Evaluating The Global Equivalence Ratio Concept for Compartment Fires: Part II – Limitations for Correlating Species Yields

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ABSTRACT: An examination of the suitability of the Global Equivalence Ratio (GER) to a compartment with prototypical building features for the prediction of carbon monoxide generation is presented. Based on an analysis of the species yields, it is seen that the GER concept is not appropriate for correlating and predicting species generation in prototypical building fires. In addition, the analysis showed that the species yields need to be calculated accounting for external burning. A new methodology to correlate the species yields from a compartment fire is presented and discussed. Good correlation for all four species examined in this study was obtained based on the new methodology.

KEY WORDS: carbon monoxide, compartment fires, species yields, global equivalence ratio.

INTRODUCTION

THIS PUBLICATION IS part of a study that aims at evaluating the applicability of the Global Equivalence Ratio (GER) concept for prediction of carbon monoxide (and other species) formation and transport in building fires with prototypical building features. The first part [1] discussed the impact of experimental techniques and measurement locations on the

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ascribed species levels exiting the compartment. Examination of data from various sources indicated that spatially uniform layers do not exist within compartments with prototypical building features; therefore, single point measurements of combustion species in the upper layer, doorway, or exhaust hood are not representative of the species generated in, and transported from, the compartment fire. New data from a recent experimental effort at Virginia Tech was presented as area averaged species mole fractions versus a new non-dimensional heat release rate. The area averaged mole fractions took into account all of the spatial variations in the species levels in the exiting portion of the doorway, while the new parameter provided a means for determining the burning conditions at the compartment exit plane.

The correlation between the species yields with the overall fuel-to-air ratio has been termed the Global Equivalence Ratio Concept (GER Concept). It was first implemented by Beyler using data from open burning fires located under an exhaust hood [2,3]. The methodology was later extended to a specially designed test apparatus used by Gottuk [4] and finally to scaled compartments by Pitts [5]. Based on limited experimental verification the methodology has been accepted by the fire protection community for predicting species generation in all fire environments.

This paper presents a detailed discussion of the GER concept, its validity for well-mixed two layer systems, and examines applicability and limitations in predicting species generation in prototypical buildings based on new data from the Building Fire Research Laboratory at Virginia Tech. A new methodology enabling to overcome the limitations and drawbacks to using the GER concept with fully featured compartments, is proposed.

THE GLOBAL EQUIVALENCE RATIO CONCEPT

Definition of Variables and Parameters

Equivalence Ratio

Toxic species generation in compartment fires is a complex function of air supply, nature of mixing, and fuel and oxidant properties [2,6]. Beyler [2] proposed that it might be possible to correlate the species yields and species production rates to an overall fuel-to-air ratio. Two key assumptions necessary for a valid correlation, according to Beyler, are:

1. The species production rate (and species yield) of major species is insensitive to the detailed structure of the flame.
2. A meaningful fuel-to-air ratio can be defined.

The focus of the current paper is on Assumption 2.

The equivalence ratio, defined in the classical way, Equation (1), determines whether a fire is fuel or oxygen limited.

$$\phi = \frac{(\dot{m}_{\text{fuel}}/\dot{m}_{\text{air}})}{(\dot{m}_{\text{fuel}}/\dot{m}_{\text{air}})_{\text{st}}} \tag{1}$$

Although typically used to define premixed combustion conditions, several different pseudo equivalence ratios have been defined for non-premixed (diffusion) flames, as occurring in typical fires.

Plume Equivalence Ratio (PER) – the ratio of the gaseous fuel generation rate at the fuel surface to the air entrainment rate into the flame between the fuel surface and the hot layer–cold layer interface normalized by the stoichiometric ratio for the fuel [2,5].

Upper Layer Equivalence Ratio – the ratio of the mass of gas in the upper layer derived from the fuel divided by that introduced from air normalized by the stoichiometric ratio for the fuel [5,7,8].

Global Equivalence Ratio (GER) – The ratio of the fuel mass loss rate within the compartment to the air flow rate into the compartment, normalized by the stoichiometric ratio for the fuel [5,8].

Under steady-state conditions, provided no air or fuel enters the upper layer except via the fire plume, and no air leaves the compartment before entering the fire plume, all three are equivalent [5]. The inherent assumption that all of the air flow into the compartment is entrained into the fire plume and pumped into the upper layer may not be valid. Species mapping, in the doorway, has shown that a spatially uniform upper layer does not exist [1]. However, typically, steady-state, well mixed, conditions are assumed and the term global equivalence ratio (GER) is used. A fire is considered over ventilated, under ventilated, or stoichiometric for $\phi < 1$, $\phi > 1$, and $\phi = 1$ respectively.

Species Yields

The generation of species in a fire has typically been defined in terms of a species yield, which is the mass of species produced per mass of fuel consumed. The species yields for the products of combustion, based on measurements of mass fuel flow rates and air flow rates, are determined by using,

$$Y_i = \frac{m_i}{m_{\text{fuel}}} = \frac{\dot{m}_i}{\dot{m}_{\text{fuel}}}$$

where

$$\dot{m}_i = y_{i,\mathrm{avg}}\dot{m}_{\mathrm{total}} = y_{i,\mathrm{avg}}(\dot{m}_{\mathrm{air}} + \dot{m}_{\mathrm{fuel}})$$

and

$$\mathrm{y}_{i,\mathrm{avg}} = \frac{MW_i}{MW_{UL}} X_{i,\mathrm{avg}}$$

which together lead to the species yield expression of:

$$Y_i = \frac{X_{i,\mathrm{avg}} MW_i(\dot{m}_{\mathrm{fuel}} + \dot{m}_{\mathrm{air}})}{\dot{m}_{\mathrm{fuel}} MW_{\mathrm{UL}}} \tag{2}$$

Since oxygen is consumed and not produced, based on a similar derivation, O_2 depletion is calculated as the amount of O_2 depleted per unit mass of fuel burned,

$$Y_{O_2} = \frac{m_{O_2,\mathrm{amb}} - m_{O_2}}{m_{\mathrm{fuel}}} = \frac{\dot{m}_{O_2,\mathrm{amb}} - \dot{m}_{O_2}}{\dot{m}_{\mathrm{fuel}}}$$

where

$$\dot{m}_{O_2,\mathrm{amb}} = y_{O_2,\mathrm{amb}}\dot{m}_{\mathrm{air}}$$

and

$$\dot{m}_{O_2} = y_{O_2,\mathrm{avg}}\dot{m}_{\mathrm{total}}$$

which leads to:

$$Y_{O_2} = \frac{MW_{O_2}(X_{O_2,\mathrm{amb}}\dot{m}_{\mathrm{air}} - X_{O_2,\mathrm{avg}}\dot{m}_{\mathrm{total}})}{\dot{m}_{\mathrm{fuel}} MW_{\mathrm{UL}}} \tag{3}$$

It is helpful to consider the normalized yields of oxygen and carbon dioxide, which are species whose reference levels are those for complete combustion. Normalized yields are determined by dividing the unnormalized yields by the theoretical maximum species yields, the maximum mass of a species produced or consumed by complete combustion of one mole of fuel, Equation (4).

$$f_i = \frac{Y_i}{Y_{i,\,\mathrm{max}}} \tag{4}$$

For example, propane (C_3H_8) has maximum theoretical yields of CO_2 and O_2 of 3.0 and 3.64 respectively. The normalized CO_2 and O_2 yields range between 0 and 1.0 and can be used as indicators of the completeness of combustion; where a value of 1.0 represents complete combustion. The normalized yields of oxygen and carbon dioxide are also referred to as depletion and generation efficiencies in literature [9].

Experimental practice has been typically based on single point measurements either in the exhaust duct of a fume hood, within the upper layer of the compartment, or in the exiting portion of the compartment vent. Therefore, the mole fractions in Equations (2) and (3) are based on local data. In the current study, a detailed mapping of the species exiting the compartment was performed and an average integrated mole fraction for each species, Equation (5), is used in Equations (2) and (3).

$$\overline{X_i} = \frac{MW_{\text{mixture}} \int \rho(x,y) y_i(x,y) V(x,y) db\, dH}{MW_i \int \rho(x,y) V(x,y) db\, dH} \tag{5}$$

This methodology takes into account all of the horizontal and vertical variations in species concentrations and velocity at the doorway. Details on this aspect can be found in the companion publication [1].

APPLICATION OF EQUIVALENCE RATIO CONCEPTS TO THREE FIRE CONFIGURATIONS

Global Equivalence Ratio Applied to Open Burning Fires Under an Exhaust Hood

Species generation from free burning diffusion flames positioned under an exhaust hood has been the subject of numerous experimental investigations, including work by Beyler et al. as reported in [5]. The most widely referenced work, and the basis for current predictive engineering tools for species generation, is the work of Beyler [2,3]. Beyler's experiments were conducted with a burner located underneath a 1-m diameter exhaust hood with gas sampling taken within the exhaust stream. The experiment was designed to simulate the upper layer of a compartment fire. Pitts [5] summarized the following major conclusions of Beyler's work.

1. Major combustion species can be correlated in terms of the GER.
2. Relatively constant concentrations of CO are generated at low and high GERs.
3. The generation of CO under rich conditions is considerably greater than for fuel-lean conditions.

4. The concentrations of CO generated for rich conditions are fuel dependent, but can be correlated with fuel structure.

In addition it is reported that:

5. A reasonably well-mixed uniform upper layer both in temperature and composition existed for steady-state conditions [8].

Beyler concluded that CO concentration was constant under fuel-lean ($\phi < 0.7$) and fuel-rich ($\phi > 1.2$) conditions, with a transition stage from the lower level to a higher level occurring in the range $0.7 < \phi < 1.2$. Beyler reported that if carbon monoxide yields are presented as a normalized yield, a fuel dependence is seen and can be correlated with the fuel structure [2]. It has to be noted that, although these conclusions are based on small-scale open fires under an exhaust hood, over the years these conclusions have been extended to reduced and full-scale compartment fires, as is presented in the following paragraphs.

Global Equivalence Ratio Concept Applied to Specially Designed Compartment Apparatus

A decade ago, in 1992, Gottuk [4] performed experiments in a specially designed scaled test apparatus. The test apparatus consisted of a 1.2 m by 1.5 m cross-section by 1.2 m high fire chamber, with a 1.2 m by 1.5 m by 0.3 m high air distribution plenum below the fire chamber. The test apparatus provided entrained air into the compartment through an inlet duct located at the base of the compartment; this allowed air to be entrained into the base of the fire over the entire circumference. The exhaust gases were vented through an opening in the upper frontal portion of the fire chamber. The area of the exhaust vent ranged between 0.0404 and 0.1615 m^2. The experiments were performed using liquid *n*-hexane in circular pans ranging in diameter from 0.15 to 0.28 m located in the center of the compartment on a false floor. With this test setup, Gottuk simulated an ideal two-layer system, where the actual air mass flow rate into and combustion species out of the compartment could be measured directly and independently.

The test apparatus used by Gottuk represents more of an idealized two-layer system, a scaled-up hood experiment, than a typical compartment scenario. Similar to free burning open fires, air entrainment into the fire occurred via the full perimeter of the fire. In addition, a well-mixed upper layer develops prior to being vented, similar to the exhaust hood experiments performed by Beyler. Good correlation between the species levels and the GER was observed, as expected.

Global Equivalence Ratio Applied to Reduced Scaled Enclosures

Bryner et al. [10] performed experiments in a reduced-scale standard room using natural gas fires. The test enclosure was a $^2/_5$-scale ISO 9705 compartment measuring 0.98 m by 1.46 m by 0.98 m high. A single doorway was located in the center of the short wall measuring 0.48 m wide by 0.81 m high. The experiments were performed using a 15-cm diameter natural gas burner, located 15 cm above the floor in the center of the compartment. The heat release rates for the fires ranged between 10 and 670 kW, corresponding to GERs between 0.1 and 1.5. Good agreement between the species mole fractions as a function of the ideal heat release rate and as a function of the GER were reported [1,5,10]. The data was not presented as species yields versus the GER. Species yields based on the reported mole fractions and GER, by Bryner et al. [10], were calculated for this review using Equation (6),

$$Y_i = \bar{X}_i \left(\frac{MW_i}{MW_{UL}} \right) \left(1 + \frac{1}{\phi(\dot{m}_{\text{fuel}}/\dot{m}_{\text{air}})_{\text{st}}} \right) \tag{6}$$

NEW COMPARTMENT STUDY AT VIRGINIA TECH

A study recently performed at the Virginia Tech Building Fire Research Laboratory included a detailed analysis of the species levels at the exit plane of a ½-scale ISO 9705 compartment under three different ventilation conditions using a single gaseous fuel. The three ventilation conditions were set by changing the doorway width and are presented as narrow (0.165 m), baseline (0.33 m), and wide (0.66 m) doorways. The three ventilation conditions resulted in variations in the equivalence ratio and the structure of the fire (reacting flow field) inside the compartment. The fuel mass flow rates, set independently, ranged between 0.002 and 0.01 kg/s. The GER ranged between 0.13 and 3.0.

Species measurements were performed at grid-points across the doorway plane. Measurements were made using a rake containing five co-located pairs of gas sampling and bi-directional probes, resulting in four measurement locations in the outflow region and one in the inflow region of the doorway at each transverse location. For the baseline ($w = 0.33$ m) and wide ($w = 0.66$ m) doorway the sampling rake was positioned at three transverse locations across the doorway, while for the narrow ($w = 0.165$) doorway only samples along the centerline were taken, since the profiles across the width were found to be uniform. A detailed description of the test facility, procedures, and results can be found in related publications [1,11].

RESULTS AND DISCUSSION

Results from a total of 28 test conditions, of which 13 were performed with the baseline doorway width (0.33 m), 4 with the wide doorway width (0.66 m), and 11 with the narrow doorway width (0.165 m), are presented, in this paper. The results are first presented and discussed based on the standard engineering practice [8], followed by a revised methodology.

Standard Engineering Practice

The calculated species yields based on standard fire protection engineering practice for oxygen, Equation (3), carbon dioxide, carbon monoxide, and unburned hydrocarbons, Equation (2), are presented in Figures 1–4 as a function of the GER. The oxygen and carbon dioxide data are presented as normalized yields, Equation (4), while the carbon monoxide and unburned hydrocarbon yields are presented as un-normalized yields. Reported data from previous studies of Gottuk [4], Belyer [2,3] and Bryner et al. [10], are also included for comparison. As mentioned previously, Bryner et al. [10] did not report yield data, therefore the species yields were

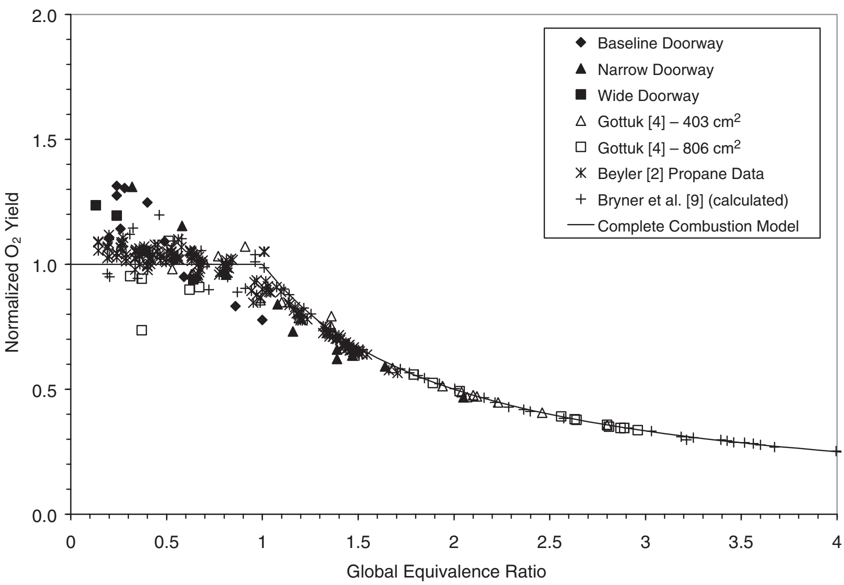

Figure 1. *Normalized O_2 yields as a function of the equivalence ratio and door width compared with data from [2,4,10] in addition to the model for complete combustion.*

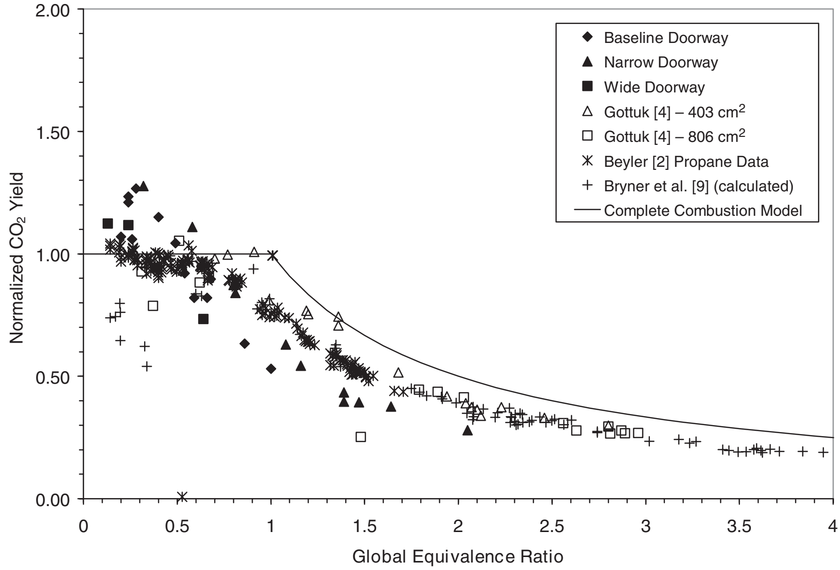

Figure 2. *Normalized CO_2 yields as a function of the equivalence ratio and door width compared with data from [2,4,10] in addition to the model for complete combustion.*

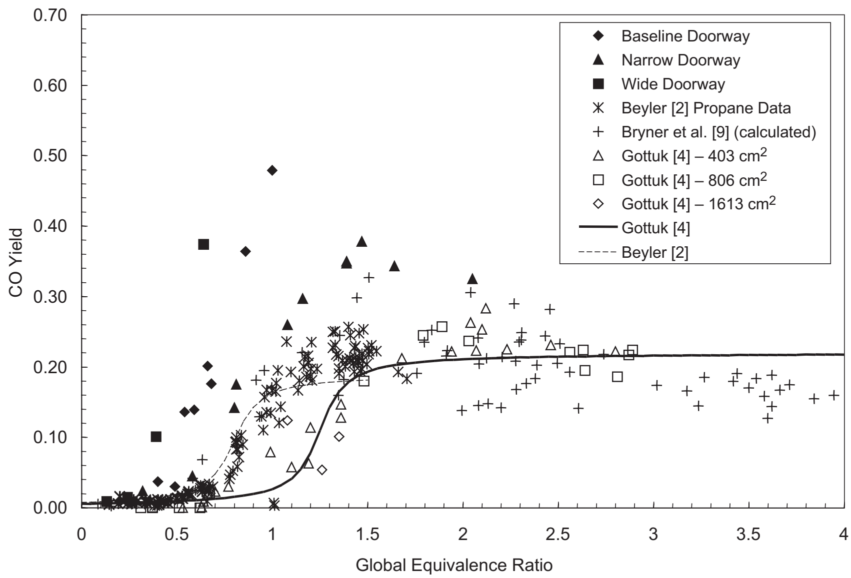

Figure 3. *Carbon monoxide yields as a function of the equivalence ratio and door width compared with data from [2,4,10] in addition to models from [2,4].*

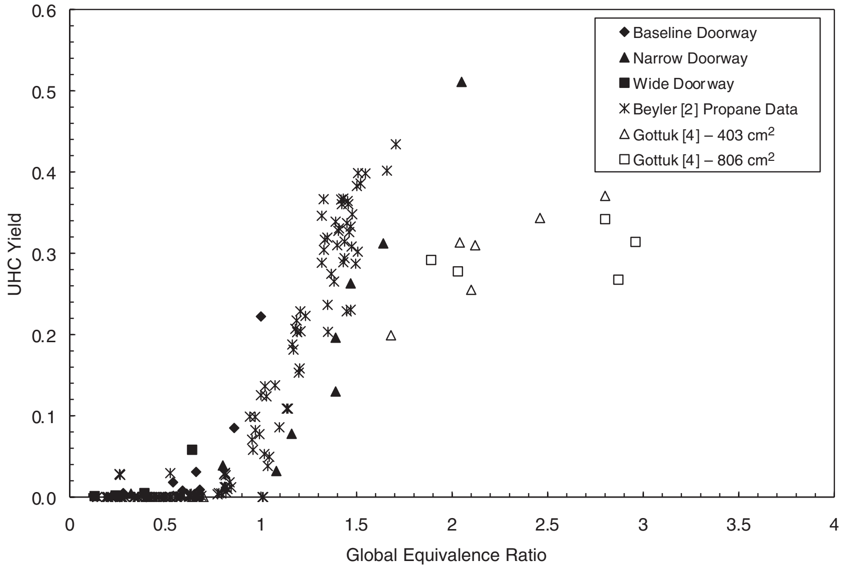

Figure 4. *Unburned hydrocarbon yields as a function of the equivalence ratio and door width compared with data from [2,4].*

calculated here based on the reported mole fraction and the local equivalence ratio, Equation (6).

The normalized oxygen data shown in Figure 1 indicate good agreement with the studies of Beyler [3], Gottuk [4], and Bryner et al. [1] and correlate well with the model for complete combustion. Similar agreement is seen for the carbon dioxide yields in Figure 2. The carbon dioxide yields are lower than the theoretical levels for complete combustion, because complete conversion of the fuel carbon to CO_2 does not happen, by the time the gases reach the compartment exit, and intermediate species, i.e. carbon monoxide and unburned hydrocarbons, are formed.

The curves for the yields of the products of incomplete combustion, CO and UHC, Figures 3 and 4, appear to have an additional dependency on the ventilation conditions, to that captured by the GER. The CO yield data as a function of the GER, shown in Figure 3, indicate a different curve for each of the three ventilation conditions. The carbon monoxide yields begin to increase at lower GERs as the width of the doorway increases. The increase in carbon monoxide yields is attributed to the start of external burning from the compartment. It was reported earlier [11], that external burning due to flame extensions begins to occur at equivalence ratios below 1.0 for the narrow, baseline, and wide doorways, Table 1. The increase in carbon monoxide levels appear at the corresponding GERs

Table 1. Minimum heat release rate and equivalence ratio for flame extension, along with the $\dot{Q}_{Stoichiometric}$, and $\tilde{Q}_{critical}$ for the present geometries [11].

Doorway Geometry	Heat Release Rate (kW)	Equivalence Ratio	$\dot{Q}_{Stoichiometric}$ (kW)	$\tilde{Q}_{critical}$
Narrow	91	0.31–0.56	183	2.01
Baseline	127	0.26	365	2.88
Wide	107–203 (155)	0.13–0.24	730	4.71

for flame extensions for each doorway. Once external burning occurs, some of the measurement points are taken directly in the flame.

The narrow doorway data appear to increase and peak at about a yield of 0.36 g_{co}/g_{fuel} and an equivalence ratio of 1.5, while both the baseline and wide doorway data have continuously increasing yields. For neither the baseline nor the wide doorway were equivalence ratios greater than 1.0 achieved; therefore, the peak CO yield and corresponding GER are unknown. It should be noted that at the lower GERs, where comparison between all three doorways can be made, the CO yield data appear to double by doubling the doorway width. Continuation of this trend at higher equivalence ratios must be investigated further.

Comparing the carbon monoxide yield data to previously published data of Beyler [2], Gottuk [4], and Bryner et al. [10] it is seen that the values for the present study are significantly higher. This is attributed to the differences in the physics of each test apparatus used in the research studies. As previously discussed, both Beyler's and Gottuk's experimental apparatuses allowed air to be entrained into the fire plume via the entire circumference of the flame. Also, the collection hood above the fire in Beyler's setup and the specially built test compartment of Gottuk generated a well-mixed layer in which there was ample time for the gases to mix and for the conversion of CO to CO_2 to take place. Both Beyler [2] and Gottuk [4] reported that the calculated GERs and the plume equivalence ratios were equal. The data from Bryner et al. [10] although taken within the compartment and reported as a function of the local equivalence ratio, are based on single point measurements, which based on the reported sampling location, are assumed to be taken within the fire plume. Therefore, the local equivalence is actually a local plume equivalence ratio and, therefore, the data agrees well with the data from Beyler [2] and Gottuk [4].

An increase in the unburned hydrocarbon yields, shown in Figure 4, is seen for all three ventilation conditions, and corresponds to the equivalence ratios at which flame extensions begin to occur. Gottuk [4] reported that the unburned hydrocarbon yields begin to plateau at GERs greater than 1.8 at a value of 0.3 $g_{C_2H_4}/g_{\text{fuel}}$. The maximum unburned hydrocarbon yield, for propane fires, when measured as equivalent ethylene, C_2H_4, is 0.96 $g_{C_2H_4}/g_{\text{fuel}}$. It is expected that the unburned hydrocarbon yields will approach this value asymptotically as the equivalence ratio increases. The present data follow the same trend as that of Beyler [2] and neither study indicates any tapering of the data. Bryner et al. [10] did not report unburned hydrocarbon data.

A competition for the available oxygen exists between the formation of CO and the oxidation of CO to CO_2. Since the levels of CO and CO_2 are directly related and are a function of the available oxygen and gas temperatures, the dependence of carbon monoxide and unburned hydrocarbons on the equivalence ratio and the size of the ventilation openings should also be seen in the carbon dioxide yields. Re-examination of Figure 2 indicates a slight dependence on the ventilation size exists, although not as obvious as with the CO and UHC data. As expected, this dependence in the CO_2 data is opposite to that of the CO and UHC yields, i.e. lower levels of CO_2 are seen for the wide doorway and increase with decreasing doorway width.

When presented in this fashion, the highest carbon monoxide yields are seen for the wide doorway and the lowest for the narrow doorway. However, when presented as species mole fractions versus the ideal fire size, Figure 5, the highest average species mole fractions are seen for the narrow doorway and the lowest for the wide doorway.

This behavior can be explained by examining Equations (1) and (2), the GER and the species yield equation. Neglecting the constants in both equations, it is seen that,

$$Y_i \propto \bar{X}_i\left(\frac{\dot{m}_{\text{fuel}} + \dot{m}_{\text{air}}}{\dot{m}_{\text{fuel}}}\right) = \bar{X}_i\left(1 + \frac{1}{\phi}\right) \tag{7}$$

and

$$\phi \propto \frac{\dot{m}_{\text{fuel}}}{\dot{m}_{\text{air}}} \tag{8}$$

Assuming a fixed ideal fire size, i.e. a fixed $\dot{m}_{\text{fuel}}$. The species yield, therefore, is directly proportional to the species mole fraction and $\dot{m}_{\text{air}}$, while the GER is inversely proportional to only $\dot{m}_{\text{air}}$. Noting that $\dot{m}_{\text{air}}$ is directly proportional to the width of the doorway results in $\phi_{\text{wide}} < \phi_{\text{baseline}} < \phi_{\text{narrow}}$ for a fixed fire size. Therefore, the shift in the data, seen between Figures 3

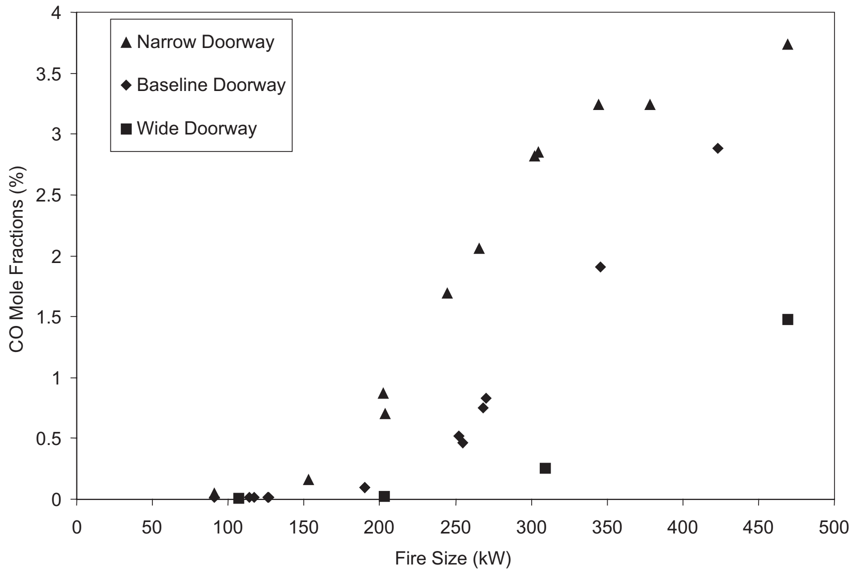

Figure 5. *Carbon monoxide mole fractions as a function of the ideal fire size and doorway width.*

and 5, must be attributed to the independent variable, the GER. This is significant since it illustrates the fact that using the GER as a correlating parameter skews the data in a counterintuitive manner, since it implies that higher yields, based on average integrated mole fractions, are seen for the wide doorway compared to the narrow doorway.

Based on the present analysis of the GER concept it has been shown that the methodology fails when extended to scaled-compartment fires. Key weaknesses in the methodology are:

1. The GER concept does not account for the burning conditions at the compartment exit plane.
2. Using the GER as the independent variable while correlating the data, shifts the data in a counterintuitive manner, indicating the highest levels of carbon monoxide yields for conditions where the lowest average mole fractions were measured.
3. Local species yields do not correlate well with a global conditions parameter (GER).
4. The data does not collapse, separate curves are observed for each ventilation condition.

In view of these limitations, a new methodology, which takes into account these issues, is required, and proposed next.

A Proposal for a New Methodology to Correlate Species Yields

Since all of the measurements were performed at the exit plane of the compartment, conditions with external burning led to species measurements directly within the fire plume. These species are not the final 'frozen' species that would be transported to remote locations, had all of the combustion occurred in the compartment. Therefore, calculating the species yield based on the total amount of fuel injected into the compartment is incorrect and the data needs to be adjusted to the burning occurring within the compartment alone, i.e. not including external burning. Based on this, a new species yield is defined as $\dot{m}_i/\dot{m}_{\text{fuel, compartment}}$.

Since the amount of oxygen consumed by the fire is known, the heat release rate occurring in the compartment is determined via Equation (9) [12].

$$\dot{Q}_{\text{compartment}} = \left(0.21 - X_{\text{O}_2,\text{scrubbed}}\right)\dot{m}_{\text{air}} \frac{MW_{\text{O}_2}}{MW_{\text{air}}} \Delta H_{c,\text{ox}} \tag{9}$$

where $X_{\text{O}_2,\text{scrubbed}}$ is the mole fraction of oxygen in the scrubbed exhaust gases and $\Delta H_{c,\text{ox}}$ is defined as the heat of combustion per gram of oxygen consumed. For propane, $\Delta H_{c,\text{ox}}$ has a value of 12,800 kJ/kg [13]. This value is based on complete combustion where the products of combustion are only CO_2 and H_2O. In compartment fires complete combustion is seldom seen and products of incomplete combustion, CO and soot, are also present. Therefore, a combustion efficiency, χ, is included to account for incomplete combustion.

$$\dot{Q}_{\text{compartment}} = \left(0.21 - X_{\text{O}_2,\text{scrubbed}}\right)\dot{m}_{\text{air}} \frac{MW_{\text{O}_2}}{MW_{\text{air}}} \left(\chi \Delta H_{c,\text{ox}}\right) \tag{9a}$$

The amount of fuel burned in the compartment is determined using the calculated heat release rate, from Equation (9a), and the effective heat of combustion of propane, $\chi\ \Delta H_c$, again accounting for incomplete combustion,

$$\begin{aligned}\dot{m}_{\text{fuel, compartment}} &= \frac{\dot{Q}_{\text{compartment}}}{\chi \Delta H_c} \\ &= \frac{\left(0.21 - X_{\text{O}_2,\text{scrubbed}}\right)\dot{m}_{\text{air}}\left(MW_{\text{O}_2}/MW_{\text{air}}\right)\left(\Delta H_{\text{c, ox}}\right)}{\Delta H_c}\end{aligned} \tag{10}$$

The calculated $\dot{m}_{\text{fuel, compartment}}$ can then be used in the denominator of Equations (2) and (3) to determine the species yields based solely on the combustion in the compartment.

Prior to applying this analysis to the data, verification of the methodology used to determine the amount of combustion occurring in the compartment is needed. The calculated heat release rate in the compartment as a function of the ideal heat release rate, for each of the three doorway widths is shown in Figure 6. Also included are the calculated maximum heat release rates possible (ventilation limit) based on each ventilation condition. If the data fall on the diagonal line below the corresponding ventilation limit, then the burning conditions are fuel limited.

The ideal heat release rate, $\dot{m}_{\text{fuel}}\Delta H_c$, is based on the amount of propane injected into the compartment and the heat of combustion of propane. The horizontal lines are the theoretical maximum heat release rate supported inside the compartment based on the ventilation limit. The theoretical maximum heat release rates are 183, 365, and 730 kW for the narrow, baseline, and wide doorways respectively. Comparison of the fuel limited heat release rates with the ventilation limited heat release rates, Figure 6, indicates that for the test conditions the baseline and wide doorways were always fuel limited. Both burning regimes were observed with the narrow doorway.

The agreement between the calculated heat release rate for combustion occurring within the compartment and the theoretical maximum heat release rate for the narrow doorway indicates that using Equations (8) and (9) to determine the amount of fuel consumed within the compartment is valid for this analysis.

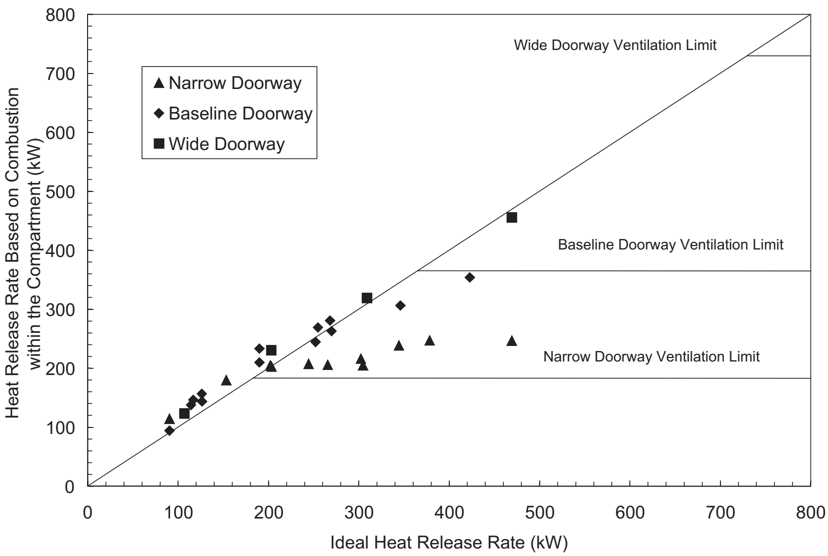

Figure 6. *Heat release rate within compartment vs. ideal heat release rate.*

The different burning regimes, highlighted in Figure 6, were next taken into account via a new analysis, to properly correlate the species formation. A new normalized heat release rate, $\tilde{Q}$, introduced in a companion publication [1] is also used here to analyze species levels. The parameter is defined as the ratio of the ideal heat release rate to the heat release rate required for the tip of fire plume to reach the compartment exit plane, Equation (11),

$$\tilde{Q} = \frac{\dot{Q}_{\text{ideal}}}{\dot{Q}_{\text{Flame Extensions}}} \tag{11}$$

Using $\tilde{Q}$ as the independent variable allows four burning regimes to be defined at the compartment exit plane [1].

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

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

Although a methodology for calculating $\dot{Q}_{\text{Flame Extensions}}$ was presented in the companion publication [1], the values used in the calculations are based on visual observations. The minimum heat release rates for which flames were experimentally observed to begin to exit the compartment are listed in Table 1, the calculated values for $\dot{Q}_{\text{Stoichiometric}}$ and $\tilde{Q}_{\text{critical}}$ are also listed. For the baseline doorway the fire size was gradually increased until the flames just began to exit the compartment. For the narrow doorway at a heat release rate of 91 kW "tiny wisps of flames" were observed to exit the compartment. For the wide doorway only four tests were performed. At the lowest heat release rate, 107 kW, no flames were observed exiting the compartment, while a continuous flame extending from the compartment was observed at a heat release rate of 203 kW. For lack of a more precise value, the average of the two values, 155 kW, will be used in the calculations as the heat release rate at which flame extensions first began to occur for the wide doorway.

The calculated species yields based on the combustion occurring in the compartment as a function of $\tilde{Q}$ for oxygen, carbon dioxide, carbon monoxide, and unburned hydrocarbons are presented in Figures 7–10

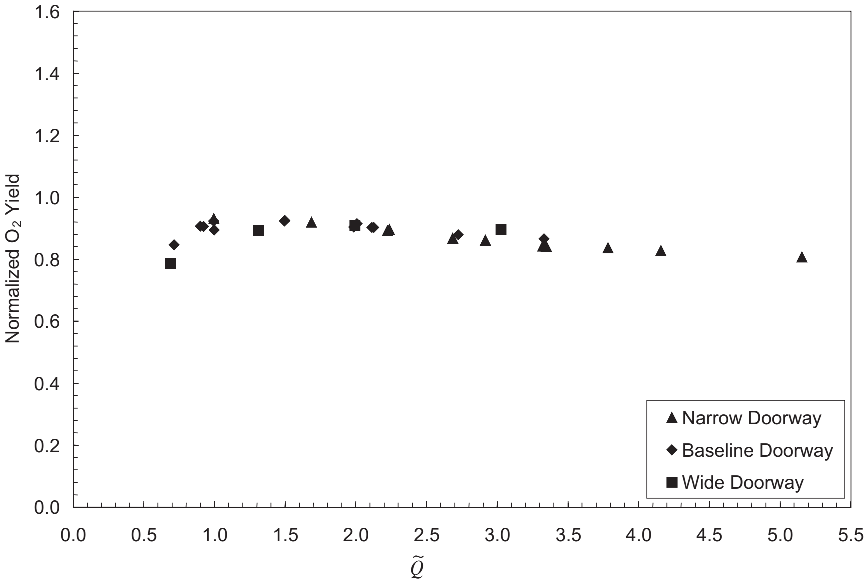

Figure 7. *Normalized oxygen species yield versus $\tilde{Q}$.*

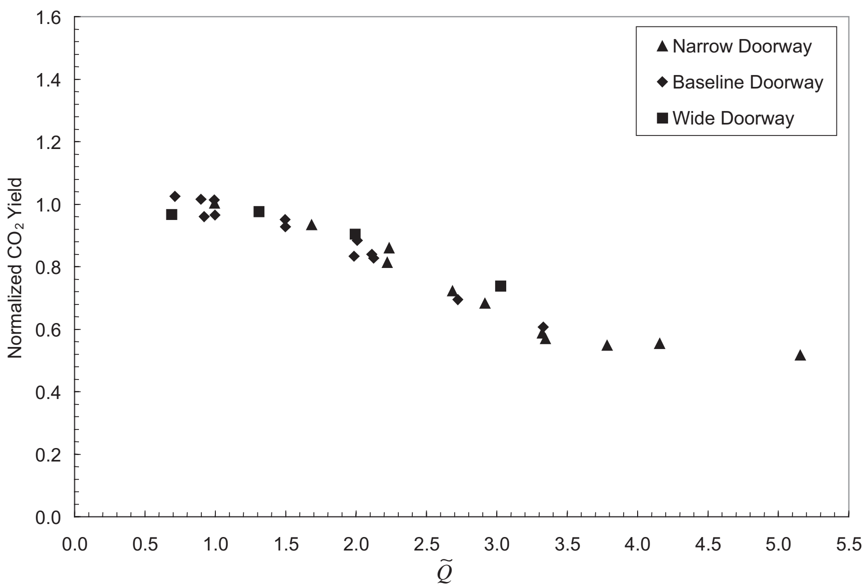

Figure 8. *Normalized carbon dioxide species yield vs. $\tilde{Q}$.*

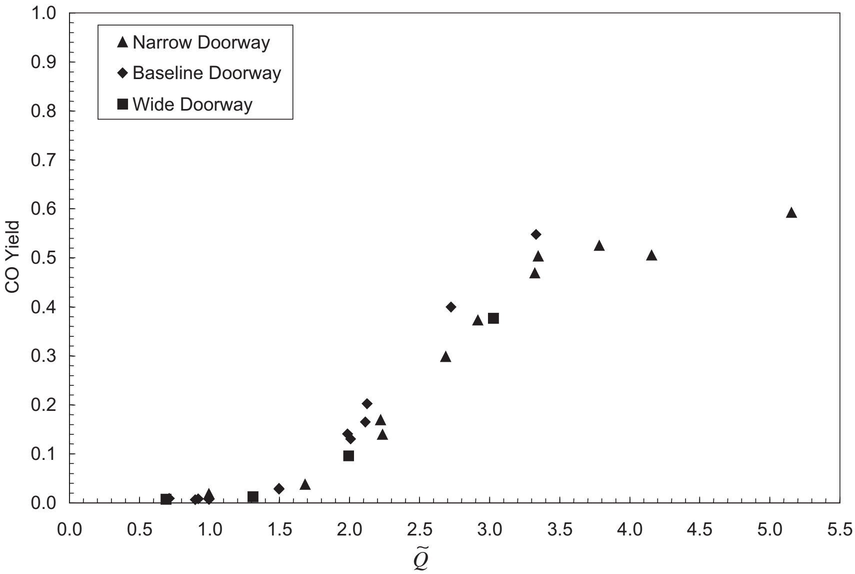

Figure 9. *Carbon monoxide species yield vs.* $\tilde{Q}$.

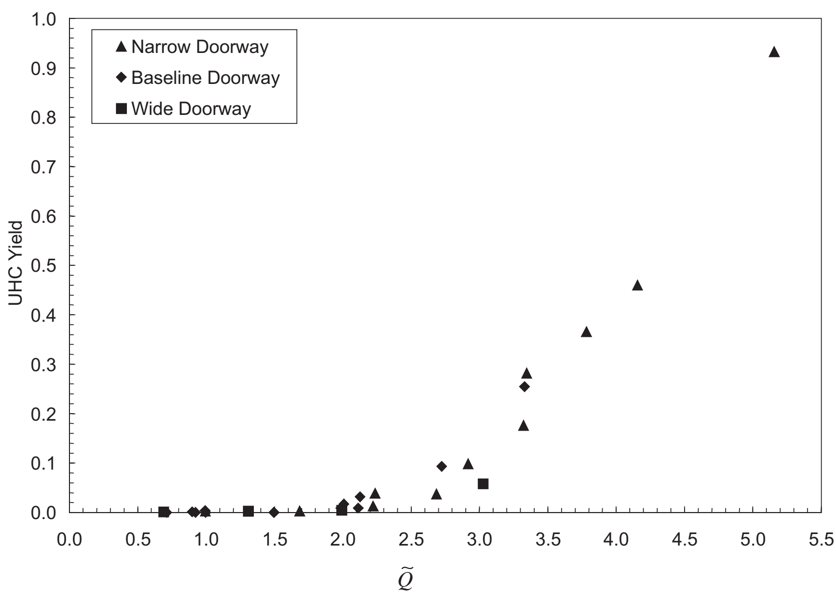

Figure 10. *Unburned hydrocarbon species yield vs.* $\tilde{Q}$.

respectively. The oxygen and carbon dioxide data are presented as normalized yields. Data from previous studies is not included since a value for $\dot{Q}_{\text{Flame Extensions}}$ could not be determined.

Presenting the data in this manner, the data collapse to a single curve for each species, respectively. The normalized oxygen yield (amount of O_2 depleted), Figure 7, indicates a near constant yield of 0.9 for all $\tilde{Q}$. This is an expected result since the yield represents the oxygen consumed within the compartment, and since the yield is normalized by the actual combustion occurring in the compartment. If perfect combustion occurring (i.e. no minor species being produced) this number would be one. It has been shown in Figure 6, that the heat release rate in the compartment is constant once the ventilation limit is reached.

The normalized carbon dioxide yields, Figure 8, appear to correlate well with $\tilde{Q}$. The data indicate a value of 1.0 for $0 < \tilde{Q} < 1.0$, and as $\tilde{Q}$ increases beyond 1.0, the CO_2 generated within the compartment decreases as more carbon exits the compartment in the form of carbon monoxide and unburned hydrocarbons as seen in Figures 9 and 10.

The carbon monoxide yield, Figure 9, indicates that incomplete combustion within the compartment begins to occur around $\tilde{Q} = 1.25$, corresponding to a $\tilde{Q}$ just beyond that for which flame extensions begin to occur. The upper bound for the CO yield is the theoretical maximum yield for propane, 1.91 g_{co}/g_{fuel}, which assumes there are no other carbon containing species generated. This limit will never be achieved, since other combustion species are present. The current data appears to plateau at $\tilde{Q} > 3.5$ approaching a species yield of approximately $0.50\,\mathrm{g_{co}/g_{fuel}}$. Similar to the carbon dioxide data, as $\tilde{Q}$ goes to infinity, only fuel will be present; therefore, it is expected that, the CO yield will begin to decrease and approach zero at higher values of $\tilde{Q}$.

The unburned hydrocarbon yields, Figure 10, begin to increase at $\tilde{Q} = 2.0$ and indicate a continuous rise. As opposed to the old analysis where the maximum UHC yield could not exceed $0.96\,g_{uhc}/g_{fuel}$, under the modified analysis there is no upper bound for the UHC yield. The unrestricted upper bound for the unburned hydrocarbons is a result of the constant value of $\dot{m}_{\text{fuel, compartment}}$ once the ventilation limit is achieved within the compartment, at higher heat release rates the numerator of Equation (2) will continuously increase as the denominator remains constant.

The new methodology provides a means for predicting toxic species generated within a compartment with prototypical building features. This methodology has a benefit over the GER methodology because it can be applied to compartment fires with prototypical building features and a non-uniform upper layer. Using this analysis the data for all four species appears to be independent of the burning conditions within the compartment and of the ventilation conditions for the range of conditions examined.

The species yields at the compartment exit plane should be viewed as the inlet boundary conditions to the hallway and not as the final species transported to remote locations. Once the onset of external burning occurs, $\tilde{Q} > 1.0$, the species transported downstream can no longer be defined based solely on compartment parameters. The final species levels will be a function of the conditions in the adjacent space, which include available oxygen, building geometry, and secondary fuel sources. These parameters are the subject of a continuing examination being performed at Virginia Tech.

SUMMARY

To date the global equivalence ratio (GER) concept has been considered to be the primary tool for predicting carbon monoxide levels formed in compartment fires. Previous studies performed under an exhaust hood or in specially designed test apparatus indicated a potential for extending the GER concept to compartment fires with prototypical building features. A detailed experimental study, performed at the Virginia Tech Building Fire Research Laboratory, examined the species exiting the compartment based on the different ventilation and fire conditions. The data is presented as species yields versus the GER, using the standard engineering practice. The analysis showed that the GER concept fails as a useful tool for predicting species levels exiting a compartment with prototypical building features. The key shortcomings are:

1. No accounting for the burning conditions at the compartment exit plane.
2. The GER shifts the data in a counterintuitive manner.
3. The data is dependent on the ventilation condition.

A new methodology which consists of the species yields based on the combustion occurring within the compartment (as opposed to the ideal heat release rate based on total mass flow rate of fuel) as a function of a normalized heat release rate, $\tilde{Q}$, was presented. This methodology accounts for each of the deficiencies observed when using the GER concept. Oxygen, carbon dioxide, carbon monoxide, and unburned hydrocarbon yields, based on combustion occurring in the compartment, appear to be independent of the degree of burning occurring within the compartment when correlated versus $\tilde{Q}$. This methodology predicts the average species level at the compartment exit plane. It is known that once external burning occurs the species levels transported away from the compartment will be different from those at the compartment exit plane.

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NOMENCLATURE

b = width of the doorway (m)
f_i = normalized species yield
H = the height of the doorway (m)
m_i = mass of species i (kg)
m_{fuel} = mass of fuel (kg)
$\dot{m}_i$ = mass flow rate of species i (kg/s)
$\dot{m}_{\text{air}}$ = measured mass flow rate of air into compartment (kg/s)
$\dot{m}_{\text{fuel}}$ = measured mass flow rate of the fuel (kg/s)
$\dot{m}_{\text{fuel, compartment}}$ = calculated fuel mass flow rate consumed in the compartment (kg/s)
$m_{O_2,\text{amb}}$ = mass of oxygen in the ambient gas stream (kg)
m_{O_2} = mass of oxygen measured exiting the compartment (kg)
$\dot{m}_{O_2,\text{amb}}$ = mass flow rate of oxygen in the ambient gas stream (kg/s)
$\dot{m}_{O_2}$ = mass flow rate of oxygen measured exiting the compartment (kg/s)
$\dot{m}_{\text{total}}$ = total mass flow rate of gases exiting the compartment (kg/s)
MW_i = species molecular weight
MW_{UL} = molecular weight of the upper layer assumed to be equivalent to that of air
$\dot{Q}_{\text{Flame Extensions}}$ = heat release rate required for fire plume to reach the compartment opening (kW)
$\dot{Q}_{\text{ideal}} = \Delta H_c \dot{m}_{\text{fuel}}$ = ideal heat release rate (kW)
$\dot{Q}_{\text{Stoichiometric}}$ = stoichiometric heat release rate (kW)
$\tilde{Q}$ = normalized heat release rate (-)
r = stoichiometric fuel to air ratio (-)
V = velocity (m/s)

$\dot{V}$ = volumetric flow rate of air (m^3/s)
X_i = measured species mole fraction (%)
$X_{i,\mathrm{avg}}$ = integrated average species mole fraction (%)
$X_{O_2,\mathrm{amb}}$ = mole fraction of oxygen at ambient (%)
Y_i = species yield
y_i = species mass fraction
$y_{\mathrm{i,avg}}$ = integrated average species mass fraction
$y_{O_2,\mathrm{amb}}$ = mass fraction of oxygen under ambient conditions
$y_{O_2,\mathrm{avg}}$ = integrated average mass fraction of oxygen exiting the compartment
ΔH_c = heat of combustion (kJ/kg)
$\Delta H_{c,\mathrm{ox}}$ = heat of combustion per kg of oxygen (taken to be 12,800 kJ/kg oxygen)
ρ = gas density (kg/m^3)
ρ_{O_2} = density of oxygen at STP (kg/m^3)
χ = combustion efficiency (-)
$(\dot{m}_{\mathrm{fuel}}/\dot{m}_{\mathrm{air}})_{\mathrm{st}}$ = stoichiometric fuel-to-air ratio for the fuel

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