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Consequence modeling using the fire dynamics simulator

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Abstract

The use of Computational Fluid Dynamics (CFD) and in particular Large Eddy Simulation (LES) codes to model fires provides an efficient tool for the prediction of large-scale effects that include plume characteristics, combustion product dispersion, and heat effects to adjacent objects. This paper illustrates the strengths of the Fire Dynamics Simulator (FDS), an LES code developed by the National Institute of Standards and Technology (NIST), through several small and large-scale validation runs and process safety applications.

The paper presents two fire experiments—a small room fire and a large (15 m diameter) pool fire. The model results are compared to experimental data and demonstrate good agreement between the models and data. The validation work is then extended to demonstrate applicability to process safety concerns by detailing a model of a tank farm fire and a model of the ignition of a gaseous fuel in a confined space. In this simulation, a room was filled with propane, given time to disperse, and was then ignited. The model yields accurate results of the dispersion of the gas throughout the space. This information can be used to determine flammability and explosive limits in a space and can be used in subsequent models to determine the pressure and temperature waves that would result from an explosion. The model dispersion results were compared to an experiment performed by Factory Mutual.

Using the above examples, this paper will demonstrate that FDS is ideally suited to build realistic models of process geometries in which large scale explosion and fire failure risks can be evaluated with several distinct advantages over more traditional CFD codes. Namely transient solutions to fire and explosion growth can be produced with less sophisticated hardware (lower cost) than needed for traditional CFD codes (PC type computer verses UNIX workstation) and can be solved for longer time histories (on the order of hundreds of seconds of computed time) with minimal computer resources and length of model run. Additionally results that are produced can be analyzed, viewed, and tabulated during and following a model run within a PC environment. There are some tradeoffs, however, as rapid computations in PC's may require a sacrifice in the grid resolution or in the sub-grid modeling, depending on the size of the geometry modeled.

Keywords: CFD; Fire; Fire dynamics simulator (FDS); Modeling; Dispersion; Large eddy simulation (LES)

Increasingly fire protection concerns are being addressed using fire modeling software tools. The software can be divided into two types which are used to solve the fundamental equations in evaluating fire scenarios, the zone fire model and computational fluid dynamics (CFD) models. Currently the zone model approach is the more prevalent in the fire protection engineering community, as it is less computationally demanding, however, as computer processing power becomes increasingly available at lower costs, CFD models are increasing in use. CFD programs are increasingly being used in all aspects of engineering and are continuously being validated for use in different types of research and design applications.

The foundation for CFD models has been around since the early 1900's when iterative numerical solutions to the fundamental conservation equations were derived. Solving for turbulence traditionally has been the biggest obstacle to overcome in CFD models. Three distinct types of CFD programs have been developed to account for turbulence, each with its own assumptions and benefits. In general, each method allows for 3-dimensional modeling of complex geometries. Codes have been written which allow for the gridding of complex geometries so that distinct physical surfaces can be gen-

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erated within the computational domain. Each method solves the Navier–Stokes equations and the fundamental conservation equations.

The fire dynamics simulator is a large eddy simulation (LES) model, which was developed by the National Institute of Standards and Technology (NIST). The primary assumption behind the LES technique is that the larger scale turbulence that carries the majority of the energy of the system, needs to be directly resolved in order to accurately represent flow. The small eddies are approximated. The modeling of the small scale eddies reduces the computational demand and thus, increases the speed in which a simulation can be performed. LES modeling does not utilize averaged parameters so a transient solution can be quickly obtained. Fire dynamics simulator (FDS) was developed specifically to deal with problems related to fire.

CFD modeling of fires is inherently complex because it incorporates aspects of bluff body aerodynamics, multi-phase flow, turbulent mixing and combustion, radiative transport, and convective and conductive heat transfer. The transport equations are simplified using techniques developed by Rehm and Baum [1] and are widely referred to as the low Mach number combustion equations within the combustion research community. These equations describe the low speed motion of a gas driven by heat and buoyancy forces. FDS solves the equations by dividing the model space into a large number of rectangular cells and calculating the temperature, gas velocity, species concentration, and other pertinent variables within each cell. The accuracy of the model is highly dependent on the grid resolution, with a smaller grid resolution producing more accurate results.

FDS can be broken up into several major sub-models; the following descriptions are taken from the fire dynamics simulator user's guide [2].

- Hydrodynamic model: The core algorithm is an explicit predictor-corrector scheme, second order accurate in space and time. Turbulence is treated by means of the Smagorinsky form of large eddy simulation (LES) [1,8].
- Combustion model: For most applications, FDS uses a mixture fraction combustion model. The mixture fraction is a non-dimensional variable that combines the fuel and oxygen conservation into a single equation. The mass fractions of fuel and the oxidizer can be derived from the mixture fraction when assuming the flame sheet approximation [9].
- Radiation transport: Radiative heat transfer is included in the model via the solution of the radiation transport equation for a non-scattering gray gas, and in limited cases using a wide band model [10]. The equation is solved using the finite volume method, similar to the finite volume methods used for convective transport. Hundred discrete angles are used in the finite volume solver.
- Geometry: FDS approximates the governing equations on a rectilinear grid. The user prescribes rectangular obstructions that are forced to conform with the underlying grid.
- Boundary conditions: All solid surfaces are assigned thermal boundary conditions as well as information about the burning behavior of the material. Material properties are stored in a database and invoked via name by the user. Material properties included in the model database have been compiled from literature sources. In many cases the necessary material properties are not contained within the model database and therefore they must be derived from experiments or obtained from other sources for use with the model.

FDS has been subjected to numerous validation and calibration studies, five of which are discussed in an article in fire protection engineering magazine [3], additional studies can be found in the literature a list of which may be found on the NIST website. These studies point out the relative strengths and weaknesses of the model for use in various fire scenarios.

Four situations are examined in this paper, which are important scenarios to evaluate for the chemical and processing industries. The first scenario is a methane gas fire with a mass flow rate of 1.26 g/s centered in a room of dimensions 2.8 m × 2.8 m × 2.18 m. This case is known within the fire field as the Steckler case and detailed information may be found in the literature [5,6]. The calculation domain is 3.4 m (length) ×2.8 m (width) ×2.35 m (height), which is larger than the room size, and the simulation grid is 100 cells (x) × 64 cells (y) × 44 cells (z), with the total number of cells equaling 281,600. The initial temperature was set to the ambient of the experiments, 31 °C. The simulation was run to 220 s with the final 20 s of data averaged together. A detailed comparison with the experimental results was made in the doorway (Fig. 1) and in the corner of the room (Fig. 2). Here only the case of a fully open door is examined, however, the other cases may be seen in the literature [10]. Temperature and velocity in the doorway and temperature in the corner of the room are compared to experimental data (Fig. 3).

Overall the model results match very well, less than 15% error, with the experimental results indicating that the model can accurately predict the velocity and temperature of a

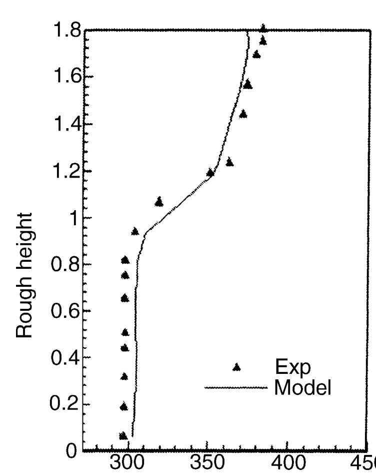

Fig. 1. Doorway temperature.

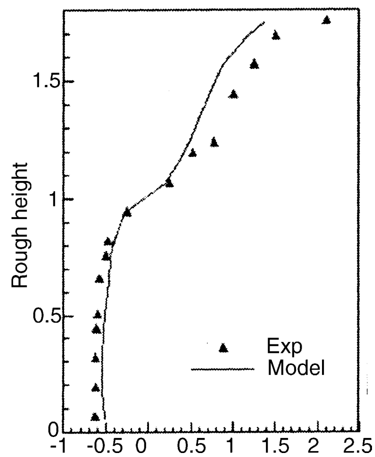

Fig. 2. Doorway velocity.

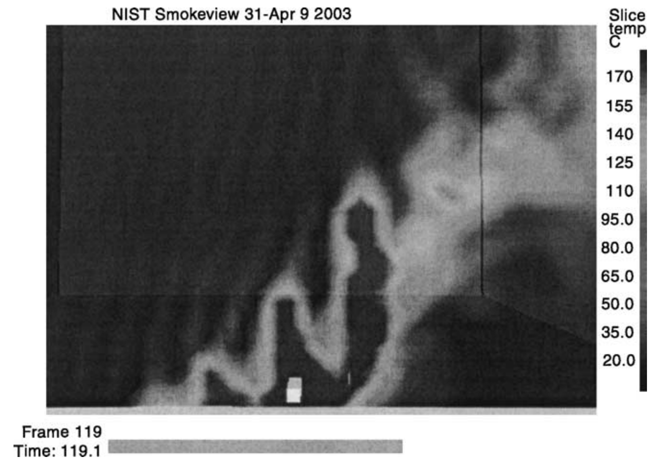

Fig. 4. Temperature profile: effect of wind on fire and target.

well-defined situation when the proper grid resolution and boundary conditions are specified. Both the temperature and velocity are grid dependent, a coarse grid often results in an overprediction of the mean velocity and the temperature.

The Steckler case is important because it is often used for model validation studies. Work by Sinai et al. and others have demonstrated the ability of other CFD codes in modeling the Steckler case, however, most studies have employed an averaging technique such as the k-epsilon. The advantage to using the LES technique employed by the FDS model is that temporal resolution is important when evaluating entrainment. Time averaged techniques can have a serious impact on the total air entrained into the fire and ignores the periodicity of the fire.

The second test series was designed to provide the information necessary to assess the hazard from radiant energy to a building, its occupants and contents due to a large fire in close proximity to the structure, in particular a pool fires effect on glass breakage. Glass breakage and breaches of other building materials may provide an entry way for the fire to gain access to other areas of the structure and thus, expose those areas to additional risk. By comparing the experimental results with model predictions and verifying their agreement, model predictions can be used to help design effective protection systems for hazardous areas [4].

The testing took place at the Energetic Materials Research and Testing Center in Socorro, New Mexico. A 15 m pool of jet fuel was used to simulate a jet fuel spill. The pool was ignited and radiant flux was measured at approximately 17 and 25 m from the pool. The biggest concerns with the testing were the environmental aspects of the large pool fire, which may not be accounted for in a design scenario. The impact of wind on the results dramatically increased the amount of radiation scene by the target, and in some cases, where the target was 8 m away it was engulfed by the fire (Fig. 4). Additionally the unburned vapors extended beyond the diameter of the pool and effectively increased the size of the fire (Fig. 5).

Heat flux was compared to the results obtained from an FDS simulation with and without wind present. The FDS model was constructed in a cube of 40,000,000 m^3 using grid

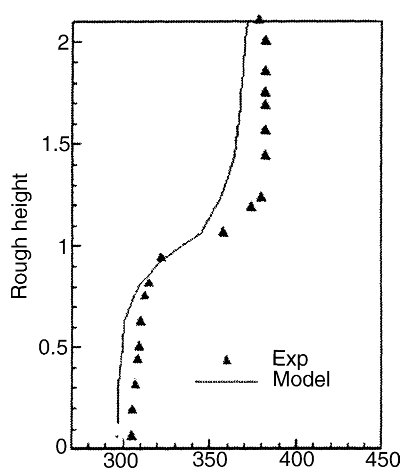

Fig. 3. Corner temperature.

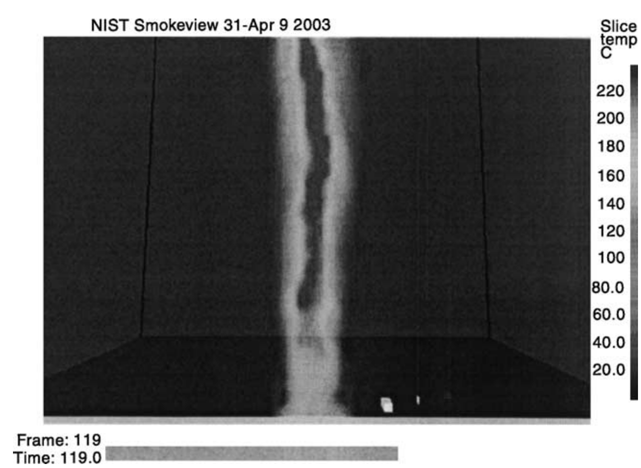

Fig. 5. Temperature profile: no wind.

Table 1
Experimental measurements and FDS predictions of heat flux to target

Comparison between pool fire data and FDS model predictions—case #1, wind			Comparison between pool fire data and FDS model predictions—case #2, no wind		
Distance to target	Experimental approximations (kW/m^2)	Model prediction (kW/m^2)	Distance to target	Experimental approximations (kW/m^2)	Model prediction (kW/m^2)
50	32	31.13	50	8	4.54
75	17	13.06	75	4	2.87

cells of 2.25 m^3. The increased size likely may result in an increased plume temperature and velocity, however, these errors were not quantified in this study.

The fuel was modeled as jet fuel and was allowed to burn as a liqued fuel. Wind was examined as a variable and was found to significantly affect the structure of the plume and flame structure. This had a significant impact on both the temperature distribution and the heat flux in both the experiments and in the model results. Table 1 shows the experimental and model comparisons of heat flux in wind and non-wind conditions.

Though the radiation model has many limitations including a poor soot production model and a large dependence on grid resolution the model results indicate fairly good comparision with the experimental data. Errors in the no wind condition are in the order of 100%, however, in cases such as this, errors of this magnitude may be acceptable, depending on the use of the model results.

The third situation is a simulation of a tank farm. In this case a single tank has had the roof partially removed and a fire was initiated inside the tank. The fire interacts with and exposes the other tanks in the area. In comparing the two previous simulations to the experimental data the results showed promise. Thus, a reasonable assumption may be made that the model may be used in other similar situations such as the tank farm. Numerous simulations can be run with varying input conditions. It is through this type of analysis that it becomes clear that differences such as a partially intact roof, wind or other environmental conditions can play a crucial role in evaluating the potential fire scenario.

FDS provides a temporal resolution that can provide important information when assessing a potential situation. For instance the temporal resolution of the thermal plume and the radiant flux incident on the adjoining tanks provides time sensitive information, which is lost in models utilizing an averaging technique. Fig. 6 shows the effect of a partially opened roof in combination with a mild wind. Effectively it can be seen that while one tank is severally exposed and at risk, tanks equally as far away are not in danger from radiant flux at this time (Fig. 7). Temperature distributions on the tanks show a similar pattern. Variables such as changing wind conditions will change which tanks or other targets may be at risk. In many cases due to the high thermal capacity of most objects the averaging techniques of other models are suitable as the heating time scales are larger than the averaging periods. The area in which this is not the case is in evaluating entrainment and its effects on the fire.

The last case is a simulation recreating a combustible gas leak. The simulation was modeled after an experiment conducted by Factory Mutual [7] (Fig. 8), in which gas filled a room and was then ignited resulting in an explosion. The gas concentration was measured at several locations within the room at varying heights and pressure was measured at the time of the explosion. The experiment addresses the explosion hazard that may occur from flammable liquid spills or heavy vapor releases. In terms of explosive power these types of explosions typically are relatively weak, however, the damage can often be substantial as buildings often are capable of

Fig. 6. Radiant flux to adjacent tanks, 5 s.

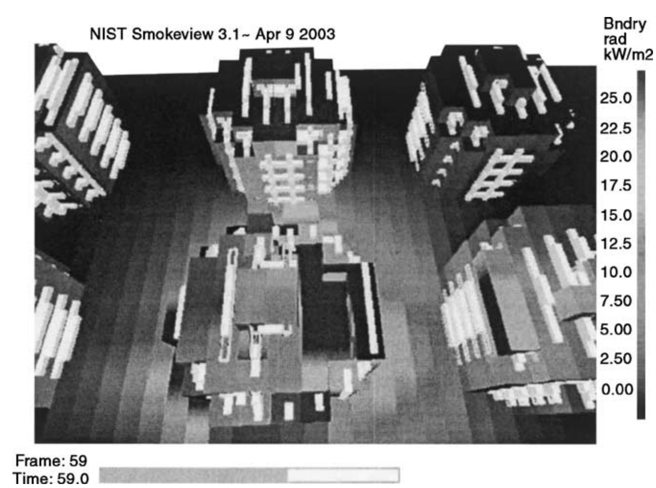

Fig. 7. Radiant flux to adjacent tanks, 59 s.

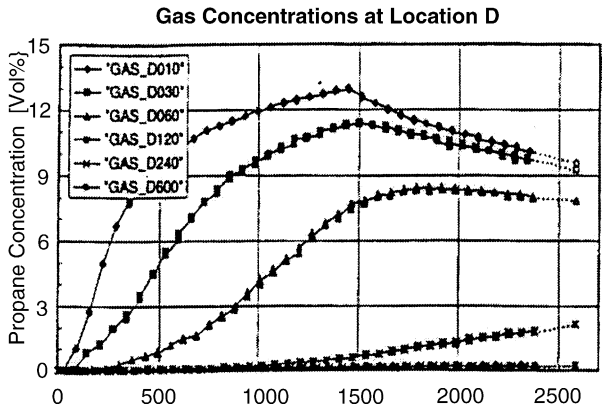

Fig. 8. Experimental propane concentrations.

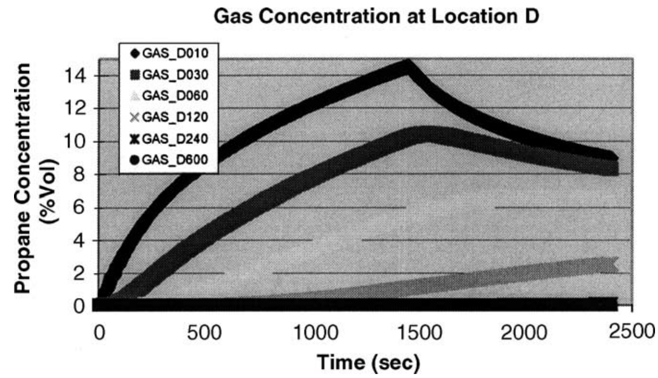

Fig. 9. FDS predictions of propane.

sustaining only minimal overpressure events without incurring damage.

At the current time FDS is unable to model the ignition and explosion of gasses, however, it is capable of modeling the dispersion of gasses throughout a space. This may be useful for planning purposes as potential areas of high gas concentrations can be identified. This can be useful in determining location of equipment, which may serve as a potential ignition source, as well as suppression and detection systems. Additionally it can show the effects that various ventilation schemes may have on the gas dispersion throughout the room.

In the experiments an explosive layer was formed at the chamber floor by slowly injecting propane through nine diffusers in the floor of the chamber. The rate of propane diffusion is equivalent to that which would be seen by the vaporization of a typical solvent. The testing facility was an enclosure of 4.57 m × 4.57 m × 3.05 m and 10 rectangular explosive vents were located in the ceiling. The tests were conducted with and without obstructions in the testing facility. The obstructions were an array of squares of 0.76 m steel plates elevated 0.46 m above the floor of the testing facility, which presented a 50% blockage to vertical expansion. The fuel was injected through 0.74 mm diameter orifices in the diffusers at a flow rate of, approximately, 10.4 slpm at an exit velocity of 14.2 mm/s. Gas was allowed to flow for 1440 s at which point the gas was turned off and settling was allowed to occur for 1160 s. At 2600 s ignition of mixture occurred using a Jacob's ladder ignition system, which was located in the center of the room. Propane concentrations were measured throughout the enclosure using a 12-port multiplexing valve, taking samples at 1, 2, 3, 4.5, 6, 9, 12, 18, 24, 60, and 120 in. above the floor. Pressure measurements within the chamber were taken during the ignition and explosion phase using a strain gauge transducer 1.5 m above the floor.

The experiment modeled had a mass volumetric flow rate of 25 slpm distributed equally through the diffusers. The experiment was modeled in FDS using approximately a 2 cm grid resolution. Gas was introduced into the space through nine vents, as in the experiment, at a rate of 25 slpm. The model was run with the default model parameters, with the exception that the combustion model was turned off. Since no combustion is being modeled the combustion model is not necessary and the elimination of it from the simulation decreases the run time. The experimental and model results are shown in Fig. 9.

As can be seen the model performs well in modeling the gas dispersion throughout the space. This technique can be used to determine flammability and explosive limits in enclosures as well as concentration data at critical locations transiently. Further this information can be used as boundary conditions for explosion models to better determine the pressure and temperature waves that would result from an explosion.

The FDS model offers the opportunity for enhanced fire modeling simulations to be performed that take into account aspects of fires, which are traditionally ignored in other models. Primarily the transient nature of the model allows the effects of entrainment to be modeled. Accurate, time dependent entrainment modeling is very important in fire scenarios as often the time scales may be short and the conditions may change rapidly, details which may be muted in a model employing an averaging technique. FDS excels in the calculation of fluid flows, however, the model requires significant improvements in the radiation sub-model prior to it extensive use. Additionally the model does not have the ability to model ventilation limited fires at this time. FDS also is highly dependent on the grid that is chosen and thus, a proper grid resolution must be chosen in order to avoid skewing of the results.

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