Development and Use of the CAFE-3D Code for Analysis of Radioactive Material Packages in Fire Environments

Carlos Lopez and Jorman Koski
Sandia National Laboratories
Albuquerque, New Mexico

Ahti Suo-Anttila
Innovative Technology Solutions, Corp.
Albuquerque, New Mexico

ABSTRACT
A computational fluid dynamics (CFD) based fire model has been successfully coupled to standard finite-element computer codes in order to permit design and risk analysis of radioactive material packages. The fire model, called Container Analysis Fire Environment (CAFE), is based on a three-dimensional finite volume formulation of basic fire chemistry and fluid dynamics. The fire model includes a variable-density primitive-variable formulation of mass, momentum, energy and species equations. Multiple chemical species and soot formation are included in the combustion model. Thermal radiation is modeled as diffusive radiation transport inside the flame zone and as view-factor radiation outside the flame zone. Turbulence is modeled with an eddy diffusivity model. The soot model can be optionally coupled to the diffusive radiation formulation with the use of the Rosseland approximation and the optical properties of soot.

Currently the CAFE-3D code is coupled to the MSC P/Thermal computer code and the coupling to the ANSYS/Mechanical finite-element code is expected to be completed in the near future. The model is normally used to represent a fully engulfing pool fire typical of regulatory qualification conditions. Other fire positions and configurations, including fires with packages that have internal passages like those in some storage casks, can also be simulated. In order to permit analysis in a relatively short time on a standard engineering computer work station, the fire model runs periodically during a package thermal calculation to update local fire conditions. The frequency and duration of the fire update calculation is user controlled with preset time and/or temperature increase criteria.

This paper outlines the key features of the CAFE-3D code and presents examples of its use. Typical fire finite volume grids are described and the methods of surface coupling to the finite element codes are also discussed.

INTRODUCTION
CAFE-3D is a computational fluid dynamics (CFD) and radiation heat transfer computer code that realistically simulates fires that has been successfully coupled to commercially available finite-element analysis (FEA) computer codes to facilitate the design and risk analysis of packages that are used for the transportation of radioactive material (RAM). The fire model, called Container Analysis Fire Environment (CAFE-3D), is based on a three-dimensional finite volume formulation of basic fire chemistry and fluid dynamics. The code is designed to run on desktop PC, UNIX, and Linux workstations with emphasis on fast-running simulations.
CAFE-3D consists of a coupled set of computer codes. The CFD fire and radiation transport models come from Isis-3d [Suo-Anttila, 2003]. The standard commercial finite element codes are either MSC P/Thermal or ANSYS Mechanical. The ANSYS version of CAFE is still in the preliminary stages of testing. Therefore, the remainder of this paper will focus on CAFE-P/Thermal applications. Nevertheless, descriptions and conclusions expressed in this paper do apply to the coupling of CAFE with either FEA code.

The finite element codes model the detailed heat transfer within the object being analyzed. The coupling between codes includes bi-directional heat transfer between the CAFE CFD finite volume fire grid and the finite element grid of the object modeled in the FEA code. Internal two-way mapping routines are used to transfer the energy between the models.

**NUMERICAL AND PHYSICAL MODELS IN CAFE-3D**

In CAFE-3D the fire phenomenon is modeled utilizing relevant physical and numerical models. The physical model is described by the following governing equations: three momentum equations for predicting the 3-dimensional velocity/momentum field, an energy equation for predicting the temperature field, and an indefinite number of scalar transport equations for tracking the flow of fuel vapor, oxygen, soot, other species of interest, and turbulent kinetic parameters.

The numerical model that CAFE-3D uses is a finite volume approach with orthogonal Cartesian coordinates for discretizing the governing equations. The use of orthogonal coordinates makes the discretization very similar to a finite difference method. CAFE-3D uses a variable density version of the PISO (Issa, 1985) pressure-based solution algorithm to solve the flow equations (Suo-Anttila, 1993). Turbulence can be modeled by the Prandlt one equation (Schlichting, 1979), a large-eddy diffusivity formulation (LES) (Smagorski 1963, Ferziger, 1993), or other algebraic formulations. Diffusive thermal radiation transport within the fire is modeled with the Rosseland approximation. Outside the flame zone radiation is treated by viewfactor methods. The rate of combustion is modeled by a combination of Arrhenius and eddy dissipation equations for the reaction rate of fuel and oxygen.

To model curved objects, such as cylinders or spheres, CAFE-3D uses a porosity method similar to the Fractional Area and Volume Object Representation method (FAVOR™) (Hirt, et. al. 1985). The CAFE-3D Porosity Method is a body fitted coordinate method that can be applied in an orthogonal Cartesian mesh. The porosity method models a curved surface by admitting a flat diagonal surface within a hexahedral finite-volume computational cell. Multiple cells with polygonal cross sections are used to represent a curved object such as a cylinder. The porosity method results in a much better representation of curved surfaces than a typical stair-step representation, which is often used with Cartesian coordinate systems. A segmented object representation has an equivalent heat transfer and flow representation as a finite-element CFD method, but it does not incur the overhead of increased processor and memory requirements associated with either finite-element methods or structured body fitted methods. With this porosity method, the flow areas on all cell surfaces are adjusted to account for the diagonal solid surface. Heat transfer occurs between the gas and solid in the same computational cell through the diagonal surface.
The primitive variables in CAFE-3D are the 3 momentum fluxes (product of density and velocity), temperature (energy equation), and mass fraction (species equations). The primitive variable momentum flux has the advantage of eliminating density interpolation error when using a pressure based solution algorithm. It also has the advantage of a better variable density implementation, which is important when solving problems with large density variations such as fires.

Various transport equations are solved for the energy and various chemical species that are present. The CAFE-3D gas energy equation includes terms for heat transfer to the coupled finite element model. Radiation transport is included in the energy equation by the Rosseland conduction formulation and utilizes energy source or sink terms for radiative boundary conditions.

CAFE-3D has several different turbulence models to choose from. All are based on an eddy diffusivity concept. There are several algebraic models wherein the eddy diffusivity is a function of Reynolds number or other flow or position parameters. Other turbulence models include a large eddy simulation (LES) model, and a one-equation transport model.

The combustion chemistry model used in CAFE-3D is a variant of a turbulent flame model developed by Said et al. (1997). The relevant species in this model are the hydrocarbon fuel vapor, atmospheric oxygen, solid carbon soot, an intermediate species, and products of complete combustion (which consists of CO2 and H2O vapor). The first reaction is incomplete fuel combustion that produces carbon soot in addition to the products of complete combustion. The second reaction is endothermic fuel cracking, which is anaerobic and produces soot and intermediate species. The third reaction is carbon soot combustion with oxygen. And the final reaction is combustion of the intermediate species. The coefficients in various reactions were determined such that complete combustion of the intermediate species and soot produces the same species and thermal energy as direct combustion of the fuel.

**THERMAL RADIATION IN CAFE**

The CAFE model of thermal radiation transport within and near large hydrocarbon fires is divided into two types, diffusive radiation inside the flame zone and clear air or view factor radiation outside the flame zone.

Within the flame zone, diffusive radiation transport is calculated by an effective gas thermal conductivity, which depends upon the local temperature, and the local extinction coefficient of the medium. The extinction coefficient is a function of the local volume fractions of soot, water vapor, fuel vapor, and intermediate species [Modest, 1993]. As an option, this formulation also includes contributions for hydrocarbons and CO2.

Outside the flame zone, thermal radiation transport is modeled by the clear air or view factor method. The calculation of the view factor between the fire and an adjacent object is complicated due to the fact that the outer surface of a fire (or smoky region) is dynamically changing due to the puffing and turbulent nature of flames. The position of the surface is found by monitoring a critical user-input soot volume fraction. The entire computational domain is examined for
locations where the soot concentration between adjacent computational cells lies both above and below the critical value. Any cell boundary that satisfies this criterion is assumed to be part of the fire surface. The surface normal vector points in the direction of the lower concentration and is perpendicular to the computational cell face. For computational cells that have more than one radiating cell surface, a normalized vector sum is performed to assign the surface unit normal vector. When the problem is set up, all surface unit normal vectors of solid objects are calculated and stored for later use. The clear air fire-surface to object view factor is calculated by the formula:

$$f_{ij} = \frac{(\mathbf{n}_i \cdot \mathbf{s}_{ij})(\mathbf{n}_j \cdot \mathbf{s}_{ij})}{\pi \cdot s^4} A_j$$

where $f_{ij}$ is the view factor of the fire cell surface to an object cell surface, $\mathbf{n}_i$ is the unit surface normal of the radiating fire surface, $\mathbf{n}_j$ is the unit surface normal of the object surface, $s_{ij}$ is the difference between the position vectors of the surface and the fire surface. “s” is the distance between the surfaces, and $A_j$ is the surface area of the object surface cell.

**USE OF CAFE-3D**

In order to use CAFE-3D, the user must first build a P/Thermal or ANSYS model of the package. When assigning boundary conditions to the object, the user should select all the external surfaces and assign a special CAFE boundary condition so that CAFE can interchange information with the FEA model.

At the present time, CAFE-3D does not have an automatic mesh generation option to build an equivalent model from the P/Thermal model. Instead the user must build a CAFE model of the object to be analyzed using the CAFE-3D solid modeler. The CAFE model should have approximately the same size, shape, and physical orientation of the external surface. The CAFE solid modeler allows the user to construct complex objects by adding and subtracting 3-d graphics primitives. Internal details of the solid object are unnecessary because they are accounted for by the P/Thermal or ANSYS FEA model.

The boundary conditions that are assigned in P/Thermal must be mapped to the equivalent object surface boundary conditions in the CAFE-3D model. The coordinate systems in P/Thermal and CAFE are co-located, which means that the X, Y, and Z axes are aligned in the same direction with respect to the object. The mapping of the P/Thermal model to the CAFE model is done automatically. The algorithm employed by CAFE-3D non-dimensionlizes both the P/Thermal and the CAFE-3D model in the X, Y, and Z directions. Using the non-dimensional positions, all of the FEM surface nodes are mapped to equivalent CAFE surface nodes.

Once the user has built an equivalent CAFE model of the object to be analyzed, CAFE is run standalone for a short period of physical (not CPU) time, typically 10-20 seconds, after which it will write a restart file. This initial CAFE run allows the object to become engulfed in flames, which form a suitable starting point for the CAFE-P/Thermal run.

During a CAFE-P/Thermal run, CAFE and P/Thermal run alternately. P/Thermal will take time steps on the order of 1 to 10 seconds, depending upon convergence of the temperature solution. At the end of each P/Thermal time step, object surface temperature data is passed to CAFE, which then runs for approximately 0.2 seconds of burn time. Finally, CAFE adds up the heat flux
from radiation and convection and computes an equivalent convection boundary condition that is position dependent and that is passed to P/Thermal for its next time step. This cycle repeats until P/Thermal reaches the desired simulation time. In a typical half-hour run, CAFE will be called approximately 1000 times, or approximately 200 seconds of physical fire burn time. Test cases have demonstrated that final results tend to be insensitive to the number of times CAFE is called, provided that CAFE is called more than several hundred times. This insensitivity is attributed to the averaging effect multiple calls have on the dynamic puffing nature of fires.

SAMPLE CAFE 3D SIMULATION
In the early stages of its development, CAFE was designed for the modeling of open pool fires that could engulf very large objects, like packages used for the transportation of spent nuclear fuel (SNF) by truck and/or rail. These packages can measure over 5 m (16ft) in length and 2 m (7ft) in diameter and can weigh over 110,000 kg (250,000lbs). Currently, CAFE has been modified so that internal fires such as tunnel fires and fire fields involving flow of combustion products through small gaps can be modeled.

For the purpose of this paper, an object the size and shape of a SNF rail cask with its impact limiters on each end was engulfed in a large CAFE fire. For simplicity, the body of the cask was assumed to be a solid stainless steel cylinder, 2.3m in diameter and 5m long, and the protecting impact limiters were assumed to be made out of aluminum honeycomb. Each impact limiter is 3.3m in diameter and one meter long. Figure 1 shows the P/Thermal and CAFE mesh. The size of the elements is usually smaller in P/Thermal when compared to the element in the CAFE finite volume mesh. The main reasons for this difference are: 1) the difference in the solution times (FEA codes usually converge much faster and easier than CFD codes), 2) there is usually more need for a finer FEA model of the object being analyzed due to the need for the modeling of relatively small features/components that are part of the design of the object, and 3) CAFE models the environment surrounding the FEA model with a computational domain that has a volume typically thousands of times larger than the FEA model. Several finite element nodes can be mapped to one finite volume CAFE cell face. Nevertheless, each finite element node receives a different heat flux due to a position-weighted distribution from the CAFE-to-FEA mapping subroutine.

![Figure 1](image)

**Figure 1.** (a) P/Thermal and (b) CAFE mesh of simulated SNF transportation package.
The simulated transportation cask shown in Figure 1 was engulfed in a large pool fire for 30 minutes. The oval fuel pool was assumed to be 9.3 by 13 meters. The cask was positioned so that the bottom of the impact limiters was one meter above the fuel pool as is specified by the regulations (e.g., 10CFR71.73). An initial temperature of 100°C was assumed for the entire transportation packaging system. Figure 2 shows a three-dimensional view of the CAFE fire and Figure 3 shows the P/Thermal results from the simulation. Note that the temperature distribution of the outer surface of the cask is completely non-uniform, reflecting the time and space varying heat flux from the CAFE fire. The lower conductivity impact limiting material on each end of the cask heats up faster than the solid stainless steel body due to the difference in their thermal masses. That is, the aluminum honeycomb has lower thermal conductivity and absorbs less energy than the solid steel body. In general, the relatively slow thermal response of this very massive object being engulfed creates a “heat sink effect” in the fire. This effect is captured by CAFE-P/Thermal due to the fact that these two codes are fully coupled and the heat transfer response of the fully engulfed object is fed back and taken into account for the next CAFE time step.

![Figure 2. CAFE fire engulfing a SNF transportation cask (temperatures in K).](image)

![Figure 3. P/Thermal results at 30 minutes (temperatures in °C).](image)

The cooler portions on the surface of the impact limiters on each end is due to the fact that those regions were not always fully-engulfed for the duration of the fire. This was caused by the necking of the fire, which reduces the fire diameter in regions above the pool.

**BENCHMARK OF CAFE 3D**

Since the development of the CAFE code (Suo-Anttila *et al.*, 1999), which initially was two-dimensional, there has been a continuing effort to benchmark and fine-tune this fire model by making use of relevant empirical data from experiments such as a 1m-diameter pipe calorimeter engulfed in a large open pool fire and a simulated airplane fuselage next to a large pool with different fire and wind conditions, among others. Results from some of these comparisons have been published by Kramer *et al.* (2003), Greiner and Suo-Antilla (2003), and Suo-Antilla *et al.* (2003). Just recently, a new set of experimental data (Gill *et al.*, 1998) was used to benchmark CAFE. This time, a much smaller pipe calorimeter (0.3 m in diameter) was
periodically engulfed in a 5 m round pool fire, with light and variable wind conditions. The calorimeter was positioned such that its axis was 1.5 m away from the center of the fuel pool. The results from this comparison are presented in Figures 4 and 5. The temperatures shown are at the center ring of this calorimeter. By looking at the temperature distribution of this very long pipe, it can be clearly seen how the external radiation algorithm worked at times when the pipe was not engulfed by the flames of the fire. This is a powerful feature in CAFE, because one can study the effect of offset fires to objects.

The differences between CAFE-3D predictions and the experimental data shown in Figure 5 are primarily due to the insufficient characterization of the wind boundary conditions. The wind was measured at a single location 10 pool diameters away from the fire. Thus considerable lead and lag time in both wind speed and direction occur between the measurement pole and the fire due to the low wind speed (0-1m/s), and variability in direction.

**SUMMARY**

While CAFE was originally designed to analyze packages that are used for the transportation of RAM in fully-engulfing pool fires, it has now evolved into a more general fire code that can be used to analyze almost any fire problem. In addition, it is coupled to finite element analysis codes, making this FEA-CFD combination a very powerful tool for the analysis and assessment of the performance of almost any object that is exposed to a fire environment, whether the object is fully-engulfed, partially-engulfed and/or not engulfed by the fire being modeled. While it is true that CAFE currently simulates fires in a realistic manner, it is important to recognize that there is a need for more benchmarking to assure accuracy of the code for various types of problems. Future fire experiments for the benchmark of the code are currently planned and are expected to refine and enhance the ability of CAFE to simulate the very complex thermal and chemical environment of a fire.
REFERENCES


1 Sandia is a multi-program laboratory operated by Sandia Corporation, a Lockheed Martin company, for the United States Department of Energy’s National Nuclear Security Administration under Contract DE-AC04-94AL85000.