Large Eddy Simulations of Fire Tests in a Large Hall

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In cooperation with the fire protection engineering community, a numerical fire model, Fire Dynamics Simulator (FDS), is being developed at NIST to study fire behavior and to evaluate the performance of fire protection systems in buildings. Version 2 of FDS was publicly released in December 2001 [1, 2]. The model is based on the low Mach number form of the Navier-Stokes equations and uses a large eddy simulation (LES) technique to represent unresolved, sub-grid scale motion. The fire is modeled by solving a transport equation for the conserved scalar quantity known as the mixture fraction, a linear combination of the fuel and oxygen that indicates the mass fraction of the gas originating as fuel. The advantage of the mixture fraction approach is that all of the species transport equations are combined into one, reducing the computational cost. Thermal radiation is modeled by solving the radiative transport equation for a non-scattering gray gas using what is known as the Finite Volume Method [3]. Using approximately 100 angles, the finite volume solver requires about 15% of the total CPU time of a calculation, a modest cost given the complexity of radiation heat transfer.

FDS has recently been applied to a series of benchmark fire tests performed as part of the "International Collaborative Project to Evaluate Fire Models for Nuclear Power Plant Applications." The tests analyzed here make up Benchmark Exercise #2. Three fire tests were performed in a large fire test hall. In each, a pool of heptane was burned for about 5 minutes, during which time gas temperatures were measured in three vertical arrays and at two points within the fire plume. The fire size and ventilation configurations were changed from test to test. Details of the tests can be found in these same proceedings.

The heat release rate of the fires in each case was calculated from the measured mass loss rate of fuel, thus the model is not making a prediction of the total energy output. While it is possible to predict the fraction of the total energy output that is emitted from the fire as thermal radiation, we chose to apply an empirical fraction of 35 % based on numerous experiments. The purpose of the numerical model in this exercise is to predict how the energy from the fire is transported throughout the test hall as a function of time. The key to handling this problem properly is to simulate well the mixing of hot combustion products and fresh air within the fire plume. The technique adopted by FDS for this purpose, Large Eddy Simulation (LES), is not widely used in the fire community because of the extensive development of various Reynolds-Averaged Navier-Stokes (RANS) models, some of which are demonstrated within these proceedings. The benefit of LES over RANS is that it renders a more faithful representation of the fire and plume dynamics because it captures fluid motion at length and time scales consistent with the underlying numerical grid. For example, animations of the fire and smoke plume show the pulsating and oscillating behavior observed in actual experiments. With the RANS approach, this motion is filtered out and the fire and plume are rendered as time-averages of the actual flow fields. While both approaches have been demonstrated to work in a variety of fire applications, we believe that that LES approach will eventually be adopted more widely because of its more faithful rendering of fire behavior.

Of course, the outcome of an LES calculation is only as good as the underlying numerical grid. If the governing equations of motion are approximated on a numerical grid whose cells are too large relative to the characteristic length scales of the fire or fire plume, not only will the realistic fluid dynamics be lost, but the mixing will be under-estimated, and in the case here, the upper layer temperatures predicted by the model will be hotter than those measured. For this reason, up to now the LES technique has not been considered of practical use to the fire protection engineer. What has made the technique useful is faster, cheaper computers and better numerical methods. A recent advancement for FDS has been the implementation of multiblock gridding, that is, the use of more than one structured numerical grid in a single simulation. Until recently, FDS used a single uniformly-spaced rectangular mesh to divide up a largely rectangular space into hundreds of thousands or millions of cells. The benefit is ease-of-use, the downside is that it is difficult to adequately resolve the numerical grid in regions of interest, like the fire plume, when a large space is to be modeled. Preliminary calculations of the benchmark fire tests required on the order of 80 CPU hours on a 1.7 Ghz Pentium IV processor. By using more than one numerical grid, the CPU time was reduced to 20 hours, and the resolution in the region of the fire and plume was improved.

The figures in the accompanying presentation show the geometry of the test hall and the layout of the various numerical grids used in the simulation. The finest grid surrounding the fire is 4 m by 4 m by 10 m high, with grid cells 13 cm on a side. Five other separate grids are used to cover the rest of the space at a resolution of 40 cm. Within each grid, the cells are uniform in size. In all, 216,000 grid cells are used in the calculation. Ten minutes of real time are simulated. Some simplifications to the geometry include making the burner and the exhaust duct square rather than round, and approximating the sloped ceiling as a series of stair steps. Otherwise, everything else is as specified in the problem description. Heptane (C_7H_{16}) is used as a fuel. Temperature and velocity predictions are recorded at all of the specified locations.

The results of the three calculations agree well with the measurements. For Test 1, the predicted temperatures at the 5 upper thermocouple locations in each array are within 10 °C of the measured temperatures, usually on the high side. The lower 5 temperature locations show good agreement as well, with the greatest difference being for the lowest two thermocouples, which under-predict the measured temperatures by roughly 10 °C. Given slightly higher temperatures in the upper layer, it is not surprising to see slightly lower temperatures somewhere else since the model is energy conserving. The model assumes that there is no air movement in the hall except for that induced by the fire or the ventilation system, thus one would expect for the level of mixing to be slightly under-predicted. The prediction of the temperature at the lower thermocouple location in the fire plume is about 100 °C higher than the measurement. The prediction at the higher location is about 10 °C higher.

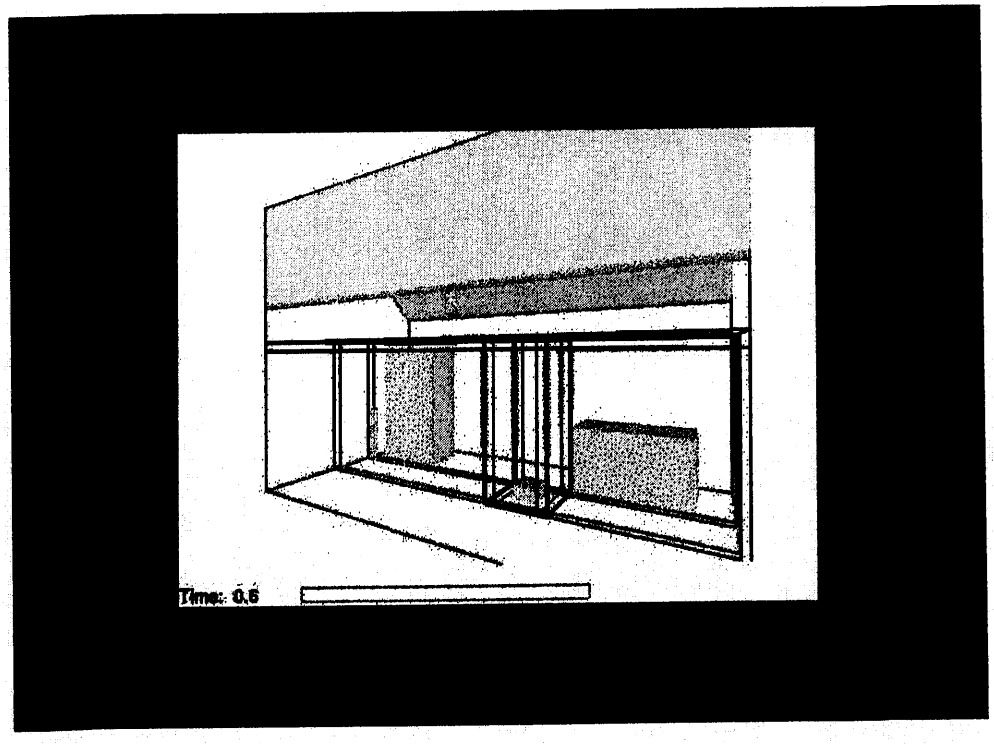
For Test 2, the agreement between model and experiment is better than in Test 1. The reason for this is that the predicted and measured temperatures within the plume are within 10 °C of one another. The simulations of Tests 1 and 2 were conducted with the exact same gridding and assumptions. The reason for the better agreement in Test 2 stems from the better agreement in the plume itself. In general, for a given level of grid refinement, a larger fire is easier to model than a smaller one, as in this instance. Another explanation of disagreement in plume temperatures is that often in large scale fire tests air movements within the test space throw the fire plume slightly off of its natural centerline, in which case numerical predictions are often high. In any case, in all three tests, the agreement between model and experiment at the upper plume thermocouple location is within 10 °C meaning that the gases filling the hot upper layer are within a very close range to the actual gas temperatures.

When these calculations were first attempted with a single numerical grid spanning the entire hall with cells between 20 and 30 cm in size, the temperatures in the upper layer were over-predicted. The difference in predicted and measured temperatures was reduced as the grid cells in the region of the fire were reduced in size. This effect is made obvious by looking at animations of temperature contour plots through a vertical centerline plane. When the grid cells are too large to resolve the eddies that entrain fresh air into the plume, the hot gases are not diluted as much in the simulation as in reality, and upper layer temperatures tend to be over-predicted. As in many studies we have performed in the past on fire plumes, we find that very good agreement with experiment is achieved when the fire is spanned by roughly 6 to 8 grid cells. Of course more is better, but this level of resolution has been found to produce very good results at a modest computational cost. Research continues to reduce computational effort by means of the multiple grids employed here, plus parallel processing of the different grids.

[1] K.B. McGrattan, H.R. Baum, R.G. Rehm, G.P. Forney, J.E. Floyd, and S. Hostikka. Fire Dynamics Simulator (Version 2), Technical Reference Guide. Technical Report NISTIR 6783, National Institute of Standards and Technology, Gaithersburg, Maryland, November 2001.

[2] K.B. McGrattan, G.P. Forney, J.E. Floyd, and S. Hostikka. Fire Dynamics Simulator (Version 2), User's Guide. Technical Report NISTIR 6784, National Institute of Standards and Technology, Gaithersburg, Maryland, November 2001.

[3] S. Hostikka, H.R. Baum, and K.B. McGrattan. Large Eddy Simulations of the Cone Calorimeter. In *Proceedings of US Section Meeting of the Combustion Institute, Oakland, California*, March 2001.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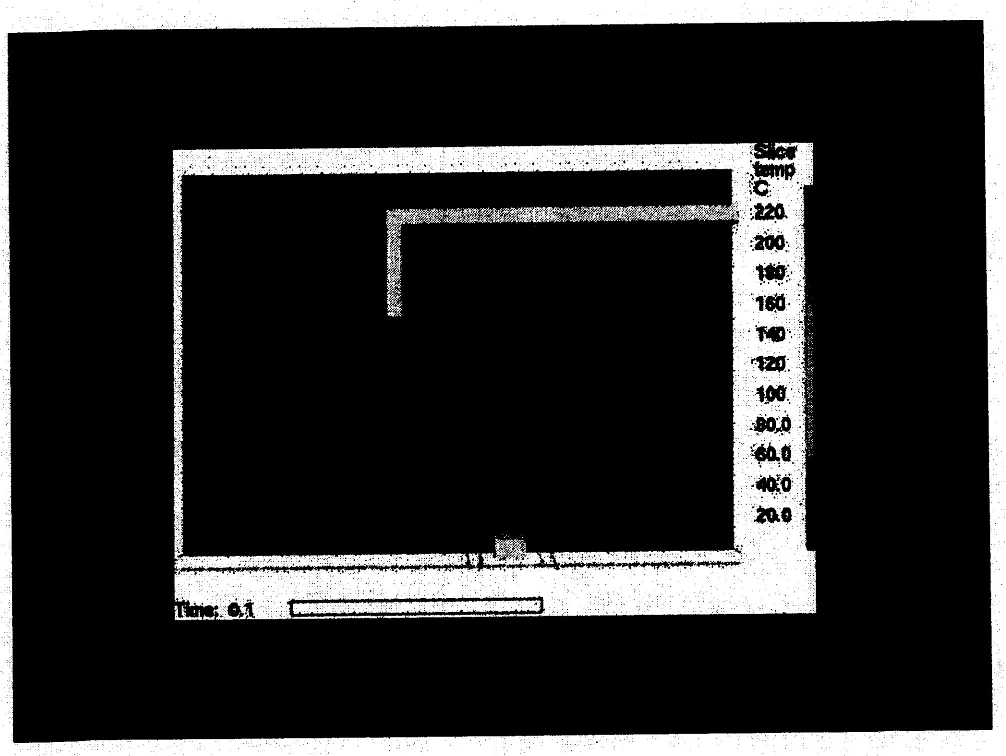
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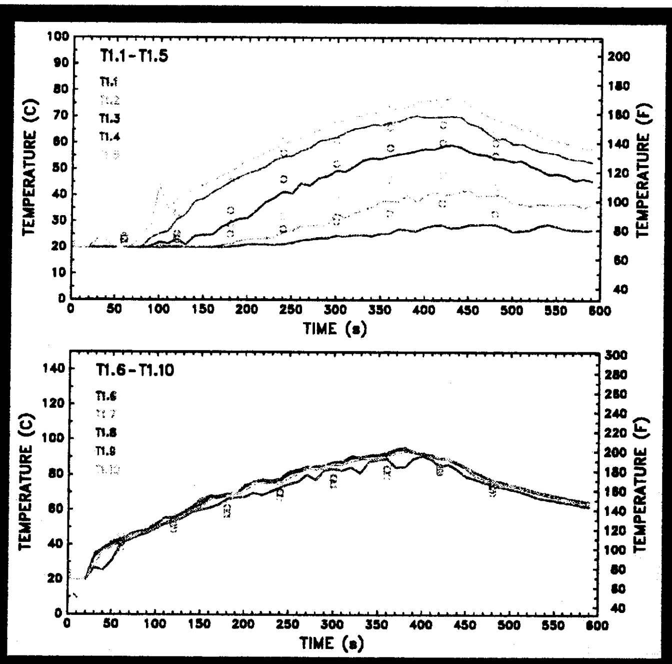

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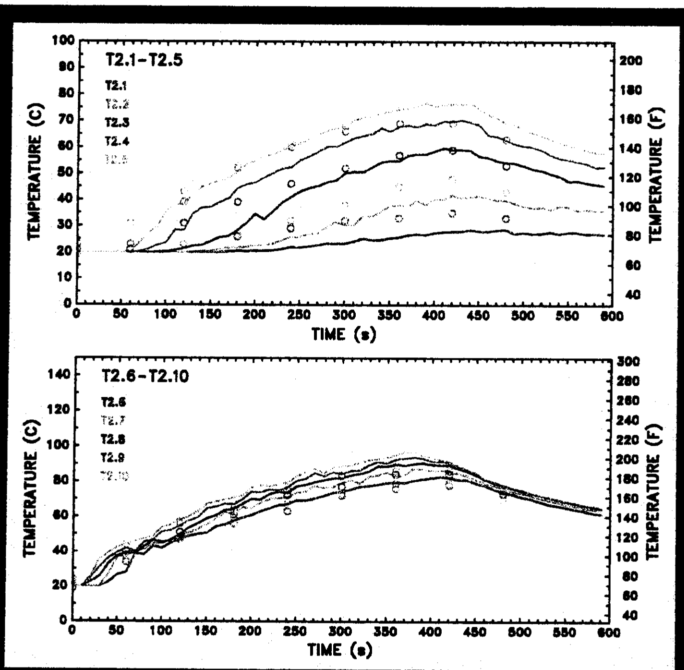

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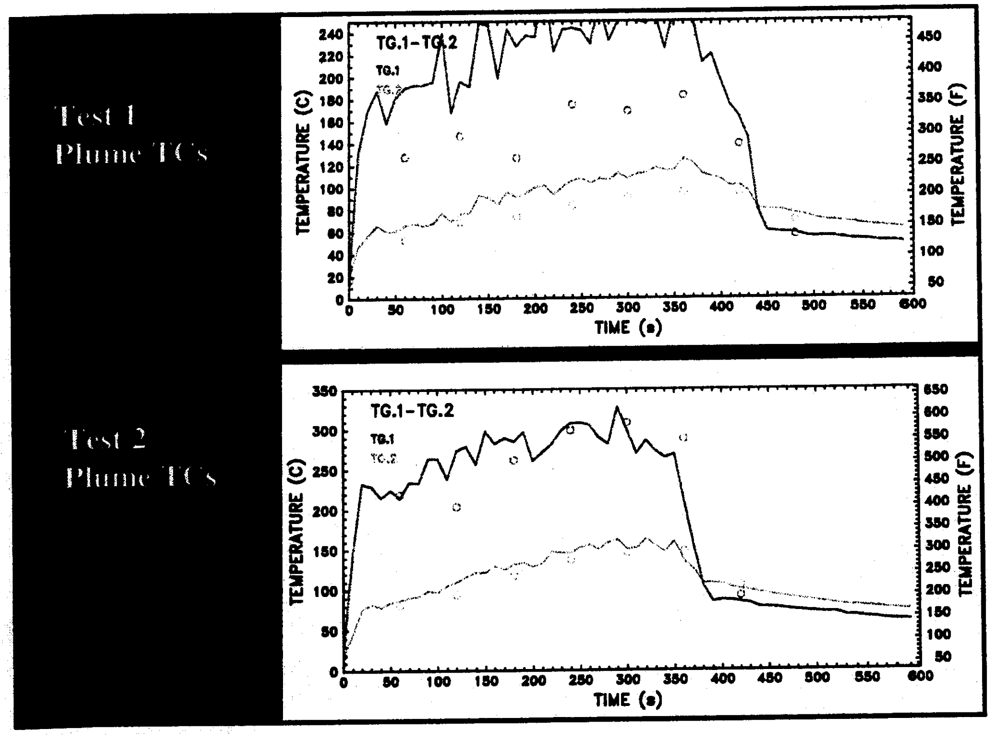
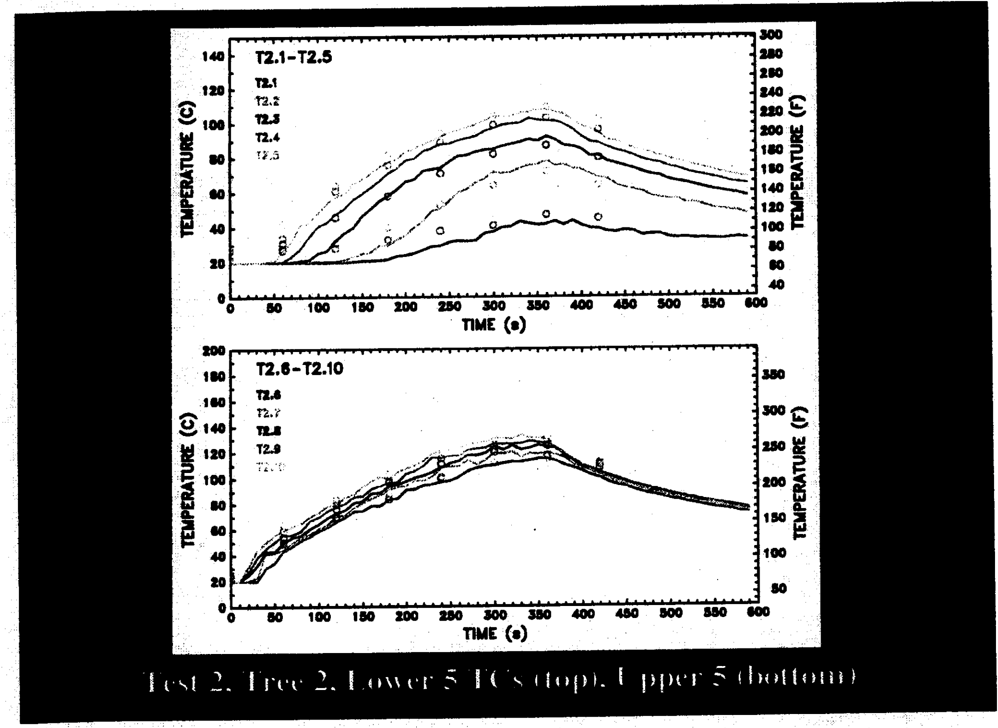


Test 1
Plume TCs

Test 2
Plume TCs



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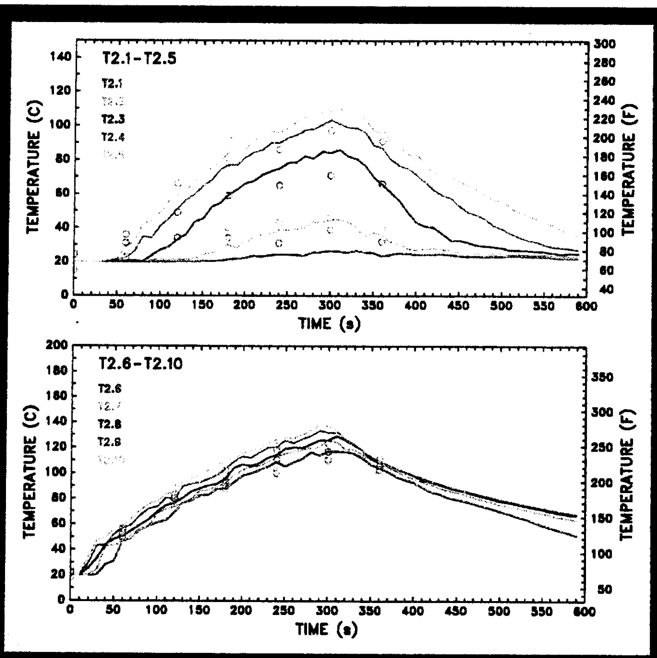

Test 3, Tree 2, Lower 5 TCs (top), Upper 5 (bottom)