Light Water Reactor Sustainability Program

FRI3D Fire Simulation Options and Verification Tasks

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ABSTRACT

The Fire Risk Investigation in 3D (FRI3D) software was developed at the Idaho National Laboratory under the Risk-Informs System Analysis pathway under the Light Water Reactor Sustainability Program. This software combines the multiple tools used by industry for fire modeling with the plant risk analysis and 3D spatial information. With this combination, FRI3D automates scenario generation and provides other tools that can reduce some fire analysis task times by more than 50%. The FRI3D software has undergone initial testing and feedback from industry to determine additional research needs before it is ready for initial industry piloting. This report outlines the work done on two of those needs, including verification against the CFAST (Consolidated Model of Fire and Smoke Transport) fire simulation tool constraints and the option to use the Fire Dynamics Simulator or FDS, fire simulation tool.

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ACRONYMS

CFAST	Consolidated Fire and Smoke Transport
CFD	Computational Fluid Dynamics
EPRI	Electric Power Research Institute
FDS	Fire Dynamics Simulator
FDT	Fire Dynamics Tools
HRR	Heat Release Rate
INL	Idaho National Laboratory
LWRS	Light Water Reactor Sustainability
NIST	National Institute of Standards and Technology
NRC	Nuclear Regulatory Commission
PDMS	Plant Data Model System
PRA	Probabilistic Risk Analysis
THIEF	The Thermally-Induced Electrical Failure
V&V	Verify and Validate

FRI3D FIRE SIMULATION OPTIONS AND VERIFICATION TASKS

1. INTRODUCTION

Fire Risk Investigation in 3D (FRI3D) software was developed over the last 3 years to research the integration of 3D spatial modeling, existing fire PRA models, and fire simulation codes. The goal was to automate many of the manual tasks in fire analysis to reduce industry efforts in initial fire modeling and fire analysis operational costs when evaluating a plant modification. By using existing tools and methods already approved by the Nuclear Regulatory Commission (NRC), only standard software verification would be required to confirm the existing methods are used correctly.

Initial work focused on ways to effectively use existing data and fire models, then incorporate 3D visualization and couple with fire simulation codes. Initial research showed that these methods could significantly reduce fire modeling time, reduce human errors, and increase fire modeling realism. These results were released in previous reports [1], [2] and published and presented at multiple conferences [3], [4] [5] and taught at three workshops, the American Nuclear Society conference in November 2021, North Carolina State University in March 2022, and the Probabilistic Safety Assessment and Management conference in June 2022.

Current work is focusing on items determined from industry feedback on what research is needed before the software can be used by industry. A preliminary licensing agreement between Idaho National Laboratory (INL) and Centroid Lab has been established to explore commercialization. This report focuses two main research and development tasks. First, the verification of the 3D model within the fire software simulation constraints of Consolidated Model of Fire and Smoke Transport (CFAST), discussed in Section 2. Second, the initial integration and use of the Fire Dynamics Simulator (FDS), a computational fluid dynamics (CFD) fire simulation software, to enable FRI3D to generate more accurate fire scenarios and advanced scenarios for complex room geometries. Section 3 reviews FDS benefits and the process used to achieve the initial integration into FRI3D.

1.1 Previous Work Overview

This section is a quick overview of previous work done on FRI3D. Detailed information on the use of FRI3D or the methods implemented can be found in papers on the LWRS website [6] or in the FRI3D training manual developed in conjunction with Centroid Lab and available upon request from Centroid Lab [7].

A majority of nuclear power utilities have existing fire models, and all have other data already available for use in fire modeling. Methods were developed for importing this existing data, including the fire PRA model format FRANX by Electric Power Research Institute (EPRI) and custom plant database information including the Plant Data Model System (PDMS).

To automate many of the fire modeling tasks, a direct correlation between existing data items and their spatial information is needed. To do this, a user interface was developed to show item information and link it with a 3D model editor and timeline visualization. The user interface provides an easy way for users to see and develop the various aspects for fire analysis and then run and visualize the results all in one location. To facilitate this ease of use the user interface, as shown in Figure 1, has the following sections:

- Compartment/Scenario Editor (top left) – Displays all the items physically in the current compartment/scenario

- Properties Editor (bottom left) – Shows the properties for the selected item and allows the user to edit them

- 3D View (center) – Allows for modeling and viewing the spatial relationships, along with fire simulation results

- FRANX or Logic View (right side) – Shows the logical mapping of raceways, cables, components, and PRA basic events

- Timeline – Displays the timing results from fire simulation and failure calculations (i.e., when items fail).
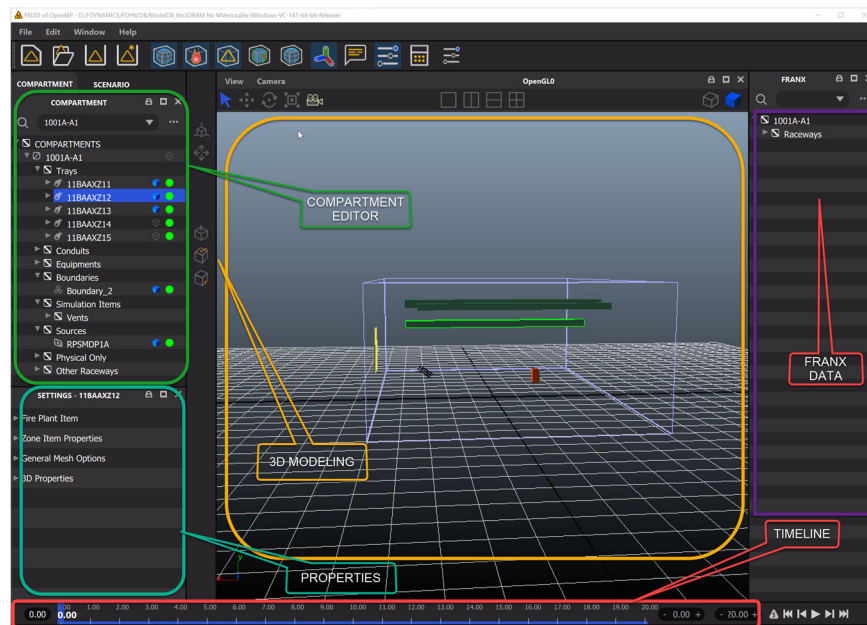
Figure 1. FRI3D graphical user interface layout with data areas labelled.

FRI3D implements several fire estimation algorithms and uses them along with the fire simulation results to determine component failures; these algorithms include FLASH-CATS [8], heat soak [9], and THIEF [10]. A user can autogenerate fire scenarios adding information on a fire source and selecting the generated scenario option then calculate the results as shown in the steps below and in Figure 2:

1. Construct a Fire Simulation Model – FRI3D constructs a CFAST model creating the vents, sources, and optimal measurement points for each item. Fire Dynamics Tools (FDTs) are not used because the FRI3D model can be constructed, and more accurate CFAST results generated in less time than performing FDT calculations. (Future option will include FDS.)

2. Secondary Combustibles – If using CFAST, use the results from step 1 and the FLASH-CAT calculation to determine any secondary combustibles. Re-run CFAST with additional HRR information.

3. Determine Failures – Use the fire simulation model results for the measurement points to determine component and cable failures. If there is no specific cable information, it uses the heat soak calculation; if some cables have details, it will automatically use the more accurate THIEF calculation.

4. Component or Basic Event Failures – The cable tracing or plant logic model is used to find all components linked to the failed cables and construct a list of all failed components for the scenario.

5. New Scenario – The scenario is added to the FRI3D model for the current compartment; each failed item is shown along with when it fails and fire simulation compartment temperature results. Now the user can assign the ignition frequency, non-suppression probability, and severity factor for the scenario.

6. PRA Results – The user can click the calculate button and select desired scenarios; these are added to the plants PRA model and solved.

Figure 2. Scenario generation and results steps.

The final work previously done in FRI3D was the visualization. This visualization allows the user to see what components fail due to a fire scenario, along with when those failures occurred. This allows for a quick qualitative validation of the results and insights about the scenario as shown in Figure 3.
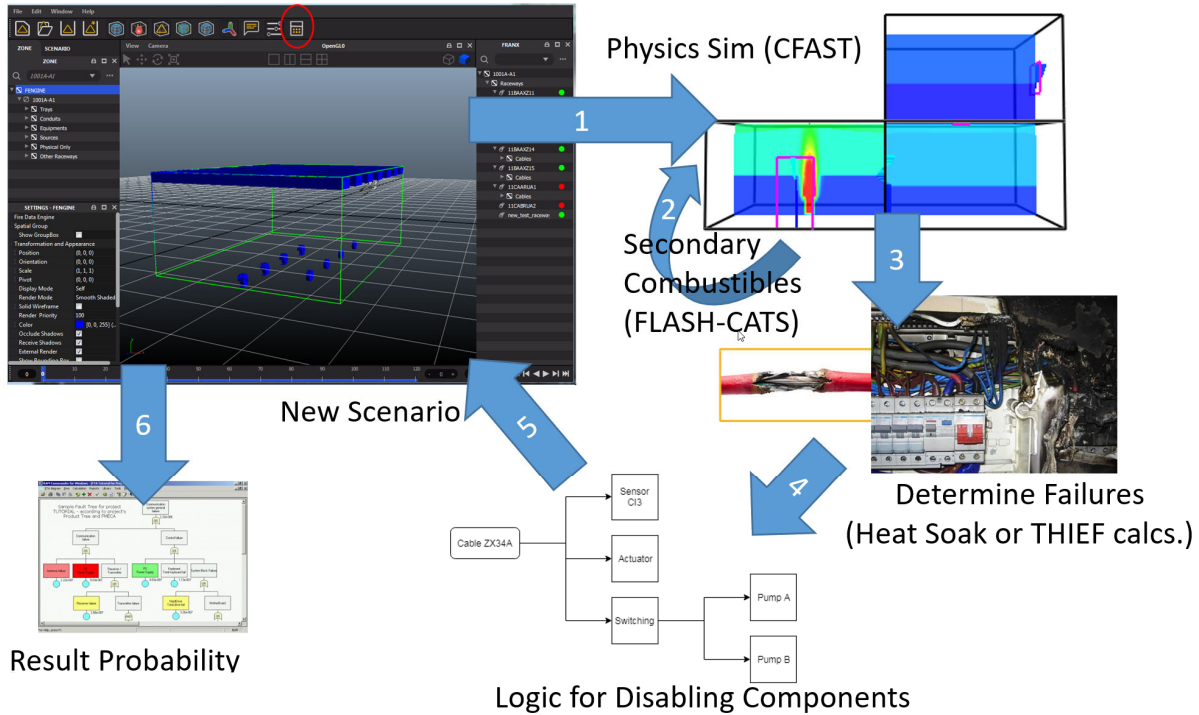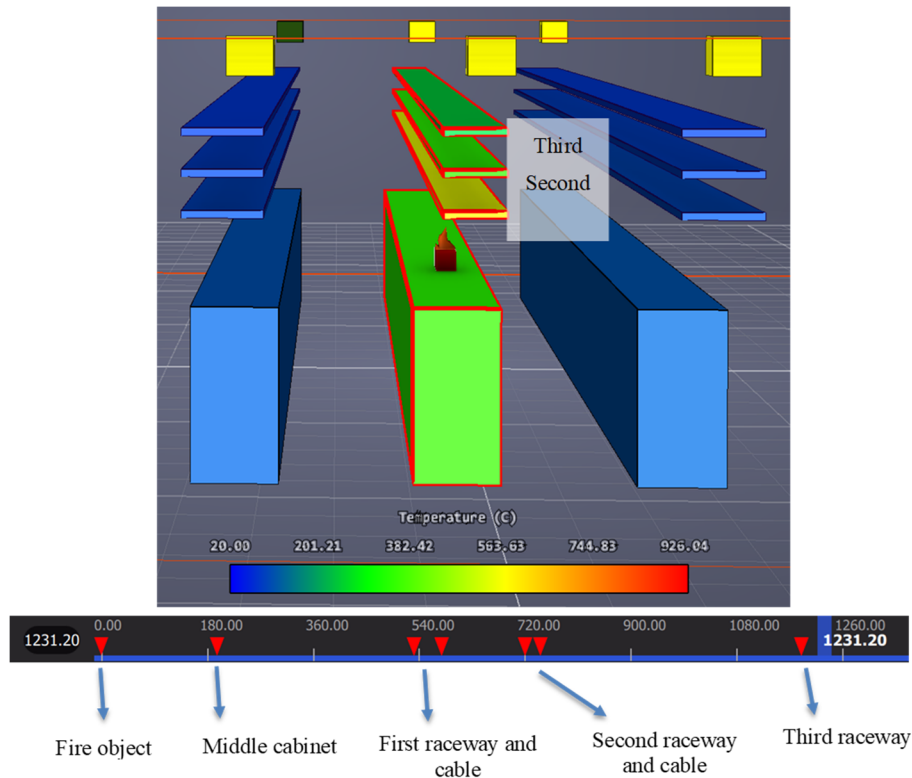
Figure 3. Component failure visualization and timeline.

2. CFAST MODEL VERIFICATION

Fire models are developed with specific underlying assumptions and limitations. For example, the traditional two-zone model used in CFAST assumes that there is an evident stratification of the hot gas layer and cold gas layer, and each layer is uniform in regard to temperature, vertical elevation, and chemical composition. This assumption limits the use of two-zone models to fire scenarios in small- and medium-sized enclosed spaces, such as rooms in residential buildings. The model may give inaccurate results when it is used to model fire scenarios out in the open since these scenarios do not have a uniform stratified hot gas layer. Similarly, the model may have limited applicability in large industrial buildings or in very small rooms where gas layers are less stratified.

CFAST employs empirical correlations to calculate flux and temperature. These correlations were developed for relatively uncluttered, flat ceilings in compartments that can be characterized as "rooms" as opposed to corridors or vertical shafts. There are no hard limits on what kind of compartment can or cannot be modeled in CFAST. The CFAST Validation Guide [11] indicates the accuracy of its predictions for compartments of various aspect ratios. Additionally, radiation from fires is modeled with a simple point source approximation. This limits the accuracy of the model within a few diameters of the fire. It is also important to note that CFAST does not model radiative exchanges between compartments. Therefore, it should not be used to calculate the target's temperature due to a fire located in another compartment.

Due to the limitations of fire models, it is necessary for the modeler to verify and validate (V&V) whether the investigated fire scenario can be analyzed using the model [12]. The V&V procedure is laid out in NUREG-1824 [13]. This procedure is explained in more detail in NUREG-1934 [14]. The V&V process is done by using normalized parameters traditionally used in fire modeling applications. The use of normalized parameters enables the modeler to benchmark results of different scenarios by normalizing the

physical parameters in those scenarios. The normalized parameters for a CFAST model V&V are listed in Table 1. Acceptance criteria from both references are listed—although the criteria used in FRI3D are from NUREG-1824 since it is the latest published standard.

Table 1. Normalized parameters for CFAST V&V.

Quantity	Normalized parameter	Acceptable V&V range
Fire Froude number	$$\dot{Q}^* = \frac{\dot{Q}}{\rho_\infty c_p T_\infty D^2 \sqrt{gD}}$$	0.4-2.4 (NUREG 1934) 0.2-9.1 (NUREG 1824)
Flame length ratio	$$\frac{H_f + L_f}{H_c}$$	0.2-1.0 (NUREG 1934) 0.0-1.6 (NUREG 1824)
Ceiling jet distance ratio	$$\frac{r_{cj}}{H_c - H_f}$$	1.2-1.7 (NUREG 1934) 0.0-8.3 (NUREG 1824)
Equivalence ratio	$$\varphi = \frac{\dot{Q}}{\Delta H_{O_2} \dot{m}_{O_2}}$$	0.04-0.6 (NUREG 1934) 0.0-0.6 (NUREG 1824)
Compartment aspect ratio	$$\text{Compartment Aspect Ratio} = \begin{cases} \dfrac{L}{H_c} \\ \dfrac{W}{H_c} \end{cases}$$	0.6-5.7 (NUREG 1934) 0.6-8.3 (NUREG 1824)
Radial distance ratio	$$\text{Radial Distance Ratio} = \frac{r}{D}$$	2.2-5.7 (NUREG 1934) 0.3-8 (NUREG 1824)
Heat release rate	-	HRR < 1 MW/m^3

Explanation of normalized parameters in Table 1:

1. Fire Froude number

   The Froude number is a measure of the buoyant strength of the fire plume. A large Froude number indicates a strong source, and given a sufficiently high Froude number, the fire plume may take on characteristics of a jet fire. Variables used to calculate the Froude number are given in Table 2.

Table 2. Variables needed to calculate fire Froude number.

Symbol	Name	Unit	Notes
$\dot{Q}$	Peak heat release rate (HRR)	kW	The peak HRR of the fire
T_∞	Ambient temperature	K	The interior air temperature
c_p	Heat capacity	kJ/kg.C	The heat capacity for air varies slightly with temperature, and, at 298 K, it is equal to about 1.012 kJ/kg-°C.
A	Fire area	m^2	
g	Gravity	m/s^2	Default at 9.81

Symbol	Name	Unit	Notes
ρ_∞	Ambient air density	kg/m³	$$\rho_\infty = \frac{352}{T_\infty}$$
D	Fire diameter	m	$$D = \sqrt{\frac{4A}{\pi}}$$
$\dot{Q}^*$	Fire Froude number	-	A typical accidental fire has a Froude number of order 1. Momentum-driven fire plumes, like jet flares, have relatively high values. Buoyancy-driven fire plumes have relatively low values.

2. Flame length ratio

The flame length ratio is a measure of the flame height relative to the upper horizontal boundary (ceiling). Variables used to calculate this ratio are given in Table 3.

Table 3. Variables to calculate flame length ratio.

Symbol	Name	Unit	Notes
H_f	Base elevation of fire	m	
H_c	Enclosure height	m	
A	Fire area	m²	
D	Fire diameter	m	$$D = \sqrt{\frac{4A}{\pi}}$$
$\dot{Q}^*$	Fire Froude number	-	
L_f	Flame height	m	$$L_f = \left(3.7\, \dot{Q}^{*\frac{2}{5}} - 1.02\right) D$$
-	Flame length ratio	-	$$\frac{H_f + L_f}{H_c}$$

3. Ceiling jet distance ratio

The ceiling jet distance ratio is a measure of the ceiling jet position at which data is sought relative to the enclosure height and is applicable primarily when the temperature and velocity of the ceiling jet are quantities of interest. A low ceiling jet distance ratio indicates that the position is within the impingement zone, and the conditions would be dominated by the thermal plume. A high ceiling jet position ratio suggests that the position is approaching the edge of the ceiling jet, at least as idealized by algebraic correlations. A high ceiling jet ratio also suggests that a considerable portion of the ceiling would need to be free of obstructions in order to conform to the underlying approximations of the ceiling jet models. The variables to calculate this ratio are given in Table 4.

Table 4. Variables to calculate ceiling jet ratio.

Symbol	Name	Unit	Notes
H_f	Base elevation of fire	m	
H_c	Enclosure height	m	
r_{cj}	Target's horizontal distance from fire centerline	m	
-	Ceiling jet ratio	-	$\dfrac{r_{cj}}{H_c - H_f}$

4. Equivalence ratio

This quantity is the ratio of the generation rate of fuel to the supply rate of oxygen. When the equivalence ratio is equal to one, the exact amount of oxygen required for complete combustion is available. The variables to calculate this ratio are given in Table 5.

Table 5. Variables to calculate equivalence ratio.

Symbol	Name	Unit	Notes
ΔH_{O_2}	Heat of combustion for oxygen	kJ / kg	Typically taken to be 13,100 kJ/kg, an average value over a wide range of common fuels. A notable exception to this convention is hydrogen, whose heat of combustion based on oxygen consumption is approximately 18,000 kJ/kg.
-	Sill	m	Height of the bottom of the opening relative to the floor of the first compartment
-	Soffit	m	Height of the top of the opening relative to the floor of the first compartment
-	Width	m	The width of the opening
A_0	Effective area of the openings	m²	$A_0 = \sum_{i=1}^{n} A_i$
H_0	Effective height of the openings	m	$H_0 = \dfrac{\sum_{i=1}^{n} H_i A_i}{\sum_{i=1}^{n} A_i}$
$\dot{V}$	Volumetric flow rate of air into the enclosure	m³/s	Sum of air flow rate from mechanical vents only
$\dot{m}_{O_2}$	Mass flow rate of oxygen into the enclosure	kg/s	Separate calculations for natural and mechanical vents: $$\dot{m}_{O_2} = \begin{cases} 0.23 \times \frac{1}{2} A_0 \sqrt{H_0} & \text{(Natural)} \\ 0.23\, \rho_\infty \dot{V} & \text{(Mechanical)} \end{cases}$$ In many compartments, both natural and forced ventilation is present. The

Symbol	Name	Unit	Notes
			recommended procedure to follow in this case is to select the dominant ventilation mode (i.e., the mode that produces the highest mass flow of oxygen). If the two modes are comparable, the oxygen masses may be added.
φ	Equivalence ratio	-	$$\varphi = \frac{\dot{Q}}{\Delta H_{O_2}\dot{m}_{O_2}}$$

5. Compartment aspect ratio

    The compartment aspect ratio is a measure of the deviation of the enclosure dimensions from a cube. It is calculated by comparing the length or width to the height of the compartment.

6. Radial distance ratio

    This ratio is the relative distance from a target to the fire. It is important when calculating the radiative heat flux. The ratio is calculated as the distance between the target and the center of the fire base divided by the fire diameter.

2.1 Verification Checks

A test function was written for the CFAST V&V module of FRI3D. The test function uses a model with a large fire within an elongated compartment having a small natural ventilation and a target located at the far end of the compartment, as shown in Figure 4. The compartment measures 10 meters long, 1 meter wide, and 0.6 meters high. The fire heat release rate (HRR) and area are given in Figure 5. The natural ventilation measures 20 cm x 5 cm. The model is expected to fail all the V&V criteria of dimensional ratios and the Froude number criteria, due to the large fire area and diameter.
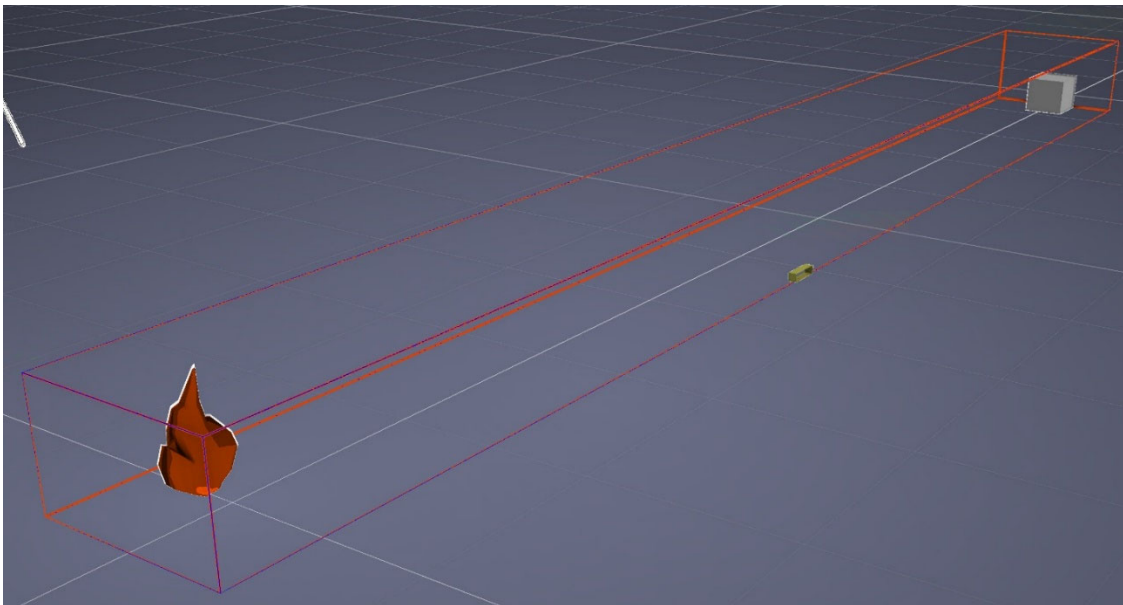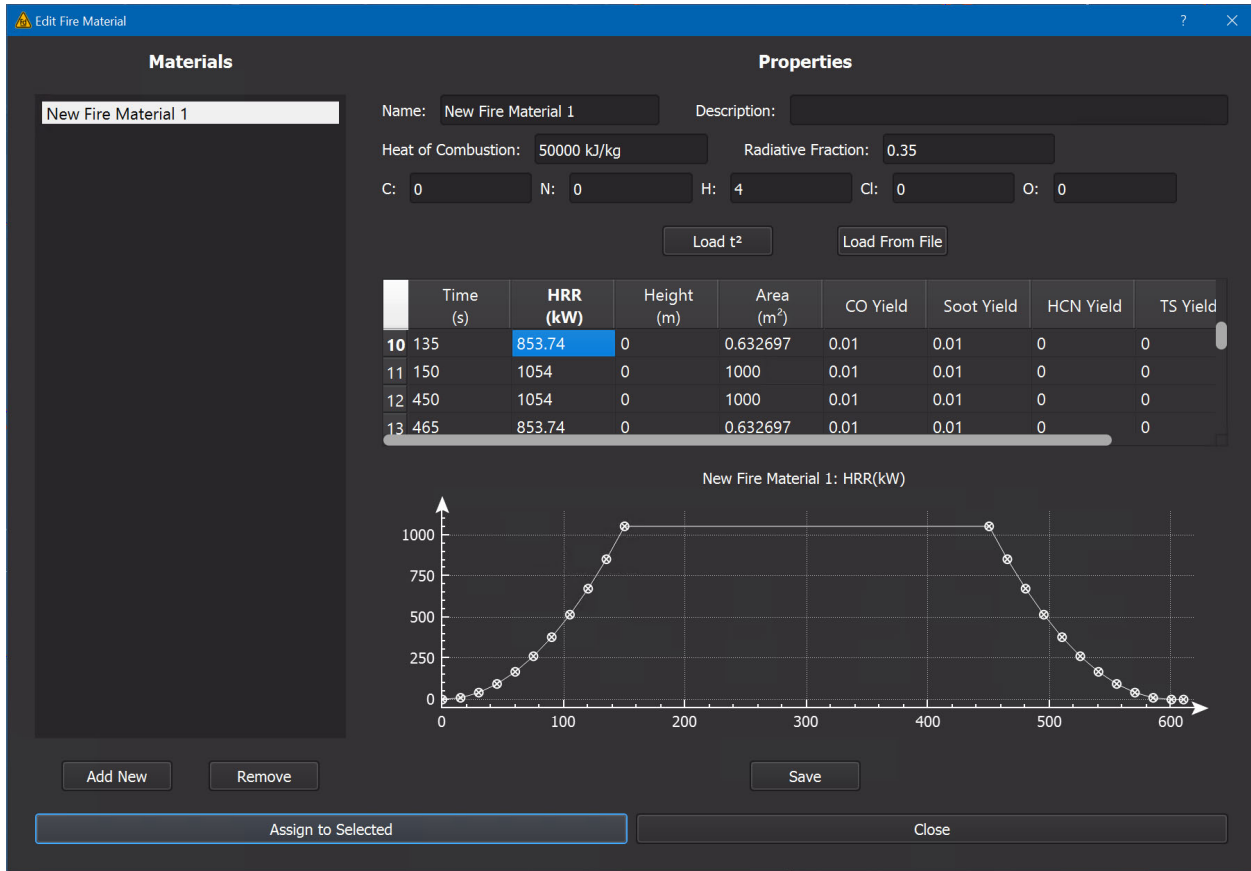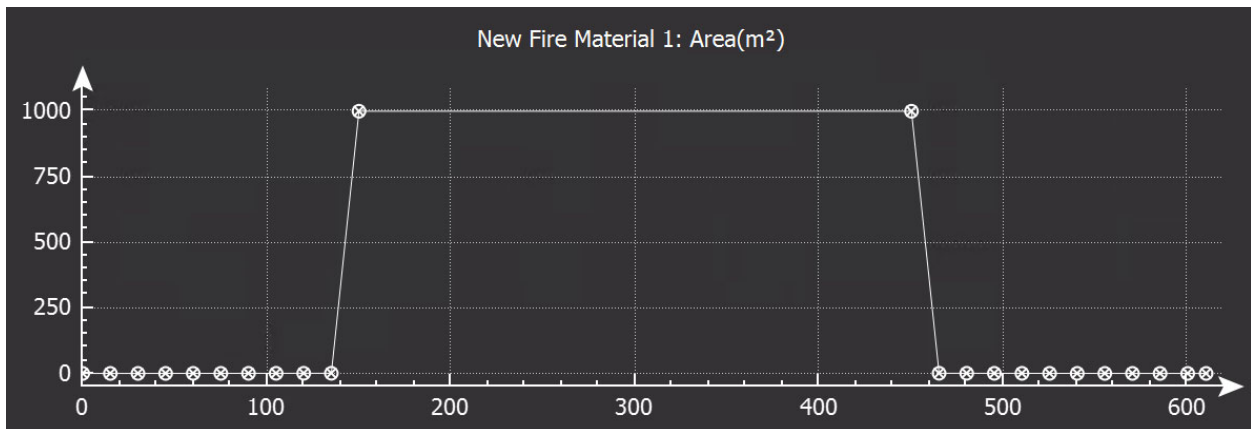

Figure 4. CFAST verificaton test model.

(a) Fire heat release rate

(b) Fire area

Figure 5. Fire parameters.

Results of the V&V process as calculated by FRI3D are compared with manual calculation results as shown in Table 6. As hypothesized, the model fails all the V&V normalized parameter criteria. FRI3D calculation results match the manual calculations.

Table 6. CFAST V&V results.

Quantity	Known parameters	Manual calculations	FRI3D calculations	V&V result
Froude number	$\dot{Q} = 1054$ $T_\infty = 293.15$ $c_p = 1.012$ $A = 1000$ $g = 9.81$	$\rho_\infty = 1.20075$ $D = 35.68$ $\dot{Q}^* = 1.24E - 4$	$\rho_\infty = 1.20075$ $D = 35.68$ $\dot{Q}^* = 1.24E - 4$	$\dot{Q}^* < 0.2$ Fire is spread over a large area and is therefore too weak.
Flame length ratio	$H_f = 0.248$ $H_c = 0.6$ $A = 1000$	$D = 35.68$ $\dot{Q}^* = 1.24E - 4$ $L_f = -32.78$ Ratio = -54.22	$D = 35.68$ $\dot{Q}^* = 1.24E - 4$ $L_f = -32.78$ Ratio = -54.22	Ratio < 0.0 Negative length ratio indicates an inexistent fire.
Ceiling jet distance ratio	$H_f = 0.248$ $H_c = 0.6$ $r_{cj} = 9.13$	Ratio = 25.96	Ratio = 25.96	Ratio > 8.3 The position is too close to the edge of the ceiling jet.
Equivalence ratio	$\dot{Q} = 1054$ $\Delta H_{O_2} = 13100$ Sill = 0 Soffit = 0.05 Width = 0.2	$A_0 = 0.01$ $H_0 = 0.05$ $\rho_\infty = 1.20075$ $\dot{V} = 0$ $\varphi = 312.8862$	$A_0 = 0.01$ $H_0 = 0.05$ $\rho_\infty = 1.20075$ $\dot{V} = 0$ $\varphi = 312.8862$	Ratio > 0.6 Fire is underventilated.
Compartment aspect ratio	$L = 10$ $W = 1$ $H_c = 0.6$	Ratio = 16.66	Ratio = 16.66	Ratio > 8.3 Compartment deviates from a cube.
Radial distance ratio	$r = 9.128$ $A = 1000$	$D = 35.68$ Ratio = 0.256	$D = 35.68$ Ratio = 0.256	Ratio < 0.3 Target is too close to fire due to the large fire radius.

When the CFAST model is built, each conditions described above is verified against the acceptable ratios. Any result outside the accepted level is saved in FRI3D's database as an issue. The example case violates each issue and has been added as a unit test in FRI3D's testing architecture.

2.2   User Interface

When running a simulation if any CFAST modeling issues are found using the validation checks, these issues are displayed to the user as shown in Figure 6. The issue descriptions provide information for the user to easily identify what is wrong with model so they can easily make adjustments to correct it or select a different fire simulation tool that may be able to handle the compartment characteristics. After selecting continue, the user can choose to make modifications and re-run the scenario simulation or keep the scenario; however, a justification should be provided as to why this scenario is still valid. Future work will provide an option for the user to attach a note to the issue for justifying why the scenario could still be acceptable.
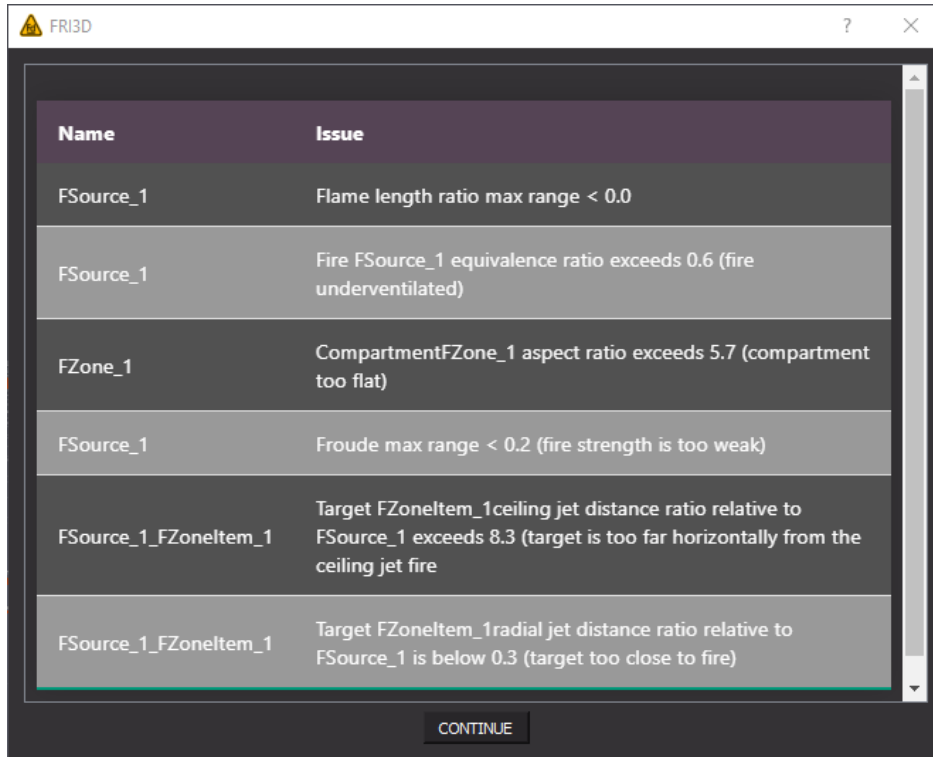
Figure 6. User interface displaying CFAST modeling issues.

3. FDS INTEGRATION

FRI3D needs a fire simulation tool that estimates the fire progression and calculates the temperature of items in the compartment over time. CFAST was used initially since it was used in more industry scenarios and is faster. However, CFAST is a two-layer heat model and has several limitations, some of which are described in Section 2. To enable the evaluation of more advanced fire configurations a full CFD capability is needed. This section reviews FDS features and how they were integrated into FRI3D to generate and evaluate fire scenarios.

3.1 FDS Background

FDS is a CFD model of fire-driven fluid flow. The FDS software solves numerically a form of the Navier-Stokes equations appropriate for low-speed, thermally driven flow with an emphasis on smoke and heat transport from fires [15]. FDS is available for free on the NIST homepage. The software was first publicly released in February 2000 and has been under active development and improvements ever since. About half of the applications of FDS have been for design of smoke handling systems and sprinkler/detector activation studies. The other half consists of residential and industrial fire reconstructions.

The basic features of FDS are the following:

1. Hydrodynamic model

    FDS uses numerical methods to solve the Navier-Stokes partial differential equations. The numerical algorithm is an explicit predictor-corrector scheme.

2. Combustion model

    FDS uses three lumped species (i.e., air, fuel, and products) to model the chemical reaction of combustion. The fuel and products lumped species are explicitly computed.

3. Radiation transport

   FDS uses the finite volume method to solve the radiation transport equation for a gray gas.

4. Geometry

   FDS approximates the governing equations on a rectilinear mesh. Rectangular obstructions are forced to conform with the underlying mesh.

5. Multiple meshes

   It is possible to prescribe more than one rectangular mesh to handle cases where the computational domain is not easily embedded within a single mesh.

6. Parallel processing

   FDS uses an OpenMP module to leverage parallel processing capabilities found in modern computers. It helps to speed up the analysis, given that CFD computations are usually time-consuming. FDS also has the message parsing interface capability to use a cluster of computers.

7. Boundary conditions

   All solid surfaces are assigned thermal boundary conditions, plus information about the burning behavior of the material. Heat and mass transfer to and from solid surfaces is usually handled with empirical correlations.

An FDS model is set up through a text input file. FRI3D translates the FRI3D model to a corresponding FDS input file. An FDS simulation produces comma-separated and binary output files. The binary output files are used by another program named Smokeview to visualize the fire, temperature, and combustion products like soot. A sample screenshot of Smokeview's visual of an FDS simulation is shown in Figure 7.
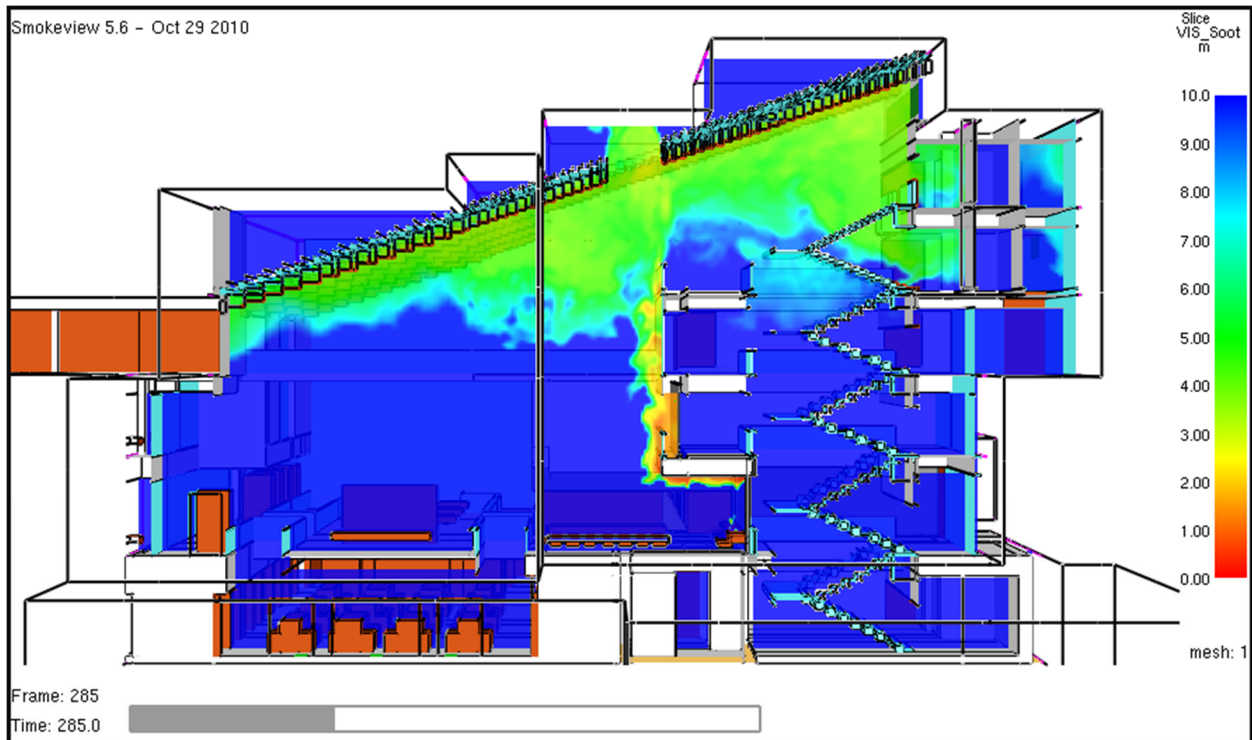

Figure 7. Sample Smokeview visualization.

3.2 User Interface Options

When the user selects a source to generate a new scenario, they have the option to now use CFAST or FDS. The general options such as simulation time, interior and exterior conditions, etc. for performing a fire simulation in both CFAST and FDS are the same and use the same user options as shown in Figure 8. If FDS is selected, then CFAST specific properties are disabled. Currently there are no FDS specific global parameters, there is however a mesh size that is specific to different areas of the model. Currently, a default value is used for the grid size in areas. More research needs to be done to determine a simple method for estimating good settings for grid size depending on fire conditions, see Section 4.
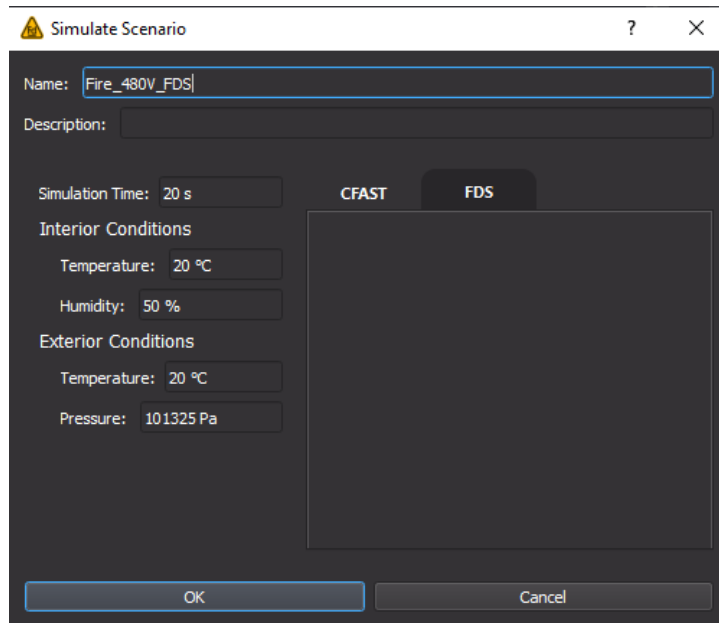

Figure 8. Common user interface options when simulating a scenario.

3.3 FDS Model Generation

The FRI3D backend was designed with the intent of having the ability to use multiple fire simulation tools. All of the code needed to construct and simulate a scenario in CFAST was put into its own project and various class structures. To create the option for FDS, a new but similar project was added to the FRI3D source code.

FDS is a full 3D CFD-based model. Since FRI3D supports both CFAST and FDS with the same model done in FRI3D, there are some limitations for the FDS models. FDS requires a full 3D representation of all boundaries and all equipment/cables/raceways in the compartment to be simulated. The FDS output can be divided into several sections or primitives. The FDS primitives and their corresponding implementation details are listed as subsections in the following section.

3.3.1 FDS Primitives

All the necessary information to perform an FDS simulation has to be contained in a single text file. Information in the input file can be found in the *FDS User Guide* [10]; the following subsections go over the main items and the properties used from FRI3D. The input file is saved with a name such as `mycase.fds`, and there should be no blank spaces in the job name.

Data is specified within the input file by using "groups." Each group record occupies a line of text and begins with the `&` character. The `&` must be first character of the line of text and should be followed

by the name of the group. Then a comma-delimited list of the input parameters is inserted. Finally, a forward slash / character closes the group, as shown in the Figure 9.
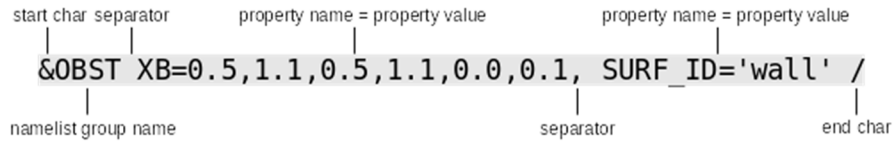

Figure 9. FDS group record format.

3.3.1.1   MESH

The computational boundary is represented by the MESH directive. The computational boundaries and its corresponding resolution are specified in this directive. In this step, domain of the simulation is set up. This is done by creating a mesh (MESH). The domain in this example is represented by a single mesh, which is specified by its coordinates XB = X1,X2, Y1,Y2, Z1,Z2, see and by the number of cells in each direction IJK = nx, ny, nz. Here, we choose the following values. Figure 10 represents the domain setup.
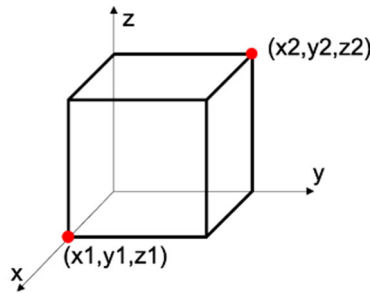
Figure 10. Computational domain.

The extent of the simulation's domain is determined automatically based on the 3D model, and resolution of the domain is specified by the user. Each boundary in FRI3D can have its own resolution specified in their properties. Currently, they are fixed to a resolution of 32x32x32. However, a future implementation would have its resolution specific to a compartment boundary primitive in FRI3D.

Backend Directive Generation

The FRI3D backend reads the 3D information provided by the front end with regards to the bounds of the simulation and generates directives like the following:

```
&MESH XB=0,2,0,4,0,2.5, IJK=32,32,32/
```

3.3.1.2   TIME

The FRI3D interface has a timeline which is updated from the user interface of FRI3D as indicated in Figure 8. This is used in the time perimeter for FDS.

Backend Directive Generation

The time for simulation is generated in seconds by the following directive:

```
&TIME T_END=20 /
```

3.3.1.3 INIT

The initial ambient temperature setting in FRI3D is specified by the user using the interface as indicated in Figure 8.

Backend Directive Generation

The initial ambient temperature for simulation is generated in seconds by the following directive:

```
&INIT TEMPERATURE=20 /
```

3.3.2 Global Outputs

FDS has various types of output files that store computed data. Some of the files are in binary format and intended to be read and rendered by Smokeview. Some of the files are just comma-delimited text files. FRI3D generates directives to generate PLOT3D files. PLOT3D files are a pair of files, generated one per time step output interval specified. The "q" files contain the value of the quantity output, and "xyz" files contain the domain. These files can be used for visualization by the frontend FRI3D application.

3.3.2.1 DUMP

The dump directive specifies an output of 3D visualization data including vector field velocities and temperature output of 1D data.

There are future plans to support multiple output options which can be used by FDS, but currently, the temperature and velocities with heat per unit volume are output and used for FRI3D calculation, see Section 3.4. The interval for writing these files are currently defaulted to each output per second.

Backend Directive

These are the generation of DT_PLT3D directives as part of DUMP command:

```
&DUMP
  STATUS_FILES=T, DT_PL3D=1.0,
  PLOT3D_QUANTITY(1:5)='TEMPERATURE',
    'U-VELOCITY','V-VELOCITY','W-VELOCITY',
    'HRRPUV', WRITE_XYZ=.TRUE. /
```

3.3.3 Geometry

In FDS, a volume is always represented by a single right parallelepiped with edges parallel to the axis. Its position and dimensions are described by the coordinates of two opposite vertices; if point A=(x_A, y_A, z_A) and point B=(x_B, y_B, z_B) are the opposite vertices, its coordinates are entered as `$x_A$, $x_B$, $y_A$, $y_B$, $z_A$, $z_B$`, for example,

```
&OBST XB=0.5,1.5,2.0,3.5,-2.0,0., SURF_ID='wall' /
```

uses the parameter `XB` to define a solid obstacle that spans the volume starting at the origin (0.5, 2.0, -2.0) and extending 1 m in the positive x direction, 1.5 m in the positive y direction, and 2 m in the positive z direction. Conversion methods described below are used to translate 3D geometry in FRI3D into FDS volumes.

3.3.3.1 OBST – Boundaries and Walls

A FRI3D model consists of items contained inside a compartment, made up of boundaries as shown in Figure 11 and Figure 12. The front end decomposes the boundary elements in FRI3D to set of obstacle elements for FDS. A set of computational geometry operations are done to consolidate all the boundary

meshes, and then a determination is made from the outer boundaries based on orientation to indicate the outer walls/ceiling and floor. They are then saved as part of the model and used to generate the FDS elements.

The following images consolidate this approach.
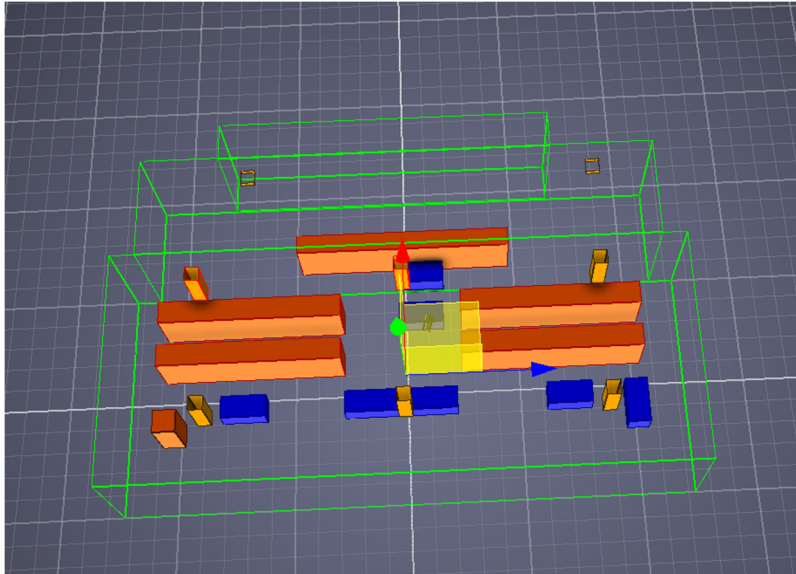
Figure 11. NUREG 1934 switch gear room example in FRI3D.
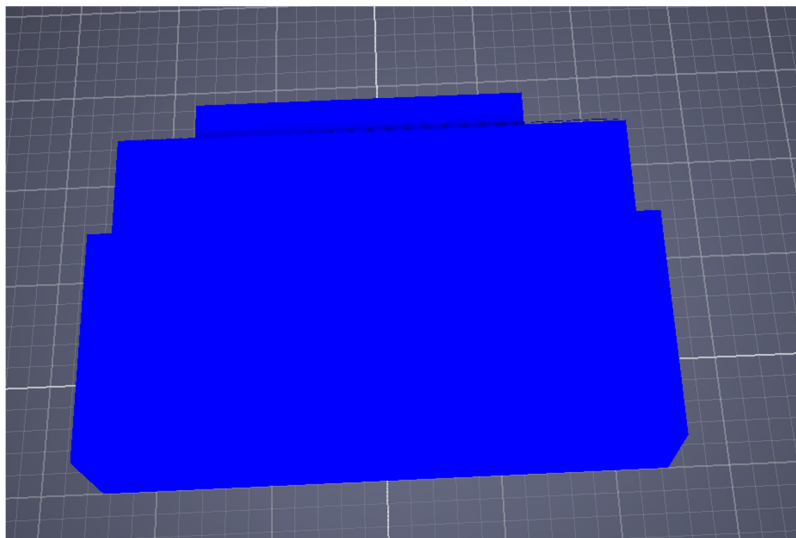
Figure 12. Bounding boxes created from the example in Figure 11.

The backend code contains lists of axis-aligned bounding boxes and generates appropriate OBST calls. The wall thickness is specified as part of the material properties of the walls.

Backend Directive

For the example in Figure 11 and Figure 12, NUREG 1934 Switch Gear Room, the following directives are generated for the walls, ceiling, and floor:

16

```
OBST ID= 'MCR_Walls_0'
   XB=10.562313079834,11.2580003738403,9.5,9.61796951293945,5.139062404
63257,5.19999980926514 SURF_ID='Wall_SURF' /
&OBST ID= 'MCR_Walls_1'
   XB=-
7.8725061416626,10.5703134536743,9.49199962615967,9.62596988677979,5.0
9999990463257,5.15937471389771 SURF_ID='Wall_SURF' /
&OBST ID= 'MCR_Walls_2'

…
&OBST ID= 'MCR_Ceiling_0'
   XB=-7.8725061416626,6.72749423980713,9.5,11.2000007629395,-
0.150000095367432,0.349999904632568 SURF_ID='ConcreteCeiling_SURF' /
&OBST ID= 'MCR_Ceiling_1'
   XB=-11.25,11.25,5,9.5,-0.25,0.25 SURF_ID='ConcreteCeiling_SURF' /
&OBST ID= 'MCR_Ceiling_2'
   XB=-12.3000001907349,12.3000001907349,-5,5,-0.25,0.25
SURF_ID='ConcreteCeiling_SURF' /
&OBST ID= 'MCR_Floor_0'
   XB=-
7.8725061416626,6.72749423980713,9.5,11.2000007629395,4.84999990463257
,5.34999990463257 SURF_ID='ConcreteFloor_SURF' /
&OBST ID= 'MCR_Floor_1'
   XB=-11.25,11.25,5,9.5,4.94999980926514,5.44999980926514
SURF_ID='ConcreteFloor_SURF' /
&OBST ID= 'MCR_Floor_2'
   XB=-12.3000001907349,12.3000001907349,-
5,5,4.94999980926514,5.44999980926514 SURF_ID='ConcreteFloor_SURF' /
```

3.3.3.2   *OBST – Equipment, Raceways, Etc.*

Each piece of equipment, raceway, or other item in FRI3D to be included in the fire simulation has the geometry in the form of cuboids. The 3D attributes are used to generate the appropriate calls to the FDS model. Currently even if the equipment have a complex shape, just their axis aligned bounding box are used to generate the FDS directive. However, presently under progress, there is an implementation which decomposes the complex shape into a number of boxes. This will result in more accurate simulations by representing the complex shape closer to the original model.

Backend Directive

The FDS directive for the equipment raceways and other similar items in FRI3D is the same as for the OBST for walls described in the previous section.

3.3.3.3   *VENT/HOLE – Passive Vents/Doors/Windows*

Doors and windows are modeled as passive vents in FRI3D with a size and location on a wall, ceiling, or floor. In FDS, they can be modeled using VENTS or HOLES. The room in Figure 13 has one door in the back; this needs to be modeled as an opening. The VENT command can be used to model openings; XB specifies the coordinates of the opening. This process will be used for vents leading to the exterior.

Backend Directive

The backend directive is:

```
&VENT XB=0.5,1.5,4,4,0,2, SURF_ID='OPEN'/
```

The geometry for this example is shown in the following figure.
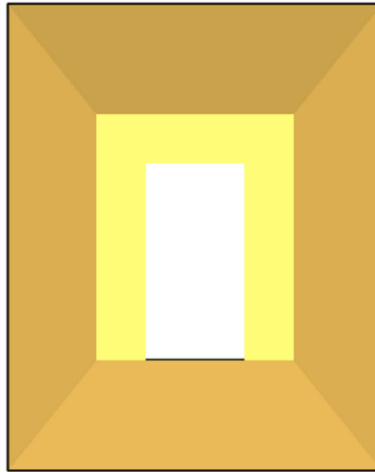
Figure 13. Example room with a door.

However, there is also the option to make the holes as part of the boundaries and is needed for doors between areas in the same compartment. The FRI3D interface could consolidate all vents with the boundaries as single exteriors. This design option and its effects on the overall model are being researched, and implementation is currently in progress, see Section 4.

3.3.4   Materials, Layers, and Sources (MATL/SURF)

FRI3D has a material properties list for things such as brick, gypsum, and concrete walls or metal properties for conduits, cabinets, or raceways. Figure 14 shows the form for editing and assigning a material to a model item.

Figure 14. FRI3D material list editing and selection form.

Backend Directive

The properties of each material used in the model are designated via the MATL name list group. These properties indicate how rapidly the materials heat up, and how they burn. Each MATL entry in the input file must have an ID that can be referred by other name list group. The MATL name list group can be used to specify thermal CONDUCTIVI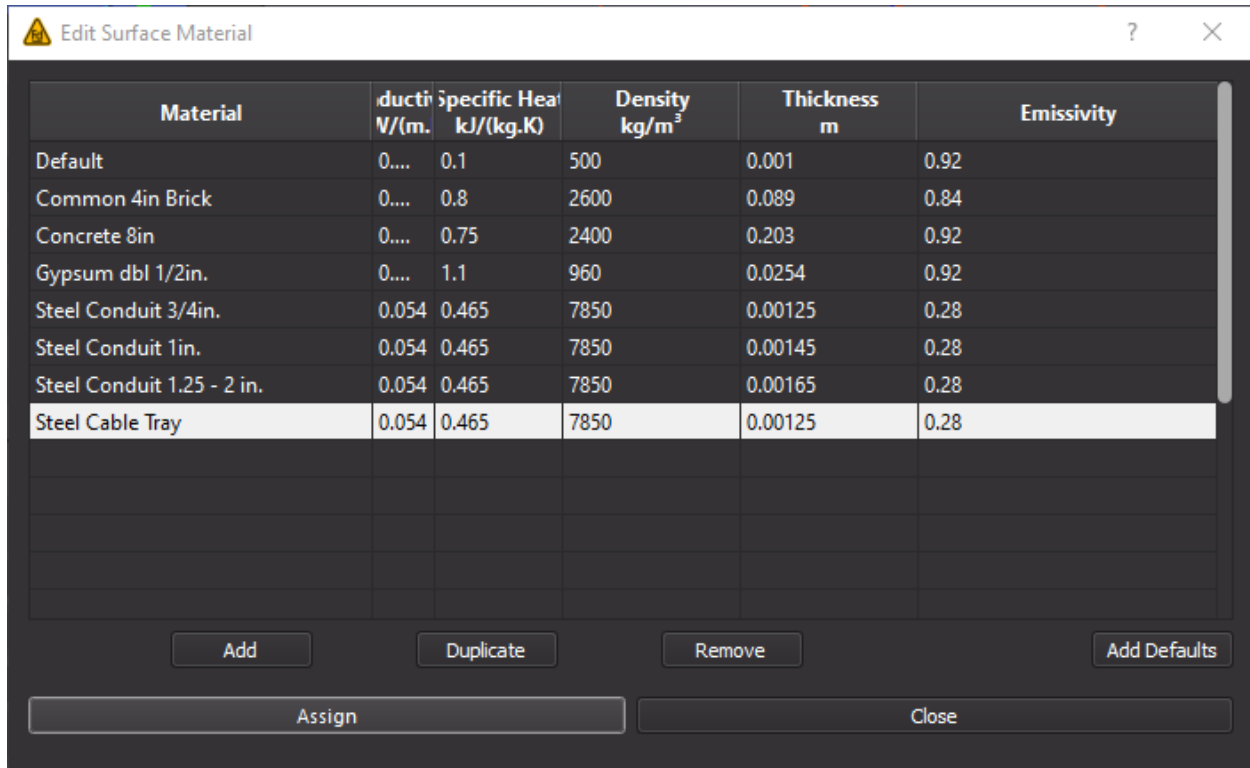TY (W m^{-1} K^{-1}), DENSITY (kg m^{-3}), SPECIFIC_HEAT (kJ kg^{-1} K^{-1}), and EMISSIVITY (0.9 by default) of materials, for example:

```
&MATL ID='steel', EMISSIVITY=.95, DENSITY=7850.,
    CONDUCTIVITY=45.8, SPECIFIC_HEAT=0.46, /
&MATL ID='concrete', DENSITY=2200.,
    CONDUCTIVITY=1.2, SPECIFIC_HEAT=0.88, /
&MATL ID='copper', SPECIFIC_HEAT=0.38,
    CONDUCTIVITY=387., DENSITY=8940. /
&MATL ID='gypsum plaster', CONDUCTIVITY=0.48,
    SPECIFIC_HEAT=0.84, DENSITY=1440. /
```

In CFAST, each object/obstacle is specified by one material line. However, in FDS, this is done in two parts. The first one specifies the material properties (MATL), and the second one specifies the surface or boundary properties (SURF). The thermal and burning properties of each material are specified via the MATL group. Then materials are invoked by the SURF group to define boundary conditions for solids.

The following is an example of a multi-layer, multi-component surface. First, materials are defined, then a boundary condition brick wall is prescribed:

19

```
&MATL ID='water', CONDUCTIVITY=0.60, SPECIFIC_HEAT=4.19,
    DENSITY=1000. / material
&MATL ID='brick', CONDUCTIVITY=0.69, SPECIFIC_HEAT=0.84,
    DENSITY=1600. / material
&MATL ID='insulator', CONDUCTIVITY=0.041, SPECIFIC_HEAT=2.09,
    DENSITY=229. / material
&SURF ID='brick wall', MATL_ID(1,1:2)='brick','water',
    MATL_MASS_FRACTION(1,1:2) = 0.95,0.05,
    MATL_ID(2,1)='insulator',
    THICKNESS(1:2)=0.1,0.2 / boundary condition
```

In FRI3D, the material and surface properties are both prescribed at once. Internal heat sources are not supported currently, and solid heat transfer to the internal points are implicit. Ignition temperature and secondary sources will be handled in a future version, see Section 4.

3.3.5 Fires & Fire Material Specifications

FRI3D has fire sources with an assigned fire material. The fire source has the spatial information, and the fire material defines properties such as the HRR as shown in Figure 15. A fire material can be assigned to multiple fire sources. These properties are used to assign fires and fire material specifications in FDS.
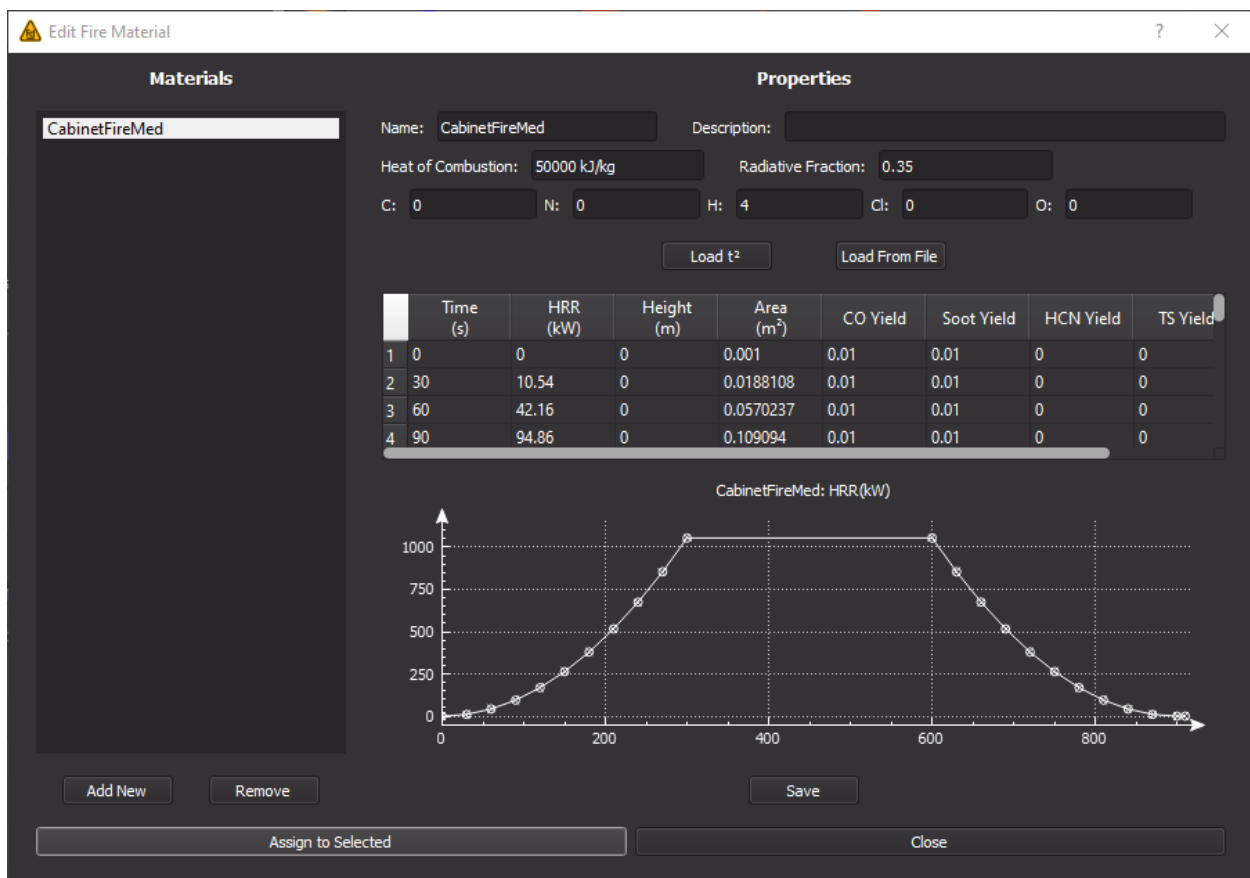

Figure 15. FRI3D form for adding, editing, and assigning fire materials to fire sources.

Backend Directive

This is done in two parts. First the fuel needs to be defined. A list with pre-defined fuels in FDS can be found in the FDS user manual.

```
&REAC FUEL = 'PROPANE' /
```
Next, the object that is burning needs to be defined. This will be done by specifying an obstacle directive to FDS, for example:

```
&OBST XB = 0.5,1.5,1.5,2.5,0,0.5, SURF_ID = 'Fire'/
```

- XB specifies the coordinates of the burning obstacle
- SURF_ID specifies which boundary conditions should be added to the surface. The input file needs to contain a line which specifies this boundary conditions. If not all surface of the obstacle have the same properties, several surface ideas can be defined.

In this example the fire is described by fixing the HRR of the obstacle. In the example, the HRR will be fixed to 600 kW/m^2:

```
&SURF ID = 'Fire', HRRPUA = 600/
```

NUREG 2232 details a list of fire heat release curves that could be used, and currently, this is a manual process of specifying the fire properties. However, a future implementation is planned where this is loaded from established databases detailing the specific kind of fire.

For a time varying HRR, if something other than a t^2 ramp up is desired, then a user-defined function must be input. To do this, a RAMP_Q, RAMP_T, RAMP_V or RAMP_MF(n) equal to a character string designating the ramp function to use for that particular surface type is set, then somewhere in the input file generates lines of the form:

```
&RAMP ID='MotorHRR_HRR_RAMP', T=0, F=0 /&RAMP ID='MotorHRR_HRR_RAMP',
T=1100, F=0.206552706552707 /
&RAMP ID='MotorHRR_HRR_RAMP', T=3100, F=0.206552706552707 /
&RAMP ID='MotorHRR_HRR_RAMP', T=3400, F=0 /
&SURF ID='MotorHRR', HRRPUA=702, RAMP_Q='MotorHRR_HRR_RAMP',
COLOR='RED'

&REAC FUEL='MotorHRR_FUEL'
   FORMULA='C1H4O0N0'
   HEAT_OF_COMBUSTION=50000
   RADIATIVE_FRACTION=0.349999994039536 /
```

3.3.6 Vents – Powered Vents

Powered vents in FRI3D are physically modeled the same as other vents; however, they have information such as air flow rate and the ability to ramp up or shut of air flow at different time points. Powered vents are currently not implemented, but that work is in progress.

Backend Directive - Supply Vent

The backend directive for the supply vent is:

```
&VENT XB=0,0,1,3,0.2,0.6, SURF_ID='supply'/
```

```
&SURF ID='supply', VOLUME_FLOW= -1, COLOR='GREEN' /
```

Backend Directive - Exhaust Vent

The backend directive for the supply vent is:

```
&VENT XB=3,3,1.5,2.5,2.6,3, SURF_ID='exhaust'/
&SURF ID='exhaust', VOLUME_FLOW=1, COLOR='BLUE' /
```

3.3.7   Cables

In FRI3D, cables are part of the logic structure, defining what cables are in which raceways. Raceways are modeled in the 3D area, but cables are not. Cable failure is determined using the heat soak or THIEF methods implemented directly in FRI3D. FDS has the option to add cables to the input as described below, but to be consistent and simplify the FDS generation, the FRI3D methods are used instead, as described in Section 3.4.

Backend Directive

In FDS, cables and raceways are considered very similar to obstacles and equipment. However, there are some additional details that have to be considered. The backend generation results in directives similar to the following:

```
&INIT ID='Cable', XB=0.01,0.01,0.,0.,0.,0., N_PARTICLES=1,
PART_ID='Cable Segment' /
&DEVC ID='Cable Temp', INIT_ID='Cable', QUANTITY='INSIDE WALL
TEMPERATURE', DEPTH=0.0015 /
&MATL ID='plastic', DENSITY=2535., CONDUCTIVITY=0.2, SPECIFIC_HEAT=1.5
/
&SURF ID='cylinder', THICKNESS=0.00815, LENGTH=0.1, MATL_ID='plastic',
GEOMETRY='CYLINDRICAL' / &PART ID='Cable Segment', SURF_ID='cylinder',
ORIENTATION=0,0,1,
STATIC=T /
&INIT ID='Cable', XB=0.01,0.01,0.,0.,0.,0., N_PARTICLES=1,
PART_ID='Cable Segment' /
&DEVC ID='Cable Temp', INIT_ID='Cable',
QUANTITY='INSIDE WALL TEMPERATURE', DEPTH=0.0015 /
```

The THIEF model assumes that the cable plastic material has a thermal conductivity of 0.2 W/(m K) and a specific heat of 1.5 kJ/(kg K). If the user changes these values, they are no longer using the THIEF model. The density is the mass per unit length of the cable divided by its cross sectional area. The THICKNESS is the radius of the cylindrical cable in units of meters (m). The LENGTH, in m, is needed by FDS because it assumes that the cable is a cylindrical segment of a certain length. It has no impact on the simulation, and its value is typically the size of a grid cell. The ORIENTATION tells FDS the direction of the prevailing radiative source. STATIC=T prevents the cable from moving. The INIT line is used to position the cable within the computational domain. The device (DEVC) line records the cables inner temperature, in this case 1.5 mm below the surface. This is typically the jacket thickness.

In the front end, the material assignment/cable assignment and option whether to use FRI3D THIEF Model or FDS THIEF model would be specified. The implementation is currently under progress.

3.3.8   DEVC – Targets

To determine failures and generate scenarios in FRI3D, temperatures over time are used. To obtain these results from the FDS fire simulation, targets are used. For each FRI3D fire susceptible item modeled

in the 3D space, in CFAST, a target is generated at the closest location to the fire source with the face oriented directly toward the fire. In FDS, just the closest location for the target is specified.

FRI3D allows the modeling of devices such as smoke detectors and sprinklers that would be modeled as DEVC items in FDS. However, these are not to be used as part of the scenario calculation because the results of detectors and sprinklers are included in the non-suppression probability. Users should only include these features to understand and help make those calculations.

Backend Directive

Devices in FDS are used to include thermocouples, sprinklers, etc. in the simulation. Every device gets several properties assigned. Every device needs to be assigned a point or a span of the computational domain. This is specified by the coordinates XYZ. Every device gets an ID. This is a label to identify the device in the output files. A device can have a specified QUANTITY, which tells FDS what should be recorded. Each device has a quantity associated with it. The time history of each quantity is output to a comma-delimited ASCII file called CHID_devc.csv.

In the front end, the dimensions of the equipment are sent to the backend. In the backend, for each equipment, the closest point to the closest fire along all the equipment's edges is generated as a device probe by the DEVC directive. Currently, only temperature is probed; however, future versions will support more probes. The following is an example of such an output generated by FRI3D.

```
&DEVC ID = 'Air Temperature', XYZ = 1,2,1.5, QUANTITY = 'TEMPERATURE' /
```

With this line, FDS will record the temperature at the point x=1,y=2,z=1.5.

3.3.9   Visualization of Failures and FDS Results

When a simulation completes just like CFAST simulations, the equipment which has failed is highlighted as we move along the timeline in the interface. The failed equipment is returned to the frontend application by the backend.

In the current version of FRI3D, CFAST heat layer results and component temperature over time are shown; this can also be done with FDS results but has not been implemented yet.

3.4   FDS Result Integration

After FDS simulation, FRI3D reads the comma-separated temperature or flux values found in the devc.csv file. This file stores the historical temperature or flux values of the devices declared in the FDS input file. FRI3D uses this data to estimate the failures of raceways and cables. The flow process is as follows:

1. Generate the FDS input file

2. Run FDS

3. Read the FDS output file to estimate component failures

4. Calculate timing of raceway failures using the heat soak method

5. Calculate failure timing of cables inside the failed raceway using the THIEF method, without calculating the heat conduction through the raceway conduit because FDS returns the temperature values at the center of each device instead of at the surface

6. Set the cable's failure time as the shortest time between raceway failure and calculated cable failure

7. Return a list of damaged raceways and cables.

A FRI3D model as shown in Figure 16 was built to test this integration methodology. A single fire occurred within an electronic room of several electrical cabinets and cable raceways running on top of the room. The fire source was set with a constant HRR with a higher heat of combustion than typical cable fires as shown in Figure 17, in order to investigate component failures. The simulation was run with an ambient temperature of 20°C for 90 seconds.
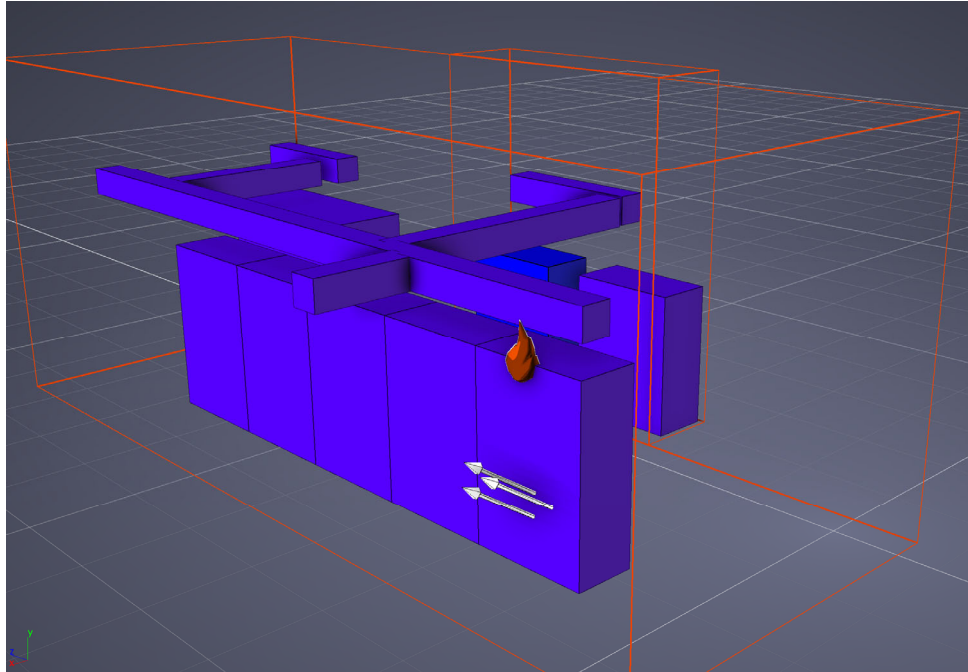
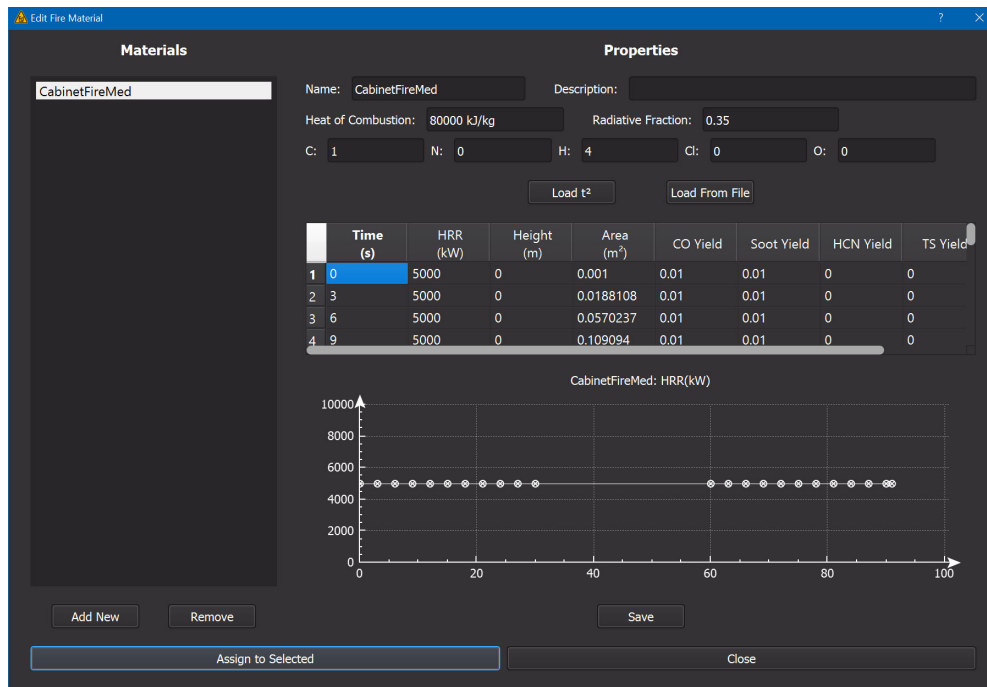

Figure 16. FRI3D test model.

Figure 17. FRI3D fire parameters.

After FDS completed its simulation, it generates a detailed output file and Smokeview file. The Smokeview visualization of the FDS result at the end of simulation (t=90 s) is shown in Figure 18. It shows a high variation of temperature inside the room, which was expected due to the high heat of combustion from the fire. It is also hypothesized that the cabinets and raceway next to the fire will experience failures. The temperature data of the devices in the simulation are plotted in Figure 19. It shows two components experiencing high temperatures: A1 and SIS.

FRI3D returns the failures of raceways and cables inside the raceways as listed in Table 7. As expected, the A1 raceway above the fire source, and the SIS cabinet next to the fire source experienced failures.
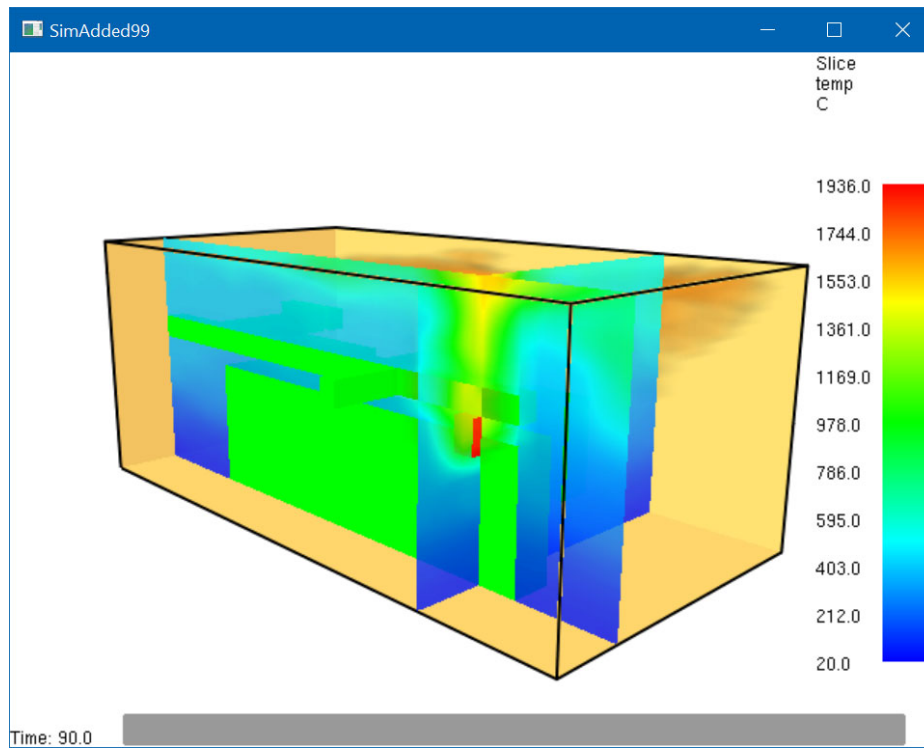
Figure 18. Smokeview visualization of FDS results.
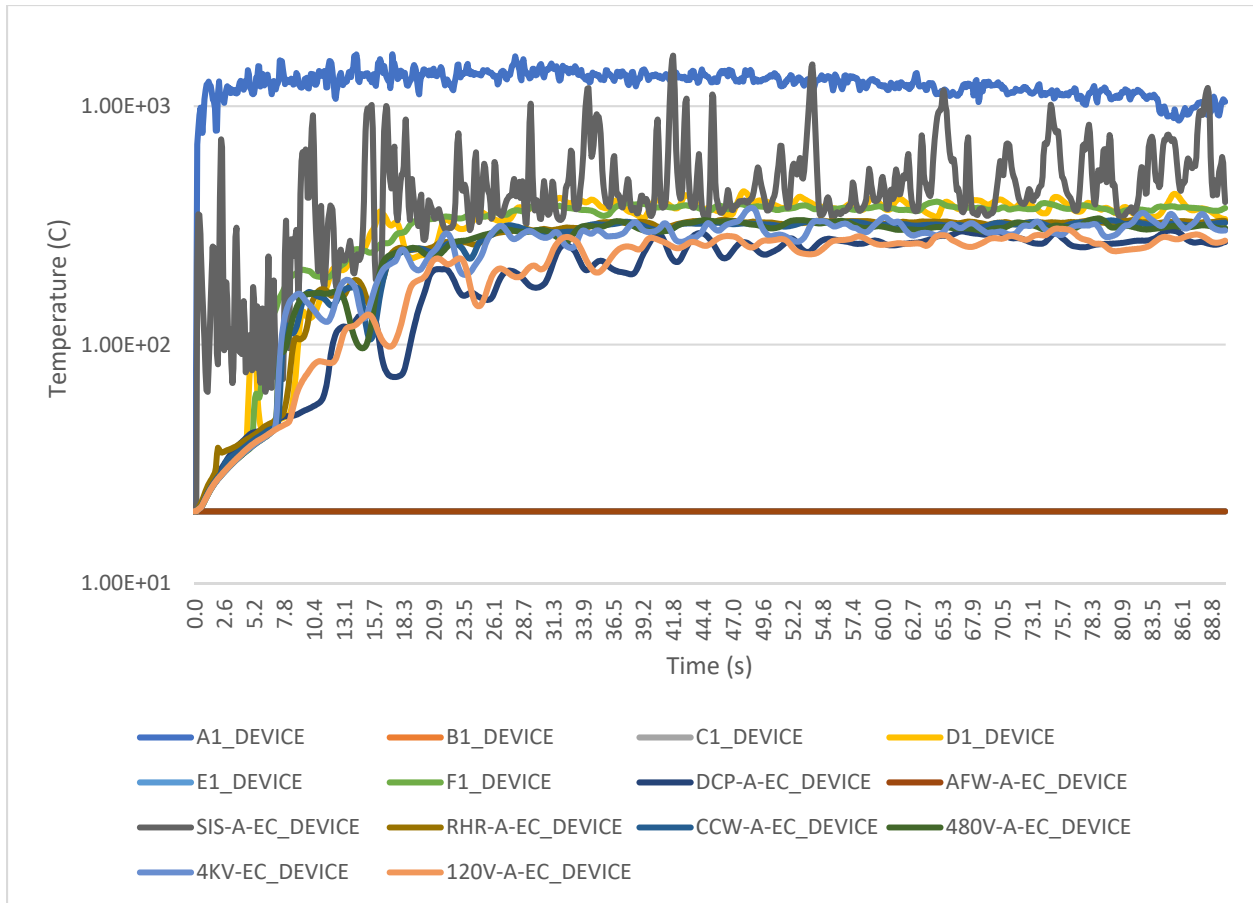
Figure 19. Plot of the DEVC FDS result file.

Table 7. Resulting failures of raceways and cables.

Number	Failed Raceway	Failed Cables
1	SIS at 83 seconds	CA-SIS-A-MDP
2	A1 at 60 seconds	CA-480-120V
3		CA-480-A-Out
4		CA-480-A-PWR
5		CA-480-DCP
6		CA-AFW-A-MDP
7		CA-AFW-A-PWR
8		CA-CCW-A-MDP
9		CA-CCW-A-PWR
10		CA-MDP-Cntrl
11		CA-RHR-A-MDP
12		CA-RHR-A-PWR
13		CA-SIS-A-MDP
14		CA-SIS-A-PWR
15		CA-SWS-A-MDP

Number	Failed Raceway	Failed Cables
16		CA-SWS-A-PWR

3.5   Summary

This research and development stage successfully performed two key tasks for the FRI3D software. The first was performing six model validation checks when autogenerating a CFAST model from the 3D structure FRI3D. These validation checks are typically part of the reports and eliminate manual effort. It also may allow some work to be done by less experienced modelers. Any validation issues are stored as part of the results and are available for automated reporting features.

An option to perform fire simulation using FDS vs. CFAST was also successful. An FDS is more difficult than CFAST to simplify the automatic generation of a model. Currently, an FDS model including the main features of the FRI3D 3D model, including walls, conduits, components, and powered vents can automatically be generated into an FDS model then solved, and the results used to determine component failures and generate a fire scenario. Some work is still being done on mesh sizing and passive vents. The addition of FDS as a fire simulation option will allow for more complex scenarios and room configurations to be performed using FRI3D.

4.   FUTURE WORK

This work focused on adding the basic capabilities for generating fire scenarios using FDS. While the basics were achieved in this project, there are additional features that need to be completed. This includes the following:

1. Venting – Work has only started on venting and is not currently being generated in the FDS model. Implementation of both powered and passive vents is in progress. Final research on the best method for implementing static vents will be determined before being implemented. Compartment exterior vents can use the normal FDS vent method, but if there are doors between geometry within the same compartment, these need to be integrated as part of the wall structures.

2. Fire Source Updates – Several fixes which need to be made for specifying fire sources and addition of other advanced reaction capabilities are to be done.

   a. Currently in FRI3D since the Fire is described based on an object which is put on the scene, its dimensions are used to calculate the bounding boxes. However, since the exact area of fire source is to be determined for specific scenarios, this is not computed and the HRRPUA output by FRI3D is not per unit area. The fix to this will be implemented in a future work.

   b. Currently there is only one reaction specification output, but in a more complex case there might need to be multiple reaction specifications.

   c. Specification of fires by the user could be a time-consuming task. This could be made easier by using the appropriate fire databases to determine the appropriate parameters for heat release rates, heat of combustions and stoichiometric coefficients for different fire scenarios. For example, using NUREG-2178 and NUREG-6931 and appropriate databases for other fire scenarios.

3. Multiple Compartments – The capability to handle multiple compartments are not yet implemented in FRI3D. FRI3D handles each room as a separate compartment and these can be modeled as a single geometry in FDS.

4. CAD Geometry – Currently CAD Geometry handling is very limited and not very usable. Several changes are identified which would enhance user experience in output of these to FDS

<ol type="a" start="1">
Import facilitation to Compartments: Ability to import CAD geometry as a full compartment and output the obstacle information to FDS.
Import facilitation to Equipment: Ability to replace each component or equipment by its corresponding CAD model
Split into multi compartments: Adding the ability to split a CAD geometry into multiple compartments to be handled by FRI3D.

<ol start="5">
Secondary Combustibles – In CFAST, the FLASH-CAT method is used to determine secondary combustibles and add new heat release rates at correct timings. FDS has a solid-phase pyrolysis modeling capability which can be used to model secondary combustibles. All pyrolysis models in FDS require the modeler to explicitly define the gas phase reaction. FDS currently supports only one pyrolysis model at a time. This limitation may pose a challenge in modeling several simultaneous cable fires. Another research topic may be how to formulate a single gas phase reaction as a surrogate for all potential cables. It is also beneficial to compare fire scenarios using FLASH-CAT and pyrolysis to model cable fires.

FDS Parameter Verification – Test cases need to be developed to verify that all the parameter options in FRI3D are being properly assigned to the FDS model. This must be manually verified and will then be added to the software unit testing.

Visualization – Usually FDS simulations are visualized using Smokeview. However, FRI3D has its own visualization system that is more integrated with the user interface and is a key aspect of the tool to link with the PRA and currently works well with CFAST. FDS outputs a more detailed set of data than CFAST, which would need to be rendered in 3D as a volume and as slices. Initial visualization features should include visualizing the temperature on the equipment, leading to when their failures occurs and displaying the temperature field across the room/volume in a meaningful format (similar to the CFAST display results). Additionally, visualization could include the display of velocity fields of the quantity involved, such as smoke as well as other quantities similar to what is displayed by Smokeview, which includes the isosurface renderings, etc. To summarize visualizations of the following may be implemented:

<ol type="a" start="1">
Visualization of Temperatures on objects (based on gas temperature at point on object).
Visualization of Temperatures on objects (based on surface temperature from .bnd files).
Visualization of volumetric temperatures on the compartment.
Visualization of Smoke from .s3d files.

<ol start="8">
Convergence Stopping Criterion – FDS is computationally expensive since it is a CFD model. It may be beneficial to add a feature in FRI3D to monitor the FDS's convergence based on user-defined criteria such as an obstacle temperature or soot density and to display the temporary results once the results converge without having to wait for FDS to finish its run. These results can be updated at the end of the FDS run.

5. REFERENCES

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