THE APPLICABILITY OF CORRELATIONS BETWEEN THE SPECIES FORMATION AND THE GLOBAL EQUIVALENCE RATIO IN A 1/2-SCALED ISO COMPARTMENT WITH NONGASEOUS FUEL

by

Christopher J. Wieczorek, Uri Vandsburger,
Christopher McKay and Sandeep Sathyamoorthy
Advanced Fuel Research, Inc.
87 Church Street
East Hartford, CT 06108, USA
and
Brian Lattimer
Hughes Associates, Inc.
Baltimore, MD 21227-1652, USA

Reprinted from the Fire Safety Science. Proceedings. Sixth (6th) International Symposium. International Association for Fire Safety Science (IAFSS). July 5-9, 1999, Poitiers, France, Intl. Assoc. for Fire Safety Science, Boston, MA, Curtat, M., Editor, 2000.

The Applicability of Correlations between the Species Formation and the Global Equivalence Ratio in a 1/2-Scaled ISO Compartment with Nongaseous Fuel

Christopher J. Wieczorek, Uri Vandsburger[*], Brian Lattimer[†], and Christopher McKay
Department of Mechanical Engineering
Virginia Polytechnic Institute and State University
Blacksburg, Virginia

ABSTRACT

Lifestyle developments on the global scale which manifest themselves in increased travel, increased elderly populations in assisted care facilities, and urbanization require increased attention to fire safety in dense occupation environments. Statistics spanning decades have shown that the key factor in fire fatalities is CO inhalation, termed loosely "smoke inhalation," not only in the fire enclosure but in areas remote from the flames. The current study was geared at developing correlations to relate the levels of CO, CO_2, and UHC produced and the amount of O_2 depleted during compartment fires to the burning compartment global equivalence ratio (GER). This is a first step in a study, which will include a study of fire products transported to adjacent enclosures, and the development of engineering correlations. Tests were conducted in a ½-scale ISO compartment with fully scaled door openings, using *n*-hexane pool fires within the center of the compartment. Two fire scenarios were simulated, a fully and partially opened door, by varying the door width. The results, in form of concentrations of the fire products as a function of equivalence ratio (corrected for various transport times) were compared with previous hood and special configuration compartment studies. The present work indicated that the residence time of the gases within the compartment has an effect on both the carbon monoxide levels and the carbon dioxide levels. The narrow door configuration yields the lowest CO levels and the highest CO_2 levels. This is expected since the residence time of the gases within the narrow door (19.5 sec) is more than twice that of the baseline door (9.3 sec), therefore the there is more time for the CO to oxidize to CO_2. The unburned hydrocarbon levels are not effected by the residence times in this study since UHC's have a higher reaction rate than CO under the present fire condition. Therefore, the levels of UHC's will be dependent only on the availability of free oxygen.

KEYWORDS : concentrations, compartment fires, global equivalence ratio, *n*-hexane

---

[*] Author of Correspondence

[†] At Hughes Associates Inc.

INTRODUCTION

Approximately two thirds of all deaths resulting from enclosure fires can be attributed to the presence of carbon monoxide (CO) [1]. Fires occurring in occupancies such as hospitals, dormitories, and nursing homes, pose a serious threat to occupants present not only in the room of origin but also to those occupants located in adjacent spaces, as well as at locations remote from the fire [1]. The ability to predict/estimate the levels of CO produced and transported to adjacent spaces during compartment fires would significantly increase occupant safety. Furthermore, it is desirable to be able to correlate these levels to primary parameters like the global equivalence ratio (GER) which incorporate physical parameters like the fuel burn rate and air entrainment rate.

Over the years several studies have been performed to better understand the development of combustion products within compartment fires. The first studies were performed with open fires situated under a collection hood. Beyler[2], Toner[3] and Morehart[4] showed reasonable correlation between the species levels and the GER. Beyler used a variety of fuels while Morehart and Toner used natural gas. Beyler and Morehart measured combustion product gas temperatures in the range of 470 to 600K[5], while Toner measured gas temperatures ranging between 500 and 870K[5]. Based on known HC chemical kinetics, at these temperatures, see Pitts[5], the levels of O_2, CO, and CO_2 are expected, and indeed were dependent on gas temperature as well as the GER.

Tewarson[6], Gottuk[7], and Bryner, Johnsson, and Pitts[8] performed studies in scaled compartments. The study performed by Tewarson consisted of using wood cribs suspended within the compartment with ventilation provided via full-width windows located at either end of the compartment. The air entrainment rate into the compartment was considered to be ventilation limited, i.e. $\dot{m}_{air} = KA\sqrt{H}$, where K is the enclosure constant typically take to be 0.5 kg/s-m$^{5/2}$, A is the opening area [m^2], and H is the height of the opening [m][9]. It should be mentioned that calculating the air entrainment rate using the ventilation limit can produce significant errors in the data.

In Gottuk's experiments air was entrained into the compartment through an inlet duct located at the base of the compartment and exhaust gases were vented through an opening in the upper portion of the compartment. With this test setup Gottuk simulated an ideal two-layer system, in which the actual mass flow rate into and out of the compartment could be measured and calculated directly. Burning, *n*-hexane, PMMA, spruce, and polyurethane, Gottuk found similar correlations between the combustion species and the GER within the compartment, as were found in the hood experiments.

A third reduced scale compartment study was performed by Bryner, Johnsson, and Pitts[8]on a 2/5-scaled ISO standard compartment. Natural gas was supplied from a burner placed in the center of the compartment floor. The concentrations of O_2 and combustion products measured within the compartment were non-uniform, especially between the front and the rear of the compartment, where high CO levels were measured in the front and high O_2 levels were measured in the rear. Therefore, Bryner, Johnsson, and Pitts stipulated that the concentrations within the compartment could not be correlated to a single GER for the compartment, instead local GER's would be required. No attempt was made to correlate the species yields to the GER. Bryner, Johnsson, and Pitts attributed the non-uniformity of the concentrations within the compartment to the presence of a door in their compartment, which was not present in the previous studies of Tewarson[6] and Gottuk.[7] Also, the compartment clearly presented a different reactor geometry than in the hood experiments of Beyler[2], Morehart[4], and Toner[3]. There is no doubt that the reacting flowfield inside the compartment is different in the presence of a door compared with the, purposeful yet artificial, separated vent system of Gottuk[7]. The fluid dynamics may have been also altered due to the use of a gaseous fuel jet instead of a vaporizing liquid or solid.

In the present paper results of a study of the correlation between the species levels from a fire in a fully featured and scaled compartment are reported. The final objective of the effort is to develop correlations between the species levels that are transported to remote locations away from the fire origin and an appropriate equivalence ratio, which is based on basic quantities like fuel and oxidizer flow rates and system geometrical factors.

EXPERIMENTAL METHODS

Facility

Experiments were performed in a half-scaled ISO 9705 standard compartment shown in Figure 1. The compartment dimensions are 1.22m wide by 1.83m deep by 1.22m high. The compartment was lined with 25.4mm thick Fire Master fiberboard. The wall thickness was scaled based on heat transfer similarity. The door dimensions were scaled based on dynamic flow similarity (ventilation and residence time parameters) to insure that the velocities and residence times of the gases within the compartment were scaled appropriately as well.

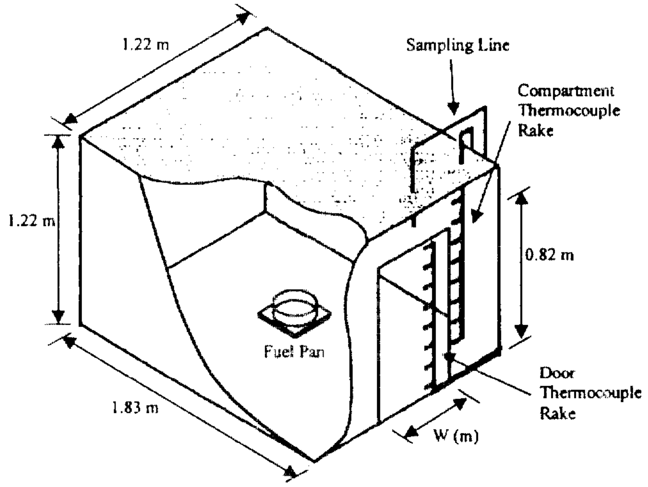

Figure 1: Half-scaled ISO 9705 Compartment with Instrumentation

Using these scaling laws the door was calculated to be 0.82m high and 0.33m wide; termed here the baseline door. To simulate a partially opened door, the width of the door was reduced to 0.165m while the height was maintained at 0.82m. In order to allow the formation of an upper layer a 0.4m deep soffit was used above the door. The fuel source was *n*-hexane placed in a pan situated in the center of the compartment for all tests. The hexane fires varied in size ranging from 65 kW to 900 kW.

The compartment was located under a fume hood in a manner ensuring the collection of all exhaust gases from the compartment upper layer. The compartment door was directly under the center of the 1.5m by 1.5m fume hood which has an exhaust fan capacity of 2.38

m^3/sec. A special gas sampling probe was constructed which enabled the measurement of local species concentrations and gas temperature simultaneously. This was accomplished using an aspirated type K thermocouple inside the tip of the sampling probe. The concentrations of product species, carbon monoxide (CO), carbon dioxide (CO_2), and unburned hydrocarbons (UHC, measured as equivalent C_2H_4), were measured along with the concentration of oxygen (O_2). The sampling probe was located 0.10m down from the compartment ceiling and at 8 different ceiling locations for the compartment upper layer mapping and at a single location for the remainder of the tests.

The mass flow rates through the door were calculated using the temperature profile method discussed by Janssens and Tran[10]. The temperature profiles were determined by using two racks of aspirated type K thermocouples. Each rack containing 8 thermocouples that were evenly spaced 0.10m apart. The racks were located in the doorway and front left corner of the compartment as shown in Figure 1.

EXPERIMENTAL PARAMETERS

The experimental parameters examined in this investigation were the fire size and door width, while the analyzed parameters were the species concentrations and the global equivalence ratio (GER). The GER for the compartment was varied by using different size n-hexane pools and by changing the door width. The narrow door limits the airflow into the compartment. This has two, potentially counteracting, effects on the fire dynamics inside the compartment. First, it limits the amount of oxygen available. Secondly, due to the lower entrained flow rate the residence time of the reacting flow increases. The importance of these effects is discussed later. Two basic definitions used later in the paper are provided below.

Global Equivalence Ratio

The amount of oxygen available to the fire relative to the fuel evaporation/supply rate determines whether a fire is fuel or oxygen limited. In the fuel limited (well-ventilated) case the fire has sufficient amount of air to burn all of the fuel produced, while in an oxygen limited (under-ventilated) case the fire has insufficient amounts of air to burn all of the fuel. The global equivalence ratio, ϕ, for the compartment quantifies whether a fire is well- or under-ventilated. The GER can be calculated by using:

$$\phi_{comp} = \frac{\left(\frac{\dot{m}_{fuel}}{\dot{m}_{air}}\right)}{\left(\frac{\dot{m}_{fuel}}{\dot{m}_{air}}\right)_{stoichiometric}} . \qquad (1)$$

A fire is considered well-ventilated, under-ventilated, or stoichiometric for $\phi<1.0$, $\phi > 1.0$, and $\phi = 1.0$ respectively.

Residence Time

The global residence time was defined, as the amount of time a unit volume of gas remains within the compartment, it is calculated using:

$$= \frac{V_{UL}}{V(T_{UL}/T_{am})} \quad (2)$$

Where,

global residence time of the gases within the compartment (s),
is the volume of the upper layer, the calculation of the upper layer volume is explained below,
volumetric flow rate of entrained air (m^3/sec),
gas temperature in the upper layer (K), and
ambient gas temperature assumed to be 293K.

In the present work, it was visually observed that during the fully developed compartment fires a single layer fire existed as opposed to a two-layer system, which is typically assumed for fires of this nature. A still photograph for one of the fires used is shown in

Figure 2: Compartment fire with baseline door configuration, the flames within the compartment extend to the floor.

The air was entrained into the compartment via an 'air tunnel.' The 'air tunnel' dimensions can be quantified as the width of the door with a height equal to the upper layer interface height (~0.35m) and extending back to the fuel pan (~0.915m). The volume of the upper layer was therefore assumed to be the full volume of the compartment minus the volume of the tunnel.

The following results represent a total of 27 tests of which 14 were performed with the baseline door width (0.33m) and 13 were performed with the narrow door width (0.165m). The *n*-hexane pool diameters varied between 0.11m and 0.28m, providing a range of GER's between 0.5 and 3.5. For each test configuration a minimum of two tests were performed. The concentrations shown represent an average over the quasi-steady-state periods of the developed fire.

The quasi-steady period was determined by examining the time traces of the air entrainment rate, fuel mass, fuel mass loss rate, GER and CO concentrations for each test. The first step for determining the quasi-steady-state period was to examine the combined time trace of the air entrainment rate, fuel mass, and fuel mass loss rate versus time. In most instances there exists a time interval for which the fuel mass loss rate and air entrainment rate are approximately constant. Examining the GER and CO concentrations versus time for the same time period, it was seen that this period also includes the CO build-up time within the compartment. The build-up time corresponds to the time required for the different species concentrations to reach a steady-state. The build-up time is a function of the transport time (on the order of 0.5 to 1 second) from the fire source to the upper layer and the mixing time within the upper layer. Both times are directly related to the fire and ventilation size. Due to the build-up period, the time interval defining the quasi-steady-state period is shifted so to include only the steady-state species concentrations.

RESULTS

Before embarking on the parametric study of the species concentrations as a function of the fire parameters, the characteristics of the upper layer inside the compartment were determined. Mapping of the species concentrations in the upper layer was performed by sampling gases at eight (8) separate locations within the compartment. The concentrations map is shown in Figure 3.

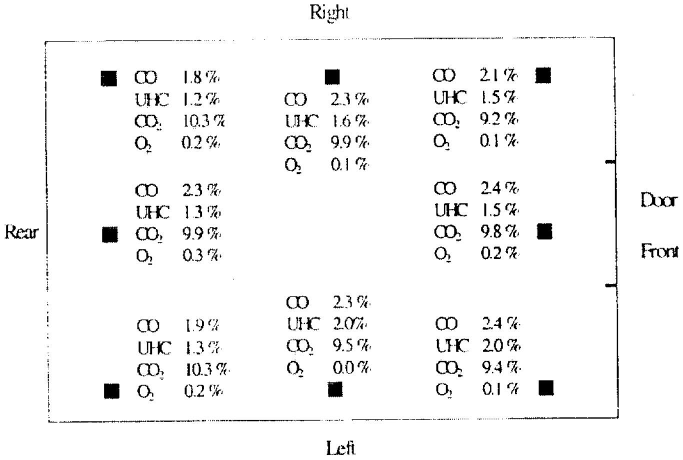

Figure 3: Wet Concentrations of CO, CO_2, O_2, and UHC in the upper layer; GER = 1.7, 576 kW fire.

Uniform concentrations, within 5-10%, for all species are seen inside the compartment. Therefore, the gases could be sampled from only one location and be representative of the entire upper layer. The sampling probe was therefore located 0.10m below the compartment ceiling and 0.20m back from the front wall. This location was chosen since (1) it guaranteed that the gases would be sampled from the upper layer and not from the upward rising gases produced by the fire plume, and (2) these are the gases exiting the compartment and transported to remote locations.

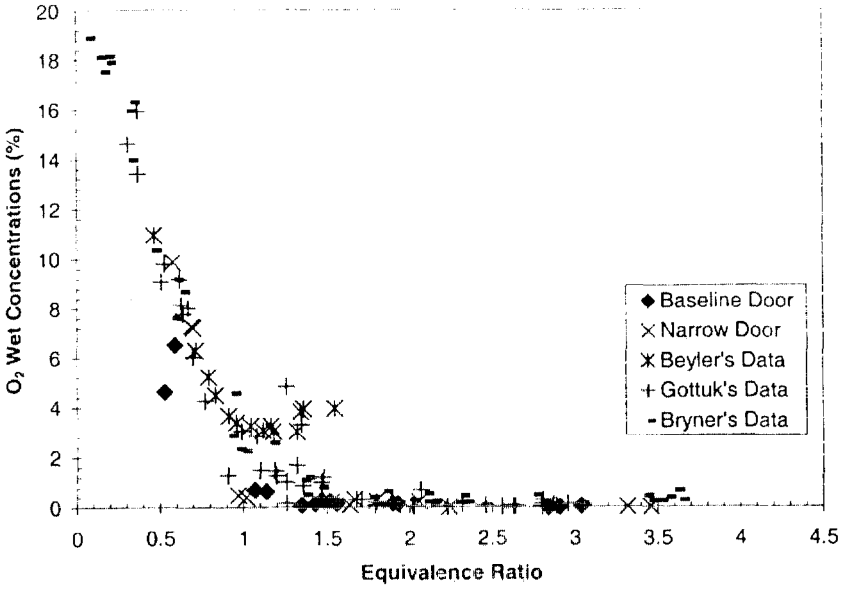

Figure 4: O_2 wet concentration versus the global equivalence ratio and door width.

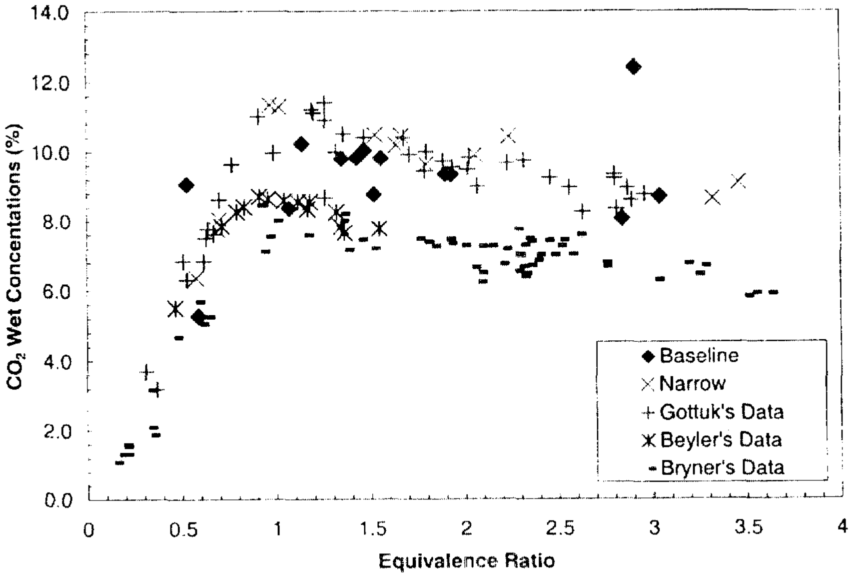

Figure 5: CO_2 wet concentration versus the global equivalence ratio and door width.

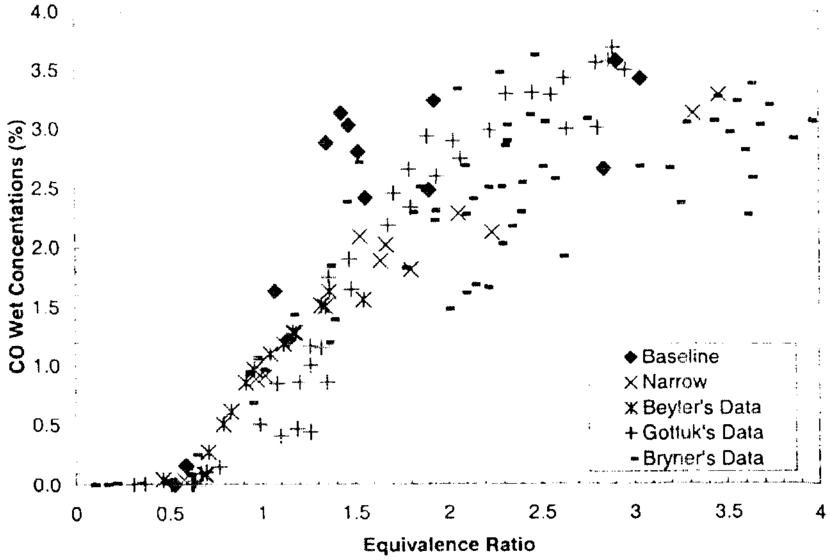

Figure 6: CO wet concentration versus the global equivalence ratio and door width.

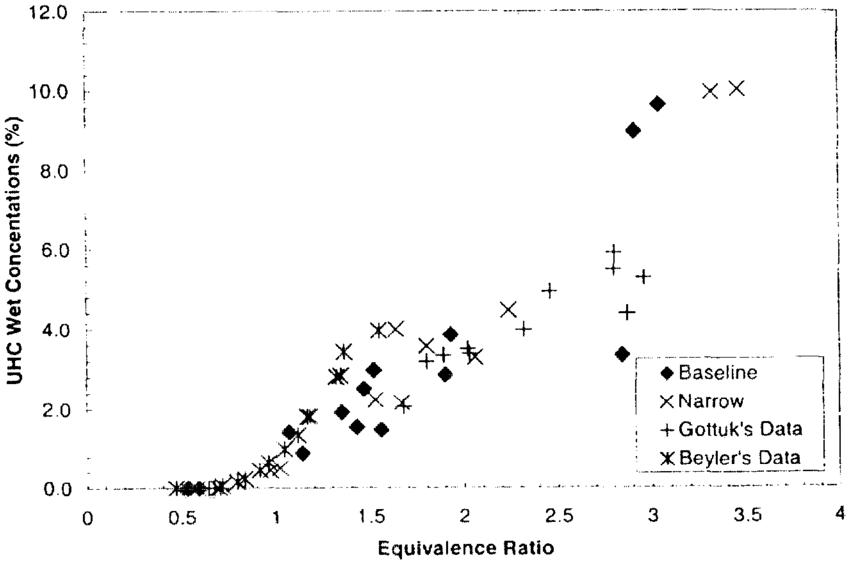

Figure 7: UHC wet concentration versus the global equivalence ratio and door width.

The concentrations of O_2, CO_2, CO, and UHC for the baseline and narrow doors as a function of equivalence ratio are shown in Figure 4 through Figure 7. Present data was compared with data available from Beyler[2], Gottuk[7], and Bryner, Johnsson, and Pitts[8]. Three points should be noted about the data taken from Bryner, Johnsson, and Pitts:

(1) Only the data taken at the front of the compartment is included. This location was chosen since this was the same location at which measurements were taken in this study.

(2) The data was digitized from the figures provided and there is an associated error of ±1.0% for the reported GER values and reported concentrations.

(3) The data is not for *n*-hexane, but for natural gas, CH_4.

DISCUSSION

During post flashover fires it is expected that the air entrainment rate through the door into the compartment will be slightly less than the ventilation limited, which is the theoretically maximum amount of air that can be entrained into the compartment and in actual situations is not reached. The ventilation limited air entrainment rates for the narrow and baseline door are 0.061 kg/s and 0.123 kg/s respectively. The air entrainment rates into the compartment, as obtained from the thermocouple measurements, for the narrow and baseline door are shown in Figure 8 versus the ideal fire size. The ventilation limit for each door width is also shown. The linear profiles observed are expected since the air entrainment rate is only a function of the size of the vent opening and not the fire size. The average calculated values for the narrow and baseline door was 0.056 kg/s and 0.109 kg/s respectively, differing by only 8.2% and 11.4% respectively from the theoretical maximum.

The GER is a function of the air entrainment rates into the compartment. Since there is no direct method for measuring the flow rates into and out of the compartment available, it is necessary to determine if the calculated GER's were accurate. For this purpose the present study must rely on some test based observations/results of previous works. In previous studies[2][7][8] it was shown that at a GER of 1.0 the oxygen concentration dropped approximately to zero. The O_2 concentration as a function of the global equivalence ratio for the present study is shown in Figure 4. The concentrations of O_2, seen in Figure 4 follow a similar trend for narrow and baseline door widths and agree well with the data from the previous studies. In all of the studies, except Beyler, the oxygen concentration does in fact decrease to approximately zero at equivalence ratios of 1.0. Oxygen concentrations in Beyler's[2] study did not approach zero at equivalence ratios greater than 1.0, which can be attributed to the lower gas temperatures in the hood experiments leading to lower reaction rates.[5] The agreement between the results indicates that the calculated GER is valid. As a consequence the method of Janssens and Tran[10] for determining the mass flow rates of air and combustible products into and out of the compartment was accepted as valid for the present configuration.

Confidence in the air entrainment rates and the GER allows the examination of the other species, CO_2, CO, and UHC as a function of the GER. The CO_2 concentrations, shown in Figure 5, indicate separate trends between the two door geometries and the other studies quoted. The CO_2 concentrations of Beyler[2] and Bryner, Johnsson, and Pitts[8] reach a maximum of approximately 8.5% CO_2 at an equivalence ratio of 1.0, while both the current study and Gottuks indicate levels as high as 11% CO_2. The lower CO_2 concentrations seen in Beyler's data can be attributed to the lower gas temperatures in the hood experiments, 470K-600K, compared with upper layer temperature of 875K-1100K in the present study. At the temperatures of Beyler's study CO to CO_2 conversion is frozen[5], at the levels generated in the fire plume below the hood. The lower CO_2 concentrations in the tests of Bry, Johnsson, and Pitts[8] were attributed to fewer carbon atoms present in natural gas (CH_4) opposed to *n*-hexane (C_6H_{14}). In all of the cases however at equivalence ratios greater than 1.0 the measured CO_2 concentrations decreased with increasing equivalence ratio. This is simply explained by the limited oxygen availability for global equivalence ratios greater than 1.0.

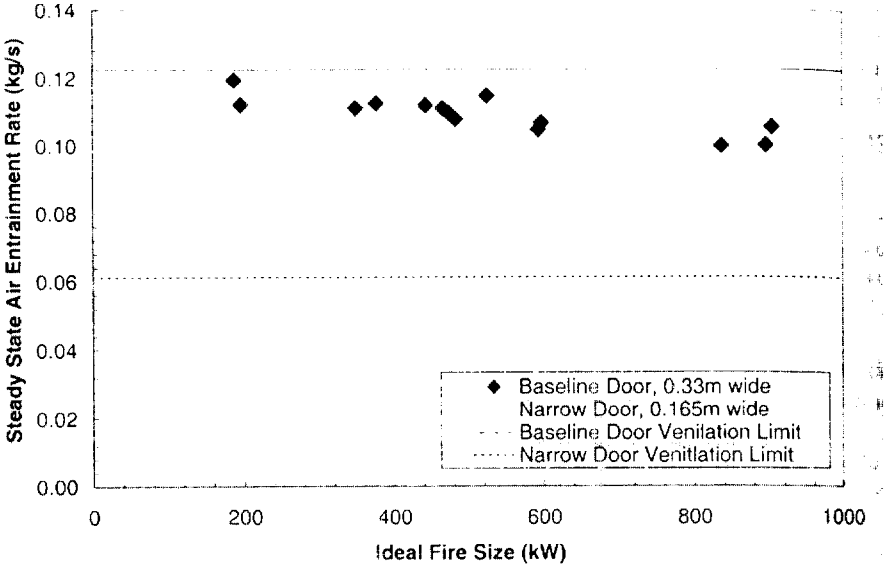

Figure 8: Steady state air entrainment verses fire size and door width.

The narrow door configuration in the current study yields the highest levels of CO_2, especially around an equivalence ratio of 1.0. Since the conversion of CO to CO_2 requires the availability of oxygen, the controlling parameter in this conversion is the present study appears to be the residence time. The residence time of the gases within the compartment was calculated to be 9.3 seconds for the baseline door and 19.5 seconds for the narrow door.

The CO concentrations are shown in Figure 6. The levels of CO are approximately zero below equivalence ratios of 0.75 and begin to increase for higher equivalence ratios. This same trend is seen in the other studies. In all three studies the CO concentration seems to plateau at equivalence ratios greater than 1.5. Significant scatter is seen however at higher equivalence ratios in the data of all of the studies quoted here.

As was seen with the CO_2 concentrations, the two door geometries of the current study indicate different concentration levels of CO. Higher levels of CO, 3.0%, are seen for the baseline door while for the same equivalence ratio, 1.5, the narrow door CO levels are only 2.0%. The UHC's levels measured in the present study compare well with data from Beyler[2] and Gottuk[7], and are shown in Figure 7. Toner[3] and Morehart[4] both reported that the UHC's increased linearly with the global equivalence ratio, a linear increase is also observed in the current study. No difference between the two door geometries is observed in the current study for UHC levels. These trends are expected since the shorter residence time within the baseline compartment provides less time for the CO to be oxidized to CO_2 with the available oxygen, however since UHC's will react with free radicals more readily than CO, consequently more CO results and less UHC.

SUMMARY

The objective of this study was to determine if the species levels within a fully scaled compartment with realistic features could be correlated to the global equivalence ratio for a condensed phase fuel. The data included two door scenarios, fully and partially open, simulated by varying the door width. The calculated air entrainment rates were shown to deviate by no more than 11.4% from the ventilation limit for both door geometries. The global equivalence ratio, which is a function of the air entrainment rate, was shown to be valid for the present geometry by comparing oxygen concentrations from the present study to those of previous studies. The current findings have shown that the combustion products and reactants correlated well over a wide range of equivalence ratios, 0.5 to 3.5 for both door geometries. The present data follows the same trends as data from previous work performed in hood experiments, special test apparatus, and reduced scale enclosures, however it has been shown that the residence time for the gases within the compartment impacts the levels of CO_2 and CO. No effect of the residence time is seen on the unburned hydrocarbon concentrations. The longer residence time of the gases within the compartment with the narrow door allows more time for the CO to oxidize to CO_2. Since the UHC's react more rapidly with free oxygen radicals, the levels of UHC's depend not on the residence time but on the available oxygen. Further development of the correlations for the evolution of these fire product gases in adjacent spaces is the subject of the continuation of the study reported herein.

ACKNOWLEDGEMENT

The present work was performed as part of a research grant by NIST, grant number, 60NANB7D0066. The project monitoring officer is Dr. W. M. Pitts.

REFERENCES

1. Gann, R.J., Babrauskas, V., and Peacock, R.D., "Fire Conditions for Smoke Toxicity Measurements", Fire and Materials, **18**, (May/June), pp. 193-199, 1994.

2. Beyler, C.L., "Major Species Production by Solid Fuels in a Two Layer Compartment Fire Environment," in Fire Safety Science - Proceedings of the First International Symposium, Hemisphere, Washington, D.C., 1986.

3. Toner, S. J. , E. E. Zukoski, and T. Kubota, "Entrainment, Chemistry, and Structure of Fire Plumes", National Institute of Standards and Technology, Center for Fire Research, Report NBS-GCR-87-528, 1987.

4. Morehart, J. H., E. E. Zukoski, and T. Kubota, "Species Produced in Fires Burning in Two-Layered and Homogeneous Vitiated Environments", National Institute of Standards and Technology, Center for Fire Research, Report NBS-GCR-90-585, 1990.

5. Pitts, W. M., "The Global Equivalence Ratio Concept and the Prediction of Carbon Monoxide Formation in Enclosure Fires", National Institute of Standards and Technology Monograph 179, June 1994.

6. Tewarson, A., "Some Observations on Experimental Fires in Enclosures. Part I: Cellulosic Materials", Combustion and Flame, Vol. 19, pp. 101-111, 1972.

7. Gottuk, D.T., "The Generation of Carbon Monoxide in Compartment Fires", Doctoral Dissertation, Virginia Tech, 1992.

8. Bryner, N., Johnsson, R. J., Pitts, W. M., "Carbon Monoxide Production in Compartment Fires – Reduced-Scale Enclosure Test Facility", National Institute of Standards and Technology, NISTIR 5568.

9. Walton, W.D., and Thomas, P.H., in SFPE Handbook of Fire Protection Engineering, ed. P.J. DiNenno, pp. 3-134 to 3-147, National Fire Protection Association Press, Quincy, MA, 1995.

10. Janssens, M. and Tran, H.C., "Data Reduction of Room Tests for Zone Model Validation", Journal of Fires Sciences, Vol. 10, Nov./Dec., pp. 529-555, 1992.