

Using Computer Fire Modeling to Reproduce and Predict FRP Composite Fire Performance

by

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Abstract

The US transportation industry has become increasingly interested in light weight vehicles due to operating costs and environmental issues. These interests combined with desires for more functional cars that have a high level of fire performance present a significant challenge for car designers. One common solution has been the use of FRP composites because they are relatively light weight and they can be customized with ease. Although there are codes and standards that regulate the use of materials in transportation vehicles, a majority of the prescriptive tests have a simplistic pass/fail criterion that do not properly assess the material in the proposed configuration and how it actually contributes to the overall hazard.

To assist car designers to properly specify FRP composites, fire engineering tools are needed that can simulate fire growth and account for material characteristics and configuration. These tools provide designers and manufacturers a cost effective methodology to predict the overall fire performance of a material. A freely available fire model developed by the National Institute of Standards and Technology (NIST) called Fire Dynamics Simulator Version 5.0 (FDS) is used in conjunction with a numerical tool to determine effective material properties for the fire model from Cone Calorimeter (ASTM E 1354) tests. FDS is calibrated based on mocked up rail car fire tests.

The simulated heat release rate, thermocouple temperatures, and heat flux levels match the experimental data closely enough that with careful model verification/validation and calibration use of FDS to make engineering estimates of mockup-scale fire development is viable. This paper presents the methodology used to simulate and predict fire scenarios with FDS with a case study example. ACMA is involved in the ICC code change process with the intent of incorporating compo-

sites into the ICC codes. By using the code provision for alternate methods and means this methodology can be adopted via a performance based analysis in those situations where compliance with the strict provisions of the code is not possible.

Introduction

The most promising long-term prospect for modeling flame spread and fire growth at building scales is the coupling of first principles-based condensed phase fuel generation models to computational fluid dynamics (CFD) models that simulate the gas-phase fluid mechanics, combustion, and heat transfer aspects of a fire. The primary advantage of this approach is its flexibility, and it has been suggested [1] that this type of fire growth modeling will become an 'invaluable tool for researchers and engineers' due to this flexibility. With a coupled pyrolysis/CFD fire model, it should be possible to consider complex geometries and ignition scenarios, evaluate the impact of design changes on expected fire behavior, and assist in forensic fire reconstruction.

Solid phase pyrolysis models have been coupled to CFD for simulating bench-scale fire tests [2-4], primarily two-dimensional upward flame spread [5, 6], reduced-scale compartment fires [6-8], and building-scale compartment fires [9-19]. Noted difficulties include strong sensitivity of model predictions to solid phase properties [12] and grid size [11, 14, 16, 18].

To date, there have been few rigorous attempts at validating CFD-based fire growth models, and flame spread prediction remains largely a research area. Most fire model validation work has involved 'gas burner' type problems where the movement of heat and smoke from a fire having a predetermined heat release rate (HRR) is predicted and compared to experimental measurements, e.g. the US Nuclear Regulatory Commission's reports [20]. Typically, a fire growth model is evaluated by comparing its predictions of large-scale behavior to experimental HRR measurements, thermocouple temperatures, or pyrolysis front position. The overall predictive capabilities of a fire growth model depends on the pyrolysis model, treatment of gas-phase fluid mechanics, turbulence, combustion chemistry, and convective/radiative heat transfer.

In this paper, Fire Dynamics Simulator (FDS) Version 5 [21] is used to simulate fire growth in a real-scale rail car mockup. Model calculations of heat release rate, temperatures, and heat flux levels are compared to analogous experimental data. The rail car mockup consists of actual seat, carpet, wall, and ceiling lining materials removed from a rail car inserted in a standard-sized fire test compartment and arranged to simulate the as-

built configuration. The material properties required to characterize these materials in terms of the FDS 5.0 pyrolysis model are estimated from bench-scale Cone Calorimeter [22] test data using an automated optimization algorithm [23, 24]. In standalone simulations, the pyrolysis behavior of these “complex” real-world materials (which contain fire retardants and char heavily) can be simulated reasonably well with the FDS pyrolysis model.

Real-Scale Rail Car Mockup Fire Test

The mockup fire test configuration is shown in Fig. 1a (pre-test) and Fig. 1b (post-test). It consists of seats, wall linings, ceiling linings, and carpet inserted in a standard sized (2.43 m by 2.43 m by 3.65 m) ISO room calorimeter. Two transverse double seats are installed against a wall of the burn room to mimic the standard seat arrangement in the actual rail car. A single seat is installed in front of the two double seats. The seats consist of a foam/fabric cushion and seat shrouds. The burn room is lined with gypsum board. A false ceiling consisting of three phenolic composite panels and one gypsum board panel is installed above the seating at a height of 2 m from the floor to mimic the as-built ceiling height. The rear wall is lined with one phenolic panel extending downward from the false ceiling.

A 1.1 m by 2.3 m section of carpet is placed in the vicinity of the seats and is fixed to the floor to prevent curling of the edges. The ignition burner (a 0.3 m by 0.6 m rectangular propane sand burner) is placed between two transverse seats located approximately 0.05 m from the wall. Instrumentation includes a single thermocouple rake consisting of 24 thermocouples installed vertically at a spacing of 0.1 m; additional thermocouples with different bead diameters are installed at five locations to allow for radiation correction of the thermocouple temperatures. Eight thin skin calorimeters are installed at floor level near the seats to facilitate heat flux measurements.

The ignition burner’s peak HRR is 500 kW, roughly approximating a flammable liquids spill. This “extreme” ignition source, unlikely to be present in an actual car fire, was selected because most of the interior lining materials are fire retardant and it was felt that a small (trash bag sized) fire would not cause significant flame propagation. Using a large ignition source strength ensures that fire spread occurs after a minimal incubation period, ultimately requiring shorter simulation times in the modeling phase of the project. Fig. 2a shows the heat release rate of the sand burner (full HRR reached after ~75 s) and the total heat release rate measured by oxygen consumption calorimetry. Fig. 2b shows the temperature measured 0.5 m below the ceiling at the door, and the heat flux measured by thin skin calorimeter at the floor. Additional experimental data are presented later in the

paper where they are compared with the model calculations.

A peak net heat release rate of 1.4 MW (1.9 MW total HRR) occurs approximately 110 s into the test. Temperatures near the ceiling approach 730 °C, and heat flux levels at the floor approach 30 kW/m². These temperatures and heat fluxes exceed the threshold rule of thumb for onset of flashover (heat flux to the floor of 20 – 25 kW/m² and upper layer temperature rise of 500 – 600 °C) yet flashover did not occur as evidenced by the unburned seats that can be seen in Fig. 1b. Flashover may not have occurred due to the relatively small section of carpet installed at the floor and the relatively small combustible wall lining area. At the time of peak heat release rate, one double seat was completely burning. It is also likely that the phenolic panels contributed significantly to the heat release rate, but smoke obscured the visual record. Post-test inspection of the burn damage (see Fig. 1b) showed that the phenolic wall panels became detached from the walls.

Solid-phase Material Property Estimation

One of the most challenging aspects of fire growth modeling is characterizing solid materials or assemblies in terms of the material properties that control their overall reaction to fire. For the present application where it is desired to simulate fire development in a compartment fire, this means quantifying each material in terms of the input parameters needed by the FDS 5.0 pyrolysis submodel. While based on a sound physical and chemical treatment of solid-phase pyrolysis as it is presently understood, material property estimation for the FDS 5.0 pyrolysis model is onerous. Each condensed-phase species (i.e. virgin wood, char, ash, etc.) must be characterized in terms of its bulk density, thermal properties (thermal conductivity and specific heat capacity, both of which are usually temperature-dependent), emissivity, and in-depth radiation absorption coefficient. Similarly, each condensed-phase reaction must be quantified through specification of its “kinetic triplet” (pre-exponential factor, activation energy, reaction order), heat of reaction, and the reactant/product species. For a simple charring material with temperature-invariant thermal properties that degrades by a single-step reaction, this amounts to ~12 parameters that must be specified.

This would not be problematic if standardized, reliable, reproducible, and inexpensive laboratory tests were available to estimate each of the required properties. Although several specialized laboratory tests are available to measure some of the properties needed by the FDS 5.0 pyrolysis model (e.g. specific heat capacity can be determined by differential scanning calorimetry), many of these tests are still considered research tools and are not standardized. Even if such tests were standar-

dized, it would likely be so expensive to conduct 5+ different specialized laboratory tests for each material that practicing fire protection engineers would be unable to apply this approach to real-world projects in an economically viable way. Furthermore, there is no guarantee that properties measured independently from multiple laboratory tests will provide accurate predictions of pyrolysis behavior in a “slab” combustion experiment such as the Cone Calorimeter.

It seems that comparison of a pyrolysis model’s predictions to Cone Calorimeter (or similar) experimental data has become the de facto standard for assessing its “accuracy”. If this is indeed the case, then it makes sense to work backwards from Cone Calorimeter data to estimate the required material properties. This basic idea (use a pyrolysis model as a “virtual” representation of a Cone Calorimeter or similar experiment and adjust the material properties until the model calculations match the experimental data) is straightforward and has been independently proposed by several researchers. The challenge stems from the number of parameters that must be simultaneously optimized. For the simple charring material example mentioned above, there are approximately 12 adjustable parameters that must be simultaneously optimized, so manual optimization is impractical.

Automated brute force search techniques suffer from the high dimensionality (large number of adjustable parameters) of the problem. Assuming each parameter could take on 10 different values (a much higher number is actually more reasonable), there are 10^{12} different combinations of model input parameters that must be explored to find the combination that best matches the experimental data. If 0.1 s of CPU time is required to evaluate each solution, it would take 32 years to calculate every solution running even when running in parallel on 100 CPUs just for a single material. Automated “gradient climbing” does not work well with nonlinear problems, and the present problem is strongly nonlinear due to temperature-dependent thermal properties and the Arrhenius nature of the reaction kinetics. It can be seen that while the basic idea seems simple, below the surface looms a considerable computer science challenge.

One method that has been proposed to estimate the material properties needed for pyrolysis modeling from Cone Calorimeter (or similar) experiments involves the application of a genetic algorithm (GA) [23, 24]. GAs are a class of stochastic search and optimization tools that operate on the principles of Darwinian evolution or natural selection, sometimes called survival of the fittest. Essentially, a random number generator is used to guess hundreds of different combinations of model input parameters (material properties). Each parameter set is then passed to the pyrolysis model and used to simulate a Cone Calorimeter experiment or experiments. The model calculations are compared to analogous experimental da-

ta (mass loss rate, surface and in-depth temperature measurements, etc.) and the “fitness” of each parameter set is determined by quantifying how well the pyrolysis model calculations match the experimental data. These fitness values are then used to rank each parameter set from highest (best fitness) to lowest (worst fitness). Next, “reproduction” occurs wherein parameter sets are combined to produce new parameter sets.

Parameter sets with higher fitness values are assigned a higher probability of reproducing, and are therefore more likely to pass their “genes” on to subsequent “generations”. This behavior gives genetic algorithms the ability to exploit promising areas of the search space, while ignoring unpromising areas. Finally, a small number of parameters are randomly “mutated”, meaning that they are slightly modified from their previous values. This preserves diversity in the population, but can slow “convergence”. The process is repeated, and the solution is said to be converged (i.e. the optimal parameter set has been found) when no further improvement of the best model calculations is seen with subsequent generations. Typically, tens of thousands of trial solutions are required for convergence. The technique is heuristic; that is, a good or near optimal solution can be found, but it does not guarantee that the best or optimal solution is found.

In the present work, an automated computer program based on genetic algorithm optimization is used to estimate the required material properties for the four materials used in the real-scale rail car mockup from Cone Calorimeter experiments. For each material, multiple Cone Calorimeter tests are conducted at irradiance levels between 15 kW/m^2 and 80 kW/m^2 . In addition to the quantities normally measured in Cone Calorimeter tests (mass loss rate, heat release rate, etc.) measurements of surface temperature and back-face temperature are made and used in the optimization process. For modeling purposes, the flame heat flux is estimated at 30 kW/m^2 based on the work of Rhodes [25] and Hopkins [26]. To accommodate temperature-dependent thermal properties in a simple manner that is compatible with genetic algorithm optimization, as was done in Ref. [27] thermal conductivity is assumed to vary as $k(T) = k_0(T/T_r)^{n_k}$ and specific heat capacity is assumed to vary as $c(T) = c_0(T/T_r)^{n_c}$ where the reference temperature T_r is 300 K.

Fig. 3 shows a comparison of the measured and modeled mass loss rate for each of the four materials. Although surface temperature and back face temperature measurements are also used in the optimization process, for clarity of presentation only mass loss rates are shown. It can be seen that the pyrolysis model reproduces the major features of the mass loss rate curves but certainly does not capture every detail. The resultant material

properties are listed in Tables 1 and 2, along with additional properties that are directly measured or inferred from the Cone Calorimeter experiments.

Comparison of Real Scale Fire Growth Calculations to Experimental Data

An FDS model of the experimental geometry shown above in Fig. 1 is assembled using cubic cells 5 cm on edge. A side view of the FDS representation of the experiment is shown below in Fig. 4 (rotated 90° from the “head on” view shown in Fig. 1). Each combustible solid surface is assigned material properties estimated above by genetic algorithm optimization and handbook values for gypsum wallboard are used. Since FDS can accommodate only a single gas-phase combustion reaction, its properties are selected to represent a mixture of propane and the combustible solid materials in the mockup. Apart from the reaction and material properties, all default FDS values are used.

Fig. 5 compares the measured and modeled heat release rate curves. The overall shapes of the curves match well, but the peak heat release rate is over predicted by ~15 % and the modeled peak occurs ~45 s later than the experimental peak. The temperature and heat flux calculations (Figs. 6 and 7) trend with the calculated HRR behavior. That is, the peak modeled temperatures and heat flux levels agree well with the analogous peak experimental quantities, but the modeled peak temperatures and heat flux levels occur later than seen experimentally. Figs. 6 and 7 show a slight bias toward under-prediction of peak temperatures and heat flux levels.

The simulations described earlier are conducted using a cubic grid 5 cm on edge. Grid dependency is checked by running a simulation (still underway) with a cubic grid 2.5 cm on edge. As shown in Fig. 8, the heat release rates calculated with both grid sizes are similar, suggesting that the calculated heat release rate is grid independent for grids finer than 5 cm.

Discussion

If a fire growth model gives sensible predictions of fire development in a rail car mockup fire test, it is reasonable to extend that model to predict the expected fire development in fire scenario involving a full rail car. While beyond the scope of the present paper, such predictions should be considered engineering estimates subject to considerable uncertainty bars rather than absolute predictions.

In addition to making engineering estimates of full-scale fire development in an as-built rail car configuration, one of the biggest promises of this type of fire growth modeling is that it allows the designer to answer “what if” questions. For example, the expected fire de-

velopment could be assessed for several different wall lining materials, allowing the designer to select a material that balances fire performance with other considerations that must be contemplated in the design of rail cars such as cost, durability, ease of maintenance, acoustic damping properties, etc. Additionally, fire development from several different initiating fires can be investigated.

As an example, the model is used here to predict the expected fire development from a trash bag fire, often used in rail industry fire tests. In this example the trash bag fire is assumed to reach a peak HRR of 290 kW after approximately 2 minutes. The heat release rate of the assumed trash bag fire and the calculated total heat release rate (including the contribution from the rail car) are shown in Fig. 9. The model predicts that only localized burning occurs, consistent with actual fire tests (not reported here). A peak net heat release rate of ~100 kW occurs around 120 s. In comparison, the peak net heat release rate is ~1,700 kW with the 500 kW ignition source (see Fig. 5 or 8). This modeling suggests that while extreme ignition sources (flammable liquids spills akin to malicious arson) may cause fire spread beyond the area of the initiating fire, “nuisance” vandalism fires such as burning trash should cause only localized burning.

Concluding Remarks and Future Work

The modeling results shown here for fire spread in a real-scale rail vehicle mockup indicate that the peak heat release rate is well-predicted, but it occurs slightly later in the model than in the experiment. The modeling results show that temperatures and heat flux levels are well-predicted when the heat release rate is well-predicted.

Fire development predictions are strongly sensitive to the specified material properties. Consequently, the material property estimation process (here, accomplished by genetic algorithm optimization) is of critical importance for predicting fire development. There are no widely accepted, standardized methods for determining all of the material properties required for fire modeling, and additional research in this area is strongly encouraged.

With careful model verification/validation and calibration, use of FDS 5.0 to make engineering estimates of mockup-scale fire development may be viable, even for non-simple geometries such as rail cars. However, no broad conclusions can be made on the basis of comparing a single set of model calculations (HRR, temperature, heat flux levels) to a single set of analogous experimental data as was done in this paper. Although FDS-based fire development predictions are potentially very useful in design applications, it is prudent to view such calculations as engineering estimates rather than

absolute predictions. The accuracy of “blind” fire growth predictions (comparing model predictions to actual-scale fire testing without prior knowledge of the test data) remains to be demonstrated with FDS 5.0, so actual-scale fire testing remains an integral part of the model calibration process. Additional research to assess the capabilities of FDS for predicting fire development for other scenarios is strongly encouraged.

Related to the fire performance of the rail car investigated in this paper, it is unlikely that a nuisance arson fire, such as a trash bag fire, would lead to fire spread beyond the area of origin. However, extreme ignition sources (flammable liquids spills akin to malicious arson) may cause fire spread beyond the area of the initiating fire. The magnitude and growth rate of such fires could potentially be investigated with FDS, subject to the caveats stated above.

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Figures:

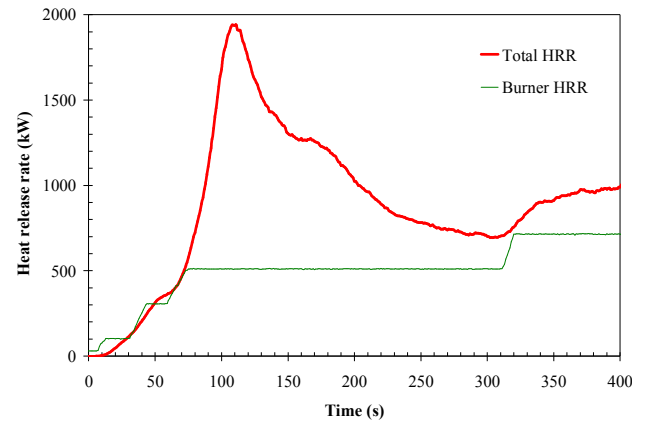


(a)

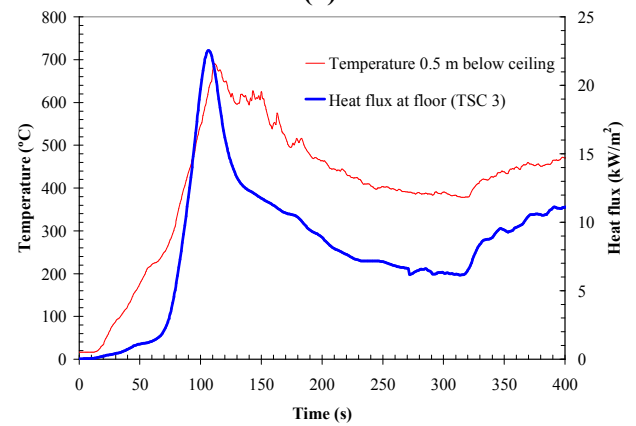


(b)

Fig. 1. Mockup fire test configuration. (a) Pre-test photograph; (b) Post-test photograph.

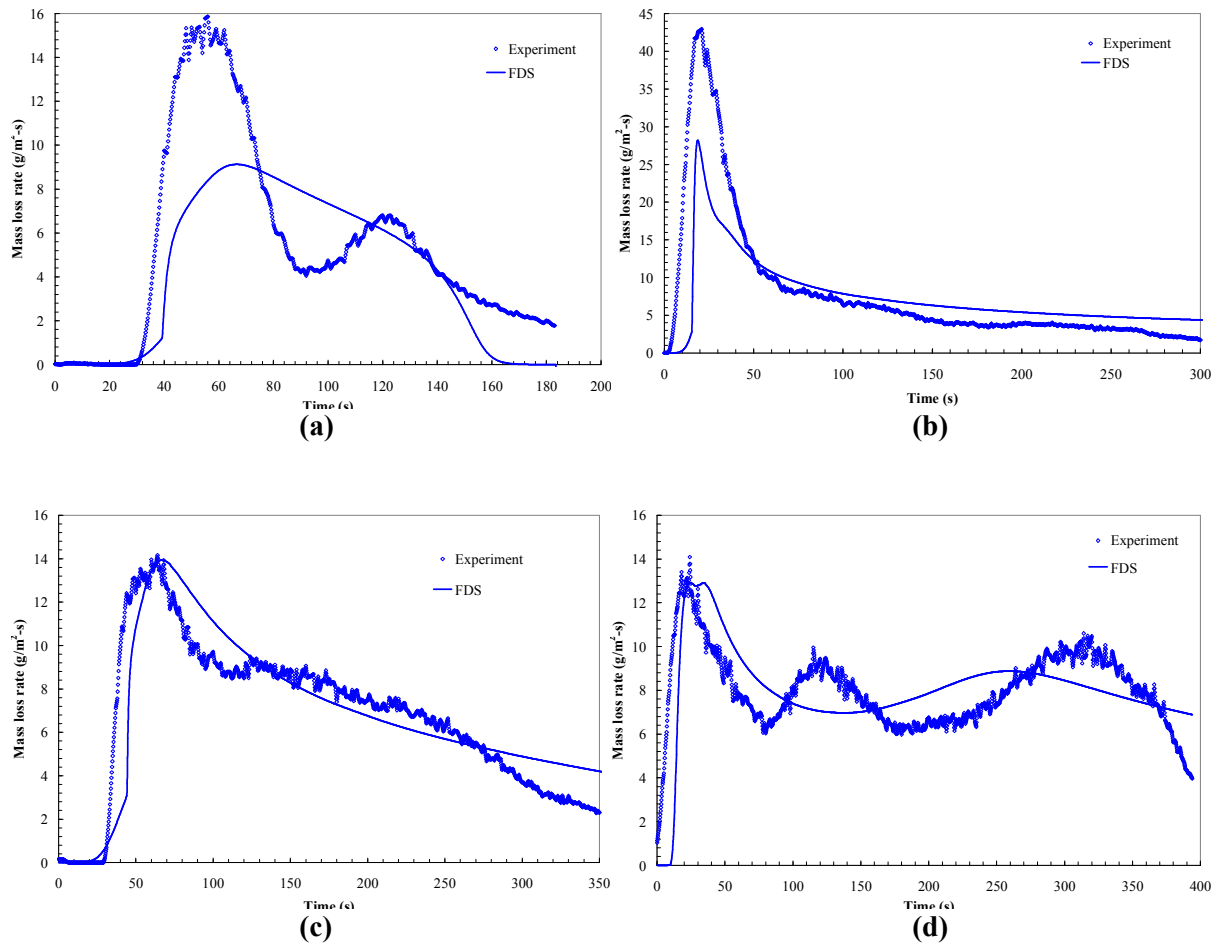


(a)



(b)

Fig. 2. Mockup fire test experimental data summary. (a) Heat release rate; (b) Temperature and heat flux.



**Fig. 3. Comparison of measured and modeled mass loss rate in Cone Calorimeter at 50 kW/m².
 (a) Phenolic liner; (b) Seat cushion; (c) Seat shroud; (d) Carpet.**

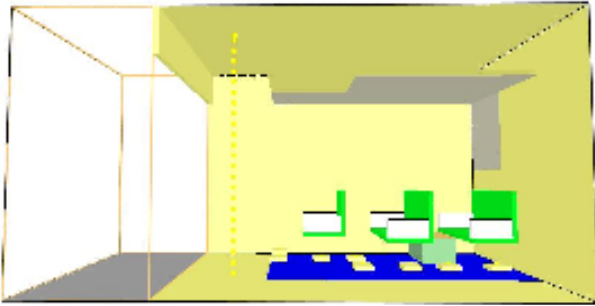


Fig. 4. FDS representation of mockup fire test.

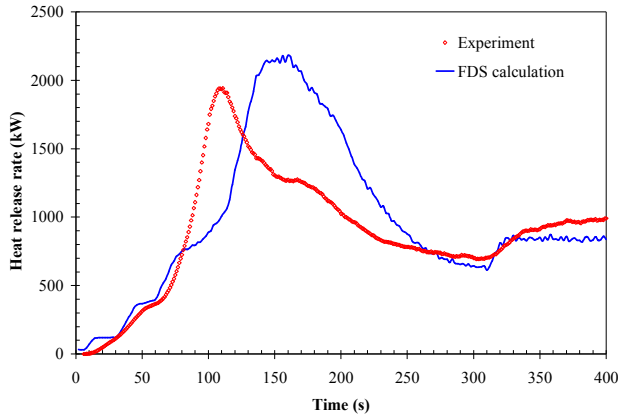


Fig. 5. Comparison of measured and modeled heat release rate.

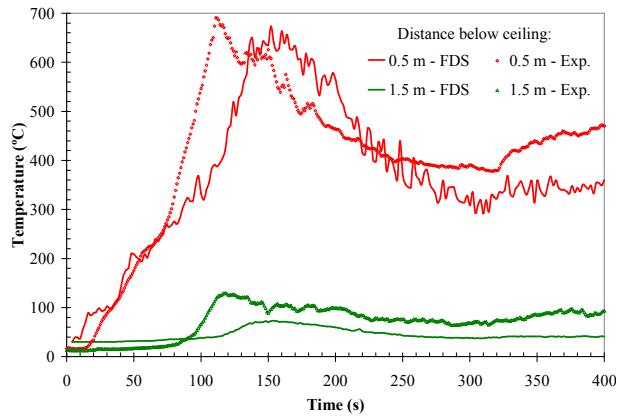


Fig. 6. Comparison of measured and modeled gas temperatures.

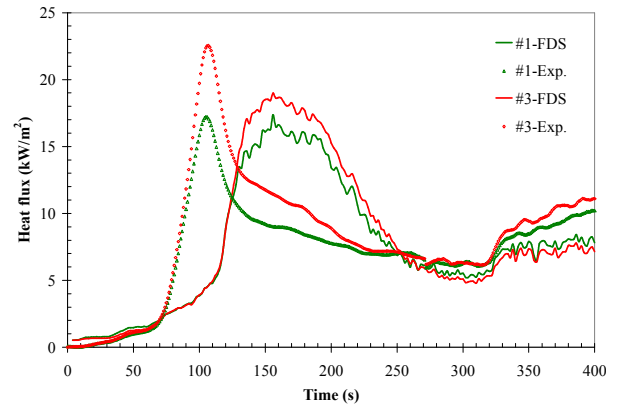


Fig. 7. Comparison of measured and modeled heat flux levels.

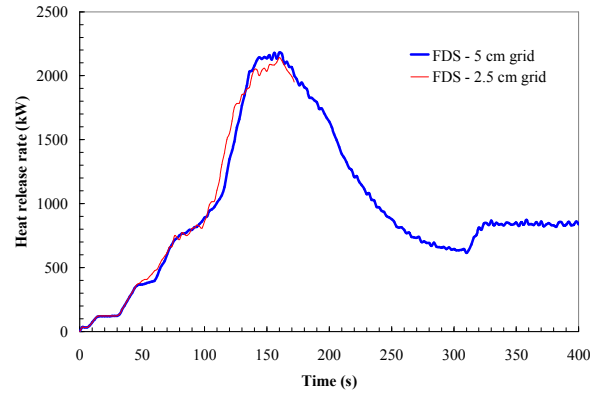


Fig. 8. Effect of grid size on calculated heat release rate for 500 kW ignition source.

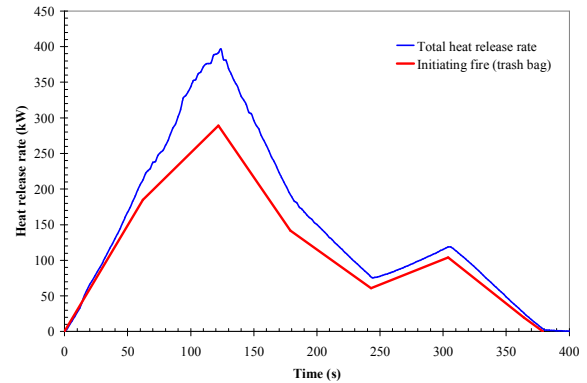


Fig. 9. Calculated heat release rate from trash bag initiating fire.

Table 1. Reaction kinetics parameters of four combustible surfaces.

| SURF | From MATL | To MATL | A (s^{-1}) | E (kJ/mol) | n (-) | ΔH_{vol} (MJ/kg) | ΔH_c (MJ/kg) | δ (mm) |
|----------|--------------|------------|----------------------|-----------------|------------|-----------------------------|-------------------------|------------------|
| phenolic | virgin | char + gas | 5.3×10^9 | 139.4 | 1.58 | 0.96 | 17.3 | 3 |
| seat | virgin | char + gas | 2.4×10^{10} | 129.1 | 1.45 | 2.17 | 9.0 | 70 |
| shroud | virgin | char + gas | 4.0×10^9 | 139.5 | 1.76 | 2.02 | 12.8 | 3 |
| carpet | virgin | char + gas | 5.4×10^9 | 154.8 | 1.83 | 1.20 | 24.3 | 20 |

Table 2. Material (MATL) thermophysical properties.

| SURF | MATL | k_0 (W/m-K) | n_k (-) | ρ_0 (kg/m ³) | c_0 (J/kg-K) | n_c (-) | ε (-) | κ (m ⁻¹) |
|----------|--------|------------------|--------------|----------------------------------|-------------------|--------------|----------------------|--------------------------------|
| phenolic | virgin | 0.30 | 0.19 | 1330 | 1489 | 0.19 | 0.9 | ∞ |
| phenolic | char | 0.25 | 0.20 | 1071 | 1622 | 0.18 | 0.9 | ∞ |
| seat | virgin | 0.22 | 0.23 | 155 | 2492 | 0.18 | 0.9 | ∞ |
| seat | char | 0.29 | 0.21 | 29 | 2258 | 0.21 | 0.9 | ∞ |
| shroud | virgin | 0.17 | 0.15 | 1320 | 1267 | 0.24 | 0.9 | ∞ |
| shroud | char | 0.08 | 0.15 | 552 | 1230 | 0.22 | 0.9 | ∞ |
| carpet | virgin | 0.37 | 0.17 | 255 | 1894 | 0.05 | 0.9 | ∞ |
| carpet | char | 0.19 | 0.17 | 32 | 1978 | 0.05 | 0.9 | ∞ |