

EFFECTS OF VENTILATION ON MATERIAL PROPERTIES

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INTRODUCTION

Vast majorities of fire deaths occur in residences because of flashover in buildings. NIST has taken initiative to reduce and eliminate these types of flashover conditions by limiting fire growth and spread by material modifications, early detection, improved active fire suppression/ extinguishment agents and systems and modeling of fire growth and spread. The modeling of fire growth and spread is being pursued such that gas temperature and concentrations of smoke and toxic compounds released in building fires could be predicted for enhancing fire safety of occupants.

For the development and refinement of model(s) for fire growth and spread in buildings, it is necessary to have an understanding of the ventilation-controlled fire behaviors. Studies on this subject have been performed in the test set ups such as the "Hood", "Enclosure", "Reduced-Scale Enclosure, RSE (ISO 9705)" and the "Flammability Apparatus" (ASTM E2058) by Beyler, Zukoski *et al*, Pitts, Gottuk *et al*, Fleischmann and Parkes, Peatross and Beyler, and Tewarson *et al* [1,2,3,4,5,6,7,8,9,10]. These studies have provided: 1) correlations of the material property data for the well-ventilated and ventilation-controlled fires with the equivalence ratio, Φ , defined as the *Global Equivalence Ratio (GER)* concept, and 2) definitions of fuel-lean well-ventilated combustion ($\Phi < 1.0$), fuel-rich ventilation-controlled combustion ($1.0 \leq \Phi < 3.5$), and highly fuel-rich ventilation-controlled combustion¹ ($\Phi \geq 3.5$). Consequently, it is now possible to introduce a *ventilation correction factor (X)*, so that commonly reported well-ventilated material property data [8,11] can be used for modeling of ventilation-controlled building fires.

In the **GER** concept, Φ is defined as the ratio of the mass flow rate of the fuel (\dot{m}_f) to the mass flow rate of oxygen (\dot{m}_o), or normal air (\dot{m}_a) into the combustion zone times the mass oxygen-to-fuel or air-to-fuel stoichiometric ratio (s_o or s_a respectively):

$$\Phi = s_o \dot{m}_f / \dot{m}_o = s_a \dot{m}_f / \dot{m}_a \quad (1)$$

It is important to account for the O_2 concentration in the calculation of Φ as demonstrated in Fig. 1, where

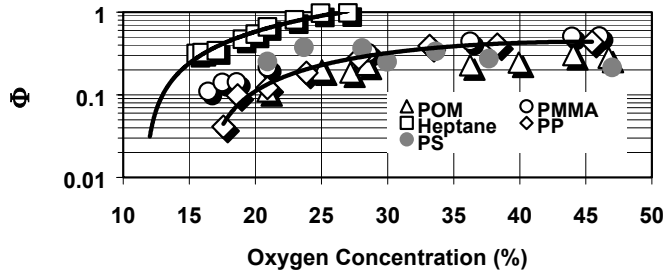


Figure 1. Equivalence ratio versus oxygen concentration in air entering the combustion zone. Data were measured in the ASTM E2058 apparatus [12].

data are taken from Ref. 12. These data were measured in the ASTM E2058 apparatus at a constant airflow rate of 1.68 g/s with variable O_2 concentration. Φ values decrease with O_2 concentration even though flow rate is constant. Experimental data for the gas temperature and concentrations of CO_2 , CO and smoke follow the Φ values [12]. Effects of reduced O_2 concentration on the reduction of \dot{m}_f values for the ventilation-controlled fires have been reported [6].

Product Concentration

The concentration of a product generated in a ventilation-controlled fire is expressed as:

$$C_{j,v} = (M_a / M_j) [\dot{m}_j / (\dot{m}_f + \dot{m}_a)] \quad (2)$$

where $C_{j,v}$ is the concentration of product j , M_a and M_j are the molecular weights of air and the product respectively and \dot{m}_j is the mass flow rate of the product, expressed as $\dot{m}_j = y_j \dot{m}_f$, where y_j is the yield of the product. From Eqs. 1 and 2:

$$C_{j,v} = [(M_a / M_j) X_{j,v} \{y_{j,\infty} / (s_a + \Phi)\}] \Phi \quad (3)$$

¹ Under highly fuel-rich ventilation-controlled combustion, flame is generally invisible and the combustion is erroneously categorized as non-flaming combustion or flame extinction.

where $y_{j,\infty}$ is the yield for well-ventilated combustion and the *ventilation correction factor for products*, $X_{j,v}$ ² is expressed as [10]:

$$X_{j,v} = 1 + [\alpha / \exp(\beta\Phi)]^{-\xi} \quad (4)$$

where α , β , and ξ are coefficients associated with the material property and generic nature of the material. The values of these coefficients have been reported in the literature [7,8,9,10]. As indicated by Eq. 3, concentration of a product in the ventilation-controlled fires has a complex dependency on: 1) the generic nature of the fuel through M_j , $y_{j,\infty}$, s , ρ_j , α , β , ξ , and heat of gasification and surface reradiation loss (through \dot{m}_f), 2) flame heat flux and heat flux from the hot walls and ceiling and heat losses (through \dot{m}_f) and 3) oxygen or air mass flow rate (through Φ).

Experimental Data

The experimental data from various studies on the ventilation-controlled fires in the "Hood" and "RSE (ISO 9705)" test set-ups are summarized in Refs. 3 and 4 and in the ASTM E2058 apparatus in Refs. 8 and 10. The product concentration data from these studies are plotted in Figs. 2 to 8. Concentrations of products in Figs. 2 to 4, 7, and 8 for gases and liquids are measured [3,4] and for solids they are calculated from Eq.3, using data measured in the ASTM E2058 apparatus [9,10]. There is a reasonable

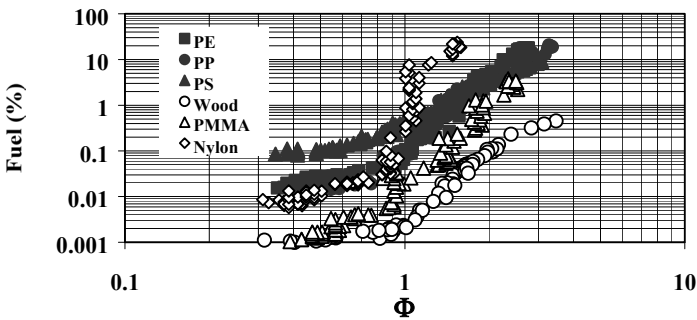


Figure 2. Unburned fuel concentration versus the equivalence ratio. Hydrocarbon data measured in the ASTM E2058 apparatus [10] were used for the estimations.

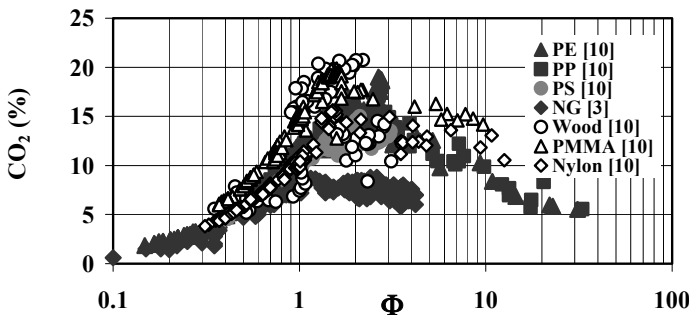


Figure 3. CO₂ concentration versus the equivalence ratio. Data were measured in the RSE for natural gas [3] and calculated from the data measured in the ASTM E2058 apparatus for solids [10].

agreement between the experimental and calculated concentration values in these figures. However, both the experimental and calculated concentrations do not collapse into a single curve as expected from Eq. 3, suggesting that: 1) $X_{j,v}$ is a strong function of the generic nature of the fuel, 2) concentration of reactive O₂ in the combustion zone affects the Φ values calculated from normal air flow rate, 3) some critical parameters are missing from Eq.3, and 4) Eq.3 is not set up properly.

Unburned Fuel Concentration (Fig 2)³

There is a sudden increase in the unburned fuel concentration as fire becomes ventilation-controlled ($\Phi \geq 1$). Fuels with lower air requirements (PMMA and wood with s values of 8.3 and 5.7 g/g respectively) have smaller amounts of unburned fuel compared to fuels with higher air requirements (nylon, PP, PE, and PS with s values of 11.1, 14.7, 14.7, and 13.2 respectively). The unburned fuel concentration remains less than about 22%, until the beginning of the highly fuel-rich ventilation-controlled combustion ($\Phi \geq 3.5$).

CO₂ Concentration (Fig 3)

CO₂ concentration increases with Φ and reaches its maximum for Φ values between

² $X_{j,v}$ is the ratio of a material property for the ventilation-controlled combustion to the material property for the well-ventilated combustion.

³ The unburned fuel concentration was estimated from the hydrocarbon data reported in Refs. 8 and 10, assuming M_j value in Eq. 3 to be similar to the molecular weight of the original fuel. For $\Phi \geq 3$, hydrocarbon concentrations could not be measured as they were beyond the range of the analyzer used in the ASTM E2058 apparatus at the time of the study.

about 1.5 to 3.5. The CO₂ concentration decreases: 1) in the highly fuel-rich ventilation-controlled combustion region ($\Phi \geq 3.5$), and 2) decrease in the s value (PMMA and wood) and molecular weight of the fuel (M_f) (natural gas versus PE, PP, and PS).

The CO₂ concentration is an indicator of the magnitude of the heat release rate, combustion efficiency, and gas temperature [8,9,10]. Expression for the calculation of the gas temperature can be set up similar to Eq. 3, using data for the convective heat of combustion and heat capacity of air, which are available in the literature [8,9,10]. Correlations between the ventilation correction factor for heat, $X_{h,v}$ and Φ are described in Ref. 10.

CO Concentration (Fig 4)

CO concentration increases with Φ , similar to CO₂ concentration, reaching its maximum value for the highly fuel-rich ventilation-controlled combustion ($\Phi \geq 3.5$). For similar Φ values, CO concentration is

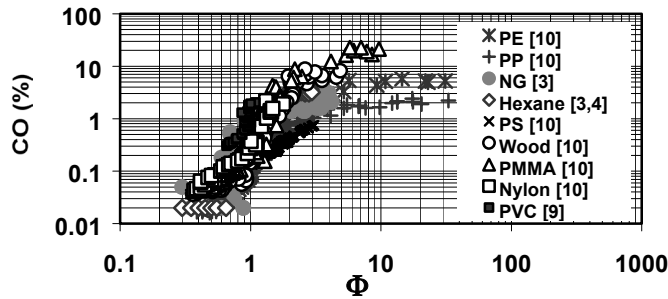


Figure 4. CO concentration versus the equivalence ratio for natural gas (NG) and hexane measured in the RSE test set up [3, 4] and for solids calculated from the data measured in the ASTM E2058 apparatus [9,10].

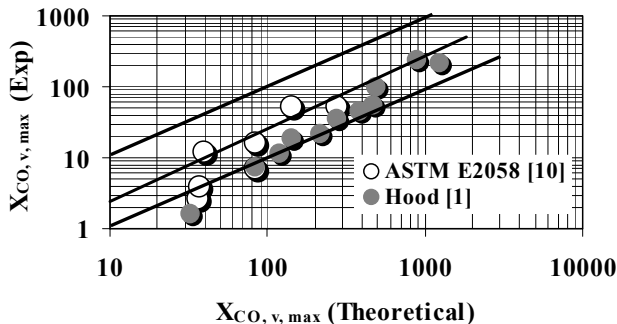


Figure 5. Experimental versus the theoretical ventilation correction factor. Data are taken from Refs. 1 and 10.

chemical bonds, however, some of the compositions and bonds may be more sensitive to changes in the ventilation than the others.

High CO concentrations observed in the "Hood" and "RSE, ISO 9705" test set-ups in the very fuel-rich ventilation-controlled fires have been suggested to be due to formation of CO by different mechanisms [3,13,15]: 1) quenching of the turbulent fire plume upon entering a rich upper layer ("Hood" test set-up); 2) mixing of oxygen directly into a rich, high-temperature upper layer with subsequent

higher for fuels with lower s values (22.6 % for PMMA, and 8.8 % for wood). High CO concentrations have also been measured in other studies, for example as high as 8% in a very heavy wood loaded enclosure fire test and 14% in the tests in RSE with walls and ceiling lined with wood [13].

The amount of CO released in the combustion of a fuel depends on the stoichiometric yield⁴ of CO, Ψ_{CO} , [8]:

$$\Psi_{CO} = 28 n_c / M_f$$

where n_c represents the number of carbon atoms in the fuel, 28 is the molecular weight of CO and M_f is the molecular weight of the fuel. This dependency is shown in Fig. 5, where experimental value of $y_{CO,v,max}/y_{CO,\infty}$ ($X_{CO,v,max, Exp}$) is plotted against $\Psi_{CO}/y_{CO,\infty}$ ($X_{CO,v,max, theoretical}$). Thus the experimental $y_{CO,v}$ values follow the Ψ_{CO} values, being lower in the "Hood" tests [1] compared to the ASTM E2058 apparatus [10] (about 1/10th and 1/5th the Ψ_{CO} values respectively).

The Ψ_{CO} value of a fuel is related to its s value as shown in Fig. 6, where data are taken from Refs. 8 and 14. For fuels with C, H, O, and N atoms, Ψ_{CO} values increase with s values up to about 14, due to increase in the number of carbon atoms relative to other atoms in the fuel. For fuels with C, H, and Cl atoms, Ψ_{CO} values decrease with increase in the s value, possibly due to increase in the linear and non-aromatic nature of the fuel. CO concentration is expected to follow these trends in the chemical composition and nature of the

⁴ Ψ_{CO} is the yield of CO for the maximum possible conversion of the fuel monomer of the material to CO.

reaction; 3) pyrolysis of wood in the high-temperature, vitiated environments, and 4) approach to full-equilibrium combustion product concentrations in a rich, high-temperature upper layer.

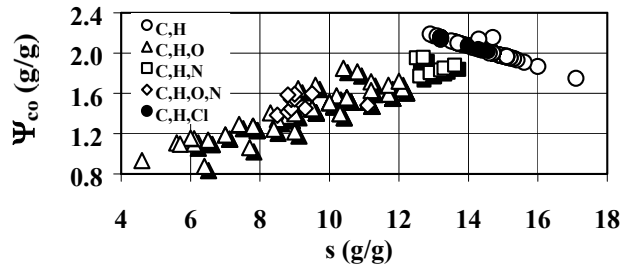


Figure 6. Stoichiometric yield of CO versus mass air-to-fuel stoichiometric ratio. Data are taken from Refs. 8 and 14.

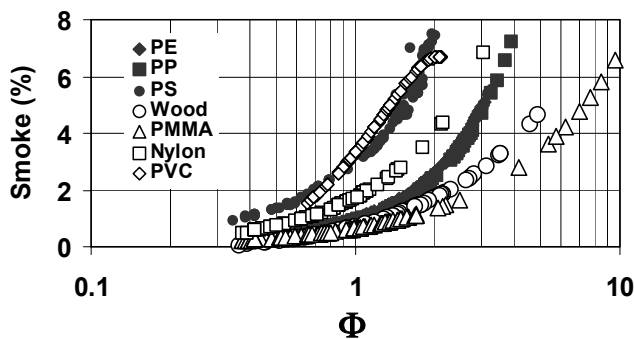


Figure 7. Smoke concentration versus the equivalence ratio. Concentration is calculated from Eq. 3, using data measured in the ASTM E2058 apparatus [9,10]. Smoke is assumed to be carbon and $\rho_a/\rho_{\text{smoke}} = 2.333$ in Eq. 3.

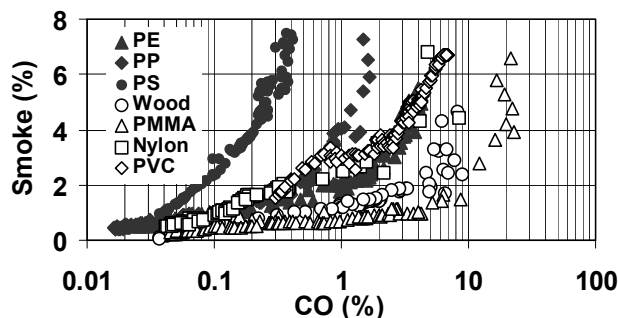


Figure 8. Relationship between smoke and CO concentrations for ventilation-controlled fires. Concentrations are calculated from Eq. 3, using data measured in the ASTM E2058 apparatus [9,10].

Ψ_j , and combustion efficiency and its radiative and convective components);

In the ASTM E2058 apparatus, high CO concentrations were observed in those experiments where normal airflow was maintained constant and external heat flux was increased and external heat flux was maintained constant and normal airflow rate was decreased [8,9,10]. All the reactions in the hot fuel vapor-product-air mixture occurred in the quartz tube in the lower section of the apparatus. The reactions were quenched as soon the mixture encountered cold ambient air, about 20 times its volume, at the top of the quartz tube.

Thus, the CO formation mechanism in the ASTM E2058 apparatus is probably closer to that in the "Hood" test set-up, except for the differences in the quenching of reactions by flowing cold normal air and rich upper layer respectively.

Smoke Concentration (Figs 7 and 8)

Smoke concentration increases with Φ and is higher for fuels with C, H atoms (PS, PE, PP) than for fuels with C, H, O atoms (PMMA and wood), similar to the trend for the unburned fuel. It is higher for the fuel with aromatic C, H atoms (PS) than for fuels with aliphatic C, H atoms (PE and PP) (this trend is expected from their smoke points). The dependency of smoke concentration on the chemical composition and nature of chemical bonds of fuels is similar to that for CO concentration.

For each generic fuel, there is a distinct change in the slope of the line at a specific Φ value or CO concentration. This distinct change in the slope is probably associated with the change in the smoke characteristics from predominantly carbon-rich to predominantly carbon-lean. Such a change is expected to have a major impact on the nature of toxic compounds and visibility.

Limitation, Deficiencies and Specific Needs to Improve the GER Concept

1. Definition of fire growth and spread using a better definition of \dot{m}_f for the ventilation-controlled fires;
2. Better definition of Φ using reduced oxygen concentration (a common feature of the ventilation-controlled fires);
3. Generalized relationship between the ventilation correction factor for products, $X_{j,v}$ and heat $X_{h,v}$ and the generic nature of the fuels (possibly using the smoke point, s , and

4. Effects of O_2 concentrations on the $X_{j,v}$ and $X_{h,i}$ values by performing ventilation-controlled combustion experiments with \dot{m}_o , \dot{m}_f and fuel types as variables;
5. Examination of the smoke characteristics for highly fuel-rich ventilation controlled combustion conditions utilizing techniques such as a particulate smoke analyzer and FTIR;
6. Further exploration of mechanisms for CO formation versus type of ventilation-controlled fire test set-ups;
7. Rigorous validation of the relationships for the product concentrations (such as Eq. 3) and gas temperature through tests for the ventilation-controlled fires.
8. Examination of the ignition behavior of fuels for the ventilation-controlled fires by establishing relationships between Φ and the ignition temperature (critical heat flux) and ignition delay parameter (defined as the thermal response parameter consisting of ignition temperature, density, thermal conductivity, and heat capacity of the fuel and a parameter⁵ associated with the changes in the chemistry due to changes in the chemical composition of the fuel-vapor-air mixture). Thermal response parameter is expected to increase with Φ due to changes in the parameter associated with the changes in the chemistry.

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⁵ The parameter is affected strongly by the presence of higher amounts of halogen atoms in the fuel and changes in the oxygen concentration of the environment.