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Using CFAST to Estimate the Efficiency of Filtering Particulates in a Building

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National Institute of
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Abstract

CFAST is a two-zone fire model used to calculate the evolving distribution of smoke, fire gases and temperature throughout compartments of a constructed facility during a fire. The modeling equations used in CFAST take the mathematical form of an initial value problem for a system of ordinary differential equations (ODEs). These equations predict quantities such as pressure, layer height and temperatures as functions of time. The model transports species produced during pyrolysis as well as the products of combustion. Eleven species are followed by the model. They can be categorized as non-reacting, particulate, reacting, and those which can agglomerate and settle. The species are: nitrogen, oxygen, carbon monoxide, carbon dioxide, hydrogen cyanide, hydrogen chloride, fuel in vapor form, soot, trace species and water vapor. A new feature of the model (version 6.1) is the capability to filter trace species and soot which flow through a fan system. Filtering is implemented through the routines that solve the ODE's. Soot and trace species which are removed from the airstream are deposited on the filter.

Keywords

Smoke movement, environmental assessment, species filtering, HVAC

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DISCLAIMER

The U. S. Department of Commerce makes no warranty, expressed or implied, to users of - CFAST and associated computer programs, and accepts no responsibility for its use. Users of CFAST assume sole responsibility under Federal law for determining the appropriateness of its use in any particular application; for any conclusions drawn from the results of its use; and for any actions taken or not taken as a result of analyzes performed using these tools.

Users are warned that CFAST is intended for use only by those competent in the field of fire safety and is intended only to supplement the informed judgment of the qualified user. The software package is a computer model which may or may not have predictive value when applied to a specific set of factual circumstances. Lack of accurate predictions by the model could lead to erroneous conclusions with regard to fire safety. All results should be evaluated by an informed user.

INTENT AND USE

The algorithms, procedures, and computer programs described in this report constitute a methodology for predicting some of the consequences resulting from a specified fire. They have been compiled from the best knowledge and understanding currently available, but have important limitations that must be understood and considered by the user. The program is intended for use by persons competent in the field of fire safety and with some familiarity with personal computers. It is intended as an aid in the fire safety decision-making process.

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Abstract

CFAST is a two-zone fire model used to calculate the evolving distribution of smoke, fire gases and temperature throughout compartments of a constructed facility during a fire. The modeling equations used in CFAST take the mathematical form of an initial value problem for a system of ordinary differential equations (ODEs). These equations predict quantities such as pressure, layer height and temperatures as functions of time. The model transports species produced during pyrolysis as well as the products of combustion. Eleven species are followed by the model. They can be categorized as non-reacting, particulate, reacting, and those which can agglomerate and settle. The species are: nitrogen, oxygen, carbon monoxide, carbon dioxide, hydrogen cyanide, hydrogen chloride, fuel in vapor form, soot, trace species and water vapor. A new feature of the model (version 6.1) is the capability to filter trace species and soot which flow through a fan system. Filtering is implemented through the routines that solve the ODE's. Soot and trace species which are removed from the airstream are deposited on the filter.

Introduction

CFAST is a two-zone fire model used to calculate the evolving distribution of smoke, fire gases and temperature throughout compartments of a constructed facility during a fire. In CFAST, each compartment is divided into two gas layers.

It is designed primarily to predict the environment within compartmented structures which results from unwanted fires. These can range from very small containment vessels, on the order of 1 m^3 to large spaces on the order of 1000 m^3. The appropriate size fire for a given application depends on the size of the compartment being modeled.

The modeling equations used in CFAST take the mathematical form of an initial value problem for a system of ordinary differential equations (ODEs). These equations are derived using the conservation of mass and energy, the ideal gas law and relations for density and internal energy. These equations predict as functions of time quantities such as pressure, smoke layer height and temperatures given the accumulation of mass and enthalpy in the two layers. The model then consists of a set of ODEs to compute the environment in each compartment and a collection of algorithms to compute the mass and enthalpy source terms required by the ODEs.

The ODEs are driven by source terms that describe the various physical phenomena. Combustion chemistry is one such source. Combustion from fires supplies both enthalpy as well as various species for transport. A fire in CFAST is implemented as a source of fuel mass which is released at a prescribed rate (the pyrolysis rate). Energy is released by the fuel and combustion products are created as it burns.

The model transports species produced during pyrolysis as well as the products of combustion. A non-reacting trace species provides the possibility to follow the effects of venting and filtering.

The model can simulate multiple fires in one or more compartments of the building. Fires are treated as independent entities, with no interaction of the plumes. These fires are referred to as “objects” and can be ignited at a prescribed time, temperature or heat flux.

Eleven species are followed by the model. They can be categorized as non-reacting, particulate, reacting, and those which can agglomerate and settle. The species are: nitrogen, oxygen, carbon monoxide, carbon dioxide, hydrogen cyanide, hydrogen chloride, fuel in vapor form, soot, trace species and water vapor.

Nitrogen is a non-reacting species. It is neither consumed nor produced during the transport process. Oxygen may be produced by pyrolysis and is consumed in regions where combustion occurs. Carbon monoxide, carbon dioxide and water are produced by the combustion process. Soot is also produced during combustion, but can settle, agglomerate or be filtered out of the system by mechanical filters such as are used in clean rooms. Hydrogen chloride (HCl) and hydrogen cyanide can also be produced during pyrolysis. HCl may be absorbed and adsorbed on boundary surfaces. This simply means that the molecules can collect on the surface of some materials, and later released, depending on its concentration on the surface and in the gas layer, as well as temperature and humidity. They are not altered by transport itself. The concentration-time product is a surrogate for the toxicity of fire gases[1]. The trace species is generated during pyrolysis and can be filtered. It too is non-reacting, that is, it is not altered during transport. The fuel, in vapor form, is generated during pyrolysis, and consumed during combustion. Neither fuel vapor nor water are filtered by the model.

Purpose

Predicting the movement of smoke and subsequent contamination of the environment resulting from a fire is one of the principal uses of a fire model. The recent addition of filtering allows one to investigate strategies to mitigate the problem. The use of this capability is illustrated in this paper.

This recent addition to CFAST was prompted by the need to qualify nuclear power plants on the basis of how much radioactive material can escape a facility after an accident, however, the implementation is general.

There are two limitations that need to be kept in mind. The first is that filters are specific to particulate size. CFAST does not track particulate distributions, so both generation and filter specification need to be kept in mind.

The second issue is that the effect on water vapor is not well understood, so this implementation applies only to particulates, that is trace species and soot.

Filtering

The transport of fire effluent is described in the CFAST Technical Reference Guide[2]. A new feature of the model (version 6.1) is the capability to filter trace species and soot which flow through a fan system.

Filtering is implemented by modifying the source terms which describe gas flow. Mass that is filtered remains in the filter and is removed from the air stream.

A Simple Example to Illustrate Filtering

First we will consider a simple case to illustrate the effect of filtering: two compartment with leaks to the outside and a mechanical ventilation (fan system) connecting the room of origin with a second compartment.

The example input script shown in Table 1 is a 50kW fixed size fire. The two compartments are 3.6m x 2.4m x 2.6m in size. Both have leaks to the outside at floor level, though in this scenario no trace material gets to the outside. A small fan pushes 0.14 m^3 per second of air from the first compartment (fire origin) to the second compartment. The fan is running throughout the simulation. The fire starts at 30 s.

By adding the filter command "EVENT,F,1,3,1,60,.90,1" we invoke a filter for fan system 1 which begins at 60 s and is 90% efficient. The input file for this example is shown in Table 1. Figure 1 shows the effect on the total mass of the trace species in the two compartments.

Since fan flow is constant, the concentration in compartment 1 is the same in both cases.

An Example of a Glove Box Disassembly Facility

CFAST is intended to predict the temperatures, gas concentrations and smoke layer heights in a multi-compartment structure during a fire. The software can be used to estimate the impact of specific events in the building fire performance such as doors or windows opening or closing. The software can also estimate the environmental conditions (e.g., temperature, combustion product concentrations, layer height) in the fire compartment and neighboring compartments. These conditions can then be used to assess the effect of fire on building occupants. Using CFAST to assess the effect on packages, containers and buildings that house radiological material is one example. Once the scenario is established, the consequences to the public and workers in neighboring facilities can be estimated.

A common room arrangement in the Department of Energy community is a laboratory compartment that can be entered through an airlock from a long hallway. Often there is a window between the process room and the corridor, but no direct access to the corridor. A schematic is shown in Figure 2 and the Smokeview rendering in Figure 3. This scenario matches the example in *CFAST Computer Code Application Guidance for Documented Safety Analysis*[3].

The assembly compartment contains a glove box and polyethelyne trash (containing radioactive waste) which is the presumed fire source. It is connected to an airlock which has doors to the corridor. In addition, an observation window connects the assembly compartment to the corridor. For this simulation, the whole building is surrounded by a container which is used as surrogate

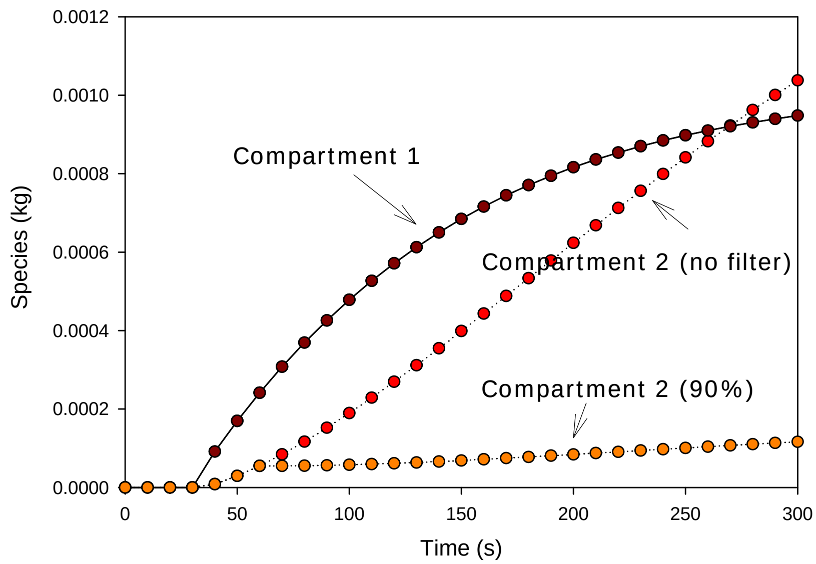


Figure 1. Comparison of species concentration by compartment, showing the effect of filtering.

for the outside world in order to measure the trace species which escapes the facility. So long as the outside compartment is large (in volume) compared to the simulated environment, and the

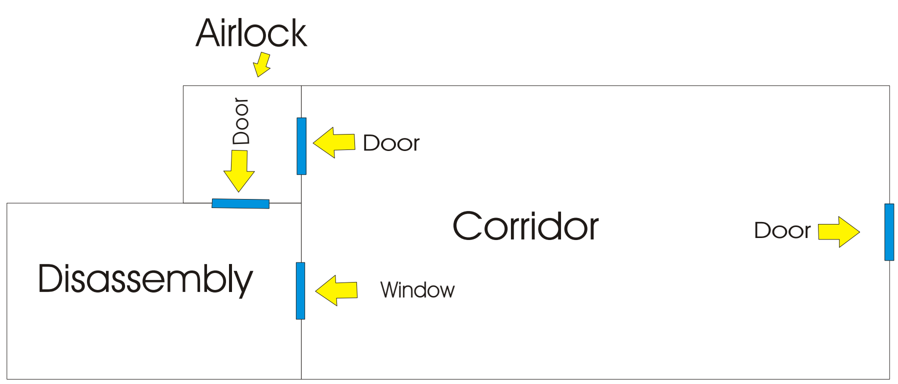


Figure 2. Schematic of glovebox/disassembly facility

openings are large enough that there is not a significant pressure increase, there will not be an effect on the flow. The data file to implement these scenarios is shown in Table 2.

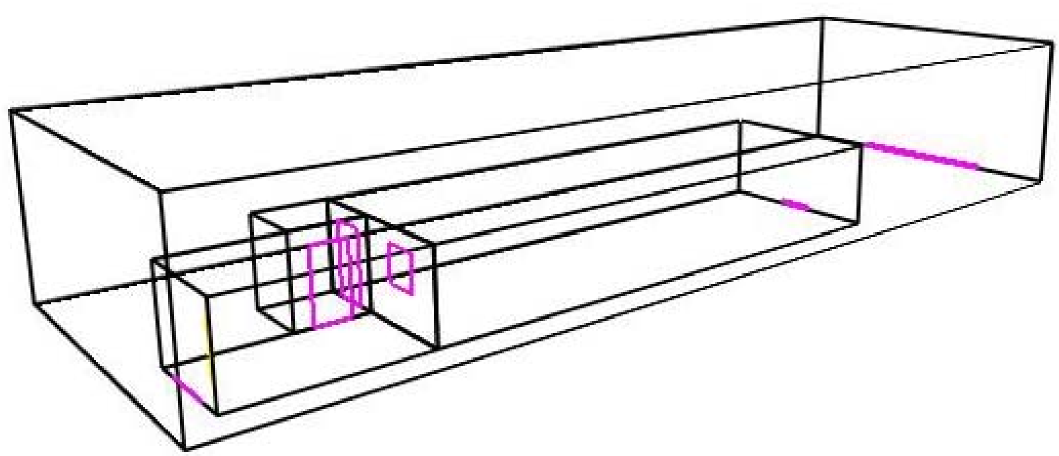
For the first scenario (no fan/filter), the airlock doors are opened 60 s after ignition to allow personnel to escape. This is followed by the observation window breaking at 120 s when the fire reaches a critical size.
To show the effect of filtering, we remove the window breakage, add a fan and duct system from the assembly compartment to the outside, and turn filtering on. The changes (added to the end of the script shown in Table 2) are

```
!!Fan and duct from assembly to the pseudo outside
MVENT,1,4,1,H,2.44,0.37,H,1.52,0.37,1.142,0,200,1
!!Filtering turned on at the beginning of the fire
EVENT,F,1,5,1,0,0.99,1
```

The results in terms of species mass are shown in figures 4a (original) and 4b (modified by a fan/duct/filter). The heat release rate is the same for both cases. Flow through the window has only a small effect on the species concentration in the corridor. Figure 5 demonstrates an alternative way to report the amount of material that has escape from the source compartment. Whereas figure 4 shows the actual amount of this material in each of the three compartments and the amount which exits the containment building, figure 5 shows this same information as a fraction of the pyrolyzed material. When the fan is used (4b), it is on continuously.

Since the filter also removes soot, so there will be an indirect effect on the temperature distribution , since soot affects the radiation balance. This effect is not illustrated since we have

Figure 3. Smokeview Rendition of the Glovebox Facility



not shown the upper/lower layer temperature distribution.

The effects of aerosol dispersal can also be seen from the graph (and report) of species concentration. Figures 4 and 5 shows how the filtering system can protect those working around

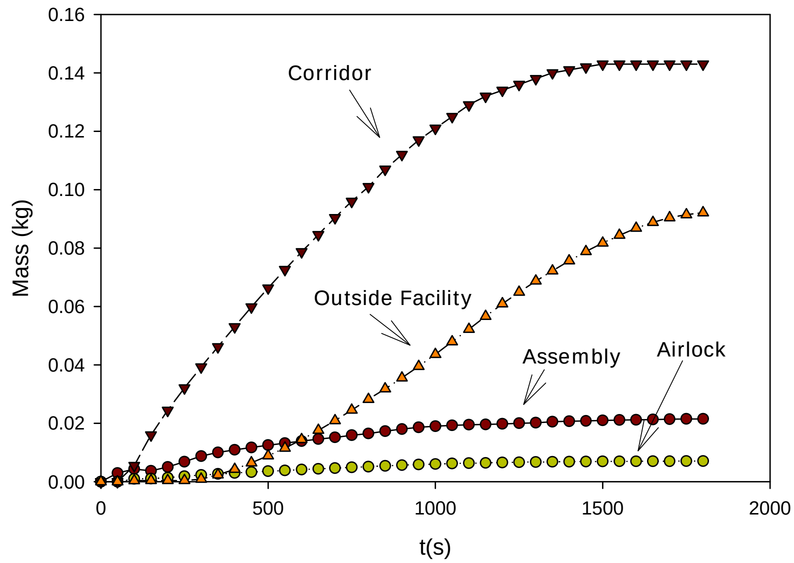


Figure 4a - Mass in each compartment - no filtering

such fires as well as the wider environment. In the first case, the amount of escaped material will continue to climb. In the second, case, the amount that escapes is reduced and declines over

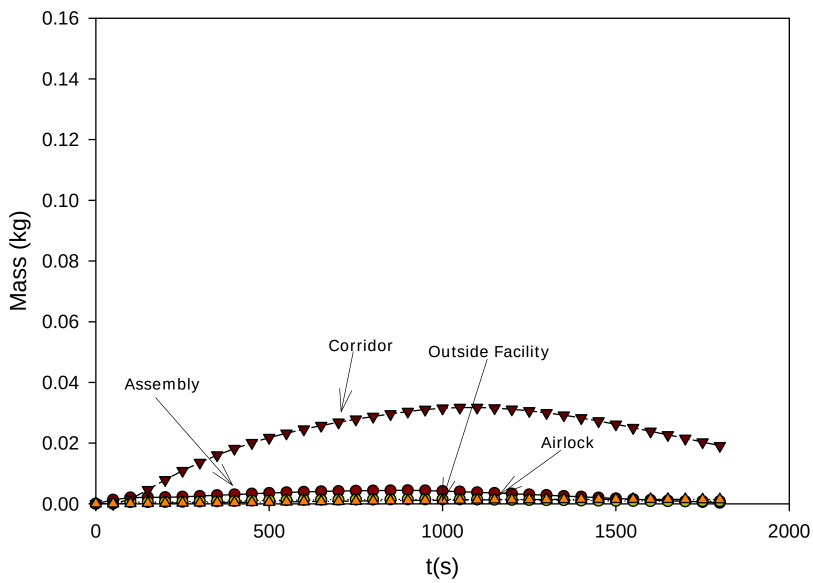


Figure 4b - Mass in each compartment - filtered

time. The progression of the fire and movement of contaminants can also be seen in figure 5. At the time of ignition, all of the fire and radioactive aerosols are in the glove-box assembly room.

As the fire grows, the contaminant moves from the assembly to the airlock to the corridor and finally to the outside. It should be noted that though there is flow from the assembly compartment to the outside through leaks, no fire gases escape through this path. When the fan/filter system is turned on, there is not even this small leakage.

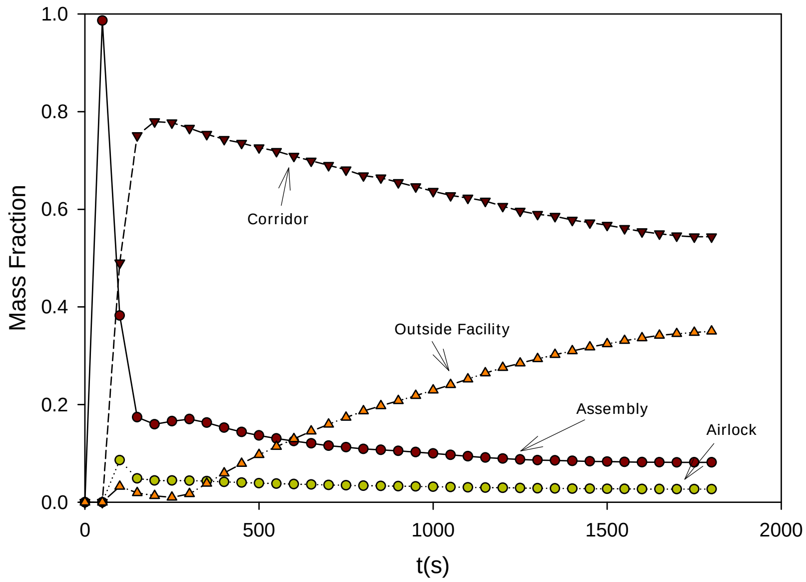


Figure 5a. Fraction of radiological material released in each compartment - no filtering.

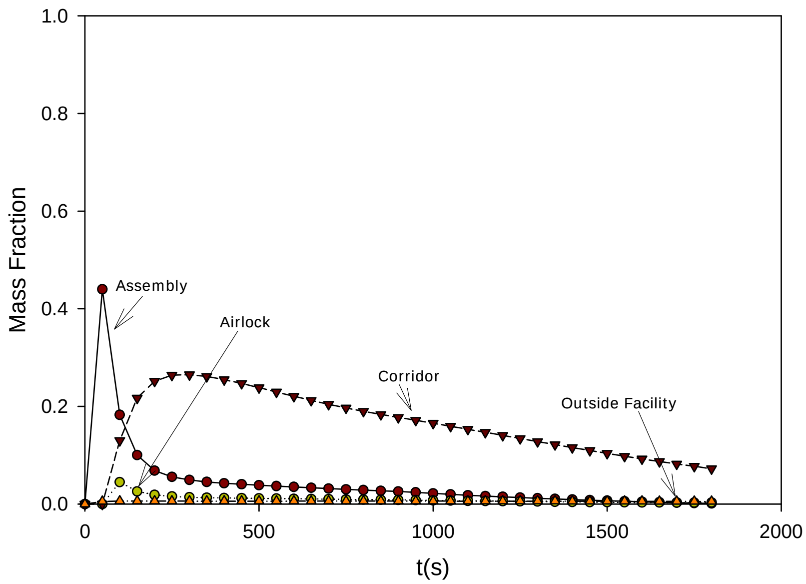


Figure 5b. Fraction of radiological material in each compartment - with filtering.

Leak Path Factor

A fire can contain pyrolysis material that is radioactive, and thus an additional hazard to occupants of a building or those within reach of a fire plume. A goal of building safety is to reduce leakage of such effluents. A leak path factor (LPF) is a measure of the fraction of the radionuclides in the fire effluent not captured by a confinement system (e.g., building rooms, ductwork) or filtration mechanism (e.g., fan filters or sand filter)[4].

The definitions the Department of Energy uses for the LPF calculations are:

> The source term (ST) represents the airborne respirable radiological material that exits a facility (or area of interest) and is defined as
>
> $$ST = MAR \times DR \times ARF \times RF \times LPF$$
>
> The Material-at-Risk (MAR) is the total quantity of radionuclides (in grams or curies of activity for each radionuclide) available that are subjected to the modeled scenario.
>
> The Damage Ratio (DR) is the fraction of the MAR actually impacted by the modeled scenario.
>
> The Airborne Release Fraction (ARF) is the fraction of a radioactive material suspended in air as an aerosol and thus available for transport.
>
> The Respirable Fraction (RF) "is the fraction of airborne radionuclides as particles that can be transported through air and inhaled into the human respiratory system and is commonly assumed to include particles 10-µm Aerodynamic Equivalent Diameter (AED) and less."
>
> The Leakpath Factor (LPF) is the fraction of the airborne respirable radionuclides that are transported through some confinement deposition system (e.g., building rooms, ductwork) and exit the building.

CFAST can be used to calculate the amount of radioactive aerosol which is transported through a building system and to assess various strategies to reduce the amount of material which escapes confinement. This is the ST as defined above.

The TS production fraction in the object data files may be calculated by

$$TS = MAR \times DR \times ARF \times RF / \dot{m}$$

TS is the term used in the CFAST User's Guide for trace species production and $\dot{m}$ is the pyrolysis rate of the object.

This input to the calculation is computed using several factors. The essence is that it is derived from the amount of material available which can subsequently made into an aerosol and then transported. This is specified in the object data file as the fraction of the pyrolysis material that is radiological and respirable. In terms of fire engineering, MAR is the mass of the object, and DR the fraction which can be affected (pyrolysized) during the incident.

The ARF and RF values may be obtained from the Release Fraction Handbook[5] and are derived from discrete experiments that typically evaluated a single release mechanism. In a severe fire there may be many mechanisms occurring simultaneously.

These sources can be combined in CFAST using several fires (objects).

The MAR term is usually expressed as time and activity distribution for each release mechanism. The components that are associated with the same release duration can be combined, but components that have different release mechanisms should be kept separate to account for time-dependent variance in atmospheric dispersion to aid consequence assessment.

Also, there are often many exfiltration routes for heated gases, so there can be multiple LPF terms applied to a single source, e.g., room leakage, ventilation system deposition, and filtration system effectiveness.

Once the source term is calculated, the consequences to the public and workers in neighboring facilities can be estimated. CFAST calculates total radiological material in each compartment of a building and the amount that has exited the containment facility, and provides this information in two forms: These are reported as absolute values (kg) and as a fraction of the species released from the fire(s).

LPF is the ratio of the mass of the trace species which flows through a vent, divided by the total released by the source term. For these examples, the fire is a ½ MW fire with the trace species (TS) being two percent of the pyrolysis. The total mass pyrolyzed as well as the total of the trace species produced are contained in the output file and the comma delimited spreadsheet. The total trace species flow through mechanical vents is shown in the listing as the last two columns for each mechanical ventilation node. "Vented" refers to the mass which passes through the duct system and "Captured" is the amount which remains on the filter. These numbers are also contained in the mass flow spreadsheet labeled "Trace Species through node nnn," and "Traced captured at node nnn."

The effect of reducing the LPF factor can be seen by comparing the total mass which flows through the fan/duct system with and without a filter, and the effect of using a fan and filter to eliminate the aerosols. Using the base case in Table 2, there are three variation:

First at 1800.0 seconds with a fan/duct but with no filtering

Upper Layer Species

Compartment	OD (1/m)	CT (g-min/m3)	TS kg
Assembly	7.474E-02	157.	1.579E-05
Airlock	0.543	196.	6.717E-04
Corridor	0.557	207.	1.208E-02
Containment B	0.00	0.00	0.00

Lower Layer Species

Compartment	OD (1/m)	CT (g-min/m3)	TS kg
Assembly	5.391E-03	0.566	5.680E-05
Airlock	1.029E-02	1.02	1.678E-05
Corridor	0.00	0.00	0.00
Containment B	0.00	0.00	0.00

Total mass flow through vents (kg)

To	Through	Upper Layer		Lower Layer		Trace Species	
Compartment	Vent	Inflow	Outflow	Inflow	Outflow	Vented	Captured
Assembly	M Node 1		1.813E+03		1.62	0.251	
Outside	M Node 2			1.814E+03		0.251	

Second at 1800.00 seconds with 10% efficient filter

Upper Layer Species

Compartment	OD (1/m)	CT (g-min/m3)	TS kg
Assembly	7.474E-02	157.	1.579E-05
Airlock	0.543	196.	6.717E-04
Corridor	0.557	207.	1.208E-02
Containment B	0.00	0.00	0.00

Lower Layer Species

Compartment	OD (1/m)	CT (g-min/m3)	TS kg
Assembly	5.391E-03	0.566	5.680E-05
Airlock	1.029E-02	1.02	1.678E-05
Corridor	0.00	0.00	0.00
Containment B	0.00	0.00	0.00

Total mass flow through vents (kg)

To	Through	Upper Layer		Lower Layer		Trace Species	
Compartment	Vent	Inflow	Outflow	Inflow	Outflow	Vented	Captured
Assembly	M Node 1		1.813E+03		1.62	0.226	2.506E-02
Outside	M Node 2			1.814E+03		0.226	2.506E-02

Finally at 1800.0 seconds with 99% efficient filter

Upper Layer Species

Compartment	OD (1/m)	CT (g-min/m3)	TS kg
Assembly	7.474E-02	157.	1.579E-05
Airlock	0.543	196.	6.717E-04
Corridor	0.557	207.	1.208E-02
Containment B	0.00	0.00	0.00

Lower Layer Spe

Compartment	OD (1/m)	CT (g-min/m3)	TS kg
Assembly	5.391E-03	0.566	5.680E-05
Airlock	1.029E-02	1.02	1.678E-05
Corridor	0.00	0.00	0.00
Containment B	0.00	0.00	0.00

Total mass flow through vents (kg)

To Compartment	Through Vent	Upper Layer Inflow	Upper Layer Outflow	Lower Layer Inflow	Lower Layer Outflow	Trace Species Vented	Trace Species Captured
Assembly	M Node 1		1.813E+03		1.62	2.506E-03	0.248
Outside	M Node 2			1.814E+03		2.506E-03	0.248

Figure 6 shows this effect graphically. The figure shows the effect of reducing the LPF by changing the filter efficiency of a fan/duct system This figure shows the fraction of the released material that escapes the containment building. The first curve is with no filter, the second shows the reduction in aerosol using a 10% efficiency filter and the third utilizes a 99% filter to extract the radiological component. Figure 7 shows the total mass of trace species captured by the filter.

Conclusion

The fire model CFAST has been modified to track radiological species and filter them out of flow through forced ventilation systems.. This capability allows one to calculate the effects of filtering radiological aerosols and illustrate the reduction in consequence of the spread of radiological products.

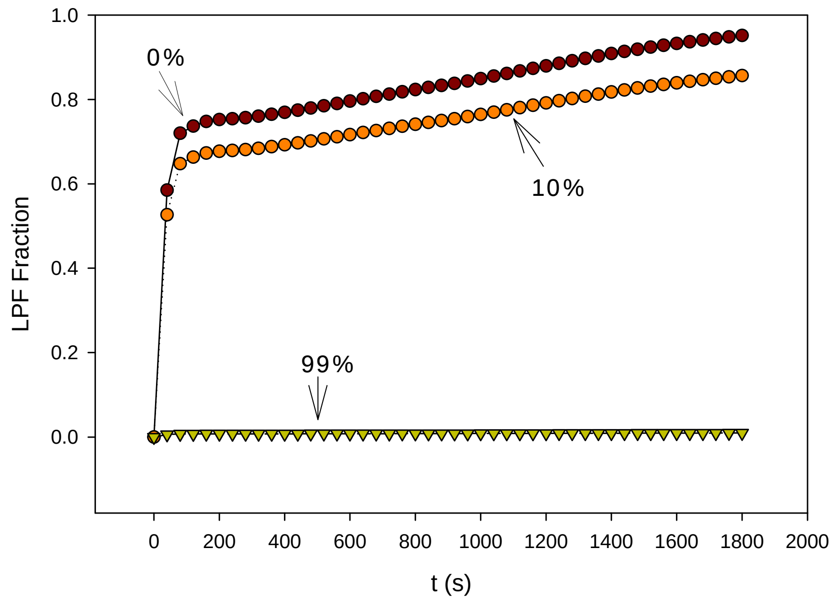


Figure 6. LPF for 0%, 10% and 99% efficient filter.

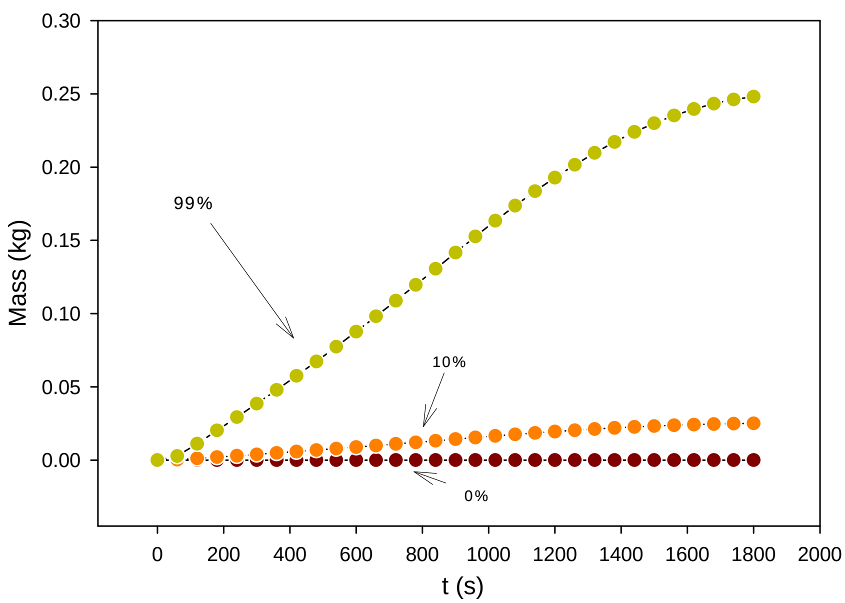


Figure 7. Radiological mass captured by the filter.

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URL is http://www.hss.energy.gov/NuclearSafety/techstds/standard/standard.html

5. Airborne Release Fractions/rates and Respirable Fractions for Nonreactor Nuclear Facilities, DOE-HDBK-3010-94 (1994).

Table 1. Simple Example Showing Movement of Trace Species

```
VERSN,6,Simple example of following trace species
!!
!!Environmental Keywords
!!
TIMES,300,-300,10,10,10
EAMB,293.15,101300,0
TAMB,293.15,101300,0,50
CJET,WALLS
CHEMI,10,393.15
WIND,0,10,0.16
!!
!!Compartment keywords
!!
COMPA,Compartment 1,3.6,2.4,2.6,0,0,0,GYPSUM,OFF,GYPSUM
COMPA,Compartment 2,3.6,2.4,2.6,3.6,0,0,GYPSUM,OFF,GYPSUM
!!
!!vent keywords
!!
HVENT,1,3,1,1,0.1,0,1,0.7,0,4,1
HVENT,2,3,1,1,0.1,0,1,0.7,0,2,1
MVENT,1,2,1,V,2.1,0.05,V,2.1,0.05,0.14,200,300,1
!!
!!fire keywords
!!
OBJECT,POSmall,1,0.3,1.2,0.5,1,1,30,0,0,1
```

Table 2. Data file for Glove Box Disassembly Facility

```
VERSN,6, Polyethylene fire - not filtered
!!
!!Environmental Keywords
!!
TIMES,1800,-60,10,10,10
EAMB,300,101300,0
TAMB,300,101300,0,5
CJET,CEILING
CHEMI,10,393.15
WIND,0,10,0.16
!!
!!Four Compartments, including a means to capture effluent
!!
COMPA,Assembly,5,3,2.44,1,1,0,GYPX5/8,CONCRETE,GYPX5/8
COMPA,Airlock,2,2,2.44,4,4,0,GYPX5/8,CONCRETE,GYPX5/8
COMPA,Corridor,15,5,2.44,6,1,0,GYPX5/8,CONCRETE,GYPX5/8
COMPA,Outside,30,10,4.88,0,0,0,GYPSUM,OFF,GYPSUM
!!
!!Doors from 1 to 2 and 2 to 3
!!Window from 1 to 3
!!Leak from 1 to 4 and 3 to 4 (pseudo outside)
!!Leak from 4 to 5 (real outside)
!!
HVENT,1,2,1,1,2,0,1,3.5,2,3,0
HVENT,2,3,1,1,2,0,1,0.5,0,2,0
HVENT,1,3,1,1,2,1,1,1,0,2,0
HVENT,1,4,1,1.5,0.05,0,1,0.75,0,4,1
HVENT,3,4,1,1,0.1,0,1,2,0,2,1
HVENT,4,5,1,5,0.1,0,1,2.5,0,2,1
!!
!!Open doors for emergency egress
!!
EVENT,H,1,2,1,60,1,1
EVENT,H,2,3,1,65,1,1
!!
!!Blow out the window
!!
EVENT,H,1,3,1,120,1,1
!!
!!Polyethylene trash fire
!!
OBJECT,pe,1,0.5,1.5,0,1,1,0,0,0,1
```