

Experimental approach to estimate species concentrations in a compartment fire

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ABSTRACT

An approach for estimating species concentration during a fire in a well-stirred compartment is investigated. A semi-empirical model based on oxygen concentration is used. It gives an estimate of the concentrations of carbon monoxide, carbon dioxide, hydrogen and hydrocarbons with a carbon chain length lower than five. Three intervals of oxygen concentration are noticed, they correspond to sufficiently ventilated, underventilated and very underventilated fires. In order to validate this model, fire experiments are performed in a reduced-scale compartment. Species concentrations predicted by the model are in good agreement with our experimental data and with those of literature. Coefficients used for the model are obtained for heptane and dodecane fires.

KEYWORDS: compartment fires; heat release rate; species concentration; reduced-scale; fire experiments.

NOMENCLATURE

ACPH	Air Change Per Hour
D	Fire diameter (m)
f_{O_2}	Normalized oxygen yield
Fr	Froude number
g	Acceleration of gravity ($m\ s^{-2}$)
h	Fuel height in the pan (m)
k_i	Theoretical maximum mass yield of the species i
L	Characteristic length (m)
LFL	Lower Flammability Limit (% vol.)
n	Number of moles (mol)
M	Molecular weight ($g\ mol^{-1}$)
\dot{m}''	Burning rate per unit area ($kg\ m^{-2}\ s^{-1}$)
MOC	Minimum Oxygen Concentration of fuel (% vol.)
\dot{Q}	Heat release rate ($kJ\ s^{-1}$)
S	Fuel pan surface area (m^2)
t	Time (s)
T	Temperature (K)
u	Gas velocity ($m\ s^{-1}$)

Y_i	Mass yield of the species i
ΔH_c	Heat of combustion (J kg ⁻¹)
Φ	Global Equivalence Ratio (GER)

INTRODUCTION

The calculation of species concentration has often been made using Global Equivalence Ratio Φ (GER) concept, which is defined as the fuel mass flow to the air entrainment mass flow into the plume, normalized by the stoichiometric ratio of fuel to air. Beyler [1], Cetegen [2], Toner et al. [3] and Morehart et al. [4] have studied oxygen, carbon monoxide and other species yields as a function of global equivalence ratio during hood experiments. It was found that, during sufficiently ventilated fires ($\Phi < 1$), oxygen yield is maximal and unburnt gas levels are low. A very underventilated fire is a fire that can stop by lack of oxygen. The heat release rate generally presents a noisy evolution (because the fire is close to extinction) and the production of unburnt species is important. When the fire becomes underventilated, unburnt gases increase following a $1/\Phi$ law. Pitts [5] has summarized a large number of these investigations. These experiments were designed to easily determine species yields and GER thanks to the steady-state nature of the hood experiments and the use of a burner. More recently, Hu et al. [6] have considered and adapted current combustion models to study the emissions of carbon monoxide and unburnt hydrocarbon mass in a compartment fire. Their model was tested for different fire room global equivalence ratios.

Experimental studies were performed in order to determine the validation of GER concept for realistic fire compartment. In this way, Gottuk et al [7] performed investigations in an ideal two-layer zone compartment and Bryner et al. [8] and Wieczorek [9] in more realistic reduced scale rooms. Gottuk et al. [7] showed that carbon monoxide production depends on the compartment flow dynamics and on the Global Equivalence Ratio. Similar tendencies were found by Beyler [1] but with higher carbon monoxide yield and lower carbon dioxide yield due to the differences of upper layer temperatures between these two types of experiments.

However, there are significant differences between phenomena encountered with upper layer environment and during fires in a compartment. In this way, Pitts [5] has studied the application of the Global Equivalence Ratio concept to the prediction of combustion gas species during enclosures fires. He has shown that the use of GER is inappropriate at intermediate temperatures ranging between 700 and 900 K. Moreover, Gottuk et al. [10] have underlined the fact that carbon monoxide production during a compartment fire as a function of GER is dependent on temperature. Beyler [1] and Tewarson [11] have also shown that the carbon monoxide yield depends on the fuel but is correlated to the fuel type.

There are not many works in the literature dealing experimentally with species concentrations during confined and mechanically ventilated fires. In this work, an approach for estimating species concentrations during a fire in a compartment (considered as a well-stirred reactor) is carried out using oxygen concentration in a fire room. This latter is obtained using the global equivalence ratio. This approach is semi-empirical and allows the estimation of oxygen, carbon monoxide, carbon dioxide, hydrogen and total hydrocarbon concentrations. It is based on fire tests performed in a 8-cubic-meter compartment with two fuels: heptane and dodecane and during ICFMP [12] heptane fire tests. A comparison between species concentrations measured during heptane fires in the 8-cubic-meter compartment and corresponding model predictions is also made to validate this model.

EXPERIMENTAL SECTION

The experimental device consists in a 8-cubic-meter room-test scaled from a 100-cubic-meter compartment. The Froude scaling technique has been widely used in reduced scale fire experiments [13] and this technique has been adopted in this work. The compartment has therefore been scaling maintaining the Froude number ($Fr = u^2 / gL$) constant. The Reynolds number is large enough to ensure the turbulence of the flow. Walls are made of reinforced concrete. Scaling heat release rate (HRR) imposes the

preservation of the quantity \dot{Q}^2 / L^5 [14]. The powers tested are lower than 130 kW, which corresponds to a maximum HRR of 1 MW at full scale. Details on the derivation of the scaling laws can be found in [15]. Picture and scheme of the experimental setup are presented in Fig. 1.

There was a square mechanical ventilation duct, measuring 0.2 m x 0.2 m, that could provide a flow of 24 or 40 m³ h⁻¹ (Air Changes Per Hour (ACPH): 3 or 5). Inlet duct is located at the bottom of the room test at a 0.3 meter high and extraction network is located near the ceiling, at a 1.7 meter height. The acquisition time is chosen at 6 s. This reduced-scale compartment has already been used in Lassus et al. [15] for the investigation of the ventilation effects in confined and mechanically ventilated fires. Let us notice that with this experimental setup air is injected at the bottom of the compartment and the extraction duct is located at the top of the compartment, on the side opposite to the air inlet duct. For this reason, we can consider that the air injected mixes well with the flame, that is to say that the mixing is not influenced by the extraction flow. We can therefore consider this compartment as a stirred reactor.

Experiments are performed with heptane and dodecane pool fires. The stainless-steel pans are located at the center of the room test, at a height of 0.5 meter, and placed on a load cell to measure fuel consumption as a function of time. Heptane used contains 71 % of n-heptane and has a density of 0.71 kg m⁻³, a flash point of 269 K and a boiling point of 644.5 K. Dodecane used contains 99 % of n-dodecane and has a density of 0.749 kg m⁻³, a flash point of 347 K and a boiling point of 489 K. In order to avoid freeboard effects, fuel quantity is determined as a function of pan diameter with the relation $h/D = 11.5 \%$, where h represents the fuel height and D the pan diameter. Indeed, before each test, water is first poured on the pan and then fuel poured onto the water until it reached 1 mm below the pan lip. During the combustion, the location of the fuel/water interface remains fixed. Therefore, since the height of the burning fuel decreases as combustion progresses, the freeboard length increases during the experiment. However, this freeboard length increase appeared to have only a minor effect on the measured combustion rate. Arai et al. [16] studied the influence of freeboard effects on the combustion velocity. The boiling point of heptane is lower than the one of water and consequently boilover is not possible. A fire test is conducted as follows: water is poured into the pan, the determined quantity of fuel is then poured in order to fill the pan up to 1 mm below the lip. Fuel is ignited with a butane torch.

Different sizes of pan diameter (0.10, 0.15, 0.23, 0.30 and 0.40 meter) are used for varying heat release rate. In this work, we just used results of heptane and dodecane fires with pan diameters of 0.23, 0.30 and 0.40 m. Results with other pan diameters are presented in Lassus [17], they lead to sufficiently ventilated fires with low HRR values and for these reasons species production is also low. HRR is measured by means of a load cell using Babrauskas' law [18]:

$$\dot{Q}(t) = S \dot{m}(t) \Delta H_C \quad (1)$$

As oxygen consumption is difficult to use during underventilated fires because of the oxygen provided by the dilution flow, HRR is measured by mass loss. Consequently, for underventilated fires, HRR is overestimated. The flow rates of gases in the inlet duct and dilution duct is measured with hot wire system placed at the entrance of these ducts. Their sensitivities are lower than 1 %.

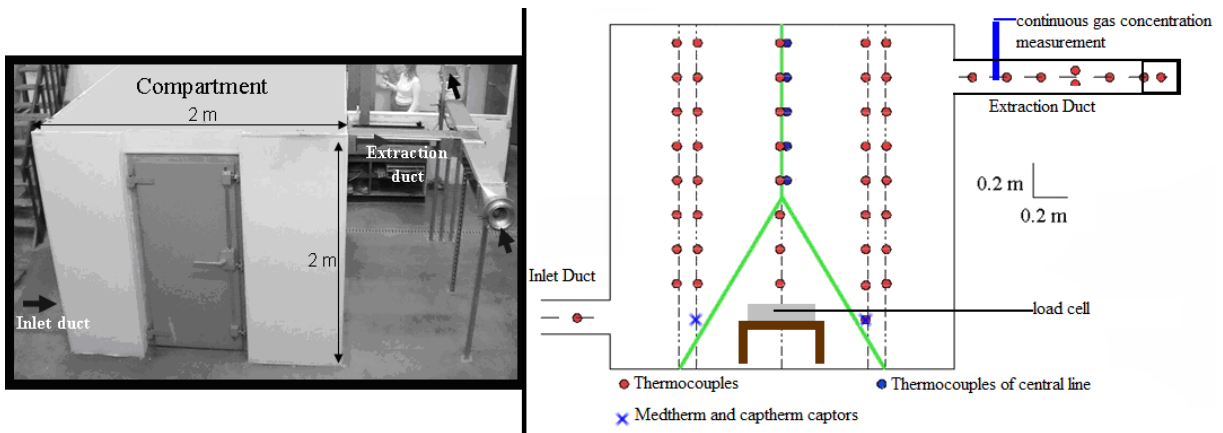


Fig. 1. Reduced scale compartment.

Oxygen, carbon dioxide and carbon monoxide concentrations are measured continuously at the entrance of the extraction duct by on-line analysis. Local measurements of oxygen, carbon dioxide, carbon monoxide, hydrogen and unburnt hydrocarbons concentrations are performed in the exhaust duct by gas chromatography (flame ionization detector and thermal conductivity detector) and mass spectrometry. Gas sampling is done using a probe. Unburnt hydrocarbons with a carbon chain length lower than or equal to four ($\leq C_4$) were identified by gas chromatography and unburnt products with a carbon chain length higher than four were identified with a mass spectrometer. All gas concentration measurements presented in this paper are performed at the entrance of the extraction duct in order to avoid dilution flow. The temperature measurements in the compartment are performed with chromel-alumel thermocouples (type K) of a 0.5 mm wire diameter; they give values with an uncertainty of ± 1.5 °C (standard NF EN 60-584).

Three fire tests for each condition are made in order to check the repeatability of the main parameters. Good agreements are found for these comparisons, which show a good repeatability of temperatures, species concentrations and HRR. The average difference of HRR between the different tests is on the order of 3.3 kW and the relative deviation between species concentration does not exceed 0.1 %.

ESTIMATION OF SPECIES CONCENTRATIONS GENERATED DURING A COMPARTMENT FIRE

A model based on oxygen concentration has been developed in order to estimate carbon dioxide and carbon monoxide concentrations as well as the whole hydrogen and total hydrocarbon concentrations. In this way, normalized oxygen yield is estimated using the global equivalence ratio. Direct calculations of oxygen concentration can also be made, providing ventilation velocities values.

Normalized yield of oxygen

The normalized yield of oxygen f_{O_2} is used to estimate oxygen concentration as a function of global equivalence ratio Φ . It is defined as the oxygen mass yield divided by the theoretical maximum mass yield of oxygen k_{O_2} for the given fuel:

$$f_{O_2} = \frac{Y_{O_2}}{k_{O_2}} \quad (2)$$

In Eq. 2, Y_{O_2} is the mass yield of oxygen and k_{O_2} is the theoretical maximum mass yield of oxygen obtained from complete reaction by:

$$k_{O_2} = \frac{n_{O_2} \cdot M_{O_2}}{n_{fuel} \cdot M_{fuel}} \quad (3)$$

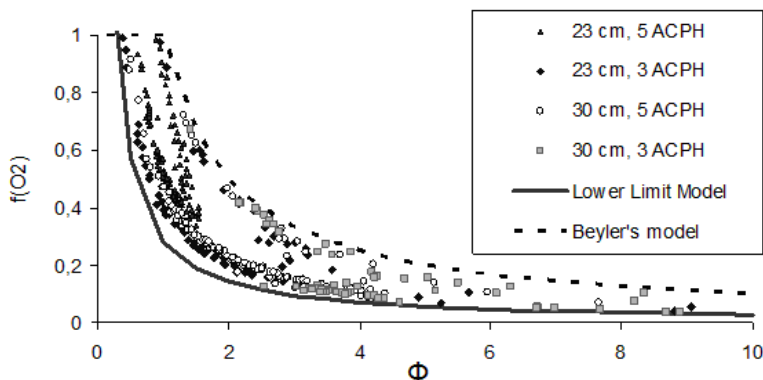


Fig. 2. Normalized oxygen yield as a function of global equivalence ratio for heptane fires at reduced scale. Comparison with Lower Limit Model and Beyer's model.

Assuming that there is no air accumulation in the compartment, the evolution of normalized oxygen yield is presented in Fig. 2 as function of the global equivalence ratio for heptane fires performed in the reduced scale room with pans of diameter of 0.23 and 0.30 meter, at 3 and 5 Air Change Per Hour (ACPH). Maximum HRR for 5 ACPH is found at 50 kW for a pan diameter of 0.23 m and at 150 kW for a pan diameter of 0.30 m. We can see in Fig. 2 that during sufficiently ventilated conditions, the normalized yield of oxygen is approximately equal to one. This shows a nearly complete reaction. It decreases with the increase of underventilated conditions. Evolutions are similar whatever the ventilation flow and the pan diameter are, which show that normalized oxygen yields are independent from the pan diameter size. For each condition applied, two curves are formed that respectively correspond to the oxygen depletion during fire and the oxygen increase at the extinction. Beyer's model is also represented for heptane in Fig. 2. It considers that normalized oxygen yield is equal to one during sufficiently ventilated fire ($\Phi < 1$) and that its evolution is $f_{O_2} = \frac{1}{\Phi}$ for $\Phi > 1$, that is to say for underventilated conditions. Comparing this method with experimental results, Beyer's model gives an upper limit of the normalized yield of oxygen during underventilated conditions. Beyer's model is presented in [1]. A model has been developed in order to obtain a lower limit of this normalized yield that is given by the equation:

$$f_{O_2} = \frac{1}{k_{O_2} \cdot \Phi} \quad (4)$$

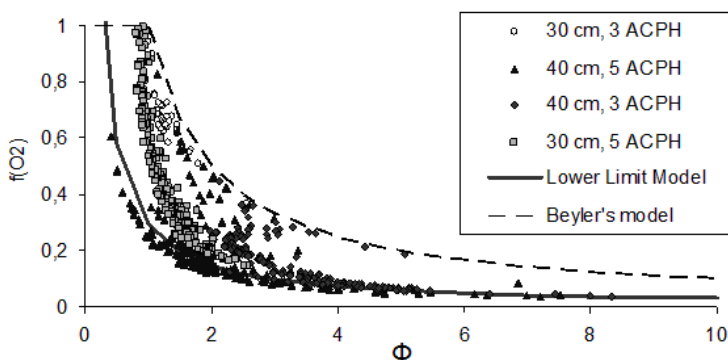


Fig. 3. Normalized oxygen yield as a function of global equivalence ratio for dodecane fires at reduced scale. Comparison with Lower Limit Model and Beyler's model.

In order to evaluate the limitation of these equations on another fuel, the evolution of normalized oxygen yield as a function of the global equivalence ratio is represented in Fig. 3 for dodecane fires performed in the reduced scale room with pans of diameter of 0.3 and 0.4 meter, at 3 and 5 ACPH. We can see from this Fig. that the normalized oxygen yield of this fuel presents the same evolution as heptane. Comparisons between calculated limits and measured values of normalized oxygen yield in the compartment show good agreement for all the initial conditions. Indeed, the relative deviation between experimental values and the closest model does not exceed 20 %. The latter are nearer of the Lower Limit Model, especially during very underventilated fires ($\Phi \gg 1$) where the relative difference between the Lower Limit Model values and experimental results is on the order of 4 % (for $\Phi > 3$). We can note that values for the case of a pan diameter of 40 cm and 5 ACPH are below the Lower Limit Model values. This case corresponds to an extreme case that can lead to fire extinction. For all the other cases, values are between Beyler's model and the Lower Limit Model.

Carbon dioxide concentration

A new approach has been developed in order to evaluate species concentration. To do so, a semi-empirical estimation of carbon dioxide concentration requires the knowledge of oxygen concentration. The Minimum Oxygen Concentration of a species i is determined using the following equation [19]:

$$MOC_i = LFL_i n_{O_2} \tag{5}$$

where LFL is the lower flammability limit of the given fuel (% vol.) and n_{O_2} is the mole number of oxygen required for a complete reaction (mol). The values of MOC for the two studied fuels are given in table 1.

Table 1. Values of coefficients a,b,c,d and of the Minimum Oxygen Concentration used in the concentration model for heptane and dodecane.

	MOC (% vol.)	$a = \frac{n_{CO_2}}{n_{O_2}}$	b	c	d
Heptane	11.55	0.64	13.90	1.96	8.00
Dodecane	11.10	0.65	14.50	1.98	8.00

When the oxygen concentration is ranging between the initial oxygen concentration and the Minimum Oxygen Concentration of carbon monoxide $MOC_{CO} = 6.25\%$, carbon dioxide concentration has a linear evolution as a function of oxygen concentration and is estimated by the equation:

$$CO_2 = -\frac{n_{CO_2}}{n_{O_2}} O_2 + b \tag{6}$$

where b is a coefficient that depends on fuel and n_{CO_2} is the mole number of carbon dioxide required for a complete reaction (mol). The values of n_{CO_2}/n_{O_2} (called a) are given in table 1 along with those of parameter b . This parameter b was obtained thanks to the linear evolution of carbon dioxide concentration as a function of oxygen concentration. It was estimated from the data shown in fig. 4 by fitting the linear

model using least squares method. Very similar results are obtained from our experiments and from ICFMP fire tests.

When oxygen concentration is below the Minimum Oxygen Concentration of carbon monoxide, carbon monoxide is no longer oxidized in carbon dioxide. Consequently, carbon dioxide concentration becomes constant and can be expressed by:

$$CO_2 = -\frac{n_{CO_2}}{n_{O_2}} MOC_{CO} + b \tag{7}$$

Evolutions of carbon dioxide concentration as a function of oxygen concentration are presented on Fig. 4 for heptane fires estimated with this model and performed in the reduced scale room and during ICFMP project [12]. Let us notice that ICFMP fire tests were performed at 5 ACPH. It shows that heptane fires performed with natural ventilation and mechanical ventilation present the same evolution of carbon dioxide concentration. Consequently, there is no influence of ventilation type. It is also found that there is no influence of fuel diameter. The model fits well with experimental observations: one can note that the relative difference between CO₂ model and experiments at 3 and 5 ACPH, with pan diameters of 30 and 23 cm respectively, does not exceed 5 %. This difference is on the order of 14 % between the model and experiments performed at 5 ACPH for a pan diameter of 30 cm. It must be noted that during these heptane fires there were no very underventilated fires ($O_2 < MOC_{CO}$) but the model is in good agreement with dodecane fires in these conditions. It is interesting to notice that the same trend was obtained with heptane fires performed during ICFMP project (Rowekamp et al. [12]).

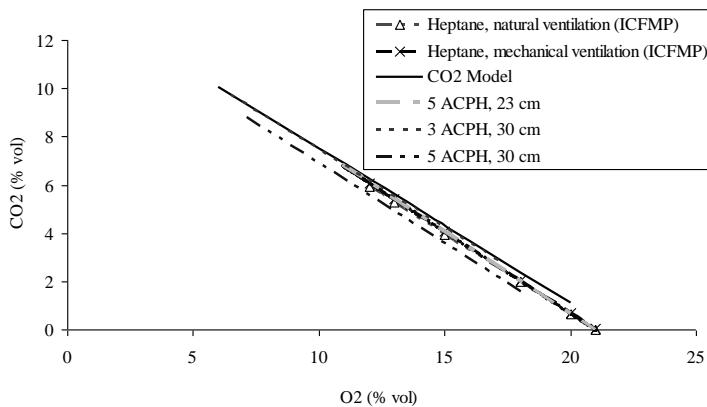


Fig. 4. Carbon dioxide concentration as a function of oxygen concentration: present measurements (heptane) for different conditions of pan diameter and ACPH, computed values and ICFMP fire test values.

Carbon monoxide concentration

The same approach is used to estimate carbon monoxide concentration as a function of oxygen concentration. These concentrations are presented in Figs. 5 and 6 for respectively heptane and dodecane fires performed in the reduced scale room at 3 and 5 air changes per hour with different pan diameters. Similar results are obtained with these two fuels. As shown in these Figs., these evolutions present three parts that are described below.

During sufficiently ventilated fires, i.e. with oxygen concentration ranging between the Minimum Oxygen Concentration (MOC) of the given fuel and the initial concentration of oxygen, fuel oxidation is almost complete. Consequently, unburnt gas production and especially carbon monoxide production is very low. In order to estimate carbon monoxide concentration in this range, the model considers that $[CO] = 0$ for oxygen concentration higher than the Minimum Oxygen Concentration of the given fuel.

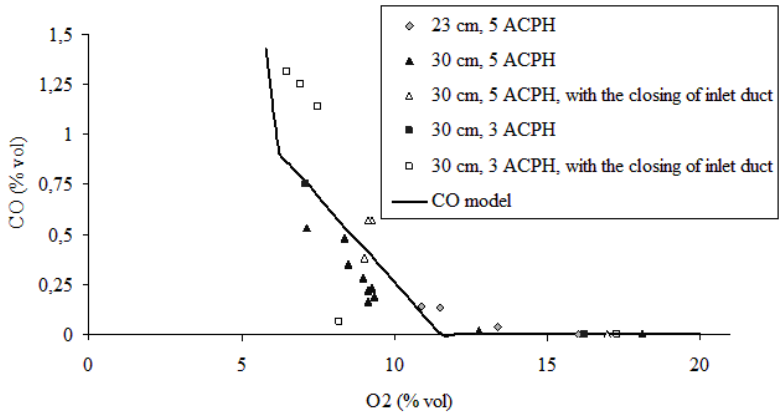


Fig. 5. Carbon monoxide concentration as a function of oxygen concentration: present measurements (heptane) for different conditions of pan diameter and ACPH compared to computed values.

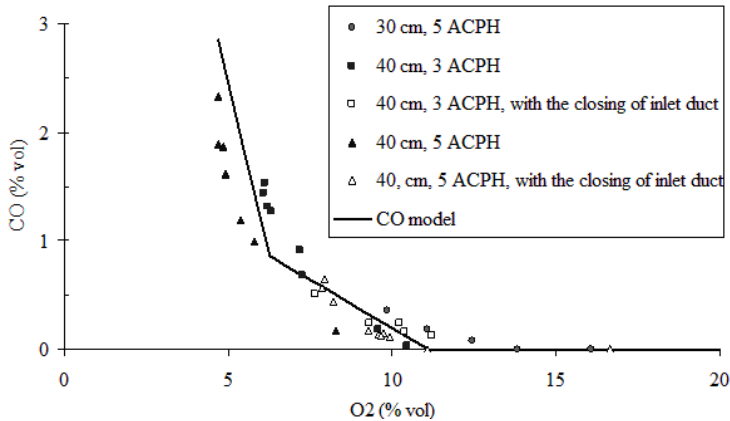


Fig. 6. Carbon monoxide concentration as a function of oxygen concentration: current measurements (dodecane fires) for different pan diameters and ACPH and estimates obtained with the model.

During underventilated fires, i.e. for oxygen concentration ranging between the MOC of carbon monoxide and the MOC of the given fuel (Figs. 5 and 6), the carbon monoxide production is proportional to the decrease of oxygen concentration. These concentrations can be estimated using the following equation:

$$CO = -\frac{c}{MOC} O_2 + c \tag{8}$$

where c is a coefficient that depends on fuel and MOC is the Minimum Oxygen Concentration of the studied fuel. Values of coefficient c are obtained for heptane and dodecane thanks to experimental data presented respectively in figures 5 and 6 and are given in table 1. It is interesting to note here that values of c are similar to k_{CO} , the maximal yield of CO species (defined similarly to k_{O_2} (eq. 3)).

During very underventilated conditions, that corresponds to oxygen concentration lower than the Minimum Oxygen Concentration of carbon monoxide, this gas is no longer oxidized in carbon dioxide. Consequently, a high level of monoxide carbon is reached and its concentration grows strongly while oxygen concentration decreases. This behavior can be modeled using the equation:

$$CO = -\frac{d}{MOC_{CO}} O_2 + d + c \left(1 - \frac{MOC_{CO}}{MOC} \right) \quad (9)$$

where d is also a coefficient depending on fuel and c is the same coefficient as in the previous equation. Values of these coefficients are given in table 1. It must be noted that these two coefficients are similar for heptane and dodecane fires, two fuels that belong to the same chemical family (alkanes): we can suppose that coefficients of this model depend on fuel type. Fire tests on other fuels should be performed in order to check this tendency. Carbon monoxide concentrations as a function of oxygen concentration obtained with this model are plotted in Figs. 5 and 6 for respectively heptane and dodecane fires. It can be noted that the relative difference between model values and experimental values for a pan diameter of 30 cm and 3 ACPH does not exceed 3 % for heptane fires. For O_2 concentrations ranging between 5 and 10 %, the difference between model and experimental CO concentrations can reach 40 % for certain conditions but is generally lower than 10 %. For O_2 concentrations higher than 12 %, the difference does not exceed 4 %, whatever the experimental conditions are.

Hydrogen and total hydrocarbon concentrations

During fire tests performed in the 8-cubic-meter room-test, hydrogen concentration as well as concentrations of hydrocarbons that have a carbon chain length lower than or equal to four are measured. This study is limited to the estimation of the sum of the concentration of these unburnt gases. Figure 7 presents this sum compared to the concentration of carbon monoxide for heptane and dodecane fires performed at 3 and 5 air changes per hour for two pool diameters: 0.3 and 0.4 meter. This Fig. clearly shows that carbon monoxide concentration as a function of oxygen concentration has the same behaviour as the concentration of the sum of the studied fuels for both of the studied ventilation conditions. Using the estimation of carbon monoxide concentration presented previously, this behavior can be estimated using the equation:

$$CO = H_2 + \sum_{\substack{i=4, j \leq 10 \\ i, j=1}} [C_i H_j] \quad (10)$$

It can be noted that only fuels that belong to alkane family were measured. Other fire tests are necessary to check the validity of this estimation on other fuel family.

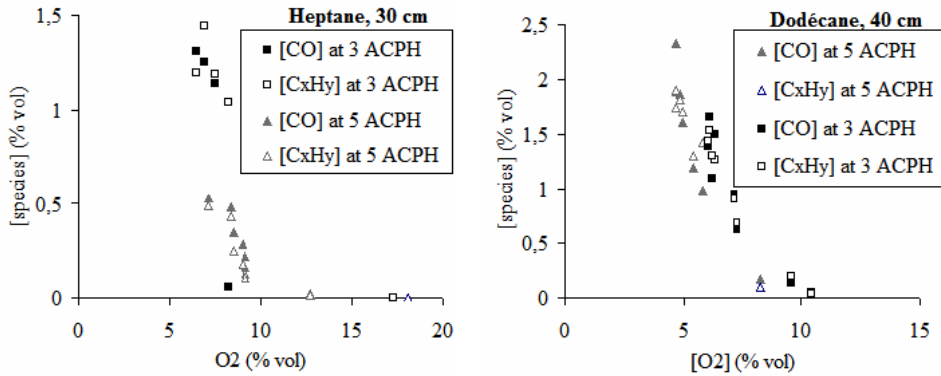


Fig. 7. Carbon monoxide and unburnt gases concentrations as functions of oxygen concentration of reduced-scale heptane and dodecane fires for different ACPH.

Procedure to estimate species concentrations as a function of time

In order to estimate the evolutions of species concentrations, three parameters have to be known:

- the evolution of fuel mass loss rate or the HRR of fire used to calculate the global equivalence ratio,
- ventilation conditions used to calculate the global equivalence ratio,
- given fuel properties, used especially to calculate the theoretical maximum mass yield of oxygen, the global equivalence ratio, the oxygen mass yield and the minimum oxygen concentration of this fuel.

These parameters are used to estimate the global equivalence ratio as a function of time. The normalized oxygen yield is obtained as a function of global equivalence ratio from the theoretical maximum mass yield of oxygen. Using the two previous calculated functions, the evolution of normalized oxygen yield can be calculated as a function of time and then the evolution of oxygen concentration can therefore be deduced. Direct calculation of oxygen concentration can also be made from ventilation velocities and mass loss rate.

Knowing the fuel nature, the coefficients $\frac{n_{CO_2}}{n_{O_2}}$, b , c and d used for this model can be estimated.

Consequently, the concentrations of carbon dioxide, carbon monoxide and the sum of hydrogen and hydrocarbons (with a carbon chain length lower than or equal to four) can be obtained as a function of oxygen concentration, using respectively Eqs. 6, 7, 8, 9 and 10. Then, species concentrations can be

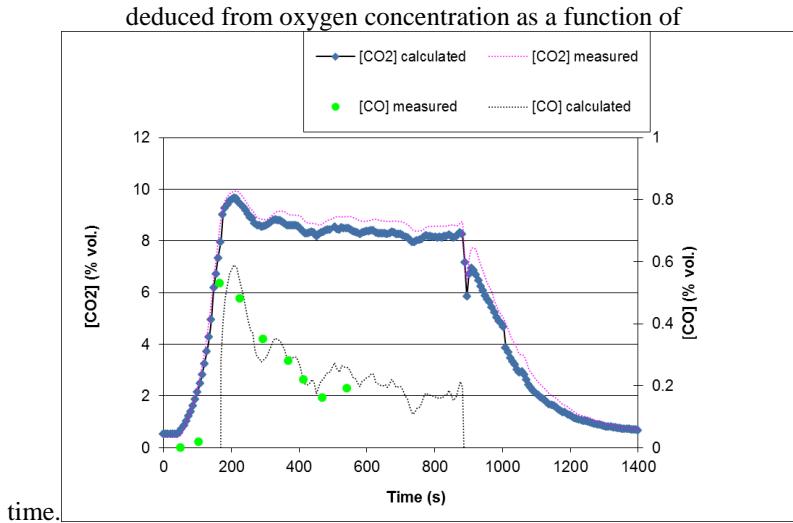


Fig. 8. Carbon dioxide and carbon monoxide concentrations as functions of time measured for dodecane fire in the reduced-scale room at 5 ACPH.

Validation of concentration estimation model

In order to evaluate the validity of the estimations of carbon dioxide, carbon monoxide and unburnt hydrocarbons concentrations, a dodecane fire was performed in the reduced scale room at 5 air changes per hour, with a pan diameter of 0.4 meter.

Carbon dioxide concentration measurements and corresponding model predictions are presented in Fig. 8. Very good agreement is found between carbon dioxide concentration measured during the experiments and the one estimated with the model: the error does not exceed 3 % between 0 and 1000 seconds. A slight difference is noticed at the fire extinction. It is due to the fact that the prediction is not able to simulate the abrupt rise of oxygen in the compartment at fire extinction moment, due to a decrease of the pressure that lets oxygen entering the room.

The evolutions of carbon monoxide concentrations are also represented in Fig. 8. During the fire test, carbon monoxide concentration was punctually measured by probe samplings and was analyzed by gas chromatography: ten measurements performed at different moments are presented in the Fig. (dots). Good agreement is found between carbon monoxide concentration estimated by the model and measured during the experiment. The relative difference between model values and experimental values does not exceed 15 % before 1000 seconds. However, a stronger decrease at the end of the fire is predicted by the model, due to the supposed complete combustion reaction for oxygen concentration higher than the minimum oxygen concentration. For this reason, the relative deviation between model values and experimental values can reach 50 %. Some fluctuations can be noted on carbon monoxide predictions: they result from the evolution of oxygen concentration during this fire.

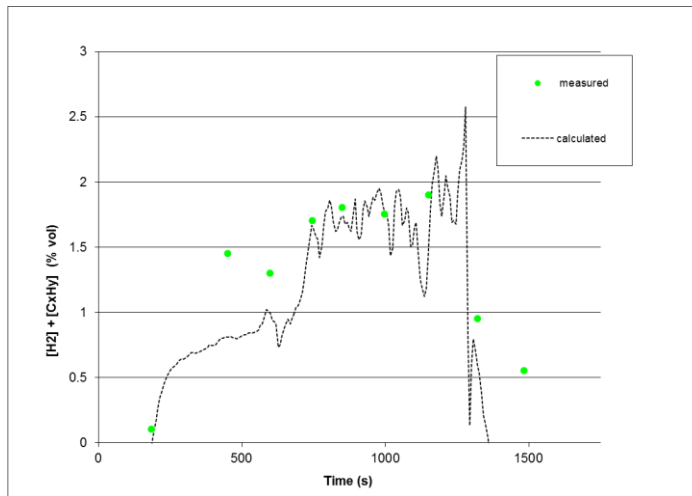


Fig. 9. Hydrogen and hydrocarbon concentrations as functions of time: present measurements for dodecane fire (pan diameter: 0.4 meter) at 5 ACPH and computed values.

Hydrogen and hydrocarbon (with carbon chain length lower than or equal to four) concentrations were measured by ten probe samplings during fire tests, following the same methodology as carbon monoxide concentration measurements. The sum of these concentrations is plotted in Fig. 9. Results predicted by the model are also presented. The model well represents hydrogen and hydrocarbon concentrations during the period where fire is very underventilated (oxygen concentration lower than the MOC of carbon monoxide): trends are similar between measured and calculated values, even if the difference between values can locally reach 40 %. During the time where fire is underventilated, with oxygen concentration ranging between the MOC of carbon monoxide and the one of the studied fuel, predicted concentration is lower than the one measured during the experiment. Lastly, since combustion reaction is considered as complete during ventilated fires, estimated unburnt gas concentration is equal to zero in the model, as soon as the oxygen concentration becomes higher than the MOC. Consequently, the decrease of unburnt gas concentration at the fire end is faster for numerical results than for experimental ones.

To support this analysis, another example is provided for a heptane fire performed with a pan diameter of 0.3 meter, at 5 Air Change Per Hour. Carbon dioxide and carbon monoxide concentrations estimated by the model and measured during experiments are presented in Fig. 10. Similar trends are found between experimental and numerical results. For the underventilated condition, carbon dioxide concentration obtained numerically is slightly higher (between 0 and 8 % higher) than the measured concentration. It can be due to the coefficients obtained for heptane. It must also be noted that, during this fire, only sufficiently ventilated and underventilated conditions are encountered. Fig. 11 presents a comparison between carbon dioxide concentration estimated by the model and performed during ICFMP project [12]. The fire test is performed in a compartment of 21.7 x 7.1 x 3.8 cubic meter with a heptane pan of 0.2 square meter, located at floor level, in the center of the compartment. One can see in Fig. 11 that carbon dioxide concentrations obtained experimentally and numerically follow the same trend. The error between measured and predicted values is on the order of 9 %. This Fig. shows that the model gives a good estimation for large scale fires.

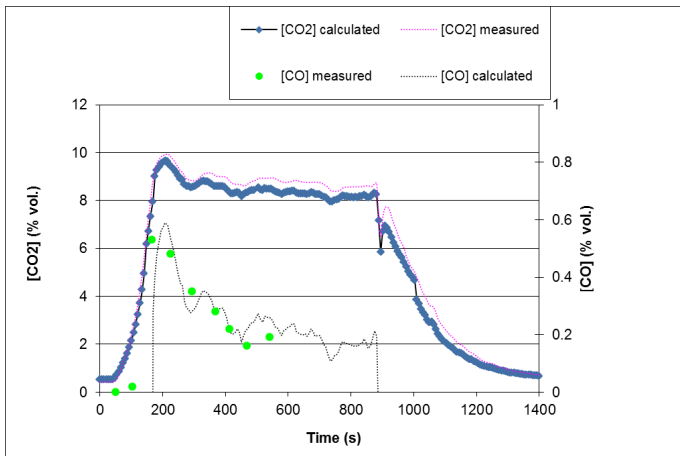


Fig. 10. Carbon dioxide and carbon monoxide concentrations as functions of time: present measurements for heptane fire (pan diameter: 0.3 meter) at 5 ACPH and computed values.

CONCLUSION

An approach to estimate species concentrations during a fire in a well-stirred compartment is developed in this study. This model needs the knowledge of three parameters: fuel mass loss rate, ventilation conditions and fuel properties. It is based on oxygen concentration obtained with oxygen balance equation, or calculated using the evolution of normalized oxygen yield as a function of global equivalence ratio. From oxygen concentration, the model estimates carbon dioxide, carbon monoxide and other unburnt gases (hydrogen and hydrocarbons with a carbon chain length lower than or equal to four) concentrations: three intervals are considered. The first interval corresponds to sufficiently ventilated fires, where oxygen concentration is higher than the Minimum Oxygen Concentration of the studied fuel. In this interval, the combustion reaction is considered as complete. Consequently, the concentrations of carbon monoxide and other unburnt gases are chosen equal to zero and the concentration of carbon dioxide increases linearly with the decrease of oxygen concentration. The second interval concerns underventilated fires, they present oxygen concentration ranging between the MOC of carbon monoxide and the MOC of the studied fuel. During this range, carbon dioxide concentration increases linearly with the decrease of oxygen concentration and there is a release of unburnt gases. This evolution decreases proportionally to oxygen concentration in the compartment and depends on the fuel type. The third interval concerns very underventilated fires, with oxygen concentration lower than the MOC of carbon monoxide. In this range, carbon monoxide is no longer oxidized in carbon dioxide that results in a constant concentration of carbon dioxide and a strong production of unburnt gases, especially carbon monoxide. Moreover, fire experiments performed in a 8-cubic-metre room-test and literature data were used to validate this model. It was found that carbon dioxide concentrations measured during fire test and predicted by the model are in very good agreement. In spite of a stronger decrease of unburnt gases and carbon monoxide concentration just before fire extinction with the model, good agreement is found for these species estimations. This model is semi-empirical and needs some coefficients that depend on the studied fuel. Coefficients have been obtained for heptane and dodecane. Other fire tests should permit the extension of this estimation at other fuels.

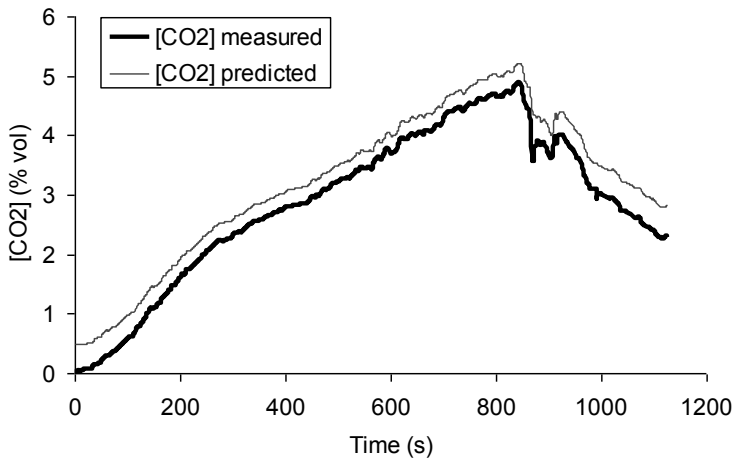


Fig. 11. Carbon dioxide concentration as a function of time estimated by the model and measured during heptane fire of the ICFMP project.

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