

CHEMICAL SPECIES AND TEMPERATURE MAPPING IN FULL SCALE UNDERVENTILATED COMPARTMENT FIRES

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ABSTRACT

Many injuries and deaths throughout the world are caused by fires each year. Many of the deaths are the result of toxic gas inhalation, such as carbon monoxide, by a victim remote from the actual fire source. In order to facilitate better building standards, forensic reconstruction, and safety design, fire models are used to predict or reconstruct the fire incident. Fire models such as the Fire Dynamics Simulator (FDS) developed at the National Institute of Standards and Technology (NIST) can predict heat transfer and gas flow through a known structural environment with relatively low uncertainty, however they utilize a very simple mixture fraction based chemistry model. This simplification is highly effective in making the code accessible and efficient enough to be used on a standard personal computer, but limits the model's effectiveness at predicting intermediate and incomplete products of combustion, such as carbon monoxide and soot, that may be generated by a real fire, especially if that fire is oxygen deficient and becomes underventilated. Recently NIST has undertaken an extensive set of measurements of the thermal and chemical environment of underventilated fires in an ISO9705 compartment to support fire model development and validation. A robust ISO9705 compartment was constructed to allow for repeated long duration underventilated compartment fire tests with repeatable boundary conditions and minimum turnaround time. The tests were conducted in the NIST Large Fire Lab (LFL), which provides a unique facility for this type of fire experiment. Temperature resistant and water cooled probes were implemented to extract gas samples for analysis, and a sturdy superstructure was constructed to facilitate positioning hardware so that the sample probes could be repositioned within the room during a test. Measurements of fuel mass loss rate and/or precise metering of fuel delivery rates were made to provide accurate data on the combustion efficiency of the system.

INTRODUCTION

Inhalation of toxic products is the primary cause of fire related injuries and deaths in residential fires [1]. Many investigations have focused on understanding the production and evolution of carbon monoxide (CO) [2– 7] and other toxic species [8] as well as the fire behavior [9] and the thermal environment [10] in a compartment for forensic analysis and hazard planning with various levels of success. Compartment fires can occur with a variety of different room configurations, fuel types, fuel distributions, and ventilation conditions, making it very difficult to understand and accurately predict the fire phenomena inside a compartment. The current study is part of a larger project aimed at making detailed measurements in an underventilated compartment fire and developing

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a better understanding of the fire dynamics, soot, and CO production, which facilitates model development [11,12]. This paper presents some of the findings related to the internal flow dynamics and species concentrations within heptane fueled compartment fires.

Previous studies [2,3] related to CO production used a well-controlled exhaust hood to simulate the upper layer effect of an enclosure fire. They found that the CO concentration can be correlated to a global equivalence ratio (GER) [6], where GER is defined as the equivalence ratio in the upper layer of a two-layered fire environment. Gottuk et al. [4,5] confirmed that the production of CO is primarily dependent on the GER and upper layer temperature in the test compartment, designed with a two-vent system to measure the GER. On the other hand, from the experimental results using a typical enclosure which included a single door opening and four walls, Bryner et al. [7] reported that the upper layer in enclosure fires is not homogeneous, and that CO is produced in greater quantities than predicted by the GER concept, depending on temperatures and flow patterns developed within the enclosure. They also noted that the geometry of the enclosure significantly impacts how the fuel and air within the room mix, heat up, and react. These studies indicated that the variation in compartment geometry, including vent (doorway) location and size, can result in significant changes in fire behavior, thermal and chemical environments and the fluid dynamics inside a compartment.

A fully-developed compartment fire can be classified into two conditions by the GER. Fires are generally discussed in terms of toxicant production and temperature measured at local points inside a compartment using the classification of over- and underventilated conditions. A $GER < 1$ represents overventilated conditions where the yields of CO or unburned hydrocarbons are very small (sometimes close to zero) due to nearly complete combustion. For $GER > 1$, underventilated conditions occur and the yields of these toxicants can increase by as much as a factor of ten compared to the overventilated conditions. Variation of ventilation can affect significant change in thermal, chemical, and fluid dynamic behavior inside the compartment. Therefore, detailed measurements of fire behavior and flow field are necessary to predict the production and evolution of CO and other toxicants. Because of the non-uniform structure of the upper layer in underventilated compartment fires, multi-dimensional effects are very important [7]. However, there have been few studies of multi-dimensional flow dynamics, thermal and chemical environments in the compartment fires due to the limited number of measurements typically made within underventilated compartment fires.

Much of this previous research has focused on a fire generated in a geometrically centered burner inside a compartment [8-10]. However, it is not well understood how the location and distribution of the available fuel materials may affect the fire growth, toxic product generation, and time to flashover as well as the internal flow dynamics and thermal environment within a compartment. A number of studies indicate that when the fuel location changes, the HRR significantly changes for an overventilated fire and time to flashover changes [11-14]. There have been few studies however, of the effects of fuel location and distribution on detailed fire dynamics and structure including the spatial distributions of temperature and combustion products in an underventilated compartment fire.

Recently, Thomas et al. [15] investigated the effects of fuel quantity and location on ethanol pool fires in an ISO 9705 room. In this study, a fuel package consisting of two or three burners was placed inside the door (front), in the center of the room (center), or adjacent to the back wall (back). They found that the variation of fuel location resulted in significant changes in time histories of HRR and temperature as well as their maximum values. For maximum HRRs, the ranking of the maximum HRR with the change in fuel location was observed to be $HRR_{front} > HRR_{back} > HRR_{center}$. This was thought to be due to difference in the combined effects of radiation feedback from the compartment walls and enhanced mixing with oxygen due to changes in fuel location. Considering that they used a full doorway, 0.8 m wide \times 2.0 m high, a maximum fuel amount of 40 L, and a total burner surface corresponding to 1.0 m², it can be estimated that the experiments were conducted in the overventilated fire regime [16]. In the field of fire safety engineering, it has been observed that underventilated fires may yield as much as ten times more toxicants, such as CO, compared to overventilated fires [17, 18]. There has been little detailed information regarding the change in the thermal and chemical environment in underventilated compartment fires as fuel is placed at different locations within a room.

This paper discusses heptane compartment fires behaviors with regard to the effect of fuel distribution on upper layer chemistry and the internal 3-D structure of the fire [16]. The main objective of the present study is to characterize these compartment fires in terms of the thermal and flow fields

and product formation using a multi-dimensional approach and to evaluate the effects of fuel distribution inside the compartment.

EXPERIMENTAL CONFIGURATION

Figure 1 presents the full scale enclosure (FSE) based on a standard ISO 9705 room, which is 2.4 m wide \times 3.6 m deep \times 2.4 m high. For some experiments a full width doorway (0.8 m \times 2.0 m) was utilized, but for most a 1/4 width doorway (0.2 m wide \times 2.0 m) or a 1/8 width doorway (0.1 m \times 2.0 m) centered at the bottom of the front wall was used to force the room to reach underventilated conditions with a smaller fire size. The uncertainty of the as-built enclosure was measured as ± 0.02 m. The floor of the enclosure was raised 0.35 m above the ground to facilitate instrumentation. The support structure of the enclosure was built using 0.89 mm (20 gauge) steel, structural studding, and 0.89 mm sheet steel. The floor of the structure was constructed of 4.8 mm thick steel sheet metal. The compartment walls, floor and ceiling were covered with two layers of 25 mm (50 mm total) thick, 128 kg/m³, high temperature ceramic fiber blanket.

Temperature and species concentrations including O₂, CO, CO₂ and total hydrocarbons were continuously measured at various locations within the compartment. Type-K thermocouples with a bead diameter of 0.5 mm \pm 0.125 mm were installed to measure the temperatures at various places in the room. Oxygen was measured using paramagnetic analyzers (Servomex[†], 4100), carbon monoxide and carbon dioxide were measured using non-dispersive infrared analyzers (Siemens, Ultramat 6E), and total hydrocarbons were measured using flame ionization detectors (Baseline-Mocon, 8800 H). The measurements of all gas species are reported on a wet basis in this paper. Detailed sampling locations are indicated in Fig. 1 and Fig. 5. A full description of the experimental apparatus and additional instrumentation including total expanded uncertainty for each measurement is given in NIST Technical Note 1603 [6].

Heat release rate (HRR) measurements were conducted using the 6 m \times 6 m calorimeter at the NIST Large Fire Laboratory (LFL) [21]. The total expanded relative uncertainty of the HRR measurements reported was ± 14 % based on a propagation of uncertainty analysis.

The present study examined several heptane fires. Different fuel locations and distributions were examined: a single centered burner (SCB), a single rear burner (SRB) and two distributed burners (TDB) as shown in Fig. 1. Pan burner(s) were used and total burner surface area was fixed at 0.5 m². In the cases of SCB and SRB, a single burner size of 0.707 m \times 0.707 m (0.5 m²) with a 10 cm lip was positioned in the geometric center of the floor (SCB) and along the centerline of the room next to the rear wall (SRB). Two 0.25 m² burners were placed at the center and rear locations in the TDB case. The total volume of fuel was fixed at 30 L (\approx 20 kg) for all cases. The fuel mass loss rate was measured using a load cell mounted underneath the burner with a measurement accuracy of ± 0.001 kg. For the 3D mapping experiments a single 0.707 m \times 0.707 m pan was utilized in the center of the room. Fuel was sprayed into the pan at a controlled rate in order to obtain highly reliable and repeatable fuel delivery rates over long durations.

UVF AND OVF RESULTS

The HRR measurement represents the total burning inside and outside of the compartment and is used to characterize the fire size. Figure 2 presents the measured real and ideal HRRs for the OVFs (0.8 m doorway) and UVF (0.2 m doorway). The real HRRs were measured by the calorimeter and the ideal HRRs were calculated using either the metered fuel flow rates or measured fuel mass loss rates with the heat of combustion for heptane fuel (\approx 44.6 MJ/kg) [25]. In the experiment for the OVFs, several different levels of steady fuel flow rate were used over 5000 s, so that the ideal HRR was increased in steps up to 2400 kW. It was observed that a time delay and large fluctuations in the HRR occurred due to intrinsic instabilities in burning rate caused by the burner design. Nevertheless, the measured HRRs showed similar values and transient behaviors compared to the ideal HRRs, in each period of pseudo-steady state. In the experiment for the UVF, a fixed volume of fuel, 30 L, was placed in a pan type burner. The real HRR increases linearly over a period of about 70 s to approach a

[†] Certain commercial entities, equipment, or materials may be identified in this document in order to describe an experimental procedure or concept adequately. Such identification is not intended to imply recommendation or endorsement by the National Institute of Standards and Technology, nor is it intended to imply that the entities, materials, or equipment are necessarily the best available for the purpose.

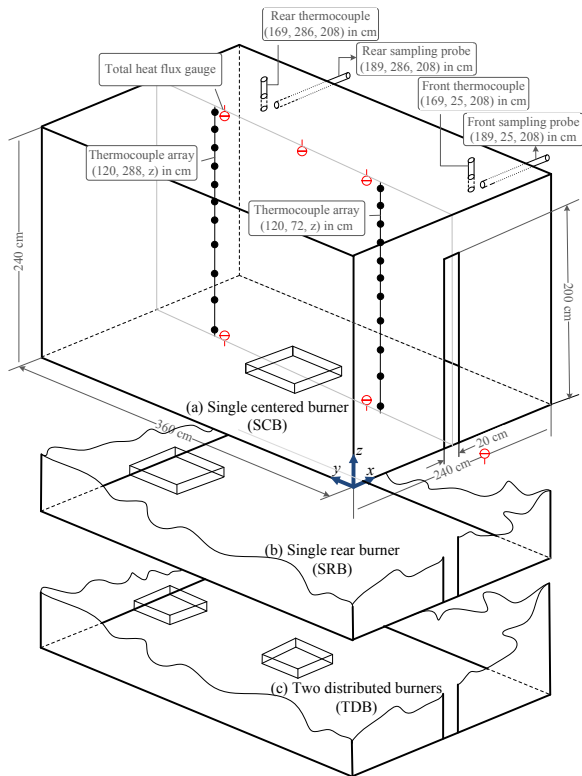


Figure 1. Schematic diagram of the ISO 9705 room for fire tests of (a) single centered burner, (b) single rear burner and (c) two distributed burners.

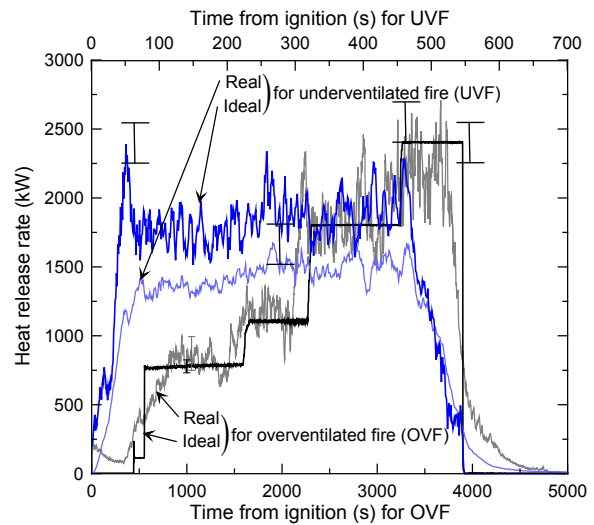


Figure 2. Measured real and ideal heat release rates for the over- and underventilated fires (total expanded uncertainties in ideal and measured heat release rate measurements are $\pm 6\%$ and $\pm 14\%$, respectively).

pseudo-steady state burning of the fuel in the pan which was maintained until the fuel evaporated completely from the pan at 700 s. The ideal HRR leads the dynamic behavior of the measured HRR and there is a proportional response of the two values. The quantitative difference between the real and ideal HRRs is attributed to the low combustion efficiency resulting in significant soot, CO and total hydrocarbons production. In addition, the quantitative differences between the real and ideal HRRs explicitly show evidence for the over- and underventilated conditions in terms of the combustion efficiency [22].

FUEL DISTRIBUTION RESULTS

Figure 3 shows images of the compartment fire after ignition for three cases with different fuel locations and distributions. Images are presented at 50 s and 150 s after ignition. At 150 s, it is obvious that most of the burning occurred outside of the enclosure. Comparing the images of the fire at 50 s and 150 s, the SRB case has burning outside the door earlier in the fire development than the other cases. This can be explained, in part, by the SRB case having the fuel located the furthest from the vent. When the burner was placed adjacent to the rear wall of the enclosure, the area through which air may be entrained was reduced and the overall fuel-air mixing rate decreased [25]. The restriction of air entrainment to the fire plume led to an increase in flame length, due to excess volatilized fuel. Consequently, the fire became underventilated earlier than the centered burner case (i.e. the SCB case). For the TDB case, smaller burners were placed at the center and rear of the compartment. The absence of external burning early was attributed to the locally decreased oxygen demand due to the distributed fuel as compared to the other cases allowing for more air to be entrained with the fuel. Even though the time to burning outside the room was different with the change in fuel placement, it was difficult to find distinct differences in flame shape once the fire was established in steady state, e.g. at $t > 150$ s.

Figure 4 compares the measured CO volume fraction at the front and rear sampling locations within the enclosure. At the front sampling location (Fig. 4(a)), CO concentration gradually increased with time for each case. The transient CO behavior for each case shows the opposite trend to the CO₂

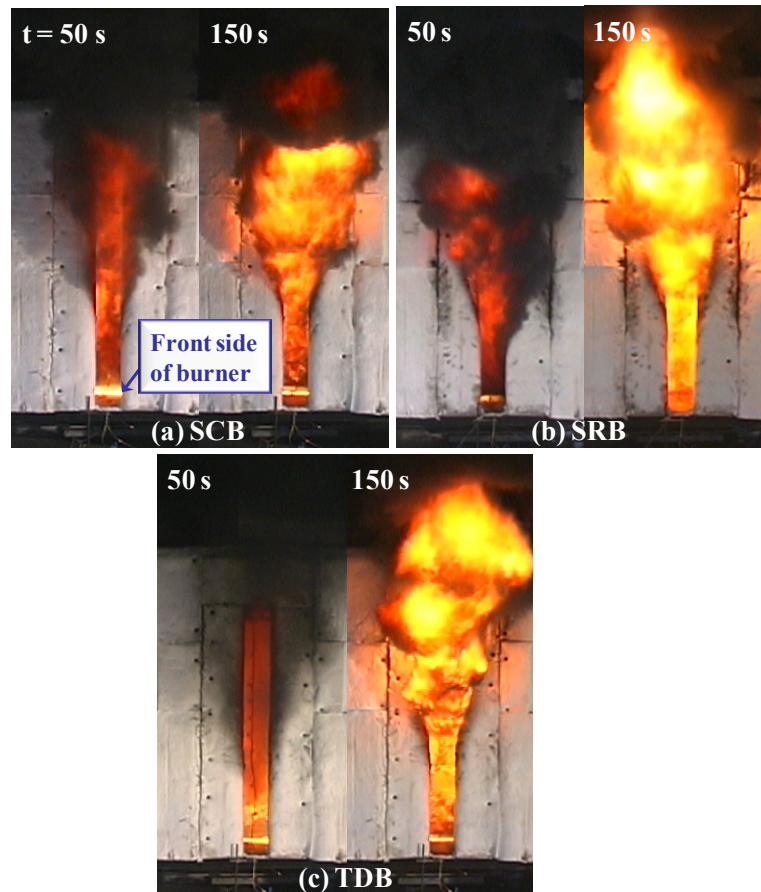


Figure 3. Temporal images of compartment fires at 50 s and 150 s after ignition for the SCB (centered burner), SRB (single rear burner), and TDB (two distributed burners) cases. Doorway width is 0.2 m.

behavior, as expected. At the front sampling location, the difference in CO volume fraction among the cases was not large and was similar to that of CO₂. On the other hand, at the rear sampling location (Fig. 4(b)), CO increased significantly in the SCB case with time, while the SRB and TDB cases showed steady CO concentration throughout the period of steady burning. Fig. 4 indicates that the variation in fuel placement played a more important role in the change in chemical environment in the rear of the compartment than in the front. This was also observed in the average species volume fractions. The O₂ volume fraction was very small in both the front and rear locations. The maximum differences in CO₂ and CO volume fractions between the front and rear sampling locations were 0.013 and 0.026, respectively. That is, the change in fuel location and distribution was accompanied by larger changes in CO and CO₂ volume fraction at the rear sampling location than at the front location. It is difficult to explain the cause of these differences with the data measured at only two local sampling

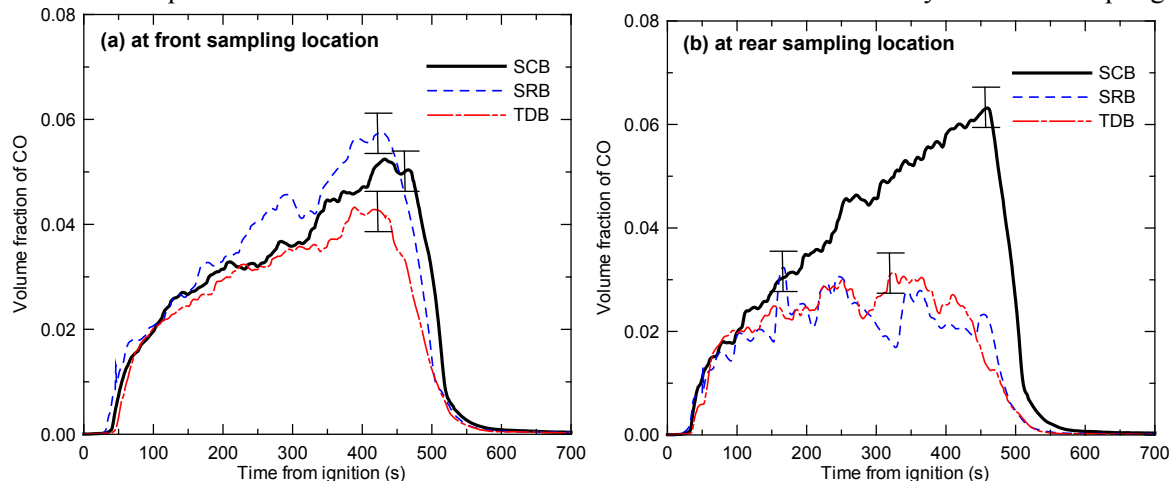
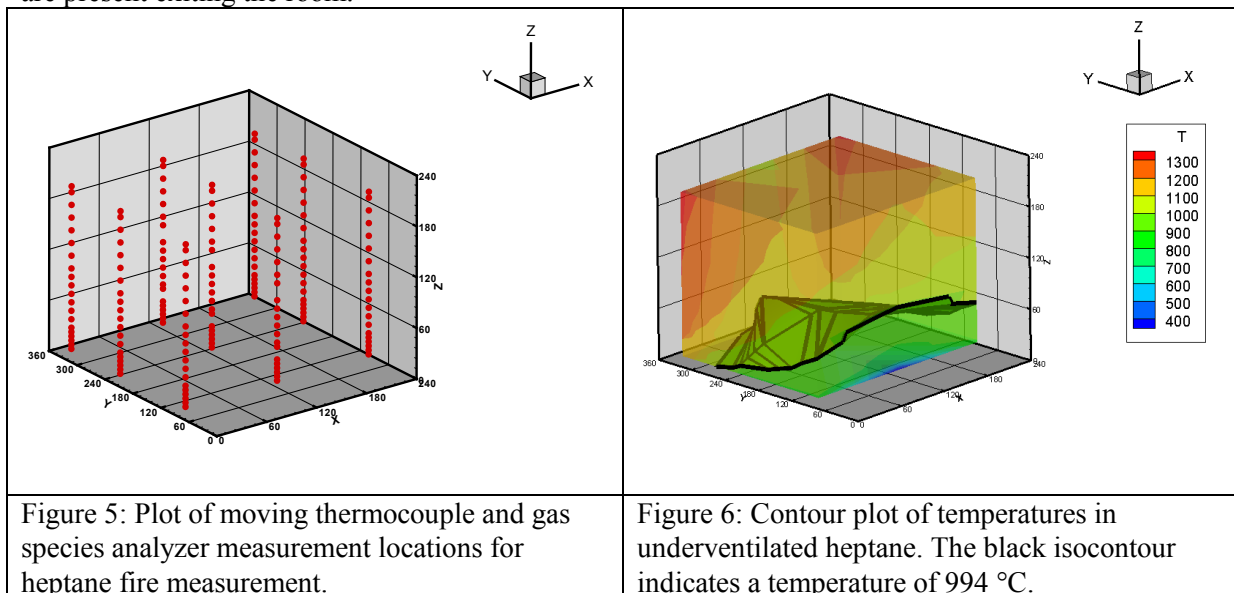


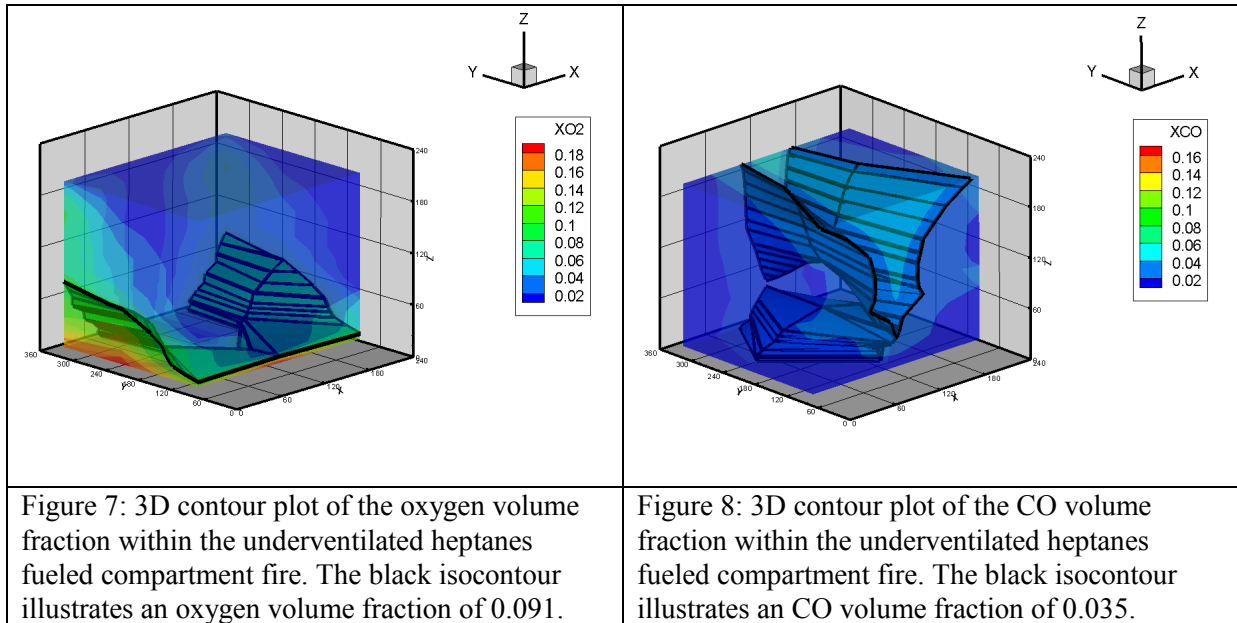
Figure 4. Comparison of CO volume fractions at the front and rear sampling probe locations.

locations. As noted earlier it was observed that product sampling at local positions in the upper layer cannot represent the fire characteristics in underventilated conditions. In particular, the CO in the underventilated compartment fire was directly related to the three-dimensional flow structure and the O₂ distribution. Therefore, the details of CO with the change in fuel placement should be discussed in the context of three-dimensional fire behaviors based on numerical simulations [22, 26].

THREE DIMENSIONAL THERMAL AND CHEMICAL MEASUREMENTS

A mapping of temperature and chemical species measurements inside an underventilated heptane-fueled compartment fire with a 10 cm doorway in order to build a map of the internal structure of the fire from experimental data. The fuel delivery rate was held constant at the volume flow rate of heptane to provide an ideal heat release rate of 1000 kW. The measured heat release rate from these experiments was 800 kW ± 50 kW. These measurements were facilitated by a set of three vertically moving probes that were built to traverse the height of the compartment. Measurements were made at two vertical slices inside the room, one at the centerline and one near the edge of the room. Symmetry was assumed in order to construct the plots presented here. The points at which measurements were made are illustrated graphically in Fig. 5. A 3-D plot of the temperatures measured inside the enclosure is presented in Fig. 6. It is evident from the plot that the cool air is entering low through the doorway. This was confirmed visually, as the upper layer was observed at the floor level during this test. The upper layer temperatures are observed to vary between 1100 °C and 1300 °C. This range was fairly consistent down to about 80 cm with smaller regions of high temperatures closer to the floor and larger regions of high temperatures close to the ceiling. Overall, the temperature contours are consistent with the configuration of the vent and the inflow of air. As mentioned in a previous paper [22] recirculation regions are expected in the upper rear corners of the compartment which may contribute to the peak temperatures measured there. Figures 7 and 8 present 3-D plots of the CO and O₂ wet volume fractions measured within the compartment, respectively. These measurements correspond to the same spatial points illustrated in Fig. 5. As expected the contours of large CO and O₂ volume fractions occupy the opposite areas of the compartment. The O₂ plot indicates that as oxygen enters the compartment it may be consumed near the burner and the excess quickly transported to the sides of the compartment where it moves up and reacts with fuel species to produce the higher concentrations of CO along the center plane of the room. The CO volume fraction contours also indicate that large volume fractions of CO are present exiting the room.





SUMMARY

Experimental data from a series of experiments on underventilated heptanes fueled compartment fires is presented. Some characteristics of overventilated (OVF) and underventilated (UVF) fires were discussed. The effect of varying the location and distribution of the burner was examined. The complex three dimensional distribution of temperature, O_2 , and CO within a underventilated compartment fire was also presented.

From the experimental results, it was observed that varying the fuel location and distribution does not play an important role in changing the global characteristics of an underventilated fire such as the fuel mass loss rate, heat release rate, combustion efficiency, global equivalence ratio and global CO emission outside the compartment. These results are different than those observed in overventilated fires [4].

The local thermal and chemical environments were different depending on the fuel location. At the front of the compartment, the thermal and chemical environment are nearly the same regardless of fuel location and distribution. However, variation in fuel placement resulted in significant changes in temperature, total heat flux, CO_2 and CO distributions at the rear of the compartment. These results are consistent with the experimental results that the thermal and chemical environments in the rear region change as the fuel placement changed inside the compartment.

Detailed three dimensional thermal and chemical measurements of the underventilated compartment fire were also presented. The 3D map of temperature indicates where regions of high temperature exist within the compartment and gives hints as to what thermodynamic phenomena and flow patterns might be contributing to the distribution. The 3D map of O_2 and CO within the enclosure indicates how the burning might be occurring within the room and also suggests some trends in the thermodynamic and flow dynamics present in the enclosure.

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REFERENCES:

1. Harwood, B. and Hall, J.R. (1989). What kills in fires: smoke inhalation or burner?, *Fire Safety Journal*, 83: 29–34.
2. Tewarson, A. (1984). Fully developed enclosure fires of wood cribs, *Proceedings of Combustion Institute*, 20: 1555–1566.
3. Beyler, C.L. (1986). Major species production by diffusion flames in a two-layer compartment fire environment, *Fire Safety Journal*, 10: 47–56.

4. Gottuk, D.T., Roby, R.J., Peatross, M.J. and Beyler, C.L. (1992). Carbon monoxide production in compartment fires, *Journal of Fire Protection Engineering*, 4: 133–150.
5. Gottuk, D.T., Roby, R.J. and Beyler, C.L. (1995). The role of temperature on carbon monoxide production in compartment fires, *Fire Safety Journal*, 24: 315–331.
6. Pitts, W.M. (1994). Application of thermodynamic and detailed chemical kinetic modeling to understanding combustion product generation in enclosure fires, *Fire Safety Journal*, 23: 271–303.
7. Bryner, N.P., Johnsson, E.L. and Pitts, W.M. (1994). Carbon monoxide production in compartment fires - reduced-scale enclosure test facility, NISTIR 5568, National Institute of Standards and Technology, Gaithersburg, MD.
8. Quintiere, J.G., Rinkinen, W.J. and Jones, W.W. (1981). The effect of Room Openings on Fire Plume Entrainment, *Combustion Science and Technology*, 26: 193-201.
9. Merci, B. and Vandevelde, P. (2007). Experimental Study of Natural Roof Ventilation in Full-scale Enclosure Fire Tests in a Small Compartment, *Fire Safety Journal*, 46: 523-535.
10. Pierce, J.B.M. and Moss, J.B. (2007). Smoke Production, Radiation Heat Transfer and Fire Growth in a Liquid-Fuelled Compartment Fire, *Fire Safety Journal*, 42: 310-320.
11. Tran, H.C. (1990). Experimental Aspects of Validating a Compartment Wall Fire Model, *Proceedings, 5th International Fire Conference, Interflam '90, London, England*, pp. 13-24.
12. Snegirev, A.Y., Makhviladze, G.M., Talalov, V.A. and Shamshin, A.V. (2003). Turbulent Diffusion Combustion under Conditions of Limited Ventilation: Flame Projection through an Opening, *Combustion Explosion and Shock Waves*, 39: 1-10.
13. Bertin, G., Most, J.M. and Coutin, M. (2002). Wall Fire Behavior in an Under-ventilated Room, *Fire Safety Journal*, 37: 615-630.
14. Lattimer, B.Y., Hunt, S.P., Wright, M. and Sorathia, U. (2003). Modeling Fire Growth in a Combustible Corner, *Fire Safety Journal*, 38: 771-796.
15. Thomas, I.R., Moinuddin, K.A. and Bennetts, I.D. (2007). The Effect of Quantity and Location on Small Enclosure Fires, *Journal of Fire Protection Engineering*, 17: 85-102.
16. Lock, A., Bundy, M., Johnsson, E.L., Hamins, A., Ko, G.H., Hwang, C., Fuss, P. and Harris, R. (2008). Experimental Study of the Effects of Fuel Type, Fuel Distribution, and Vent Size on Full-scale Underventilated Compartment Fires in an ISO 9705 Room, NIST Technical Note 1603, National Institute of Standards and Technology, Gaithersburg, MD.
17. Leonard, S., Mulholland, G.W., Puri, R. and Santoro, R.J. (1994). Generation of CO and Smoke during Underventilated Combustion, *Combustion and Flame*, 98: 20-34.
18. Pitts, W.M. (1994). Application of Thermodynamic and Detailed Chemical Kinetic Modeling to Understanding Combustion Product Generation in Enclosure Fires, *Fire Safety Journal*, 23: 271-303.
19. McGrattan, K., Hostikka, S., Floyd, J., Baum, H. and Rehm, R. (2008). *Fire Dynamics Simulator (Version 5) Technical Reference Guide*, NIST SP 1018-5, National Institute of Standards and Technology, Gaithersburg, MD.
20. Pitts, W.M. (1994). Application of Thermodynamic and Detailed Chemical Kinetic Modeling to Understanding Combustion Product Generation in Enclosure Fires, *Fire Safety Journal*, 23: 271-303.
21. Bryant, R.A., Ohlemiller, T.J., Johnsson, E.L., Hamins, A., Grove, B.S., Guthrie, W.F., Maranghides, A. and Mulholland, G.W. (2004). *The NIST 3 Megawatt Quantitative Heat Release Rate Facility - Description and Procedure*, NISTIR 7052, National Institute of Standards and Technology, Gaithersburg, MD.

22. Hwang, C.H., Lock, A.J, Bundy, M., Johnsson, E., Ko, G.H., Studies on Fire Characteristics in Over- and Underventilated Full-scale Compartments, *Journal of Fire Sciences*, (2010)
23. Tewarson, A. (1995). Generation of Heat and Chemical Compounds in Fires, *SFPE Handbook of Fire Protection Engineering*, Society of Fire Protection Engineers.
24. Ceramic fiber blanket K-Lite™, <http://www.gltproducts.com>.
25. Turns, S.R. (2000). *An introduction to combustion: concept and applications*, 2nd edn, McGraw Hill.
26. Hwang, C.H., Lock, A.J, Bundy, M., Johnsson, E., Ko, G.H., Effects of Fuel Location and Distribution on Full-Scale Underventilated Compartment Fires, *Journal of Fire Sciences*, Accepted (2010)