14th International Symposium on the Packaging and
Transportation of Radioactive Materials (PATRAM 2004),
Berlin, Germany, September 20-24, 2004

Paper # 096

CALIBRATION OF THE CAFE-3D FIRE CODE WITH CONTROLLED INDOOR FIRE DATA

Carlos Lopez, Sandia National Laboratories[1], Albuquerque, NM 87185, USA
Ahti Suo-Anttila, Alion Science and Technology, Albuquerque, New Mexico, USA
Jorman A. Koski, Consultant to Sandia National Laboratories, Albuquerque, New Mexico, USA
Imane Khalil, Sandia National Laboratories, Albuquerque, NM 87185, USA

ABSTRACT

The Container Analysis Fire Environment (CAFE) code contains a computational fluid dynamics (CFD) based fire model that has been successfully coupled to standard finite element computer codes. This coupling of CFD and finite element codes allows for a more realistic modeling of the thermal performance of objects engulfed in fire, which aids in the design and risk analysis of radioactive material packages. The CAFE fire model is based on a three-dimensional finite volume formulation of basic fire chemistry and fluid dynamics. This 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 is coupled to the diffusive radiation formulation using the Rosseland approximation and the optical properties of soot.

In order to verify and improve the accuracy of computers codes, they should be benchmarked against test data. This paper describes a set of experiments that were performed at the Fire Laboratory for Accreditation of Modeling by Experiment (FLAME) fire facility of Sandia National Laboratories in Albuquerque, New Mexico, USA. The paper also describes how the data collected from the experiments was used to calibrate and benchmark the CAFE-3D fire code. Detailed description of the tests performed and comparisons between the calculated results and the collected data from the experiments are provided.

1. INTRODUCTION

The Container Analysis Fire Environment (CAFE) fire model has reached a point in its development that demands the design and performance of tests to calibrate and benchmark the various models in the code that, together, permit the realistic simulation of fires. CAFE is a three-dimensional computational fluid dynamics (CFD) and radiation heat transfer computer code that realistically simulates fires and has been successfully coupled to commercially available finite-element analysis (FEA) computer codes. This coupling facilitates the design and the study of the performance of packages that are used for the transportation of radioactive material (RAM) when exposed to fires. The CAFE fire model 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, or Linux workstations with emphasis on fast-running simulations. The FEA-CFD coupling is a very powerful tool that can be used 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, or not engulfed by the fire being modeled. Extensive testing of the coupling of CAFE with MSC PATRAN/Thermal (P/Thermal) has been performed thus far. Therefore, the CAFE-P/Thermal was used for the coupled analyses presented in this paper.

Benchmark efforts in the past demonstrate that CAFE simulates outdoor fires adequately. However, data from indoor controlled fires have never been used before to calibrate the code. It was for this reason that a set of indoor and controlled fire tests were designed and recently performed. The main purpose of this series of tests is to calibrate CAFE models of variable fuel evaporation and heat transfer to objects both inside and outside the flame zone. This paper contains discussions of the progress made so far on the calibration of CAFE by making use of the data collected from the recently performed tests and from another set of experiments that were performed at the same facility and had the same size of fire but included other valuable benchmark data. The benchmarking and calibration of CAFE with regard to heat transfer to objects, as well as how well the code is predicting the generation of combustion products and temperatures, are the main points of discussion in this paper. Calibration of the variable fuel evaporation model was not performed as part of the work presented in this paper. This data will be presented in future papers when these efforts are completed.

2. DESCRIPTION OF THE FLAME FACILITY AND CONTROLLED TESTS

The Fire Laboratory for Accreditation of Modeling by Experiment (FLAME) facility at SNL was constructed for the purpose of generating data for validation of fire CFD codes. A schematic of this facility is shown in Figure 1. The facility is an enclosure, which allows the experimenter to burn a controlled large two-meter fire without the complications encountered when performing outdoor fire test such as wind. A large chimney is located above the ceiling to provide an exit path for the products of combustion. The walls of the facility are water cooled to simulate the radiative environment of an outdoor fire. A set of 4 fans provides 7.55 m^3/s of combustion air at standard conditions, which is injected vertically at floor level through a series of honeycomb flow straighteners. The flow straighteners provide a uniform upward flow condition to simulate an outdoor no-wind environment. Additional details of the FLAME facility and the characterization of the air source at this facility are discussed in Blanchat [1]. A 2.7 m high pedestal is located in the center of the room upon which a 2 m diameter pan fire is situated. Generally, JP8 jet fuel is floated upon a layer of water within the pan to perform the fire tests.

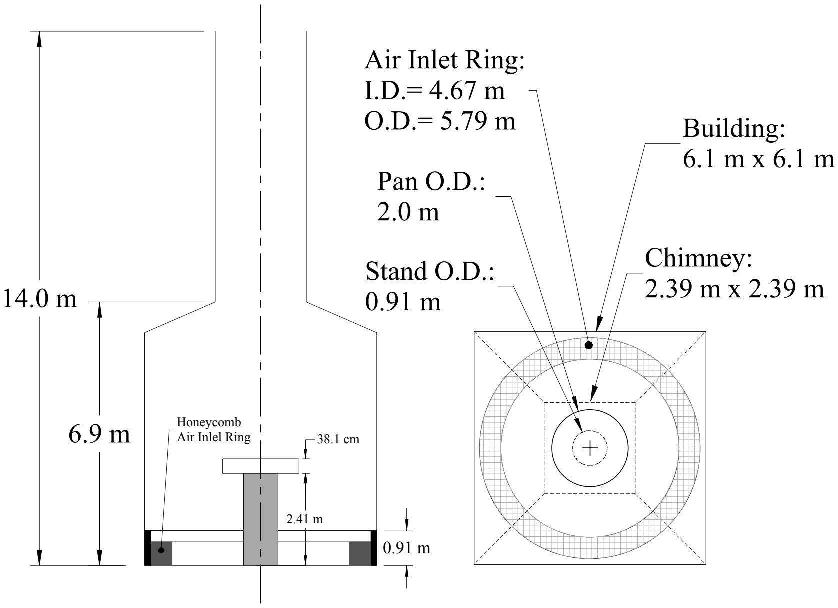

Figure 1. Schematic of the FLAME facility at Sandia National Laboratories

Experimental measurements include heat fluxes and temperatures at various locations within the room and within the fire. In addition, within the fire, measurements of the soot volume fraction and extinction coefficient were made at several locations using lasers and other optical diagnostics. Two-color optics provide a measurement of the soot temperature, and an independent measurement of the soot volume fraction. Outside the fire, heat fluxes were measured with both Gardon and Sandia Heat Flux gauges [2]. Measurements were made for a number of fires and the results were compiled into a report by Murphy and Shaddix [3]. The experimental data were repeatable from one fire to the next, thus these data can be used for validation of fire models such as CAFE. Additional detail on experiment conduct, data reduction and results can be found in Murphy and Shaddix [3, 4].

In addition to the earlier tests of Murphy and Shaddix, several new tests were run with additional diagnostics. Several floating thermocouples were placed along the centerline of the fire at various heights to measure temperature within the fire field. Three independent and concentric annular fuel pool rings of equal area were used as fuel pans to allow for the measurement of the evaporation rate of fuel as a function of pool radius. The evaporation rate in each concentric pool was measured with differential pressure gauges. In each test, fuel was added until a small layer of fuel covered all concentric pools. This was done to ensure a common starting point for all pools and monitor the recession rate of each pool as they started to burn independently. The information gathered from these experiments will help in characterizing the variations of the fuel recession rate within the pool. This information is valuable for the benchmark of the variable evaporation model in CAFE.

To measure the heat transfer from the fire to an engulfed object, two small calorimeters (approximately 0.3 m diameter, 0.4 m length, attached at one end to each other) with multiple thermocouples mounted on the interior walls were placed 0.5 m above the center of the pool in two of the tests. In addition to the new diagnostics, heat flux data was obtained using both Gardon and Sandia heat flux gauges outside the fire at various locations. Heat flux to the surface of the pool was estimated using 12 Sandia HFGs mounted in the pool facing up to measure the heat transfer from the fire to the pool surface. Figure 2 contains three pictures from a test in this new series of experiments. Figure 2(a) shows the calorimeter inside the fire at ignition, while Figure 2(b) and Figure 2(c) show the calorimeter partially and fully engulfed, respectively, as the fire spreads and grows with time. Figure 2(c) also illustrates fire puffing which is the reason for the mushroom shape near the top of the picture. The calorimeters were fully engulfed within a minute after initial fuel ignition.

Figure 2. Controlled indoor fire (a) at the moment of ignition, (b) spreading over the pool, and (c) fully developed.

The fire durations were fairly short, on the order of 10 minutes. However, the period of useful data was about 5 minutes. Within the first minute, the fire is in a transient growth stage, and the fuel level is above the lip of the annular rings in the fuel pan. Early in the fire, the three annular fuel pans communicate their depths and independent recession rates do not occur. After 5 minutes the innermost ring of fuel burns out reducing the overall fuel evaporation rate and the subsequent burn data. Data after 5 minutes was not considered in this report for comparison with CAFE predictions.

The fire tests were conducted with and without the cylindrical calorimeters in place. Transient temperature data on the inside surface of the calorimeters was obtained. The recorded temperature response of the calorimeter was used to compare and benchmark the predictions from CAFE.

3. DESCRIPTION OF NUMERICAL MODEL

A CAFE code input file describing the interior of the FLAME facility was constructed. The enclosure was modeled to its measured dimensions. The chimney was shortened although the cross sectional area was kept the same. A shorter chimney was used to reduce the number of computational cells. The shortened chimney does not affect the fire because the air flow rate through the structure was set by the combustion air fans, not natural ventilation. The number of computational cells was 43 by 43 in the horizontal plane by 34 cells high. A variable grid structure was used throughout to better resolve the details of heat transfer in the region of the calorimeter. A coarser cell structure was used in locations away from the fire. This CAFE model is illustrated in Figure 3.

The air flow into the facility was injected vertically as a constant air flow velocity boundary condition in an annular ring on the floor, quite similar to the actual air injection method. The annular ring had the same geometry as the actual honeycomb mesh that was used in the experiment. The pan fire was approximated by three annular rings, which inject fuel vapor at the measured rates. No attempt was made to allow the model to predict the evaporation rate since all other diagnostics depend upon the fire burn rate, thus a small error in evaporation rate would lead to errors in all other measurements. Future simulations will include a prediction of the fuel evaporation rate based upon local fuel surface heat fluxes.

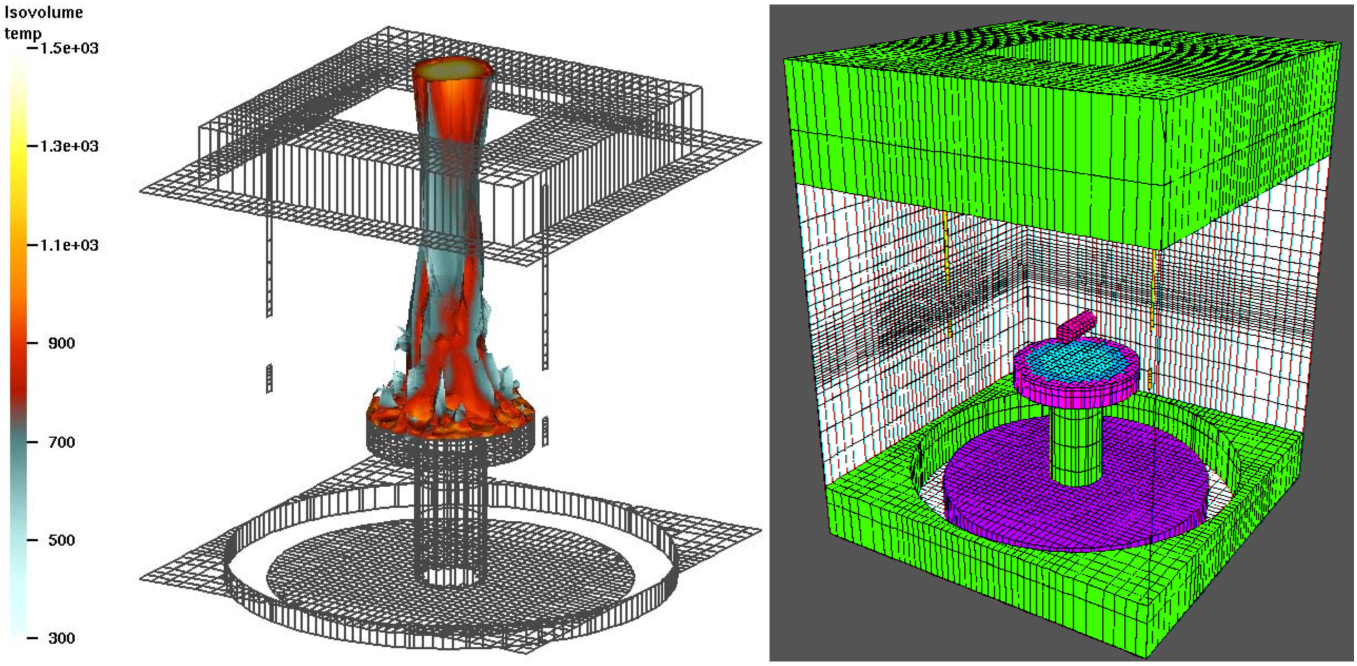

Figure 3. CAFE model of the FLAME facility with and without fire present, respectively. Strips to the left and right of the pedestal represent heat flux gauge arrays.

The external Sandia heat flux gauges were modeled in one-dimension. The one-dimensional model included the thin faceplate, a one-dimensional approximation of the 1/8-inch thermocouple, and the backing insulation. This allowed a prediction of both the transient heat-up and the steady state temperature of the Sandia heat flux gauges.

The cylindrical calorimeter was modeled with its actual geometric size and shape. Temperature dependent thermophysical properties of 304 stainless steel were used in the simulations. Three floating thermocouples placed at 0.25, 2, and 4m above the center of the pool were not explicitly modeled, however the local gas temperature at the same location as the thermocouples were compared to the experimental data. The thermocouple temperature is a balance between incoming radiation, outgoing radiation, and convective effects. When temperature gradients within the fire are small, the local gas temperature and radiation temperature are very close to one another due to the short radiation mean free path (approximately 8 cm). However, when large thermal gradients are present, the thermocouple temperature is not expected to equal the local gas temperature since the thermocouple can radiate to cooler surroundings as well as receive heat from hotter surroundings.

The combustion/soot formation model that was used in the simulations presented in this paper was the same as that of Greiner and Suo-Anttila [5], with slight modifications in the reaction coefficients. Previously, the reaction coefficients were determined by comparison to a single data point, Gritzo [6]. The reaction coefficients were modified based upon new soot volume fraction data that has become available with the set of experiments by Murphy and Shaddix. Modifying the reaction chemistry allows the present model to predict soot volume fractions within the fire that are similar to those measured by Murphy and Shaddix [4].

The turbulence model affects the combustion chemistry through the eddy breakup model in CAFE. Adjustments were made to the turbulence length scale such that better agreement between predicted and measured soot volume fraction and extinction coefficients were obtained. The CAFE combustion model is not very sensitive to the turbulence model because it includes both Arrhenius and eddy breakup effects. For intense turbulence levels, the Arrhenius model dominates the combustion rate, whereas for low levels of turbulence the reaction rate is slowed by the eddy breakup model. The combination of both models reduces the combustion rate sensitivity to turbulence levels. In the model, species and temperature dependent thermophysical properties were used for air, fuel vapor, soot, and products of combustion. Convective heat transfer to the calorimeter was modeled as crossflow over a cylinder.

4. COMPARISON TO FLAME FACILITY EXPERIMENTS WITHOUT CALORIMETER IN FIRE

Results from the stand-alone CAFE code were compared to the experiment designated DOE-RW3 and to previous experiments conducted in the same facility under similar conditions by Murphy and Shaddix [4]. For these experiments, the central zone of the fire was open, without the presence of the calorimeter. In the results of Murphy and Shaddix, tunable dye laser absorption spectroscopy was used to measure soot properties and species concentrations in the FLAME facility. This also enabled Murphy and Shaddix to report fire temperatures, soot volume fraction and extinction coefficients as a function of height above the pool fires.

For the CAFE simulations, fuel mass fluxes of 0.022, 0.025 and 0.037 kg/m^2-s were used for the outer, middle and inner fuel rings, respectively. These values were taken from inspection of Figure 4 as typical of the fuel evaporation rate during the first 300 s of the fire. Mass fluxes shown in Figure 4 were derived from a smoothed first derivative with respect to time of the static pool pressure that was measured for each fuel ring during the fire. Later fluctuations in the mass flux are likely caused by water evaporation as the fuel is exhausted. The inner fuel ring was exhausted approximately 500 s after ignition.

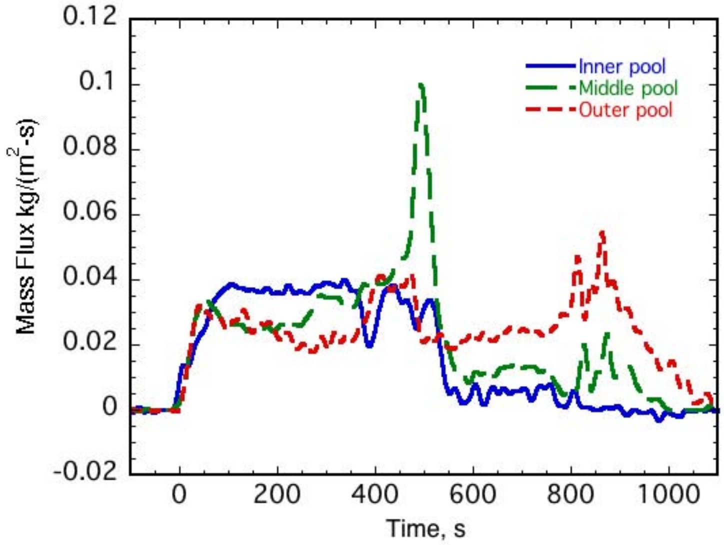

Figure 4. Mass flux from pool surface as a function of time.

To compare the data from experiment and CAFE simulations, approximate probability density functions (PDFs) were constructed for both simulation and experiment. Data were counted into fixed-width bins and the probability for each bin was determined by dividing the individual bin counts by the total number of data points. For consistency, the same binning scheme used by Murphy and Shaddix was also used for the CAFE results. Bins of 20 Kelvin width for temperature and 0.05 ppm width for soot volume fraction were used. For all comparison plots in this section, heavy lines are used to represent experimental data, while thinner lines represent CAFE simulation results. Line style and color is consistent at each elevation above the fire.

Figure 5 shows temperature PDFs for both CAFE and experiment at various heights above the center of the pool. The CAFE temperatures exhibit narrower, higher peaks than the experimental data, but peak temperatures are in the same 1100 to 1300 K range. CAFE soot temperatures also exhibit the same general pattern as the experimental data. The peak temperatures and general distributions are also generally consistent with the PDFs calculated by Koski [7] with data from large outdoor pool fires. Soot volume fraction data from CAFE output and Murphy and Shaddix [4] experimental values are shown in Figure 6. This figure shows that the CAFE data are significantly more peaked than experiment. However, the CAFE soot volume fraction values with higher probability of occurrence are in the same numerical range of those mean values reported by Murphy and Shaddix[4].

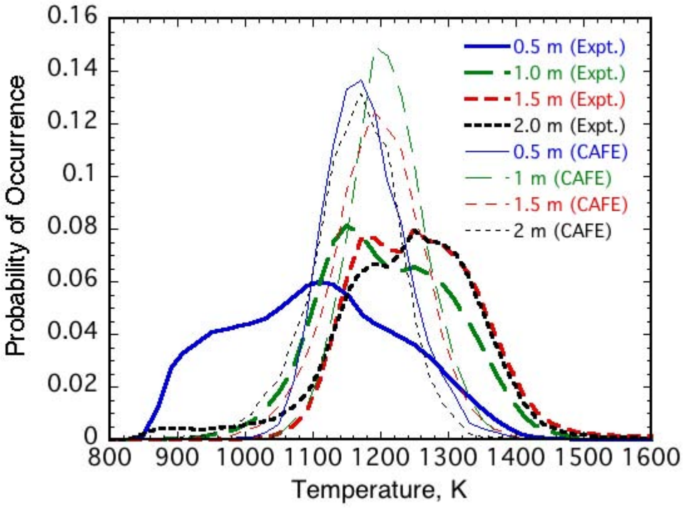

Figure 5. Comparison of temperature distributions at various heights above pool center for experimental results and for CAFE simulations.

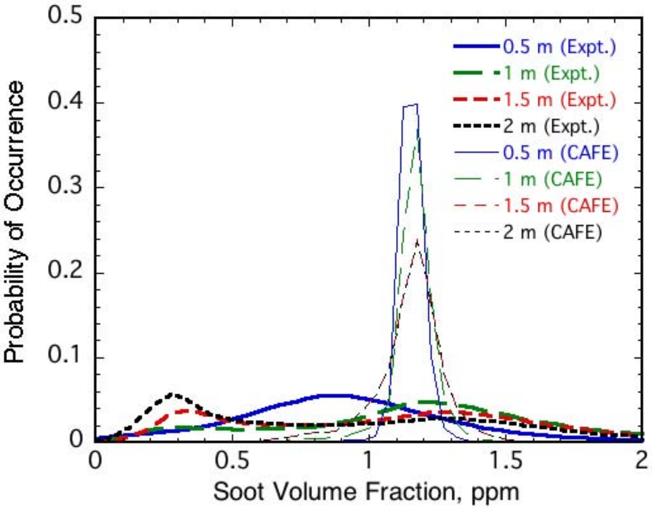

Figure 6. Comparison of soot volume fraction distributions at various heights above pool center for experimental results and for CAFE simulations.

Extinction coefficient distributions at various elevations above the pool center during the simulated fire are presented in Figure 7. The highest values of extinction coefficient occur at the 0.5 m elevation, and decrease with elevation. A plot of the mode values (peaks) of the CAFE data are compared to values reported in Murphy and Shaddix [4] in Figure 8. CAFE simulation values are again within the range of experimental results. These results indicate that radiant thermal energy emitted from the fire drops by a factor of 1/e (e = 2.718…) over a distance shorter than 0.1 m. High attenuation over short distances confirms the validity of the Rosseland approximation for optically thick media that is used for thermal radiation transport in the CAFE fire model.

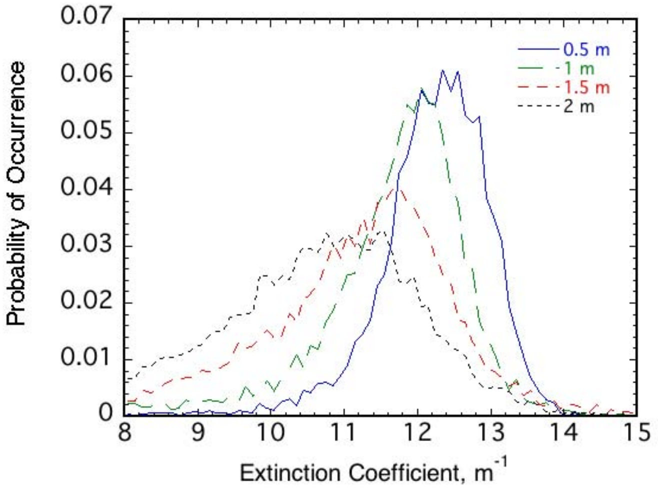

Figure 7. Distribution of extinction coefficient values for various elevations above pool center calculated from CAFE simulations.

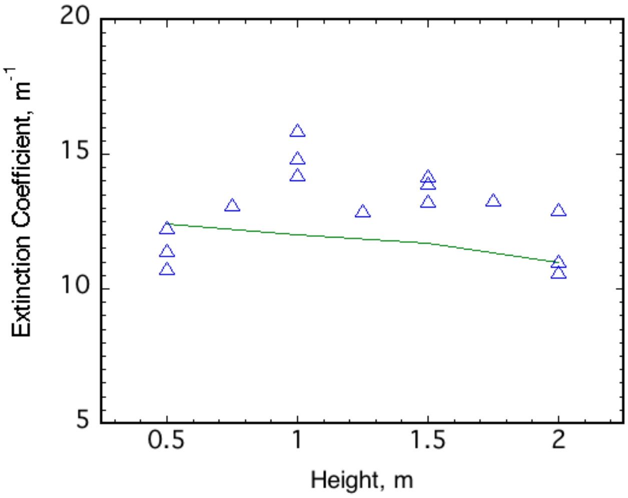

Figure 8. Extinction coefficient values for various locations above pool center. Experimental values are triangles. The line represents peak values calculated by CAFE.

CAFE simulations for temperatures at 0.25, 2, and 4m above the center of the pool are compared to bare sheathed thermocouple data for those locations from experiment DOE-RW3 in Figure 9. Good agreement is seen at the elevation of 2 m above the fire, but experimental values are consistently lower than the 0.25 and 4 m CAFE simulations. Note that the trends are consistent, in that both CAFE and experiment have peak temperatures near 2 m, and lower temperatures above and below that elevation. The thermocouple temperatures measured at the extreme locations (0.5m and 4m) may be in the range where significant thermal gradients exist in the fire. If this is the case, then thermocouple temperatures are not a reliable indicator of local gas temperature.

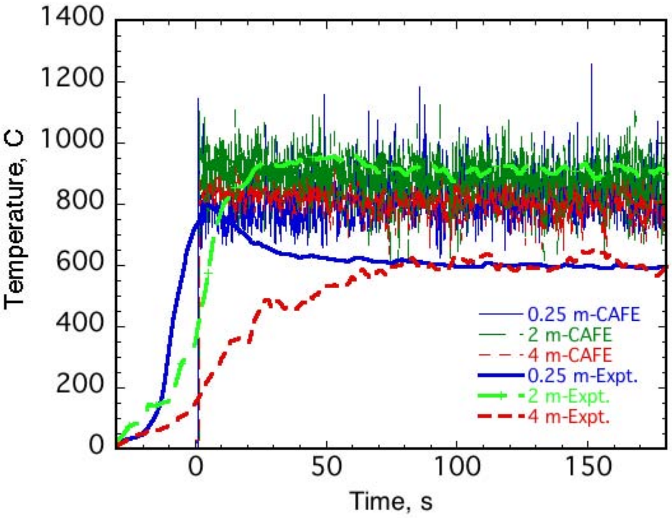

Figure 9. Experimental thermocouple measurements above the pool center compared to CAFE calculated temperatures for the same locations.

Data from the Heat Flux Gauges (HFGs) compared to CAFE simulations is shown in Figure 10 and Figure 11. Two vertical arrays of four HFGs each were placed outside the fire with active faces toward the fire. Four HFGs elevations were evenly spaced from 0.2 m below pool level to 3.3 m above pool level on a pole located 0.4 m from the pool edge. The other four HFGs were mounted on the wall of the test facility about 1.75 m from the pool edge. HFG 1 is at the lowest elevation.

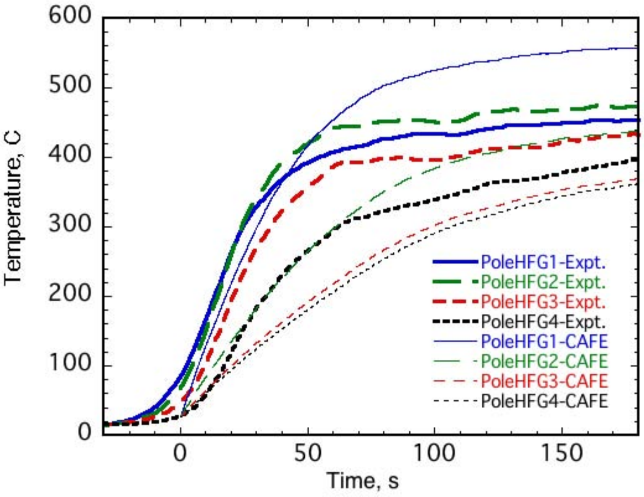

Figure 10. Experimental heat flux gauge temperatures compared to CAFE values at a pole adjacent to fire.

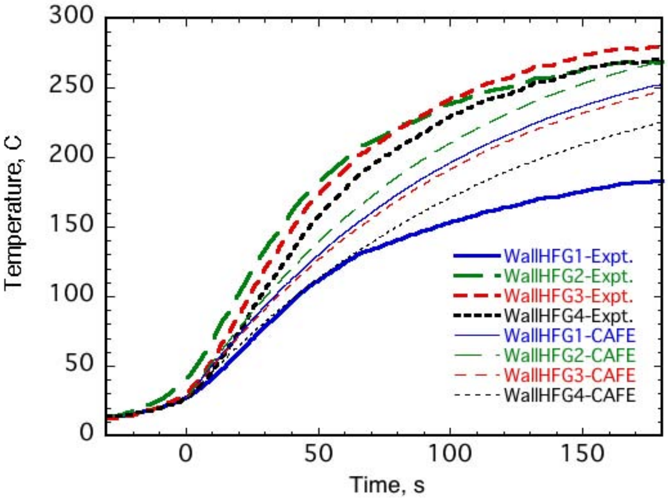

Figure 11. Experimental heat flux gauge temperatures compared to CAFE values on the wall of FLAME.

Note that because the HFGs are mounted outside the fire zone, the CAFE code calculates the heat transfer to these objects with a gray diffuse thermal radiation (T^4 law) model. The view factor from the fire to the object is calculated in the CAFE code by placing a hypothetical isosurface at a soot volume fraction of 0.5×10^{-6} within the fire zone, and then calculating a fire temperature to apply to the hypothetical surface. Thermal radiation heat transfer to objects outside the fire can then be calculated. The soot volume fraction used for the calculation is an input parameter, and the value of 0.5×10^{-6} has been empirically determined to yield reasonable results.

Heating of the pole mounted HFGs is shown in Figure 10, where both experiment and CAFE simulations heat into the same general 300 to 500°C range at similar heating rates. Again, experimental values are thick lines, and comparable CAFE values are thinner lines. In order to make a direct comparison, a 30-second delay to allow for fire ignition was subtracted from the ignition start time of the experimental data. By adjusting the geometry, material density, and specific heat in the one-dimensional model of the Sandia HFG in the CAFE simulation, the curves could be brought into better alignment. The Sandia HFG is actually a three-dimensional device, which can be approximated as a one-dimensional device as done in this work. However, such simplification introduces errors in the thermal response of the system. Nevertheless, the unadjusted results are shown here to give an idea of the general accuracy of the approach without such adjustments.

The wall-mounted HFG results from the CAFE model are compared to the experimental values in Figure 11. Agreement is generally better than for the pole locations, with the temperatures heating into the same 200 to 300°C band. The departure from the group of the experimental trace for Wall HFG 1 is attributed to detachment of the thermocouple from foil surface of that HFG prior to the experiment.

5. COMPARISON TO FLAME FACILITY EXPERIMENTS WITH CALORIMETERS IN FIRE

The heat transfer response of two calorimeters was monitored in the tests identified as DOE-RW1 and DOE-RW2. In these two tests, two small calorimeters were attached at one end to each other and the junction of the two placed 0.5 m above the center of the fuel pool. Each calorimeter is approximately 0.4 m long and 0.3 m in diameter with a wall thickness of 3.2 mm. Each calorimeter was instrumented with multiple thermocouples mounted on the interior wall to measure the heat transfer from the fire to an engulfed object. Repeatability of the results was confirmed with the redundant tests. Because of the similarity of the response of the calorimeters between themselves and between the two tests, the response of only one calorimeter and during test DOE-RW1 was used for the comparisons presented in this paper. For additional simplicity, temperature histories measured from only four out of the twelve internal thermocouple locations in the selected calorimeter are presented. These four thermocouples were spaced 90 degrees apart starting at the upper most point. Figure 12 shows a comparison between the measured and calculated temperatures at these four locations. The experimental data is shown from the time when the calorimeter stared to heat up and was truncated to about 400 seconds after that, which is when the fuel in the pools started to burn out. The calculations shown were performed using CAFE in stand-alone form and coupled with P/Thermal.

As shown in Figure 12, the calculated temperature around the inside wall of the calorimeter are in good agreement with the measured temperature data. The calculated temperatures at the four locations seem to be converging to a steady state value of about 900 K, which agrees with measured data at two locations (lower and right) but is hotter than the measured temperature at two other locations (upper and left). The hotter temperature predictions suggest that the fire may have been somewhat tilted to the right and CAFE didn't predict such behavior. CAFE appears to be predicting nearly uniform conditions around the calorimeter, indicating a simulation of a perfectly straight up fire. It is currently unknown if the fire actually tilted in any way to one side. It is possible that some of the test diagnostics such as HFGs and non-uniformities in the combustion air injection may have caused or contributed to the asymmetries. Future investigation of the available test data and videos of the fire test will be performed to try to understand the behavior of the test data.

The calculated temperatures from CAFE stand-alone and CAFE-P/Thermal agree very well as expected. Relatively minor differences between these two calculations are understood to be due to the fact that CAFE-P/Thermal calculated three-dimensional response of the engulfed object while CAFE uses a one-dimensional heat conduction model to track the heating of the engulfed object when run in stand-alone form. These differences could be magnified if a thick-walled object were to be used instead of the thin-walled calorimeter used in these experiments. Therefore, the use of CAFE-P/Thermal is highly recommended when analyzing thick-walled and multilayered objects such as spent fuel transportation casks.

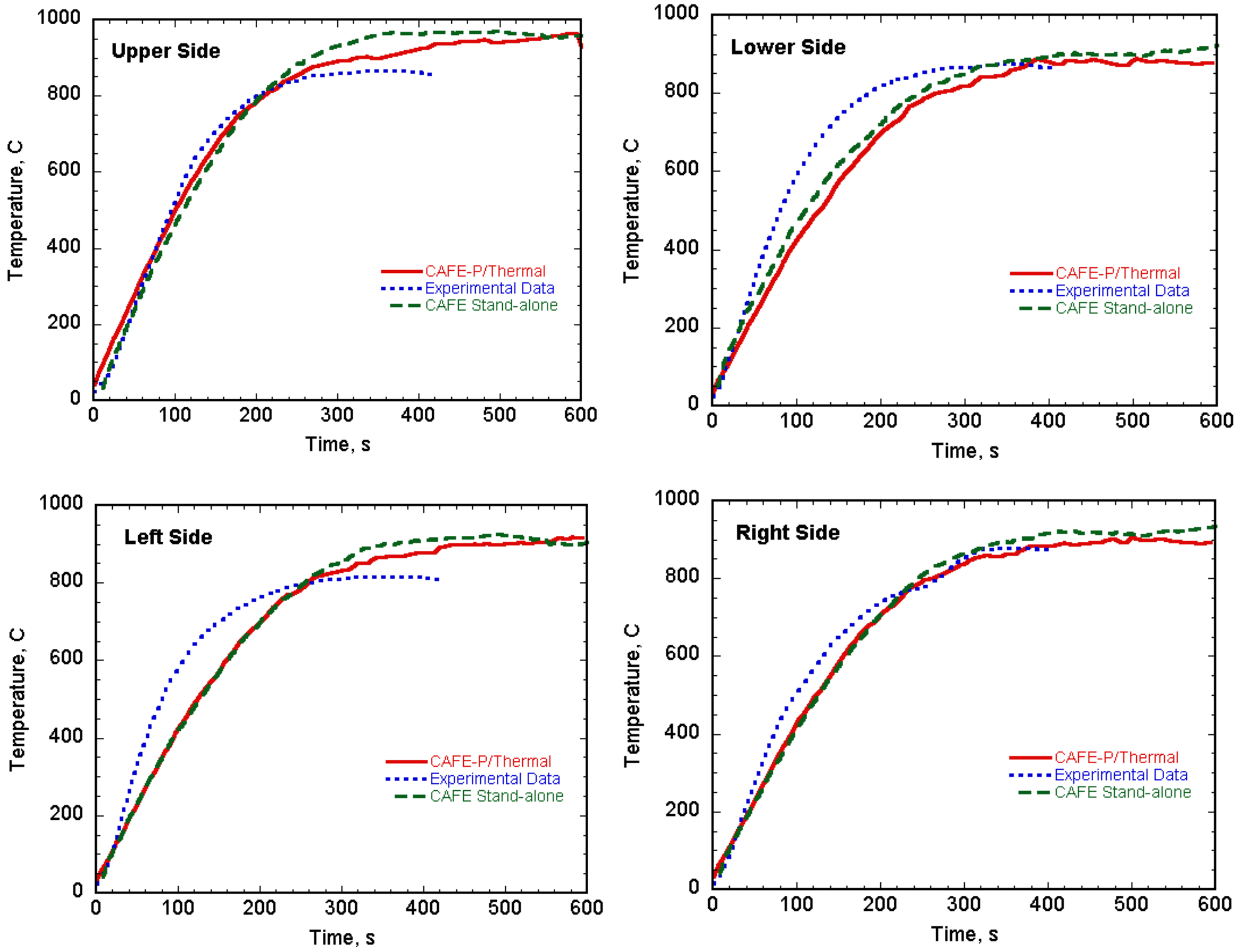

Figure 12. Comparison of the temperature history predicted by CAFE stand-alone and CAFE-P/Thermal against experimental data collected at four locations 90 degrees apart around the inside wall of the engulfed calorimeter.

6. SUMMARY AND CONCLUSIONS

Data indicated that the center fuel ring had the highest evaporation rate and burned out first. Although mass fluxes vary greatly from ring-to-ring and from time-to-time, constant evaporation rate values were used for each ring in these simulations. Future CAFE development efforts will concentrate on the calibration of the variable fuel evaporation rate model using the data collected in these experiments.

Comparison of approximate distributions of data for temperature, soot volume fraction, and extinction coefficient demonstrates that values calculated within the CAFE code are in the same general range as the experimental values reported by Murphy and Shaddix [4].

Sheathed thermocouples above the pool center had good agreement with CAFE values 2 m above the pool, but, while the overall trends were consistent, experimental temperatures were lower at 0.25 and 4 m above the pool. The lower values are in the locations where temperature gradients in the fire are significant and thermocouple measurements are unreliable as an indicator of local gas temperature.

Wall and pole HFGs located outside the fire zone yielded experimental values for temperature and heating rates that compared well with the CAFE calculations. Although the agreement could have been improved through adjustment of properties and other parameters within the CAFE input file, these adjustments were not made to show the general level of accuracy that could be expected.

CAFE comparisons to an engulfed calorimeter show good agreement for the heat flux on the top and one side of the calorimeter. Discrepancies are noted for the bottom and the other side of the calorimeter. It is not known why the experimental data showed an asymmetry in the heat flux since fire conditions were designed for symmetry. This unexpected asymmetry will be further investigated.

In general the CAFE predictions agree quite well for a large number of experimental diagnostics ranging from temperatures, soot volume fractions, radiation extinction coefficients and heat fluxes at a wide range of positions. The CAFE code in its present state is reasonably well calibrated for indoor fires in the two-meter diameter range. Comparisons for larger fires have been made [5] but a significant number of experimental data for larger fires is not yet available. Larger and outdoor pool fire tests are planned for the near future to further benchmark the CAFE code.

7. REFERENCES

[1] T.K. Blanchat, *Characterization of the Air Source and the Plume Source at FLAME*, SAND2001-2227, Sandia National Laboratories, Albuquerque, NM, July 2001.

[2] T.K. Blanchat, L.L. Humphries, and W. Gill, *Sandia Heat Flux Gauge Thermal Response and Uncertainty Models*, SAND2000-1111, Sandia National Laboratories, Albuquerque, NM, May 2000.

[3] J.J. Murphy and C.R. Shaddix, *Soot Properties and Species Measurements in a Two-Meter Diameter JP-8 Pool Fire*, SAND2003-8246, Sandia National Laboratories, Livermore, CA, June 2003.

[4] J.J. Murphy and C.R. Shaddix, *Soot Properties and Species Measurements in a Two-Meter Diameter JP-8 Pool Fire: 2003 Test Series*, SAND2004-8085, Sandia National Laboratories, Livermore, CA, March 2004.

[5] M. Greiner and A. Suo-Anttila, *Validation of the ISIS-3D Computer Code for Simulating Large Pool Fires Under a Variety of Wind Conditions*, Proc. of the 2003 ASME Pressure Vessel and Piping Conference, Cleveland, Ohio, PVP2003-2146, PVP-Vol. 467, pp. 101-112, July 2003. (To appear in the J. Pressure Vessel Technology)

[6] L.A. Gritzo, Y.R. Sivathaunu, and W. Gill, "*Transient Measurements of Radiative Properties, Soot Volume Fraction, and Soot Temperature in a Large Pool Fire,*" Combustion Science and Technology, Vol. 139, pp. 113-136, 1998.

[7] J.A. Koski, *Measurement of Temperature Distributions in Large Pool Fires with the use of Directional Flame Thermometers*, in Proc. 2000 ASME Pressure Vessels and Piping Conference, Seattle WA, July 23-27, 2000.

---

[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.