Application of a simplified pyrolysis model to predict fire development in rack storage facilities

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ABSTRACT

The simplified (thermal) pyrolysis model is applied to simulate flame spread and fire growth in the rack storage facility using the FDS software. Pyrolysis in the combustible material is not explicitly considered, and the ignition temperature and the burning rate are used as the input parameters. Once the fuel surface temperature reaches the ignition temperature, the material ignites and burns at a prescribed burning rate. This approach is found to reasonably replicate both the transient development of the heat release rate and flame dynamics observed in the full-scale rack storage fire with 2x4x3 cardboard boxes in the rack, provided the model parameters (thermal properties of the fuel, ignition temperature, average heat release rate per unit area, burn-out time, and heat of gasification) are properly selected.

Distinct flame propagation regimes including buoyancy-driven upward flame spread, horizontal flame spread, and buoyancy-opposed downward flame propagation are observed in the simulations of the rack-storage fire development. Both measured and predicted HRR growth rates appear to be faster than that in a t-squared fire, mainly because of the developed combustible surface densely packed within the compact volume and due to availability of vertical gaps creating chimney-like effect and horizontal gaps providing permanent supply of fresh air.

It is shown how the full-scale test data enable selection of the model parameters. In particular, average value of the heat release rate per unit area is evaluated by joint consideration of the measured dynamics of the growing heat release rate and the surface area engulfed in fire. The burn-out time and the effective thickness of the fuel layer is estimated as the period from ignition to the time instant after which the measured heat release rate starts to decay. The heat of gasification is selected by fitting the predicted transient dependence of the heat release rate to that measured in the full-scale tests. Optimum values of the model parameters are consistent with the literature data for cardboard, and this indicates possibility of the simplified thermal pyrolysis model to predict rack storage fire dynamics with an alternative fire load, for which the full-scale test data may not be available. Further work is required to validate this approach for a wider range of full-scale fire tests.

KEYWORDS:

flame spread; ignition, rack-storage fire; fire growth; FDS; coupled simulations
INTRODUCTION

Rack storage fires are special because of the following issues greatly affecting the overall fire dynamics and growth rate: extremely high accumulation of fire load causing enormous peak heat release rates; developed surface area of the combustible items densely packed within the compartment volume; close face-to-face location of burning surfaces, high view factors, intensive radiative exchange causing rapid ignition; chimney-like effect facilitating intensive ventilation of the in-rack area. Obstructions hinder early detection of fire which often activates the suppression system only after engulfing considerable amount of combustibles. Design and efficiency assessment of fire detection and suppression systems could benefit from quantitative predictions, hence the efforts invested to develop comprehensive CFD models during the recent decade.

Time-dependent design fire selected as the input for engineering calculations of detection and alarm systems as well as smoke and heat venting routinely implies time-squared fire growth rate as recommended by NFPA 72, 92B, 204, among other codes. It is also used in the analysis of fire hazards in rack storages, for example, see Ref. [1]. The t-squared law was extensively validated for the performance of compact combustible items such as furnishings, and slow to ultra-fast fire types have been defined to allow for the variety of the growth rates. However, the different topology of fire load characteristic for high-rack storages would imply deviation from this law towards much higher growth rates. Indeed, early rack-storage fire tests conducted in Refs. [2, 3], indicated that the dependence on time for convective heat release rates produced in the initial fire growth period obey the third power; an even faster growth rate is possible due to the above-listed specific features of the rack storage fires, and this substantiates the need in detailed predictive simulations.

Simulations with most comprehensive modeling approaches applied to predict pyrolysis, charring and even exfoliation of practical combustibles burning in the rack-storage configurations have been recently undertaken in Refs. [4, 5, 6, 7], in which FireFOAM software tool with the bespoke pyrolysis model was applied. This series of works demonstrate that excellent replication of the heat release rates measured at the large-scale tests as well as of the realistic fire dynamics can be achieved as a result of the careful and long-term model refinement. Being tuned for a particular combustible material, such a comprehensive model might require recalibration of a large number of model parameters if applied to alternative fire load. As such, a simplified approach incorporating as few as possible model parameters, yet capable of replicating the realistic heat release dynamics, should also be explored.

The simplified approach that describes ignition and burning of a flammable material in terms of the ignition temperature and prescribed burning rate (thereby avoiding consideration of the finite-rate pyrolysis) is applied here to predict the fire growth in the rack storage configuration. The examples of successful application of this approach in predicting upward flame spread over the vertical slab and in room-corner tests can be found in Refs. [8] and [9], respectively. It is of practical interest to understand whether this approach could potentially be applied in the rack storage occupied by the variety of materials for which pyrolysis kinetics may not be readily available. To explore this simplified approach by comparing the FDS predictions to the published measurements and to the results of more comprehensive simulations is the objective of this work.

It is worthy of note that the very few previously published studies used FDS to predict the rack-storage fires. The example of fully coupled simulations of this kind is Ref. [10] in which, however, an obsolete version 4 was applied. Taking into account all the improvements introduced in FDS submodels during recent years, it is necessary to validate it against a practical rack-storage fire scenario.

MODEL DESCRIPTION

Turbulence, combustion and thermal radiation

Fire Dynamics Simulator (FDS 6.6) numerically solves the Navier-Stokes equations for a multi-component reacting mixture in the low-Mach number limit. The large eddy simulation approach is used to simulate turbulent flow with the default Deardorff sub-grid model. For turbulent combustion modeling, the eddy dissipation concept is utilized, and the single-step fast irreversible reaction is considered. Constant soot and CO yields are assumed. The rate of fuel consumption is set proportional to both the local limiting reactant concentration and the local rate of mixing, and the subgrid mixing time is evaluated taking subgrid kinetic energy, molecular diffusivity, and buoyancy into account.

Radiative transfer is simulated by solving the radiative transfer equation using the finite volume method with 104 discrete solid angles. Spectral properties of the gas-soot media are accounted for by the mean (gray) absorption coefficients, which are simulated by the RadCal procedure as a function of composition and
temperature. The ratio of the radiation emission in the flame to the chemical heat release is set equal to the pre-assumed radiative fraction. Unless otherwise stated, default heat transfer options of FDS 6.6 are used.

Two distinct approaches are applied in this and the earlier author’s work to account for thermal decomposition of a solid combustible material.

**Finite-rate pyrolysis model**

This model employs the single step irreversible n-th order reaction of material decomposition. Temperature dependence of the reaction rate is described by Arrhenius type equation. Using this approach, the upward spread of the turbulent flame over the 5 m height PMMA slab is replicated in Ref. [11].

**Simplified (thermal) pyrolysis model**

This approach uses the ignition temperature, $T_{ign}$, and the mass loss rate, $m_{fuel}^{\tau}$, as the input parameters. 1D heat conductivity equation without the reaction term is solved in the material layer of a constant thickness in the direction normal to the surface. The boundary condition at the surface takes into account conductive heat transfer to the material, absorbed radiation, reradiation, and the convective heat flux from the gas phase. Transparency of the material for the radiative flux is accounted for, and radiative transfer inside the material layer is solved by the two-flux method.

Once the surface temperature reaches the value of $T_{ign}$, the ignition occurs, a constant prescribed mass loss rate, $m_{fuel}^{\tau}$, is set at the surface, and the net heat flux received by the surface is decreased by the value of $\Delta m_{fuel}^{\tau}$, where $\Delta m_{fuel}^{\tau}$ is the effective heat of gasification. Note that in FDS 6.6 surface temperature is still calculated after ignition by solving the same heat conductivity equation with the corrected net heat flux at the boundary. This enables predicting considerable surface temperature growth in burning of charring materials. This default option is, therefore, retained in this work.

In order to account for the fuel burn-out, the corresponding heat release rate per unit area is ramped down to 0 kW/m² after the burn-out time, $\tau_b$, is reached. The latter depends on burning rate and layer thickness and is defined by a user in the input data. The following estimate is used in this work for the burn-out time after ignition: $\tau_b = \rho \delta / m_{fuel}^{\tau}$, where $\rho$ and $\delta$ are the material density and the layer thickness.

Thus, it is possible to include heating up, ignition, developed and fire decay stages in the simulation in a simplified way, while still being able to capture most of the significant thermal feedback effects. The input parameters are as follows: thermal properties of the fuel (conductivity, specific heat, and heat of gasification), ignition temperature, heat release rate (or mass loss rate) per unit area of the burning material, burnout time.

**RACK STORAGE FIRE SIMULATIONS**

**Simulation set-up**

The experimental scenario studied in Ref. [6] is considered, with 2x4x3 combustible boxes in the rack. Each box has the dimensions of 1.07x1.07x1.07 m (see Fig. 1) and is simulated as a solid obstruction, for which a simplified pyrolysis model is employed as a boundary condition. The flues in the horizontal directions are 15 cm, in the vertical direction – 46 cm, the wooden pallets (often used in rack storages) are not considered. The first tier is elevated by 13 cm above the floor level. To initiate burning, four ignitors with constant heat release rate (22.5 kW each) were placed in the center of the rack so that 4 center bottom boxes are heated from different sides. Free-born scenario (no fire suppression) is considered.

Computational domain has the dimensions of 10.7x8.3x8 m (length, width, height). The grid is composed of 2.5, 5, and 10 cm size cubic cells. Nested rectangular zone with the finest grid surrounds the rack (see Fig. 1). The central area (4 central columns of boxes) is spanned by 2.5 cm cubic cells (6 cells across the horizontal flue). The cell size is increased to 5 cm in the vicinity of side columns and above the central columns where the main plume develops. At the periphery of the computational domain, 10 cm cells are used. The total number of cells is 3 103 220. It takes 125 hours of the wall clock time to compute 320 s of simulation time using 54 CPU cores (2 CPU Intel Xeon E5-2697 v3).
Model calibration

The following model parameters have to be defined: (i) material thermal properties and layer thickness, $k$, $\rho$, $c$, and $\Delta h_f$; (ii) ignition temperature, $T_{ign}$; (iii) heat release rate per unit area after ignition, which is coupled with the mass burning rate as $Q^* = m_{fuel}^* \Delta h_f$; (iv) burn-out time, $\tau_s$.

For the cardboard fuel considered in this work, we use the values of density, $\rho = 184$ kg/m$^3$, specific heat, $c = 2700$ J/(kg K), and pyrolysis heat of combustion, $\Delta h_f = 14.2$ MJ/kg provided in Ref. [6]. For thermal conductivity, we adopt the value of $k = 0.1$ W/(m·K), which is closer to the literature data for cardboard (for example, see [13]) than the value of 0.42 W/(m·K) used in Ref. [6].

The ignition temperature, $T_{ign}$, is taken 360 °C as a representative value consistent with the literature data [14]. Note, that with the average net heat flux of 15 kW/m$^2$ time to ignition estimated in thermally thick limit is $t_{ign} = (\pi/4)k\rho c \left( (T_{ign} - T_0) / q_{net}^* \right)^2 = 20$ s. Consistent with the simulations performed in this work, during this time period the total measured heat release rate exceeds that provided by the igniters (90 kW) thereby indicating the beginning of sustained fire growth.

The HRRPUA value can be directly estimated from the HRR growth dynamics observed in Ref. [6], which shows that at time instant 85 s the HRR approaches 10 MW, and two central columns at the second and third tier are engulfed in fire. The latter implies that the burning area equals to the total surface area of 8 boxes, i.e. $1.07^2 \times 6.8 = 55$ m$^2$, which results in $Q^* = 10000 / 55 = 182$ kW/m$^2$. Also, at time instant 150 s 16 boxes are engulfed in fire, which indicates that the burning area roughly doubles (mainly due to the horizontal flame spread to the outside columns). The measured HRR at 150 s is about 20 to 23 MW, which indicates that the value of HRR per unit area remains nearly the same. Based on these estimates, we use the HRRPUA value of 200 kW/m$^2$. Recall that this is the average heat release rate per unit area of the box surface, which is much lower than the peak value of HRR per unit area of the horizontal cross-section of the rack.

The burn-out time, $\tau_s$, determines the onset of the decay of the heat release rate. Transient variation of the HRR recorded in Ref. [6] shows that the burn-out time can be estimated as $\tau_s = 290$ s. In fact, by assigning the burn-out time, we define the fuel mass per unit area, $m_{fuel}^* \tau_s = \rho \delta$. For the given material density, mass burning rate and heat of combustion, it corresponds to the equivalent layer thickness $\delta = \tau_s m_{fuel}^* / \rho = \tau_s Q^*/(\rho \Delta h_f) = 0.022$ m. This value is larger than the actual cardboard thickness (for example, 8.4 mm thick cardboard is used Ref. [12]), and this difference accommodates possible variation of the burning rate in time.

Finally, the heat of gasification, $\Delta h_g$, has to be estimated. In the model, the heat of gasification is subtracted from the net heat flux received by the material thereby reducing the predicted surface temperature. Thus, an underestimated value of $\Delta h_g$ causes overestimated surface temperature, radiative flux emitted by the burning surface, and, therefore, radiative flux incident to the non-burning surfaces. In its turn, it causes earlier ignition of the non-burning surfaces and faster total heat release rate. This is shown in Fig. 2 where transient dependences of the predicted heat release rate are shown for three pre-assumed values of $\Delta h_g$. It can be seen that the value of $\Delta h_g = 1$ MJ/kg results in a reasonable agreement with the measurement.

Simulation results

Predicted fire development is visualized in Fig. 1. As highlighted in Ref. [7], the HRR growth rate is higher if flame propagates vertically upwards compared to that occurring if flame propagates horizontally: the growth rate, therefore, varies in time because of the varying direction of primary flame propagation. The following periods can be identified after the lowest boxes are ignited at time instant 16 s. Period 1 (16 – 50 s): flame spreads upwards over the vertical surfaces of the central boxes, and the flame tip appears above the upper tier. Period 2 (50 – 80 s): flame spreads horizontally covering the bottom surfaces of the central boxes in the upper tiers. The flame tip impinges the ceiling. Period 3 (80 – 120 s): flame spreads both vertically and horizontally: all vertical sides of the central boxes, 2nd and 3rd tier, burn. Period 4 (120 – 140 s): flame spreads horizontally towards the side boxes between 2nd and 3rd tier. Period 5 (140 – 190 s): flame spreads both vertically and horizontally. Note, that downward flame propagation over the external vertical surfaces of the side boxes at the second tier is also predicted. Finally, all vertical sides of the boxes in the 2nd and 3rd tiers
burn, and the heat release rate attains its maximum. This fire dynamics corresponds well to experimental observations and simulation results presented in Refs. [6, 7], where a more complicated model was utilized.

Fig. 1. Predicted flame snapshots (200 kW/m² heat release rate iso-surface) for the 2×4×3 rack-storage free-burn fire. The left upper figure shows the computational mesh in the central plane.

Fig. 2. Heat release rate history in the 2×4×3 rack-storage free-burn fire.

Fig. 3. The temperatures of the inner box surfaces (facing inside the rack) predicted with different values of the heat of gasification: a) – 0 MJ/kg; b) – 0.5 MJ/kg; c) – 1 MJ/kg at time instant 150 s and (d) the corresponding flame snapshot (200 kW/m² heat release rate iso-surface, the heat of gasification–1 MJ/kg).

Predicted temperature distributions at the inner surfaces of the burning boxes is shown in Fig. 3. As expected, it appears to be much higher than that of the outer surfaces as presented in simulation results in Ref. [7]. This can also be attributed to the significantly different thermal conductivities used in these simulations.

CONCLUSIONS

A simplified (thermal) pyrolysis model enables approximate replication of the fire dynamics observed in full-scale fire tests of rack-storage fires. This can be achieved provided the model parameters (ignition temperature, HRRPUA, burn-out time, and heat of gasification) are properly selected for a given type of fuel load. In this work, thermal properties and the ignition temperature of the cardboard are selected based on the published measured values. The average HRRPUA value is evaluated by joint consideration of the measured dynamics of the growing heat release rate and the surface area engulfed in fire. The burn-out time and the
effective thickness of the fuel layer is estimated as the period from ignition to the time instant after which the measured heat release rate starts to decay. The heat of gasification is selected by fitting the predicted transient dependence of the heat release rate to that measured in the full-scale tests. Optimum values of the model parameters are consistent with the literature data for cardboard. This implies potential capability of the simplified thermal pyrolysis model to predict rack storage fire dynamics with an alternative fire load, for which the full-scale test data may not be available.

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