An Evaluation of the Global Equivalence Ratio Concept for Compartment Fires: Data Analysis Methods

CHRISTOPHER J. WIECZOREK AND URI VANDSBURGER*

Department of Mechanical Engineering
Virginia Polytechnic Institute and State University
Blacksburg, Virginia 24061 USA

JASON FLOYD

Hughes Associates Inc.
3610 Commerce Dr., Suite 817
Baltimore, MD 21227-1652 USA

ABSTRACT: An experimental effort at Virginia Tech was initiated with the aim to evaluate the applicability of the Global Equivalence Ratio (GER) concept to compartment fires with prototypical building features. The present paper contains an in depth review of previous studies, which are contrasted with a new data set. The data are presented as integrate average mole fractions exiting the compartment correlated versus a new nondimensional heat release rate. In addition to presenting good correlations for depleted oxygen, carbon dioxide, carbon monoxide, and unburned hydrocarbons, the new parameter provides an indication of the degree of burning occurring up to the compartment exit plane.

KEY WORDS: compartment fires, species generation, spatial variations, carbon monoxide.

INTRODUCTION

CARBON MONOXIDE POISONING has been shown to be the primary cause of death from fires in many occupancies [1]. Carbon monoxide (CO) generation is a complex function of air supply, air–fuel mixing patterns, and

*Author to whom corresponding should be addressed. E-mail: uri@vt.edu

1042-3915/04/01 0009–23 $10.00/0 DOI: 10.1177/1042391504034743

fuel type [2]. Determining the levels of toxic species generated under different fire scenarios has been the focus of several recent studies. Species data available stems primarily from bench-scale and hood experiments, with limited data obtained directly from full-scale and scaled compartment fires.

The primary objective for a recent study being conducted at the Virginia Tech Building Fire Research Laboratory is to evaluate the transport of toxic species generated in compartment fires with prototypical building features to remote locations. The first phase of the project was aimed at determining the proper inlet boundary conditions in order to examine the transport of combustion species down a hallway. Three different inlet conditions may exist; combustion product gases, a combination of combustion products and flames, and complete flaming.

Species formation in fires occurring in enclosures has been the focus of research efforts for the past thirty years. Examination of the existing data, however, indicated that although extensive data from these studies are available, consistency in experimental techniques and data reduction was not maintained. Experimental variations included sampling techniques, i.e. single versus multiple sampling points, and sampling locations, i.e. measurements in the compartment gas layer, in the doorway, and in an exhaust hood. Although, no single study has been performed that examines all of the potential measurement techniques for the same fire conditions, together, all of the studies provide a foundation for understanding the complexity of species formation. A detailed discussion of the different experimental techniques and their effect on the deduced combustion species levels is presented.

The data set that formed the foundation for the field was reported by Beyler [3] who performed a series of experiments using gaseous, liquid, and solid fuels burning in the open under an exhaust hood. Beyler proposed the concept of correlating the combustion products as a function of the global equivalence ratio. This methodology was termed the GER concept. The simplicity of the GER concept for predicting species levels led Pitts [4] and Gottuk [5] to extend the methodology to scaled-compartment fires. This has led to the current practice for evaluating the hazardous conditions generated by fires occurring in compartments. The methodology is based primarily on the data from Beyler and Gottuk, in which species yields are presented as a function of the global equivalence ratio [2,6,7].

Based on the previous data, experimental and data reduction methods were developed and applied in the present study to properly evaluate the species levels at the exit plane of a compartment. The new data were collected for four different ventilation conditions with propane fires in a half-scale ISO 9705 compartment. This paper provides the foundation for the evaluation of the global equivalence ratio concept with a detailed review of previous experimental techniques and data measurements. In addition, new experimental data, obtained from detailed measurements at the compartment exit plane, are presented and analyzed based on the three possible boundary conditions at the compartment exit.

PARAMETERS AFFECTING SPECIES LEVELS QUANTIFICATION

Measurement Locations – Summary

Guidelines for performing species measurements in compartments are limited to ISO 9705:1993(E) and ASTM 603-98a [8,9]. Neither standard was developed to prescribe the detailed analysis of toxic combustion products generated from compartment fires. Typically measurements are performed in the exhaust hood, as prescribed by both standards. These data, however, are intended for the use of determining the heat release by means of oxygen (O_2) consumption techniques and not for the evolution of toxic products from the fire. ASTM 603-98a states that additional measurements of carbon monoxide and carbon dioxide (CO_2) in the test room, sampled 0.025 m below the top of the doorway, ''may yield useful information'' [9]. ISO 9705:1993(E) states that the guide is intended for well ventilated conditions and does not provide any guidance on evaluating toxic products of combustion generated by compartment fires.

Over the years, small scale and full scale experiments have been performed based on the experimental setups outlined by both standards. Both standards state that hood measurements should be made at a position where the combustion products are uniformly mixed [8,9]. It must be noted that hood measurements are not necessarily representative of the species exiting the compartment since additional reactions can (and usually do) occur as O_2 rich ambient air is entrained into the hood along with the compartment exhaust gases. The occurrence of additional reactions up to the hood and in the hood, has a strong dependence on the gas temperatures; therefore, as noted by Lönnermark et al. [10] the most distinct changes in the smoke gas composition between the compartment opening and hood exhaust duct take place with under-ventilated conditions in the compartment, when burning occurs outside the opening.

To overcome the limitations of performing gas sampling in the exhaust hood, some studies have performed measurements in the upper layer or the exit plane of the compartment. Species distributions within the compartment almost always exhibit spatial variations, therefore single point measurements of the species are not representative of the entire compartment environment, or the gases exiting the compartment.

Comparison Between Upper Layer Compartment and Exhaust Hood Measurements

Variations between species levels measured in the upper layer of a compartment versus those measured in the exhaust hood can be quantified with the experimental work of Gottuk [5]. Gottuk performed scaled experiments in a special test apparatus that separated the incoming and exiting flows. Gottuk simulated an ideal two-layer system, where the actual mass flow rate into and out of the compartment could be determined directly. Gottuk reported that based on a series of measurements within the upper layer, a well-mixed, uniform layer existed; and therefore positioned a sampling probe horizontally 0.13 m into the compartment through the center of the exhaust vent [5]. Gottuk performed measurements within the upper layer of the compartment, referred to as layer data, and in the exhaust hood, referred to as hood data.

Data for three exhaust ventilation conditions, one for measurements in the hood (625 cm^2) and two for layer measurements (403 and 806 cm^2) are presented in Figure 1. Data at both locations for the same ventilation conditions are not available; therefore a direct comparison between the two measurement locations cannot be made. One would anticipate that results for the 625 cm^2 vent would lie between the other two vents, however, this is

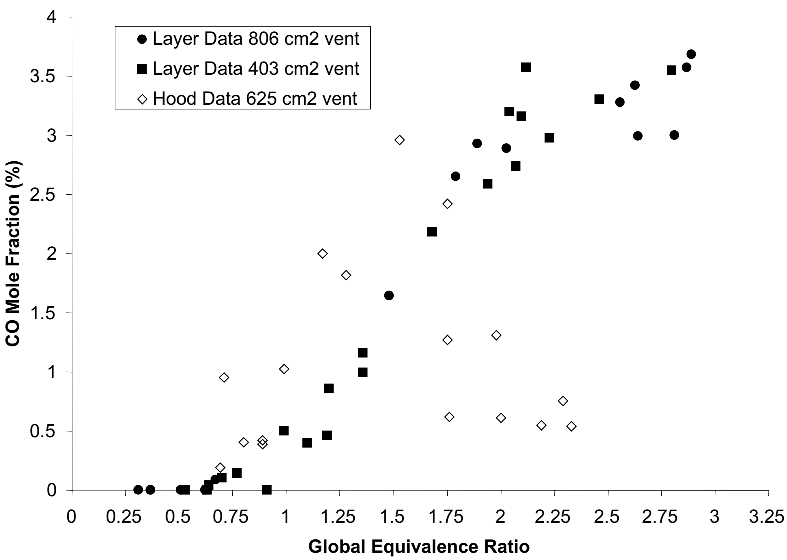

Figure 1. *Comparison between carbon monoxide levels measured in the compartment upper layer and the exhaust hood by Gottuk [5].*

not the case. Data for the 403 and 806 cm^2 vents show the CO mole fraction rising starting at an equivalence ratio, ϕ, near 0.6 and peaking near $\phi = 2.0$ with a mole fraction of 3.5%. The exhaust hood data peaks near $\phi = 1.5$ at 3.0% and drops rapidly thereafter.

Agreement between the layer data and the hood data is seen for $\phi < 1.5$. The differences seen between the layer and hood data, beyond $\phi = 1.5$, can be attributed to external burning. Gottuk reports that initial flashes of external burning were first observed at an equivalence ratio of 1.4 ± 0.4 and sustained external burning occurred at an average equivalence ratio of 1.9 ± 0.3 [5]. Examination of the layer data, beyond $\phi = 1.5$, shows that the constant CO levels correspond to the condition where maximum burning with available O_2 has occurred within the compartment; additional reactions will only occur externally where more O_2 is available. This is seen in the hood data where at higher equivalence ratios, lower CO levels were measured as a result of additional reactions occurring between the exit of the compartment and the measuring location. These CO levels do not represent the species production within the compartment.

Comparison Between Compartment Exit Plane and Exhaust Hood Measurements

Recently, full-scale tests were performed at the Swedish National Testing and Research Institute (SP) in an ISO 9705 room using solid and liquid fuel sources [11]. The compartment ventilation was varied by maintaining the same door width and changing the sill height. Species measurements were performed at two locations, in the exit plane of the compartment opening and in the exhaust hood. The measurements in the exit plane were performed using a probe with 7 equally spaced holes; the probe was positioned diagonally across the exiting flow of the opening, thereby spatially averaging any potential species distributions.

Data for chlorobenzene at three equivalence ratios (1.51, 1.88, and 2.51) measured at the exit plane of the compartment and in the hood, indicate that the yields of CO measured in the exhaust hood are lower than those measured in the exit plane. This is expected since the high temperatures and the presence of additional O_2 in the hood provides favorable conditions for the conversion of CO to CO_2. This is also seen in the measured CO_2 yields, which show higher CO_2 yields in the exhaust duct, an indication of the conversion of CO to CO_2.

Lönnermark et al. [10] did not report at what equivalence ratio, if any, external burning occurred. It is expected, based on the definition of the global equivalence ratio and prior experience with compartment fire dynamics that at equivalence ratios greater than 1.0 external burning will have occurred. These data, therefore, agree qualitatively with data from Gottuk [5].

Spatial Variations Within the Compartment

The specially designed test apparatus used by Gottuk [5] provided a well-mixed uniform hot upper layer for which a single point local measurement represented the upper gas layer composition. In compartments with prototypical building features, a well-mixed upper layer is not necessarily achieved and spatial variations in the species levels are expected within the layer.

The only study known to the authors where a detailed mapping of the horizontal and vertical species variations was made was performed at the National Institute of Standards and Technology. Bryner et al. [12] performed tests within a 2/5-scale ISO 9705 compartment, using a natural gas burner located in the center of the compartment. A portion of the study consisted of performing horizontal and vertical scans of species measurements in the compartment. Horizontal measurements were taken 0.2 m below the ceiling for two different heat release rates, 400 and 600 kW. A fixed probe continuously monitored the species levels, in the front of the compartment (0.29 m from the left wall, 0.1 m in from the front, and 0.1 m below the ceiling).

Horizontal variations existed within the compartment for both heat release rates. The highest concentrations of CO, between 3.0 and 4.0%, were reported in the front of the compartment for both heat release rates. For the 400 kW fire the measured CO concentrations varied between 1.0 and 3.0% depending on the horizontal distance from the front wall. Data for the 600 kW fire indicate fairly uniform CO concentrations within the compartment at this elevation. Data for both the 400 and 600 kW fires show a region of high CO concentration at a horizontal distance of 0.51 m from the front of the compartment, which is attributed to the location of the natural gas burner, positioned 0.71 m from the front wall.

Data for vertical variations in the species levels were presented by Bryner et al. [12], for 250 and 600 kW fires. The probe was positioned inside the doorway and moved vertically from the top to the bottom. The data indicate vertical variations in the species levels, as opposed to the typically assumed uniform composition of the upper layer. For the 250 kW fire, at distances greater than 0.15 m below the ceiling the CO levels decrease rapidly from approximately 2.5–3.0% to less than 1.0%. For the 600 kW fire the CO levels appear to be uniform but lower, for distances between 0.15 and 0.41 m below the ceiling, than those measured by the fixed probe. Based on the species mapping, Bryner et al. [12] concluded that in the upper layer gas species concentrations can vary significantly over small vertical and horizontal distances.

NEW DATA FROM PRESENT WORK

The data from previous studies indicate the importance of proper measurement procedures for evaluating species generation in compartment fires. Horizontal and vertical variations in gas composition prevent single point measurements from being taken as representative of the layer composition, while experimentally generated, well mixed uniform layers do not properly represent the environment in a prototypical building compartment. To obtain a full understanding of species formation in compartment fires a detailed analysis of the gas composition, including O_2, CO_2, CO, and unburned hydrocarbons (UHCs), at the exit plane of a ½-scale ISO 9705 compartment was performed. Horizontal and vertical variations were examined and an integrated average mole fraction for each species was obtained, based on the local velocities and temperatures. Four ventilation conditions were examined. Propane was used as the fuel.

Experimental Facility

The experiments were performed in a ½-scaled ISO 9705 compartment, shown schematically in Figure 2. The compartment frame dimensions are

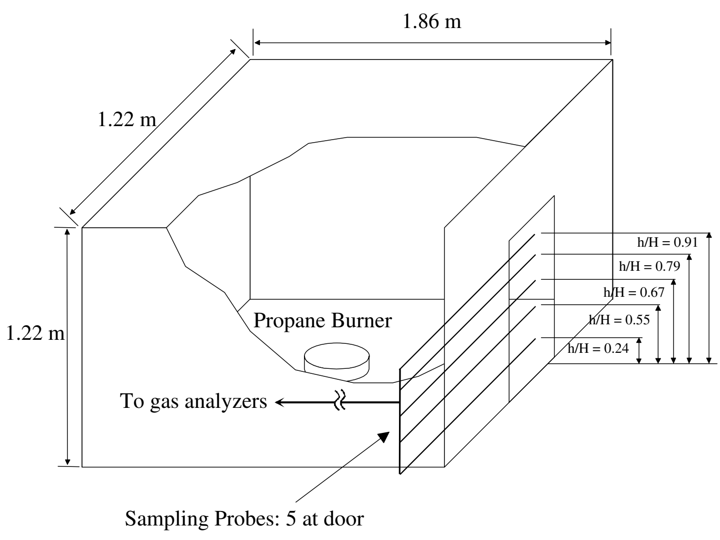

Figure 2. *Half -scaled ISO 9705 compartment arrangement.*

1.22 m wide × 1.83 m deep × 1.22 m high, the interior of the compartment is lined with 0.0254 m thick fiberboard, the actual interior compartment dimensions are 1.17 m wide × 1.78 m deep × 1.17 m high. In order to allow the formation of an upper layer, a 0.4 m deep soffit was used above the door. Three ventilation conditions were examined; the area of the openings were 0.06, 0.15, 0.27, and 0.54 m^2. Maintaining a fixed doorway height of 0.82 m, while changing the doorway width generated the three ventilation conditions. The three ventilation conditions are presented in the paper as narrow (0.165 m wide), baseline (0.33 m wide), and wide (0.66 m wide) doorways. The three ventilation conditions influenced the flow and mixing patterns in the compartment.

Continuous Gaseous Fuel Supply System

The fire source was a 0.305 m diameter diffusion flame burner, fed through 1″ SCH 40 pipe from a 500 gallon propane (LPG) storage tank. The burner, located at the center of the compartment at the floor, was 0.102 m high. This allowed space for a 0.05 m inlet plenum topped by a perforated plate, covered by a wire mesh and a 0.04 m layer of fine marble chips. This construction was devised to create a top hat velocity profile at the burning surface and to generate a buoyancy and not a momentum driven diffusion flame. The fuel mass flow rates ranged between 0.002 and 0.01 kg/s, providing heat release rates ranging between 50 and 500 kW.

Gas Sampling System

Gas sampling was performed by a rake of five probes constructed of 1/4″ (6.4 mm) stainless steel tubing. The probes were located at nondimensional heights, h/H, of 0.28, 0.45, 0.70, 0.80, and 0.93, as shown in Figure 3. This resulted in four samples from the outflow stream and one sample from the inflow region of the doorway for each lateral position. For the baseline and wide doorways the sampling rake was positioned at three locations across the doorway width, $w/W = 0.25$, 0.5, and 0.75. The narrow doorway was only sampled at the centerline, as the profiles across the width were found to be uniform. Samples from the rake were sent to three analyzers, an O_2 analyzer, CO/CO_2 gas analyzer, and flame ionization detector (FID) to determine UHCs, reported as C_2H_4 levels.

Temperature Measurements

Temperature measurements within the compartment and at the doorway were obtained via 16 aspirated type-K thermocouples. The aspirated

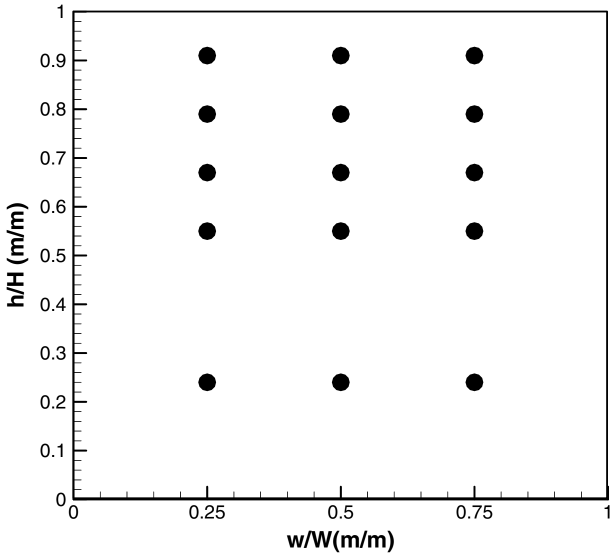

Figure 3. *Sampling point grid in doorway plane.*

thermocouple rakes were designed and constructed based on the recommended suction velocities of Blevins and Pitts [13]. The body of the thermocouple rake is insulated with 37.2 mm thick Durablanket Strip from Fiberfrax, and the inlet ports are insulted using Fiberfrax 970 Paper insulation. The insulation is used to reduce the thermal radiation loading on the inlet port tubes and the rake body.

Velocity Measurements

Velocity measurements were obtained using bi-directional probes located at each of the gas sampling locations discussed above. The bi-directional probes were designed based on the probe description discussed by Emmons [14] and McCaffrey and Heskestad [15]. Each probe was connected to a differential pressure transducer. Measurements of the local temperature and differential pressure allow the local velocities to be determined based on a simple Bernoulli analysis.

Test Procedure

At the start of each test series, the burner was ignited and a 20–30 min compartment heat up time was provided. Once near steady-state conditions were reached, determined by observation of the change in compartment temperature $\Delta T/t \approx 1$ K/min, data were collected at each sampling location for 180–240 s. In general there was no cool-down period between successive tests, so successive testing in the same day did not require a lengthy warm-up period. To verify repeatability of the results, sampling at some locations was repeated at the end of the test series. In addition, several tests were repeated in their entirety. A detailed description of the test facility, procedures, and results can be found in the final report [16].

The results from a total of 28 tests, of which 11 with the narrow doorway width (0.165 m), 13 with the baseline doorway width (0.33 m), and 4 with the wide doorway width (0.66 m) are presented in this paper.

Data Reduction

The detailed mapping of the species in the doorway, along with the species velocity, and temperature allows for the determination of an average species mole fraction exiting the compartment. The data for each species are reduced based on the methodology described in the following section.

Species Measurements – Integrated Average Doorway Species Mole Fractions

The current data have been reduced based on the time-averaged, spatially integrated species mass flux in the exiting plane of the compartment. For each measurement location the temperatures, velocities, and species data were time averaged over the sampling interval. These values were used to calculate the species mass flux, using Equation (1),

$$\dot{m}_{\text{out},i} = \int \rho Y_i V dA_{\text{out}} = \overline{Y_i} \int \rho V dA_{\text{out}} \tag{1}$$

where

$$Y_i = \frac{\mathrm{X}_i MW_i}{MW_{\text{mixture}}} \tag{2}$$

and

$$\overline{Y_i} = \frac{\int \rho Y_i V dA}{\int \rho V dA} = \frac{\int_x \int_y \rho(x,y) Y_i(x,y) V(x,y) dxdy}{\int_x \int_y \rho(x,y) V(x,y) dxdy} \tag{3}$$

The average mole fraction is determined by substituting $\bar{Y}_i$ into Equation (2) and solving for $\bar{X}_i$. This methodology takes into account all of the horizontal and vertical species and velocity variations within the doorway.

RESULTS – SPATIAL VARIATIONS IN THE EXIT PLANE

Mole fraction maps for each of the measured species for each doorway width are shown in Figures 4–6. Each figure consists of four spatially nondimensional plots of (a) O_2, (b) CO_2, (c) CO, and (d) UHC mole fractions at the doorway. The heat release rates for the narrow, baseline, and wide doorways were approximately 153, 270 and 470 kW respectively, resulting in the same global equivalence ratio** for all three doorways of approximately 0.6. The solid black line in each of the figures indicates the calculated neutral plane elevations in the doorway.

Although the global equivalence ratio for all three doorways was approximately 0.6, it should be noted that for all three doorways external

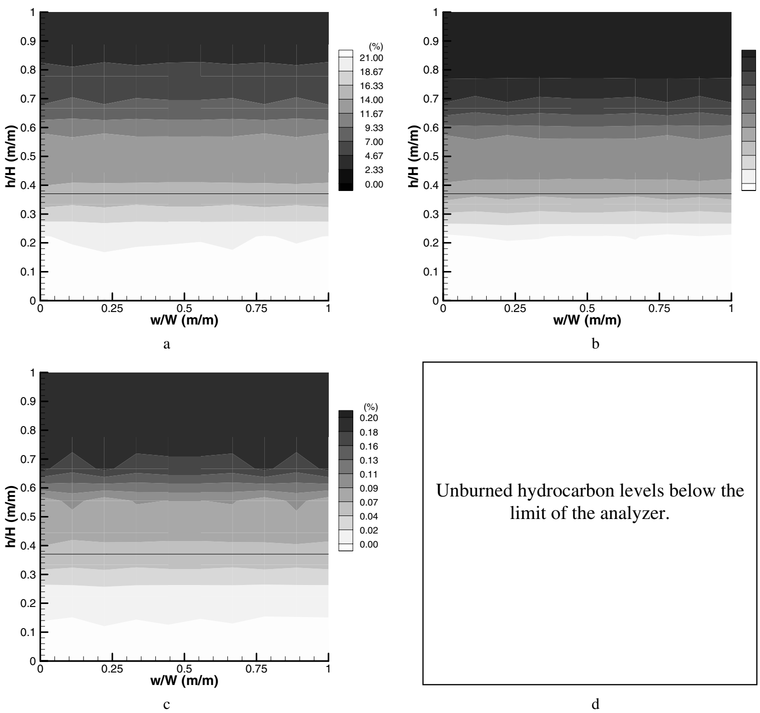

Figure 4. *Narrow doorway species mapping of: (a) O_2; (b) CO_2; (c) CO; and (d) UHC mole fractions (%), 153 kW (GER of 0.58), neutral plane determined from velocity probe data.*

**The global equivalence ratio, ϕ, is defined as the fuel to air ratio for the compartment normalized by the stoichiometric fuel to air ratio for propane. A more detailed discussion can be found in [16].

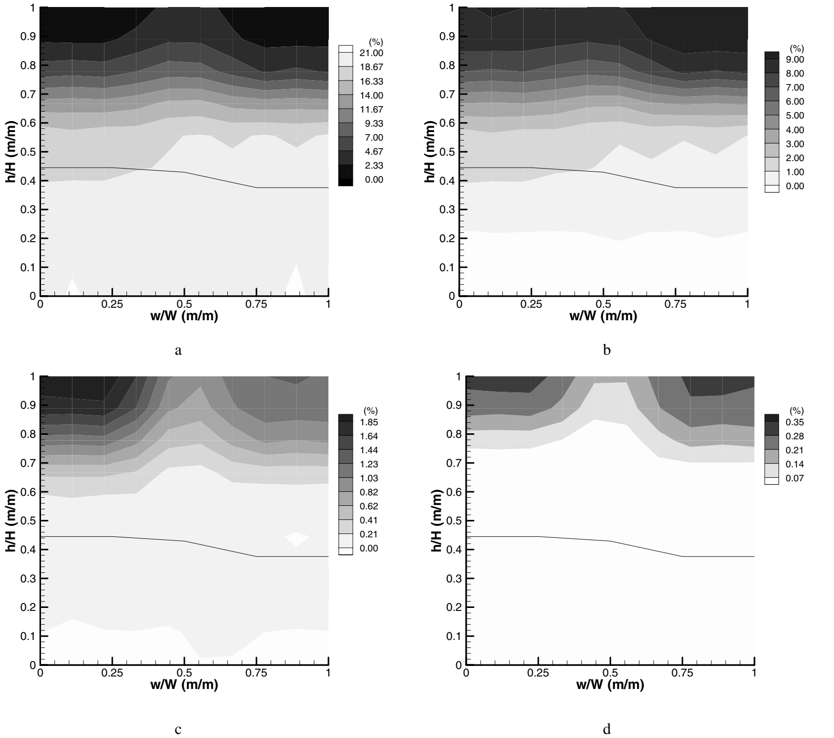

Figure 5. *Baseline doorway species mapping of: (a) O_2; (b) CO_2; (c) CO; and (d) UHC mole fractions (%), 270 kW (GER of 0.56), neutral plane determined from velocity probe data.*

burning due to flame extensions had occurred. The theoretical fire size and global equivalence ratios at which external burning begins to occur for each doorway are listed in Table 1 [17].

Therefore, in the exiting portion of the doorway, i.e. above the neutral plane, in Figures 4–6, the data include measurements that are both within the fire plume and in the hot combustion product gases.

The data shown in Figures 4–6 indicate that as the doorway width increases the uniformity of the upper layer diminishes. Spatial variations in the vertical direction appear with the narrow doorway, Figure 4. O_2 mole fractions in the upper layer range between 2.0 and 16%, with CO_2 levels ranging between 2.8 and 8.5%. It is interesting to note that although the most substantial external burning occurred with the narrow doorway, CO levels were below 0.2% and UHC levels were below the range of the gas analyzer.

Spatial variations in both the vertical and horizontal directions are seen with the baseline and wide doorways, Figures 5 and 6. The highest levels of

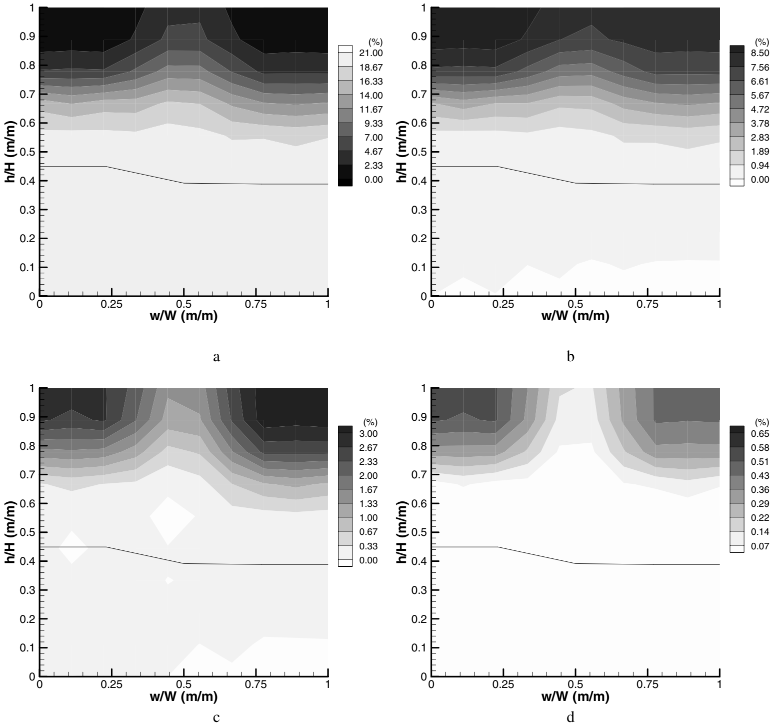

Figure 6. *Wide doorway species mapping of: (a) O_2; (b) CO_2; (c) CO; and (d) UHC mole fractions (%), 470 kW (GER of 0.64), neutral plane determined from velocity probe data.*

Table 1. Minimum fire size and equivalence ratio for flame extensions [17].

Test Configuration	Fire Size Theoretical	Equivalence Ratio Theoretical
Narrow	95	0.51
Baseline	127	0.34
Wide	190	0.26

combustion products, CO_2, CO, and UHCs and lowest levels of O_2 are seen in the upper corners of the doorways, which correspond to measurements taken directly in the flame. Although the exact contour of the flame was not documented during any of the tests, one would expect, based on the commonly accepted assumption that a uniform upper layer exists within the compartment, that below the fire plume a well-mixed uniform environment would exist. This well-mixed, well-defined layer does not exist. Instead, for the baseline doorway, above the calculated neutral plane $h/H \approx 0.42$, O_2 levels vary between 18.7 and 0.0% and CO_2 levels vary between 1.0 and 9.0%.

The wide doorway data, Figure 6, exhibit a similar trend to that of the baseline doorway; however, the levels of CO and UHCs are significantly higher than seen with either the narrow or baseline doorways. CO levels as high as 3.0% along with UHC levels of 0.5% are seen in the upper corners of the doorway. The high levels of CO and UHCs indicate that although the global equivalence ratio is the same for all three doorways, the species levels at the doorway are primarily dependent on the fire size. In the upper region of the doorway, measurements for both the narrow and wide doorways were taken directly in the fire plume, however, the heat release rate for the wide doorway was more than three times greater than the heat release rate for the narrow doorway, and resulted in CO levels that are 15 times higher. Although the global equivalence ratio indicates that the same fuel and air ratio exists for all three doorways, the combustion occurring in the compartment is not the same.

Species levels within the narrow doorway for a heat release rate of 470 kW (the corresponding global equivalence ratio is 2.05) are shown in Figure 7. This is the same heat release rate as for the wide door data shown in Figure 6.

Under the present conditions the compartment with the narrow doorway is completely ventilation limited, i.e., postflashover. Therefore, all of the measurements were taken in the fire plume. The data shown in Figure 7 represent a cross-sectional slice of the fire plume. Very little variation in each species is seen above the neutral plane, with some mixing due to shear forces between the in-flowing and out-flowing gases occurring at the neutral plane.

Although, the data presented in Figures 6 and 7 are for the same heat release rate, the upper layer CO levels are significantly higher with the narrow doorway than those seen with the wide doorway. High CO levels, greater than 2.0% are seen throughout the upper layer, the maximum measured CO mole fraction was 4.4%; while with the wide doorway the maximum CO mole fraction was 3.0%. The most important observation is the extremely high levels of UHCs with the narrow doorway, 4.5–7.0%, Figure 7, compared to the highest levels reported previously of 0.7%, Figure 6, for the wide doorway. This is attributed to the fact that although the UHCs are measured in the fire plume, with the wide doorway only "small wisps" of flames are exiting the compartment and the measurements are being taken in the flame tip; while for the narrow doorway substantial external burning is occurring and the measurements are taken deep within the fire plume.

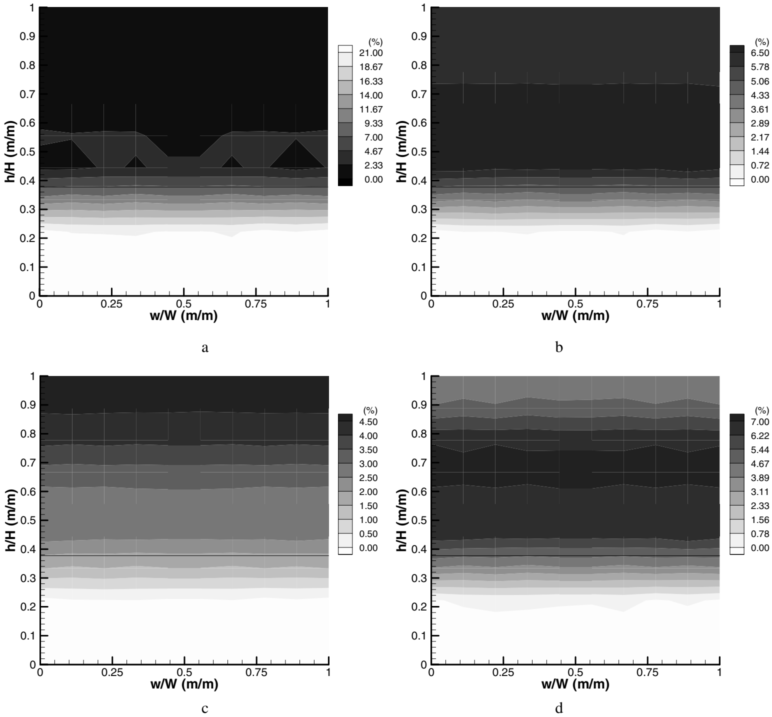

Figure 7. *Narrow doorway species mapping of: (a) O_2; (b) CO_2; (c) CO; and (d) UHC mole fractions (%), 470 kW (GER of 2.05), neutral plane determined from velocity probe data.*

DATA ANALYSIS AND DISCUSSION

The use of the global equivalence ratio to characterize the combustion occurring in a compartment provides no indication of the degree of burning occurring up to the compartment exit. Flashover occurs at an equivalence ratio of 1.0, however, external burning due to flame extensions may occur at global equivalence ratios well below 1.0, as reported in Table 1, depending on the size of the ventilation [17].

A new parameter that quantifies the degree of external burning occurring at the compartment exit plane is required. The proposed parameter is a non-dimensional heat release rate, $\tilde{Q}$, Equation (4), defined as the ideal heat release rate, $\dot{Q}_{\text{ideal}}$, divided by the heat release rate required for the flame to reach the compartment doorway, $\dot{Q}_{\text{Flame Extensions}}$.

$$\tilde{Q} = \frac{\dot{Q}_{\text{ideal}}}{\dot{Q}_{\text{Flame Extensions}}} \tag{4}$$

where $\dot{Q}_{\text{Flame Extensions}}$ is given by:

$$\dot{Q}_{\text{Flame Extensions}} = \left(\frac{\beta}{360^\circ}\right) 1090 H^{2.5} \left(\sqrt[0.3266]{\frac{1}{2.886}\left(\frac{L_f}{H}\right)} \right) \tag{5}$$

and,

$$\dot{Q}_{\text{ideal}} = \dot{m}_{\text{fuel}} \Delta H_c \tag{6}$$

The first term in Equation (5) accounts for the fact that walls bound the fire plume; therefore, air entrainment into the base of the flame does not occur via the full 360° circumference of the fire plume. An angle of 90, 120, and 180° was used for β for the narrow, baseline, and wide doorways respectively in the present calculations. Equation (5) was developed based on an extension of a correlation from Hasemi et al. [18]. (More details can be found in [17].)

There are four important regions to consider for $\tilde{Q}$:

$$\tilde{Q} = \begin{cases} < 1.0 - \text{Combustion within the compartment} \\ = 1.0 - \text{Flame tip at the compartment doorway} \\ > 1.0 - \text{External burning due to flame extensions} \\ \geq \tilde{Q}_{\text{critical}} = \dfrac{\dot{Q}_{\text{Stoichiometric}}}{\dot{Q}_{\text{Flame Extensions}}} = \dfrac{r\dot{m}_{\text{air}} \Delta H_c}{\dot{Q}_{\text{Flame Extensions}}} \\ \qquad -\text{External burning due to flashover} \end{cases}$$

where, $\dot{Q}_{\text{Stoichiometric}}$, is the heat release rate required for flashover.

The four conditions for $\tilde{Q}$ are illustrated in Figure 8. For the case of $\tilde{Q} < 1.0$ the fire plume is completely contained within the compartment, and only product gases generated by the fire are exiting the compartment. For $\tilde{Q} = 1.0$ the length of the flame is such that the tip of the flame reaches the compartment opening. When $1.0 < \tilde{Q} < \tilde{Q}_{\text{critical}}$ the conditions at the compartment exit plane will comprise of both a flaming region and a hot gas region; therefore, species measurements performed in the out flowing gases will be taken both inside and outside of the flaming region. Beyond $\tilde{Q}_{\text{critical}}$ all measurements at the exit plane will be in the flaming region.

For the present compartment and ventilation geometries, the calculated $\dot{Q}_{\text{Flame Extensions}}$, $\dot{Q}_{\text{Flashover}}$, and $\tilde{Q}_{\text{critical}}$ are given in Table 2.

The integrated species mole fractions as a function of $\tilde{Q}$ are shown in Figures 9–12. It should be noted that the O_2 mole fractions shown are

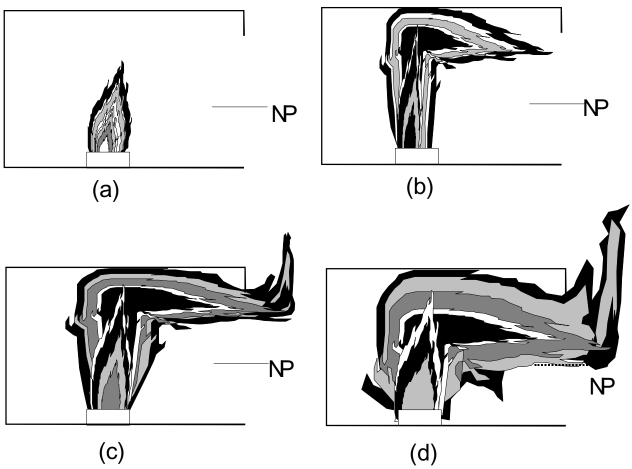

Figure 8. *Illustration of four $\tilde{Q}$ conditions: (a) $\tilde{Q}<1.0$; (b) $\tilde{Q}=1.0$; (c) $1.0<\tilde{Q}<\tilde{Q}_{\text{critical}}$; (d) $\tilde{Q}>\tilde{Q}_{\text{critical}}$. NP = Neutral plane elevation in the doorway.*

Table 2. Calculated $\dot{Q}_{\text{Flame Extensions}}$, $\dot{Q}_{\text{Flashover}}$, and $\tilde{Q}_{\text{critical}}$ for the present geometries.

Doorway Geometry	$\dot{Q}_{Flame\ Extensions}$ (kW)	$\dot{Q}_{Flashover}$ (kW)	$\tilde{Q}_{critical}$
Narrow	95	183	1.92
Baseline	127	365	2.88
Wide	190	730	3.84

the amount of O_2 depleted in the compartment, since it is a consumed species.

Examination of the O_2 and CO_2 mole fractions as a function of $\tilde{Q}$, Figures 9 and 10, indicates that the data for all three ventilation conditions follow the same trends but three separate curves, one for each doorway, are seen. The wide doorway data indicate the lowest depleted fraction of O_2 and lowest CO_2 mole fraction, while the highest depletion of O_2 and highest mole fraction of CO_2 is seen for the narrow doorway. The baseline doorway data fall in-between.

Using this methodology the CO and the UHC levels, Figures 11 and 12, appear to be independent of the degree of burning within the compartment. This is a consequence of the overall balance between the entrained air, consumed O_2, and the species generated within the compartment for the different burning conditions of each doorway. The CO levels, Figure 11, begin to increase at approximately $\tilde{Q}=1.5$, while the UHC do not increase until $\tilde{Q}=2.5$. The CO mole fractions, Figure 11, increase linearly

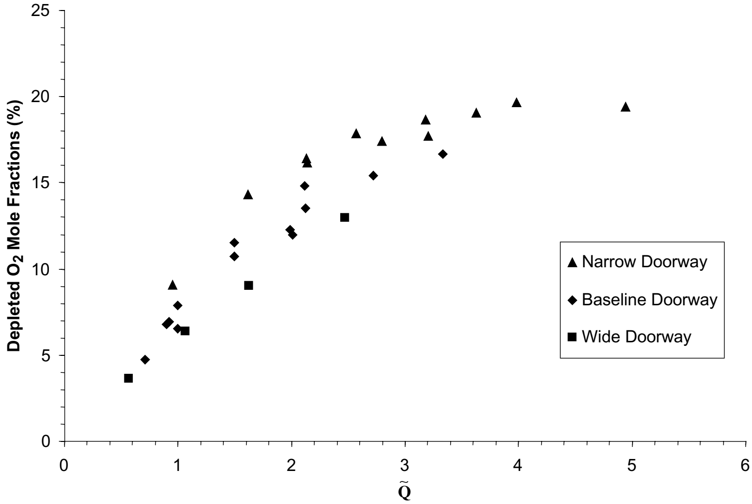

Figure 9. *Integrated average oxygen mole fractions (depleted) as a function of the non-dimensional heat release rate parameter,* $\tilde{Q}$.

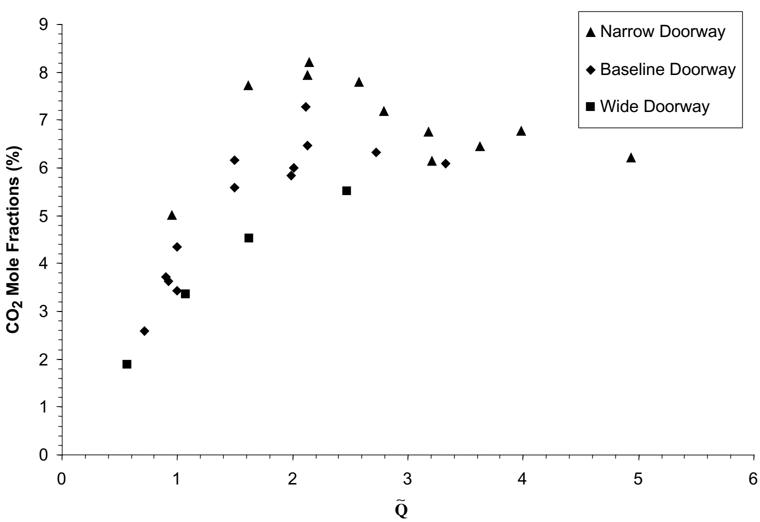

Figure 10. *Integrated average carbon dioxide mole fractions as a function of the non-dimensional heat release rate parameter,* $\tilde{Q}$.

and begin to taper off slightly at $\tilde{Q} = 3.6$. Similarly, the UHC mole fractions, Figure 12, increase linearly. It is anticipated that this trend would continue as $\tilde{Q}$ increases, and that the UHC levels will approach 100% as $\tilde{Q}$ approaches infinity.

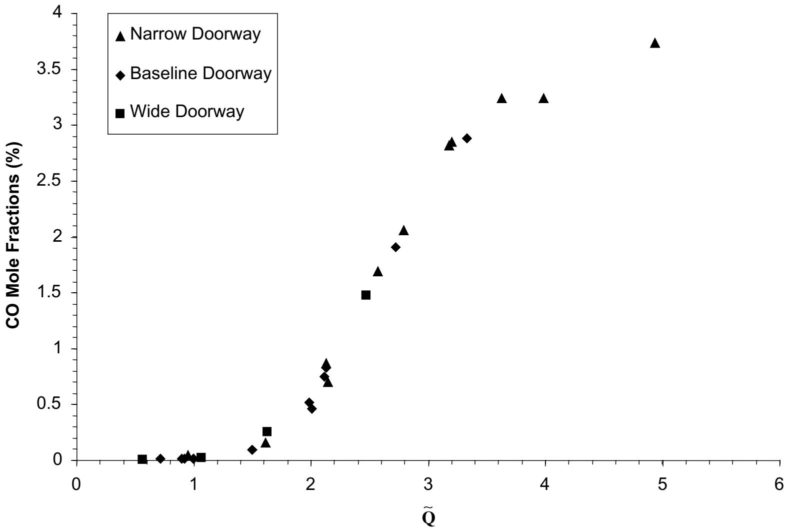

Figure 11. *Integrated average carbon monoxide mole fractions as a function of the non-dimensional heat release rate parameter,* $\tilde{Q}$.

The entire fire plume was contained within the compartment for five data points, 1 narrow, 3 baseline, and 1 wide, indicated by $\tilde{Q} < 1.0$. From the data it can be determined that the hot gases exiting the compartment consisted only of O_2 and CO_2, no CO or UHCs were present.

In general most tests in the present study fell into $1.0 < \tilde{Q} < \tilde{Q}_{\text{critical}}$ range indicating that the exiting hot gases from the compartment consisted of hot combustion gases and a flaming region. It is interesting to note, that within this range for the narrow doorway, where $\tilde{Q}_{\text{critical}} = 1.92$, the gases exiting from the compartment consisted of O_2, CO_2, and CO, no UHCs were present. For the baseline and wide doorways all four species were present, once $\tilde{Q}$ exceeded 2.5, which is lower than $\tilde{Q}_{\text{critical}}$ for all three doorways.

For the narrow doorway, conditions that exceeded $\tilde{Q}_{\text{critical}}$ were also achieved. The most interesting observation in the data for this condition is the decrease in CO_2 levels beyond $\tilde{Q}_{\text{critical}}$. Examination of Figure 10 indicates that at $\tilde{Q}_{\text{critical}}$ for the narrow doorway, the CO_2 mole fraction peaks at 8.0 %, beyond $\tilde{Q}_{\text{critical}}$ the CO_2 mole fractions decrease. It is assumed that similar results would be observed for the baseline and wide doorways.

Unlike the products of incomplete combustion, depleted O_2 and CO_2, are a function of both $\tilde{Q}$ and the doorway width. Examining the mole fractions of O_2 depleted in the compartment, Figure 9, it is seen that the least amount of O_2 was depleted under the wide doorway conditions and the most under

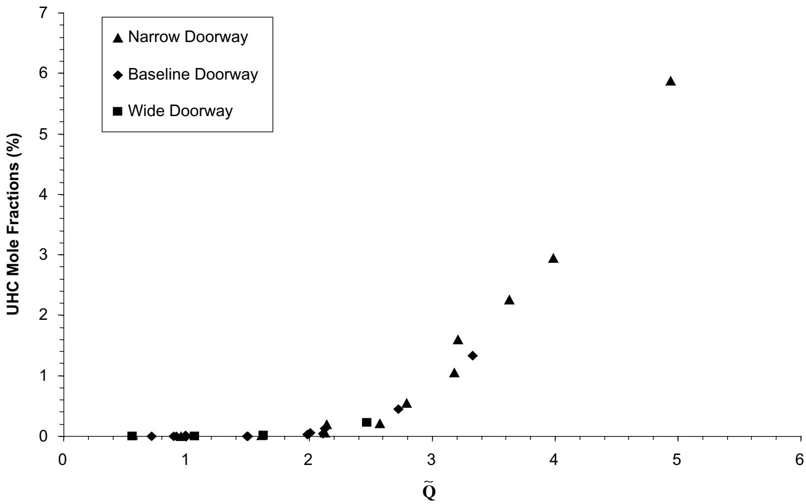

Figure 12. *Integrated average unburned hydrocarbon mole fractions as a function of the nondimensional heat release rate parameter, $\tilde{Q}$.*

the narrow doorway conditions. Therefore, noting that the CO and UHC mole fractions are the same independent of the doorway width, it can be reasoned that the lowest levels of CO_2, formed in the compartment, will be seen for the wide doorway and the highest for the narrow doorway. Examining Figure 10, these trends are indeed observed.

Due to the external burning that begins to occur once $\tilde{Q}$ exceeds 1.0 for all three doorway widths, the species levels transported downstream of the compartment exit plane will be different than those observed at the exit plane. The final downstream species levels will be a function of not only the conditions in the compartment but also of additional O_2 and fuel sources available in the adjacent space.

SUMMARY

A detailed experimental study was undertaken at Virginia Tech Building Fire Research Laboratory to develop appropriate prediction methodologies for species formation in compartment fires. It has been shown in this paper, based on a review of previously published work, that measurement locations are critical in obtaining representative data. The study consisted of mapping species levels, gas temperatures, and gas velocities at the exit plane of a compartment under conditions with and without external burning.

Data reduction based on an integrated average of the species exiting the compartment was performed and was presented as average species mole fractions versus a new normalized heat release rate parameter. A new parameter, $\tilde{Q}$, was defined as the ratio of the ideal heat release rate and the heat release rate required for the flame to reach the compartment opening. This new parameter provides an indication of the burning conditions at the compartment exit.

Good correlation between the integrated average species mole fractions and $\tilde{Q}$ was found. Correlation between the depleted O_2 mole fractions and CO_2 mole fractions versus $\tilde{Q}$ indicated three separate curves, corresponding to the three ventilation conditions. For both the depleted O_2 mole fractions and carbon dioxide mole fractions the three curves followed the same trends. Excellent correlation with $\tilde{Q}$ was seen for the CO and UHC mole fractions. For both gases the average mole fractions appear to increase linearly with $\tilde{Q}$. As $\tilde{Q}$ goes to infinity it is expected that the UHC data will continue to increase and asymptotically approach 100%, while the CO data are expected to peak and decrease to 0%.

NOMENCLATURE

A_{out} = exiting flow area of doorway (m^2)
x = width of the doorway (m)
y = the height of the doorway (m)
$\dot{m}_i$ = mass flow rate (kg/s)
MW_i = species molecular weight
$MW_{mixture}$ = molecular weight of the upper layer assumed to be equivalent to that of air
$\dot{Q}_{Flame\ Extensions}$ = heat release rate required for fire plume to reach the compartment opening (kW)
$\dot{Q}_{ideal} = \Delta H_c \dot{m}_{fuel}$ = ideal heat release rate (kW)
$\dot{Q}_{Stoichiometric}$ = stoichiometric heat release rate (kW)
$\tilde{Q}$ = normalized heat release rate (–)
r = stoichiometric fuel to air ratio (–)
V = velocity (m/s)
X_i = measured species mole fraction (%)
Y_i = species mass fraction
β = sector angle over which air entrainment into the fire plume occurs
ΔH_c = lower heating value for fuel (kJ/kg)
ρ = gas density (kg/m^3)

ACKNOWLEDGMENTS

This work was supported by the Fire Research Division, Dr. Gann and Dr. Grosshandler directors, of the Building and Fire Research Laboratory of the National Institute of Standards and Technology under Grant Number 60NANB7D0066, Project Officer Dr. W.M. Pitts.

REFERENCES

1. Gann, R.J., Babrauskas, V. and Peacock, R.D., ‘‘Fire Conditions for Smoke Toxicity Measurements,’’ Fire and Materials, Vol. 18, 1994 (May/June), pp. 193–199.
2. Karlsson, B. and Quintiere, J., Enclosure Fire Dynamics, CRC Press, 2001.
3. Beyler, C., ‘‘Major Species Production by Diffusion Flames in a Two-layer Compartment Fire Environment,’’ Fire Safety Journal, Vol. 10, 1986, pp. 47–56.
4. Pitts, W., The Global Equivalence Ratio Concept and the Prediction of Carbon Monoxide Formation in Enclosure Fires, NIST Monograph 179, National Institute of Standards and Technology, 1994.
5. Gottuk, D.T., ‘‘The Generation of Carbon Monoxide in Compartment Fires,’’ Doctoral Dissertation, Virginia Polytechnic Institute and State University, 1992.
6. Drysdale, D., Introduction to Fire Dynamics, Wiley-Interscience, New York, 1994.
7. Gottuk, D. and Roby, R., ‘‘Effect of Combustion Conditions on Species Production,’’ in The SFPE Handbook of Fire Protection Engineering, 2nd Edn, National Fire Protection Association, Quincy, MA, 1995.
8. ISO 9705:1993, Fire Tests – Full-Scale Room Test for Surface Products, International Organization for Standardization, 1993.
9. ASTM E603-98a, Standard Guide for Room Fire Experiments, Annual Book of ASTM Standards, Vol. 04.07.
10. Lönnermark, A., Blomqvist, P., Mansson, M. and Persson, H., ‘‘TOXFIRE – Fire Characteristics and Smoke Gas Analysis in Under-Ventilated Large-Scale Combustion Experiments: Tests in the ISO 9705 Room,’’ SP Swedish National Testing and Research Institute, SP REPORT 1996:45, 1996.
11. Blomqvist, P. and Lönnermark, A., ‘‘Characterization of the Combustion Products in Large-scale Fire Tests: Comparison of Three Experimental Configurations,’’ Fire and Materials, Vol. 25, 2001, pp. 71–81.
12. Bryner, N., Johnsson, R.J. and Pitts, W.M., ‘‘Carbon Monoxide Production in Compartment Fires – Reduced-Scale Enclosure Test Facility,’’ National Institute of Standards and Technology, NISTIR 5568, December 1994.
13. Blevins, L. and Pitts, W., ‘‘Modeling of Aspirated Thermocouples (Suction Pyrometers) for Fire Research’’, Building and Fire Research Laboratory, National Institute of Standards and Technology, 1997.
14. Emmons, H., ‘‘Vent Flows,’’ in The SFPE Handbook of Fire Protection Engineering, 2nd Edn, National Fire Protection Association, Quincy, MA, 1995.
15. McCaffrey, B.J. and Heskestad, G., ‘‘Brief Communications: A Robust Bidirectional Low Velocity Probe for Flame and Fire Application,’’ Combustion and Flame, Vol. 26, 1976, pp. 125–127.
16. Vandsburger, U., ‘‘Evolution of Compartment Exhaust Gases Providing Evaluation Criteria and Design Tools,’’ Final Report, NIST/BFRL Contract No. 60NANB7D0066, 2001.

17. Wieczorek, C., ‘‘Carbon Monoxide Generation and Transport from Compartment Fires,’’ Doctoral Dissertation, Virginia Polytechnic Institute and State University, Mining and Minerals Engineering, to be published May 2003.
18. Hasemi, Y., Yokobayahi, S., Wakamatsu, T. and Ptchelintsev, A., ‘‘Firesafety of Building Components Exposed to a Localized Fire-Scope and Experiments on Ceiling/Beam System Exposed to a Localized Fire,’’ in Proceedings of ASIAFlam 1995, 1st International Conference, 1995, pp. 351–361.