peak heat release rate of approximately 1.7 MW, which was insufficient to create flashover.
- Fire 3 is identical to Fire 2, except that a three-seat sofa of the same set was tested. The same ignition source was used as in the Fire 2 experiment but in the Fire 3 experiment a peak heat release rate of 2.25 MW was reached in approximately 8 minutes. The upper layer temperature exceeded the flashover limit of 500 °C but only slightly and for less than 2 min.

The sensitivity study involved five CFAST simulations of each of the three compartment fires. In all simulations it was assumed that the compartment walls and ceiling consist of a single layer of 12.7 mm gypsum board backed by an air gap. For the first simulation (base case), we specified the mean values for density ρ , thermal conductivity k and specific heat c from Table 2. For the remaining simulations (cases R1-R4), we increased or decreased the three properties by one standard deviation. Calculated averages (Fire 1) or maximum values (Fires 2 and 3) of the upper- and lower-layer temperature rise (ΔT_{UL} and ΔT_{LL}), upper gas layer depth (ΔZ_{UL}) and incident heat flux to targets on the back wall at 1.8 m and 0.3 m above the floor ($\dot{q}_{UL inc}''$ and $\dot{q}_{LL inc}''$) are given in Tables 3–5.

The sensitivity analysis shows that the upper gas layer depth is not sensitive to the thermal property values that are assumed in the simulations. However, the use of incorrect thermal property values can result in significant errors in the temperature and heat flux predictions. A possible approach to reduce these errors involves measuring the density based on the mass and dimensions of gypsum board samples taken from the fire scene that have not been exposed to heat from the fire. The magnitude of the remaining error can be estimated from a sensitivity analysis, similar to the analysis discussed here.

4.2.2 Calcination study

In 1983, James and Eleanor Posey introduced the idea of using calcination depth mapping to identify burn patterns [65]. Since then, the technique has been refined and reliable methods for measuring calcination depth have been developed [66-70]. Calcination depth mapping is now a well-established resource to assist fire investigators in determining the cause and origin of a fire, as is evident from the detailed guidance provided in NFPA 921 [7]. In this work, we examined the extent to which this technique can provide quantitative information about the severity of exposure to heat from the fire at a given location.

Table 3. Summary of CFAST simulation results for Fire 1

Case	ρ (kg/m ³)	k (kW/m·K)	c (kJ/kg·K)	Averages between 4.5 and 14.5 min				
				ΔT_{UL} (°C)	ΔT_{LL} (°C)	ΔZ_{UL} (m)	$\dot{q}_{UL inc}''$ (kW/m ²)	$\dot{q}_{LL inc}''$ (kW/m ²)
Base	730	0.24	990	1070	402	1.31	176	156
R1	812	0.30	1121	1029	364	1.31	156	137
R2	648	0.30	859	1061	394	1.31	171	151
R3	812	0.18	1121	1080	411	1.31	182	161
R4	648	0.18	859	1113	443	1.31	199	178

Table 4. Summary of CFAST simulation results for Fire 2

Case	ρ (kg/m ³)	k (kW/m·K)	c (kJ/kg·K)	Peak Values				
				ΔT_{UL} (°C)	ΔT_{LL} (°C)	ΔZ_{UL} (m)	$\dot{q}_{UL inc}''$ (kW/m ²)	$\dot{q}_{LL inc}''$ (kW/m ²)
Base	730	0.24	990	433	63	0.71	15.3	12.8
R1	812	0.30	1121	411	55	0.72	13.4	11.3
R2	648	0.30	859	436	64	0.71	15.6	13.0
R3	812	0.18	1121	435	64	0.71	15.5	12.9
R4	648	0.18	859	463	75	0.71	18.1	15.2

Table 5. Summary of CFAST simulation results for Fire 3

Case	ρ (kg/m ³)	k (kW/m·K)	c (kJ/kg·K)	Peak Values				
				ΔT_{UL} (°C)	ΔT_{LL} (°C)	ΔZ_{UL} (m)	$\dot{q}_{UL inc}''$ (kW/m ²)	$\dot{q}_{LL inc}''$ (kW/m ²)
Base	730	0.24	990	532	101	1.01	26.2	22.4
R1	812	0.30	1121	497	85	1.01	22.0	18.7
R2	648	0.30	859	538	104	1.01	26.9	23.1
R3	812	0.18	1121	534	102	1.01	26.5	22.7
R4	648	0.18	859	568	117	1.00	30.7	26.6

4.2.2.1 Composition of gypsum board

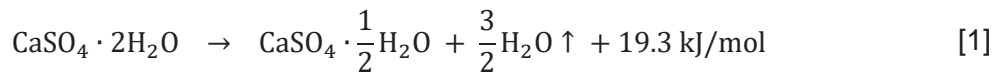
Gypsum board consists of a non-combustible core sandwiched in between two layers of paper. The thickness of the paper is approximately 0.4-0.5 mm [71, 72]. Based on the research studies that were reviewed, it appears that between 60 and 90 percent of the core consists of gypsum (calcium dihydrate, CaSO₄·2H₂O). Some boards also contain smaller amounts (generally less than 10 percent) of calcium carbonate (CaCO₃), magnesium carbonate (MgCO₃) or dolomite [CaMg(CO₃)₂]. The balance consists of inert materials.

In addition to the chemically bound water in the gypsum, the core also contains some free water in the pores. In the research studies that were reviewed, the free water ranged from a fraction of a percent [73] to as much as seven percent [48]. To optimize agreement between model predictions of the thermal conductivity of gypsum board and k_0 values reported for 10 boards used in various fire research studies, de Korte and Brouwers found that 2.8 percent of free

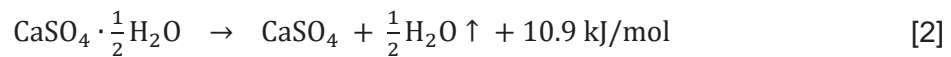
moisture provides the best fit [74]. This appears to be a reasonable value for generic use in modeling.

4.2.2.2 Thermal degradation of gypsum board

Gypsum board is very efficient as a fire-resistant barrier material because of the large amount of energy (approximately 560 kJ per kg of gypsum [75]) required for complete dehydration of gypsum to anhydrate (calcium sulfate, CaSO_4) and evaporate the resulting free water. The dehydration occurs in two endothermic reaction steps. In the first step, the gypsum decomposes to form hemihydrate ($\text{CaSO}_4 \cdot \frac{1}{2}\text{H}_2\text{O}$, also known as plaster of Paris):

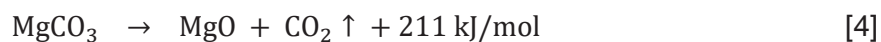
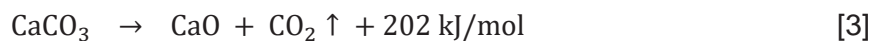


This reaction occurs between 80 and 180 °C, with the exact range depending on the heating rate [76]. The second step consists of further dehydration of hemihydrate to anhydrate:



The second reaction occurs between 110 and 220 °C, with the exact range again depending on the heating rate [76]. The heats of reaction for the two steps are based on measurements reported by Kontogeorgos [75].

Boards that contain calcium carbonate, magnesium carbonate, or dolomite lose additional mass at higher temperatures (between 600 and 750 °C [76]) as a result of the thermal decomposition of these components:



The heats of reaction for Equations 3–5 are based on values reported in the literature [49, 76, 77]. The decomposition of dolomite consists of two steps. In the first step, magnesium oxide and calcium carbonate are formed. In the second step, calcium carbonate decomposes according to Equation 3.

Finally, mass loss due to evaporation of free moisture becomes noticeable in thermogravimetric analysis (TGA) experiments at approximately 70 °C; consequently, it is hard to distinguish from the first step in the gypsum dehydration. The latent heat of evaporation of free water in gypsum board was measured by Kontogeorgos to be approximately 2260 kJ per kg of water [75].

4.2.2.3 Numerical model

The pyrolysis model in FDS [4] was used to model the dehydration of gypsum board. The model allows the user to specify temperature-dependent properties. A survey of the literature was conducted to determine how the thermal conductivity of gypsum board varies with temperature [47-49, 52, 53, 56, 58, 59, 62, 76, 78, 79]. Figure 3 shows normalized k_0 (which varied among the different studies) as a function of temperature.

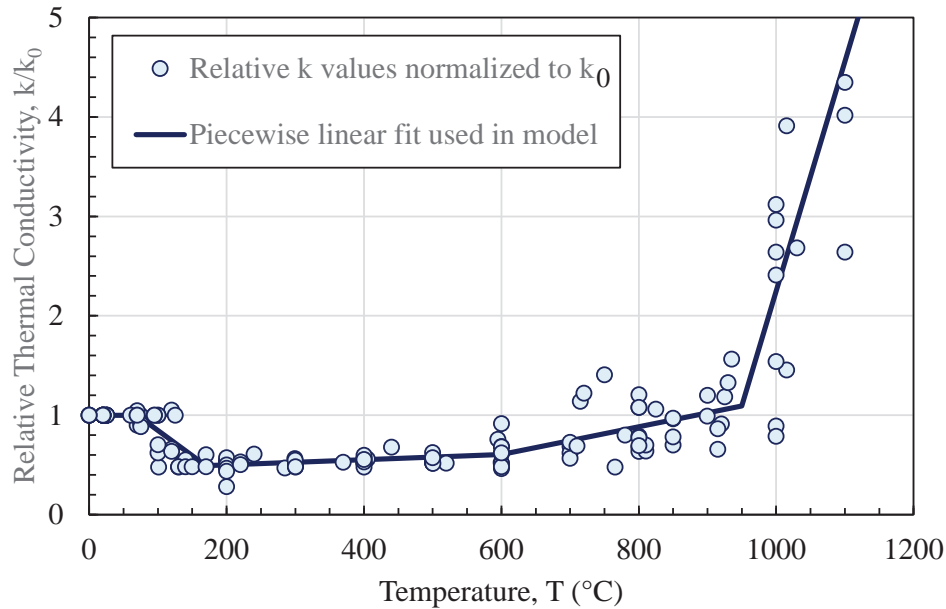


Figure 3. Relative thermal conductivity of gypsum board as a function of temperature

Based on the survey, it was determined that it is reasonable to assume a constant value for the specific heat: $c = c_0 = 0.99 \text{ kJ/kg}\cdot\text{K}$. Shrinkage is neglected based on data reported by Bénichou and Sultan [47]. Consequently, the density of the board is assumed to decrease based on the mass loss associated with the generation of water vapor and carbon dioxide in the thermal degradation reactions.

FDS uses an Arrhenius reaction equation to model the thermal decomposition of the active components. The dehydration of gypsum is assumed to take place as a single step, as proposed by Craft [73]. The kinetic parameters and the heat of reaction for gypsum, calcium carbonate, and dolomite are provided in Table 6.

Arrhenius reaction rate parameters for the decomposition of magnesium carbonate could not be found. Instead, the specific heat is increased between 600 and 680 °C to account for the heat of reaction associated with its decomposition. A similar adjustment is made to the specific heat

between 340 and 420 °C to account for the enthalpy change associated with the transition from soluble anhydrite III to insoluble anhydrite II.

Table 6. Kinetic parameters and heat of reaction for thermal decomposition reactions

Model Parameter	CaSO ₄ ·2H ₂ O		CaCO ₃		CaMg(CO ₃) ₂	
	Value	Ref.	Value	Ref.	Value	Ref.
Frequency Factor, A (s ⁻¹)	5.7·10 ¹²	[73]	1.84·10 ⁸	[80]	1.63·10 ⁷	[81]
Activation Energy, E (kJ/mol)	116		194		191	
Reaction Order, n	1.00		1.91		0.404	
Heat of Reaction (kJ/kg)	560	[75]	2000	[49]	4280	[76]

4.2.2.4 Sensitivity study

A sensitivity study was performed to determine whether there is a relationship between calcination depth and the total irradiance to which gypsum board has been exposed. We simulated exposing a sample of gypsum board with a thickness δ of 12.7 mm to the radiant heater of the Cone Calorimeter [35]. For all simulations, we assumed that the exposed surface of the specimen is cooled by convection to the surrounding air with a convection coefficient h_c equal to 12 W/m²·K [82]. Four sets of simulations were performed.

1. In the first set, we examined the effect of the intensity of thermal exposure. Simulations were performed for 12.7 mm gypsum board with a density of 730 kg/m³, a gypsum content of 80 percent, a free moisture content of 2.8 percent, and a balance of inert material, exposed to irradiance levels of 10, 30, 50, 75 and 100 kW/m². At each level, the duration of exposure was adjusted so that total irradiance was 18 MJ/m² (i.e., the

specimen was exposed for 1800 s at 10 kW/m², 600 s at 30 kW/m², etc.). The results of the first set of simulations are given in Table 7. Calcination depth δ_c is defined as the depth from the exposed surface to where 95 percent of the chemically bound water has evaporated. Q is the total irradiance in MJ/m² and $\delta_{c,max}$ is the maximum calcination depth.

2. For the second set of simulations, the irradiance and duration of exposure were fixed at 50 kW/m² and 360 s, respectively, but the density of the board was varied. Simulations were performed for board densities of 610, 670, 730, 790 or 850 kg/m³. Results are presented in Table 8.
3. The third set of simulations is similar to the second set except that the density was held constant and gypsum content was varied between 70 and 90 percent. Results are presented in Table 9.
4. In the fourth set of simulations, we examined the effect of adding calcium carbonate (10 or 20 percent) or dolomite (10 or 20 percent) to gypsum board with a density of 730 kg/m³ and a gypsum content of 70 percent. These simulations were performed at two irradiance levels: 50 kW/m² with an exposure time of 360 s and 100 kW/m² with an exposure time of 180 s. The difference in behavior compared to the baseline without calcium carbonate or dolomite was negligible.

The results of the first set of simulations show that there is no unique relationship between calcination depth and total irradiance because the former also depends on the heating rate. The second and third sets of simulations indicate that, with known density and gypsum content, the model can be used to obtain a reasonably accurate estimate of the severity of fire exposure. The density of the gypsum board can be calculated based on measurements of the mass and dimensions of samples taken from a wall section at the fire scene that has not been exposed to

heat. The gypsum content can then be determined by first removing the paper from one of the samples and measuring the mass loss after 2 days of heating in an oven at 200 °C [50].

Table 7. Summary of results of the first set of FDS simulations

Irradiance (kW/m²)	Duration (s)	Time at $\delta_c = \delta/2$ (s)	Q at $\delta_c = \delta/2$ (MJ/m²)	$\delta_{c, \max}$ (mm)
10	1800	1412	14.1	8.0
30	600	404	12.1	8.5
50	360	273	13.7	8.0
75	240	209	15.7	7.5
100	180	174	17.4	7.0

Table 8. Summary of results of the second set of FDS simulations

Board Density (kg/m³)	Time at $\delta_c = \delta/2$ (s)	Q at $\delta_c = \delta/2$ (MJ/m²)	$\delta_{c, \max}$ (mm)
610	243	12.2	8.5
670	266	13.3	8.5
730	273	13.7	8.0
790	300	15.0	7.5
850	322	16.1	7.5

Table 9. Summary of results of the third set of FDS simulations

Gypsum Content (% by mass)	Time at $\delta_c = \delta/2$ (s)	Q at $\delta_c = \delta/2$ (MJ/m ²)	$\delta_{c, \max}$ (mm)
70	270	13.5	8.0
75	279	14.0	8.0
80	273	13.7	8.0
85	297	14.9	7.5
90	306	15.3	7.5

4.2.3 Effect of temperature dependency of surface material thermal properties

CFAST assumes that the thermal properties of the compartment interior surface materials are constant. Typically, the user specifies the property values at ambient temperature, but the thermal properties of these materials vary with temperature. Consequently, assuming ambient temperature properties may result in significant errors in the heat loss calculations. This is of particular concern for gypsum board, whose ambient temperature properties do not reflect the core's capacity to absorb large amounts of energy required for the dehydration of gypsum. To assess the magnitude of this potential error, two FDS simulations were performed for each of the three fires described in Section 4.2.1.3. For the first simulation, it was assumed that the 12.7 mm gypsum board on walls and ceiling had the same temperature-dependent properties as the board used for the first set of FDS simulations described in Section 4.2.2.4. The FDS calculations were then repeated assuming the average ambient temperature properties from Table 2.

A comparison between the upper layer temperature predictions for the two sets of properties are shown in Figure 4, Figure 5 and Figure 6 for Fires 1–3, respectively. Based on these figures, it appears that assuming constant ambient temperature properties (slightly) overestimates the upper layer temperature during the peak burning period, and for the pre-flashover fires also during the decay period. For Fire 1, which had a 10-minute post-flashover period of relatively steady burning rate, agreement can be improved by increasing the specific heat in the constant property simulation from 0.99 to 1.60 kJ/kg-K, as shown in Figure 7. The value of 1.60 kJ/kg-K was obtained by distributing the heat required for evaporation of all free water (assumed to be 2.8 percent) and full dehydration of the gypsum over the temperature range over which the thermal conductivity is relatively constant (20-950 °C, see Figure 3). This also improved agreement for Fire 2 but not for Fire 3. It should be noted that the upper layer temperatures calculated with FDS are well below those calculated with CFAST (see Section 4.2.1.3). This is because the layer height and temperatures in FDS were calculated at a location close to the walls where the temperatures are lower while CFAST calculates average temperatures over the entire interior upper- and lower-layer gas volumes.

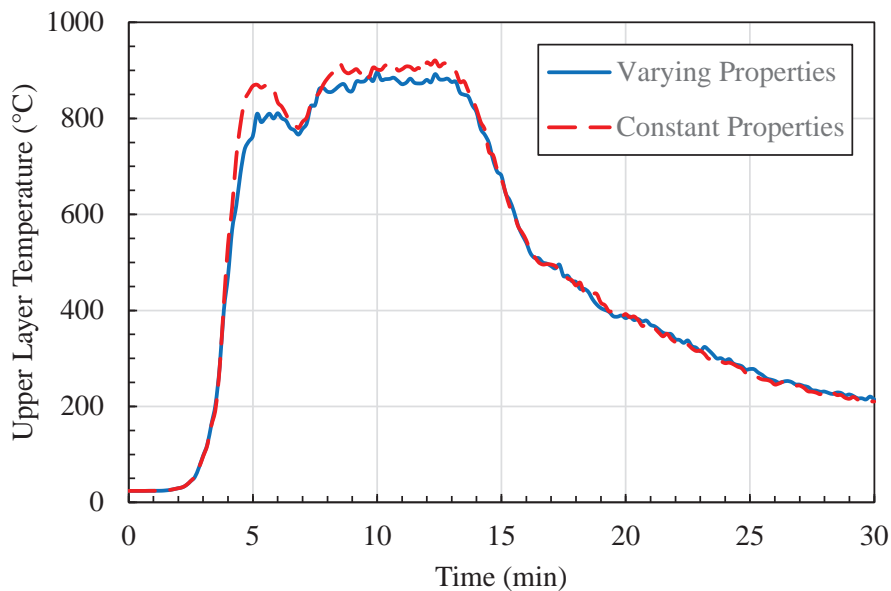


Figure 4. Effect of temperature-dependent wallboard properties on T_{UL} predictions for Fire 1

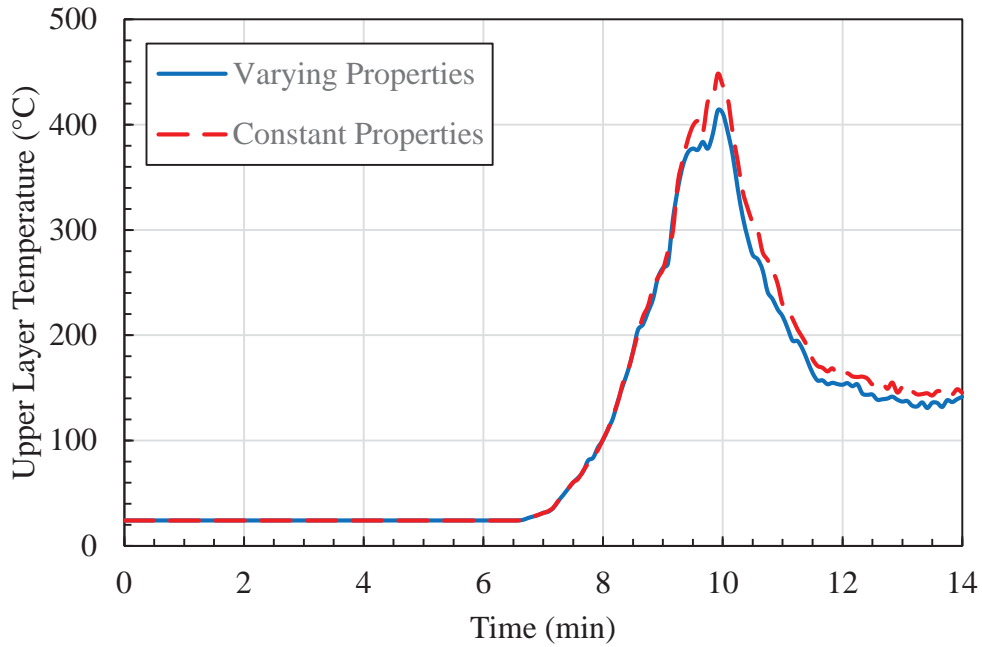


Figure 5. Effect of temperature-dependent wallboard properties on T_{UL} predictions for Fire 2

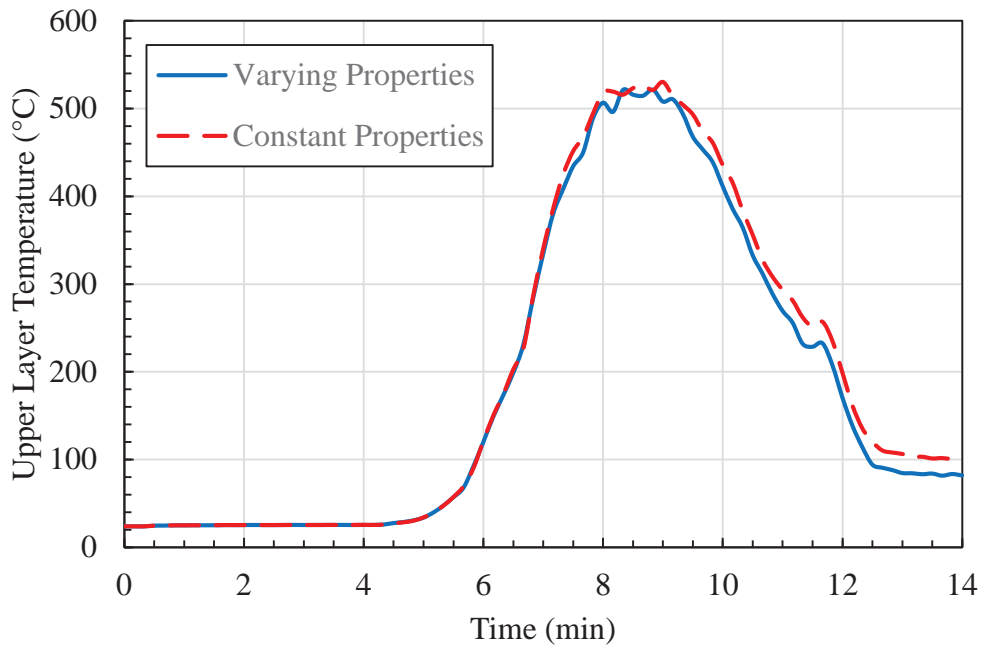


Figure 6. Effect of temperature-dependent wallboard properties on T_{UL} predictions for Fire 3

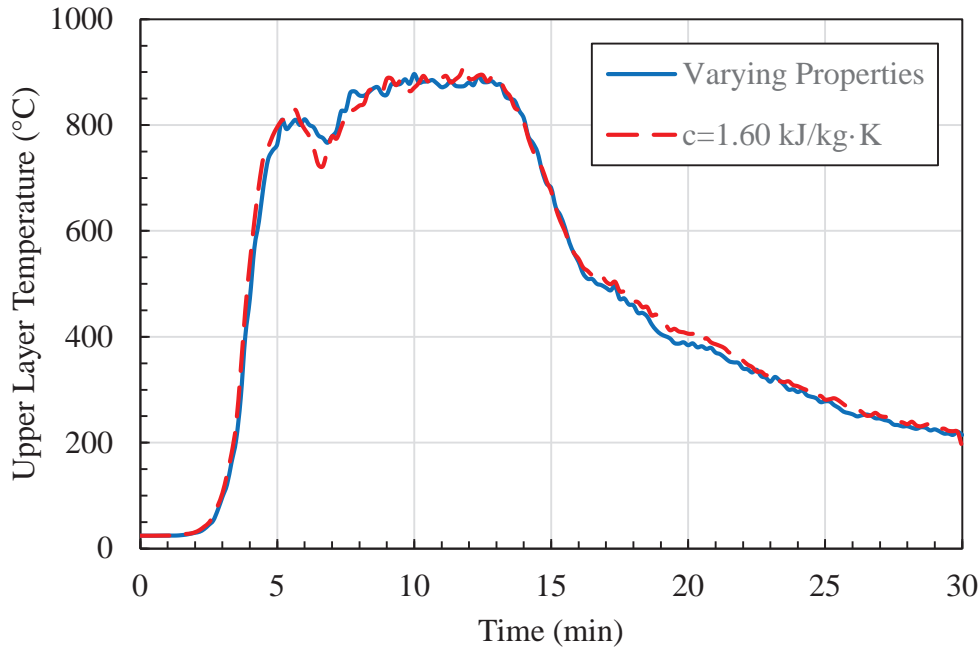


Figure 7. Proposed correction to constant wallboard properties to improve T_{UL} predictions

4.2.4 Effect of substrates

Finally, FDS simulations of Fires 1–3 were performed for 12.7 mm gypsum board walls and ceiling with constant properties backed by one of four different substrates (air gap, glasswool insulation, concrete and solid softwood). The substrate has a significant effect on the upper layer temperature predictions for the post-flashover fire (Fire 1), as shown in Figure 8. The effect is insignificant for the pre-flashover fires (Fires 2 and 3). The current version of CFAST (7.5.2) does not allow the user to specify multiple surface layers. However, the next version of CFAST (7.6, release TBD) will include this capability, which will address this limitation.

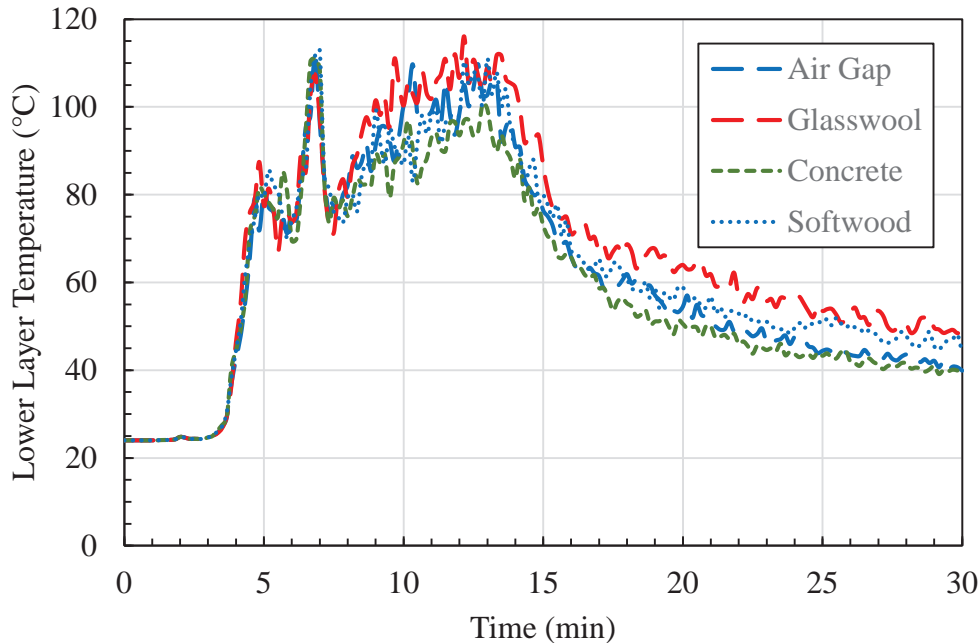


Figure 8. Effect of the substrate on T_{UL} predictions for a post-flashover fire

4.3 Limitations

CFAST has some inherent limitations in its ability to accurately predict the effects of a fire because of the fundamental simplifying assumption that the gases inside the compartment stratify in two layers of uniform composition and temperature: a lower layer of relatively cool air and an upper layer of hot smoke. For this reason, CFAST cannot accurately predict smoke detector actuation time, which depends on the concentration of particulates at the detector. This limitation can be addressed by using a field fire model, also referred to as a computational fluid dynamics or CFD model, such as FDS [4]. Field models subdivide the gas volume inside the compartment in a large number (typically a few hundred thousand) of small cells; increased resolution enables more accurate predictions. Another approach to obtain more accurate predictions of smoke detector activation in the room of fire origin involves using a simplified algebraic thermal plume model, such as that described in Chapter 11 of NUREG 1805 [3] (see Section 3.0 for additional discussion). Although CFAST is a powerful fire simulation tool, its

usefulness can be significantly enhanced by supplementing it with spreadsheet calculations and FDS simulations.

Some additional work is needed to make the toolkit more useful to fire investigators. For example, upholstered furniture accounts for more than 60 percent of the items in the fire object database. A fire investigator often does not have detailed information about the furniture involved in the fire and will have a hard time finding “representative” items in the fire object database. Another example is the simulation of post-flashover fires. During the post-flashover period, the fire is fully developed and all exposed contents and furnishings are involved. Under those conditions it is not possible, nor would it be practical, to estimate the total burning rate from the heat release rates of the individual items. In the coming year (2021), we will prepare a journal article in which we will provide guidance to fire investigators on how to address these outstanding issues.

5.0 ARTIFACTS

5.1 List of Products

5.1.1 Short Course Materials

The educational materials for the short course consist of two PowerPoint presentations (144 slides for day one and 129 slides for day two), a 107-page instructor’s manual and CFAST input files and results for six case studies.

5.1.2 Conference papers and journal articles

Based on the results of this investigation, we intend to prepare up to four publications.

- The first publication is a conference paper that provides a general overview of the work. This paper, entitled “CFAST-based Fire Simulation Toolkit for Fire Investigators” was submitted for presentation at the 16th Fire and Materials conference, originally to be held

February 1–3, 2021 in San Francisco, California. Unfortunately, this conference was postponed until 2022 due to the COVID-19 pandemic.

- The second publication is a conference paper that will describe the methods that were developed to obtain “equivalent” constant thermal property values for interior surface and target materials, whose actual thermal properties vary significantly with temperature. An abstract will be submitted for presentation at the ASTM E05 Committee Symposium on “Obtaining Data for Fire Growth Models” to be held December 9–10, 2021 in Atlanta, Georgia. Selected papers will be considered for publication in ASTM’s *Selected Technical Papers (STP)*, an online and printed, peer-reviewed publication for the international engineering community.
- The third publication is a journal article that will provide guidance for using the fire object database in the toolkit to obtain CFAST input parameters for upholstered furniture and post-flashover fires. This paper will be submitted to one of the major peer-reviewed fire journals (e.g., *Fire and Materials*, *Fire Safety Journal*, *Fire Technology*, or *Journal of Fire Sciences*).
- The research that was done on calcination of gypsum board (see Section 4.2.2) would be useful to the fire community, too. To the extent practicable, this element of the research will be submitted to one of the aforementioned peer-reviewed fire journals.

5.2 Data Sets Generated

Two databases were developed but are not ready for general use. The databases will be updated and finalized in 2021, after the release of the next major version of CFAST (7.6), which is expected to require some adjustments to the databases. No social science data were generated in this work.

5.3 Dissemination Activities

Dissemination activities has been limited as a result of restrictions associated with the COVID-19 pandemic.

The primary mechanism of dissemination of this work to date is through the short course. Instructure, maker of the popular online learning management platform Canvas, has given Dr. Ilove a website to publish the course. This makes it accessible throughout the U.S. at no charge. Most recently, the course was offered in December 2020 as State of Tennessee Police Officer Standard and Training (POST) Course #20-452. The course is now “Certified” in Tennessee for fire and arson investigators, and has been incorporated into the Graduate Certificate Course, ECE 564 – Enclosure Fire Dynamics, which is offered via distance education both on-campus and remotely at the University of Tennessee, Knoxville. The novel distance educational interstate compact (NC-SARA) allows anyone in the U.S. to register for this course.

Results of the work also will be disseminated through conference papers and journal articles (see Section 5.1).

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