Fire Modeling for the Fire Research, Fire Protection, and Fire Service Communities

Kevin McGrattan, Randall McDermott, Glenn Forney, Kristopher Overholt, and Craig Weinschenk National Institute of Standards and Technology

Jason Floyd Hughes Associates, Inc., Baltimore, Maryland

The Fire Dynamics Simulator (FDS) was first publicly released in 2000, and it has recently undergone its fifth major revision. Since its first release, FDS has been applied in three major areas: basic research in fire dynamics, performance-based design, and forensic reconstructions of actual fires. As its applications widen in scope, there is a need to develop new capabilities, while at the same time to verify and validate new and existing algorithms. This is a difficult task because the variety of applicable scenarios is vast and growing. Take, for example, the images shown in Figure 1 through Figure 3. The first figure shows a few snapshots of a simulation of a house fire that were used to assess the consistency of eyewitness accounts. Figure 2 provides an example of how FDS was used to complement field experiments that were designed to study the impact of crew size, alarm assignments, and vertical response modes on occupant survivability, firefighter safety, and property protection for high-rise fire scenarios [1]. Safety concerns prevented live fires during the experiments, so FDS was used to simulate potential thermal and toxic hazards representative of fires in a high-rise office building. Figure 3 shows a simulation of the dispersion of toxic gases in the atmosphere. The model includes a portion of the FDR Drive along the East River in New York City where there were concerns about the accumulation of carbon monoxide from a partially enclosed roadway that was part of planned new construction.

These three examples highlight very different applications, with length scales varying from tens to thousands of meters and physical phenomena ranging from millimeter scale pyrolysis of common household materials to kilometer-scale atmospheric boundary layer phenomena. Applications such as these have driven the development of FDS since its first release, and this article reviews some of the major changes in the most recent version.

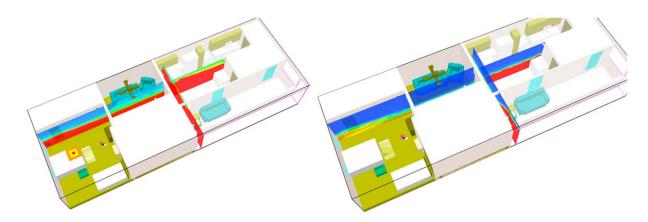


Figure 1. Smokeview snapshots of two simulations of a house fire that were intended to assess the consistency of eyewitness accounts. Courtesy, Hughes Associates.

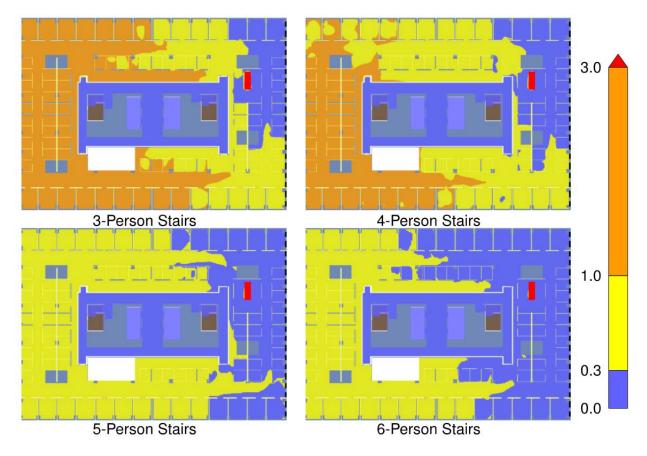


Figure 2. Predicted fractional effective dose contours on the high-rise fire floor. Higher values represent more toxic environments. Courtesy, NIST.

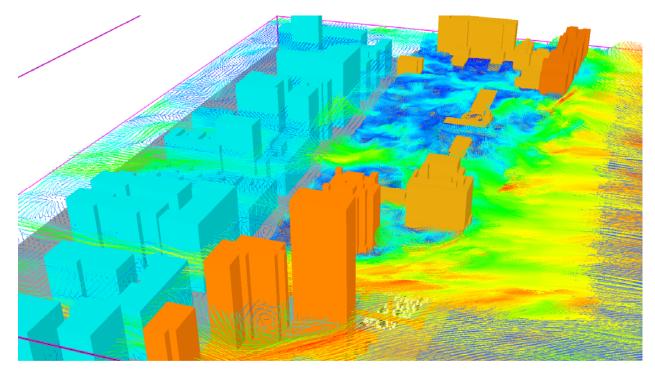


Figure 3. Smokeview snapshot showing the wind field over a proposed semi-enclosed roadway along the east side of Manhattan. Courtesy, Hughes Associates.

Improvements in FDS 6

Many of the improvements in FDS 6 are not immediately obvious. Most of the input parameters remain the same, as does the overall look and feel of the graphics program Smokeview. However, some very important changes have been made to improve the basic flow solver, in particular how the governing equations are approximated on the numerical grid and how the subgrid-scale turbulence is represented. In addition, algorithms have been added to Smokeview for solving the fractional effective dose equation in a slice plane (contours in Figure 2) and the radiative transport equation for visible light (volume rendered smoke and fire in Figure 4).

The flow model in FDS is essentially a set of partial differential equations known as the Navier-Stokes equations. These equations cannot be solved exactly. Instead, the partial derivatives are written in approximate form as finite differences, and the accuracy of the approximation is determined by the size of the numerical grid. There are many different ways of writing the finite difference terms, and versions 1 through 5 of FDS used a simple central difference scheme that was reasonably fast and accurate. It did have one drawback, however, for regions where temperatures would change rapidly, such as the edge of the fire, the numerical scheme would allow the temperature, density and species concentrations to oscillate above and below their ambient values. This was, of course, simply a numerical artifact related to the fact that the finite difference scheme is only an approximation, but it was nevertheless noticeable and could sometimes lead to spurious results, especially when the numerical grid was relatively coarse. To correct this problem, a more sophisticated finite difference scheme was implemented that

removes the spurious oscillations. This scheme is more costly in terms of CPU time, but it was decided that the improvement in accuracy was more important than speed, especially because the steady increase in computer speed will soon make up the difference.

The second major change to the flow solver is the turbulence model. FDS uses a technique known as large-eddy simulation (LES) to represent the fluid motion that is too fine to resolve on the numerical grid. This technique has been around since this 1960s, when it was first developed for weather simulations. Since that time, a number of enhancements have been made to its treatment of subgrid-scale turbulence. FDS versions 1 through 5 used the original LES turbulence model developed in 1963 by meteorologist Joseph Smagorinsky [2]. However, this technique proved to be overly dissipative, meaning that simulating realistic plume dynamics on a relatively coarse numerical grid was difficult. Several variations of the Smagorinsky approach were investigated, and a simplified form of the model of another meteorologist, James Deardorff [3], was chosen on the basis that it is relatively cheap and performs reasonably well at both coarse and fine resolution.

Other improvements in FDS 6 include:

<u>Combustion</u>: There is increased flexibility to define a detailed combustion scheme that goes beyond the simple "fuel meets air and burns" approach. For many typical fire applications, much of the new combustion machinery is not needed and one can specify a predetermined design fire with little change from past versions. However, for topics such as CO production, underventilated fires, suppression, and soot growth and oxidation, the new chemistry and combustion framework will make it easier to explore alternative reaction schemes.

<u>Radiation</u>: FDS uses a set of subroutines called RadCal to calculate the absorption and emission properties of hot gas mixtures. One limitation of RadCal had been its use of methane as a surrogate for all fuel types. FDS 6 now includes the radiative absorption properties for fuel gases other than methane. These properties are based on measurements by Prof. Greg Jackson and students at the University of Maryland [4], and the implementation in FDS was done by Vivien Lecoustre. This can improve the radiation calculations in detailed flame simulations or fuel-rich fires.

<u>Ventilation</u>: In previous versions of FDS, one could only specify pre-defined inlet and outlet flows. To improve the ability of FDS to model buildings, a heating, ventilation, and air conditioning (HVAC) sub-model was added, based on the solver in MELCOR, which is a U.S. Nuclear Regulatory Commission code for analyzing containment buildings. This model treats an HVAC system as a collection of nodes and junctions. With the HVAC model, one can define the following components:

• Ducts with forward and reverse flow losses (ASHRAE and other handbooks contain tables of flow loss data for various types of ducts)

- Nodes (e.g., tees, inlet and outlet vents, plenums) with flow direction dependent losses (as with ducts, values can be found in various handbooks)
- Fans with three options: constant flow, quadratic, and user-defined. The quadratic and user-defined options change the fan flow rate based on its inlet and outlet pressure. This, for example, would reduce the flow into a compartment with a growing fire.
- Dampers (currently only fully open or fully closed)
- Filters with the ability to define different removal efficiencies for different species as well as the impact of filter loading on the pressure drop across the filter
- Heating and cooling coils with either a fixed amount of heat exchange or an amount computed with a simple heat exchanger efficiency model

<u>Soot Deposition</u>: An accurate prediction of smoke concentration and smoke deposition to surfaces is important in various fire model applications, including visibility for human tenability studies and fire patterns for forensic reconstructions. Smoke that deposits to surfaces can reduce the gas-phase smoke concentration and affect visibility and detector activation time. The deposition of particulate matter is also important for predicting the dispersion characteristics of aerosol toxicants (e.g., ash, radionuclides, or other particulate matter). In FDS 6, soot and aerosols can accumulate on surfaces due to gravitational settling, thermophoretic deposition (where temperature gradients near walls push particles towards or away from walls), and turbulent flows near surfaces (where particles impact surfaces due to turbulent motion). Figure 4 is a simple example showing soot deposition to surfaces.



Figure 4. Simple demonstration of smoke deposition to surface.

Verification and Validation (V&V)

In 2007, the U.S. Nuclear Regulatory Commission (NRC) and the Electric Power Research Institute (EPRI) published the results of a validation study of five different fire models commonly used by the commercial nuclear power industry [5]. The study was prompted by the NRC's adoption in 2004 of the National Fire Protection Association standard, NFPA 805, *Performance-Based Standard for Fire Protection for Light-Water Reactor Electric Generating Plants* [6]. In particular, NFPA 805 requires fire models to be verified and validated. The standard does not state explicitly what is meant by this. Guidance documents, like the SFPE *Guidelines for Substantiating a Fire Model for a Given Application* [7], and standards documents like ASTM E 1355, *Standard Guide for Evaluating the Predictive Capabilities of Deterministic Fire Models* [8], and ISO 16730, *Assessment, Verification and Validation of Calculation Methods* [9], all provide a basic framework for evaluating models. However, these documents do not have specific requirements as to how the model uncertainty is to be reported and how this information is to be used in a regulatory context. As a result, the NRC and EPRI took it upon themselves to develop a relatively simple framework for reporting and applying model uncertainty in day-to-day design analyses.

With the support of the NRC, FDS and the NIST zone model, CFAST, have adopted the basic framework of the NRC/EPRI V&V study. In addition, the way in which FDS is developed, tested, and released has greatly improved in recent years because of the boom in free and open source software development tools. Using a procedure that is commonly referred to as *continuous integration*, an automated script runs hundreds of FDS test cases and regenerates all of the plots and figures for the FDS manuals each night. This greatly reduces the likelihood that new bugs will be created with each new routine.

Fire Service Applications

Even before it was publicly released, the Fire Research Division at NIST has used FDS to provide insight on the development and thermal conditions of fires that have caused injuries or fatalities [10, 11, 12, 13, 14, 15, 16]. In addition, FDS has been used in firefighter staffing studies, firefighter training studies, and the impacts of various tactical operations such as ventilation or suppression operations. The overall objective of the use of fire models in these studies is to improve firefighter safety and operational effectiveness. These applications are challenging to model because they incorporate advanced features such as the pyrolysis of real materials, under-ventilated combustion, and complex geometries. In fact, much of the current FDS development activities are driven by the fire service applications, primarily because fire growth and spread are to be *predicted*, and not just *specified* as in most fire protection design applications. This demands a more thorough knowledge of material properties and complex fire physics.

References

- J. Averill, L. Moore-Merrel, R. Ranellone, C. Weinschenk, N. Taylor, R. Goldstein, R. Santos, D. Wissoker and K. Notarianni, *Report on High-Rise Fireground Field Experiments*, NIST Technical Note 1797, National Institute of Standards and Technology, Gaithersburg MD, April 2013.
- 2. J. Smagorinsky. General Circulation Experiments with the Primitive Equations. I. The Basic Experiment. *Monthly Weather Review*, **91**(3): 99–164, March 1963.
- 3. J.W. Deardorff. Numerical Investigation of Neutral and Unstable Planetary Boundary Layers. *Journal of Atmospheric Sciences*, **29**: 91–115, 1972.
- K. Wakatsuki, G. Jackson, J. Kim, A. Hamins, M. Nyden, and S. Fuss. Determination of Planck mean absorption coefficients for hydrocarbon fuels. *Combustion Science and Technology*, 180: 616–630, 2008.
- K. Hill, J. Dreisbach, F. Joglar, B. Najafi, K. McGrattan, R. Peacock, and A. Hamins. Verification and Validation of Selected Fire Models for Nuclear Power Plant Applications, NUREG 1824, United States Nuclear Regulatory Commission, Washington, DC, 2007.
- 6. NFPA 805, *Performance-Based Standard for Fire Protection for Light-Water Reactor Electric Generating Plants*, National Fire Protection Association, Quincy, Massachusetts, 2001.
- 7. SFPE G.06, *Guidelines for Substantiating a Fire Model for a Given Application*, Society of Fire Protection Engineers, Bethesda, Maryland, 2011.
- 8. ASTM E 1355-04, *Standard Guide for Evaluating the Predictive Capabilities of Deterministic Fire Models*, American Society for Testing and Materials, West Conshohocken, Pennsylvania, 2004.
- ISO 16730, Fire Safety Engineering Assessment, Verification and Validation of Calculation Methods, International Organization for Standardization (ISO), Geneva, Switzerland, 2008.
- 10. D. Madrzykowski and R.L. Vettori, *Simulation of the Dynamics of the Fire at 3146 Cherry Road NE Washington D.C., May 30, 1999.* NISTIR 6510, National Institute of Standards and Technology, Gaithersburg, Maryland, April 2000.
- 11. D. Madrzykowski, G.P. Forney, and W.D. Walton, *Simulation of the Dynamics of a Fire in a Two-Story Duplex Iowa, December 22, 1999.* NISTIR 6854, National Institute of Standards and Technology, Gaithersburg, Maryland, January 2002.
- R.L. Vettori, D. Madrzykowski, and W.D. Walton, Simulation of the Dynamics of a Fire in a One-Story Restaurant – Texas, February 14, 2000, NISTIR 6923, National Institute of Standards and Technology, Gaithersburg, Maryland, October 2002.
- 13. D. Madrzykowski and W.D. Walton. Cook County Administration Building Fire, 69 West Washington, Chicago, Illinois, October 17, 2003: Heat Release Rate Experiments and FDS Simulations, NIST Special Publication SP-1021, National Institute of Standards and Technology, Gaithersburg, Maryland, July 2004.

- 14. W.L. Grosshandler, N. Bryner, D. Madrzykowski and K. Kuntz, *Report of the Technical Investigation of The Station Nightclub Fire*, NIST NCSTAR 2, National Institute of Standards and Technology, Gaithersburg, MD, June 2005.
- 15. N. Bryner, S.P. Fuss, B.W. Klein, and A.D. Putorti, *Technical Study of the Sofa Super Store Fire, South Carolina, June 18, 2007*, NIST Special Publication 1118, National Institute of Standards and Technology, Gaithersburg, MD, March 2011.
- 16. A. Barowy and D. Madrzykowski, *Simulation of the Dynamics of a Wind-Driven Fire in a Ranch- Style House, Texas*, NIST TN 1729, National Institute of Standards and Technology, Gaithersburg, MD, 2012.