Influence of Gas Species on Backdraft Probability Using a Diffusion Flame Limits Criterion

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ABSTRACT: Backdraft is a limited-ventilation fire phenomenon closely linked to the unburnt gases accumulated in the fire compartment just before creating an opening that allows a new supply of oxygen to enter the compartment. The aim of this article is to help understanding the influence of gas species such as hydrocarbon C_mH_n, water, carbon dioxide, oxygen, and nitrogen on backdraft probability. The influence of increasing the number of moles of the above gas species as well as the number of atoms of carbon, hydrogen, and oxygen in the fuel composition is analyzed. For this purpose, a diffusion flame limit criterion based on Le Chatelier's rule is used. In order to verify the obtained results, validation with 41 backdraft experiments is carried out.

KEY WORDS: backdraft, under-ventilated fire, flammability limits, diffusion criterion, gas species.

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INTRODUCTION

BACKDRAFT CAN DEVELOP from fires of either ordinary combustibles or ignitable liquids that become oxygen starved yet continue to generate a fuel-rich environment in a building with limited ventilation. If fresh air is allowed to flow into the vitiated space, such as by opening a door or breaking a window, a gravity current of air will flow into the compartment while the hot fuel-rich gases flow out through the top of the opening. Once a localized flammable mixture is formed and is in contact with an ignition source, the fuel-rich gases will combust acutely, the temperature will rise rapidly and the fire will develop into a deflagration. The deflagration will cause the gases to heat and expand within the compartment, thus forcing unburnt gases out of the opening ahead of the flame front. These gases will mix with additional air outside the fire compartment. As the flame crosses through the building and penetrates the doorway, it ignites the gases outside the space resulting in a fireball and a blast wave.

Several authors have studied this fire phenomenon [1–4]. One of the main conclusions obtained from these studies shows that backdraft is closely linked to the mass concentration of hydrocarbon C_mH_n accumulated just before the opening time. For that reason, in the following sections the influence of gas species as well as the number of atoms of carbon, hydrogen, and oxygen in the fuel composition is analyzed using a diffusion flame limit criterion.

DIFFUSION FLAME LIMITS CRITERION

Flammability limits for diffusion flames were first examined by Simmons and Wolfhard [5]. In their experiments, they determined the minimum level of dilution of the oxidant stream necessary to prevent the stabilization of a diffusion flame for a variety of gas and liquid fuels. The oxygen mole fraction, χ_{O_2}, of the oxidant stream at the flammability limit is known as the limiting oxygen index. They observed that the limiting oxygen index of their diffusion flames equaled to the ratio, $\chi_{O_2}/(\chi_{O_2} + \chi_{\mathrm{diluent}})$, found in a premixed stoichiometric limit mixture involving the same fuel. This implies that the adiabatic flame temperature for the limit diffusion flame, calculated on the basis of stoichiometric combustion of the fuel and oxidant stream, is equal to the adiabatic flame temperature at the stoichiometric limit of a premixed system involving the same fuel, oxidant, and diluent.

Ishizuka and Tsuji [6], verified Simmons and Wolfhard's results for methane and hydrogen, and showed that the adiabatic flame temperature at the flammability limit is small whether the dilution is of the fuel or oxidant stream. This conclusion forms the basis of a method for the evaluation of diffusion flame limits for fuel mixtures. In essence, the ability of a fuel and oxidant pair to react in a diffusion flame is evaluated by examining the flammability of a premixed stoichiometric mixture of the fuel and oxidant [7].

To do this, it is assumed that Le Chatelier's rule holds at the stoichiometric limit, Equation (1), and that the adiabatic flame temperature at the stoichiometric limit for each fuel is a constant. These lead to Equation (2).

$$\sum\left(\frac{C_i}{SL_i}\right) \geq 1 \tag{1}$$

$$\sum_{1}^{n}\frac{(C_i/100)\Delta H_{c,i}}{\int_{T_o}^{T_{f,SL,i}} n_p C_p \mathrm{d}T} \geq 1 \tag{2}$$

where

- C_i is the percent volume of fuel species i, when the fuel stream is mixed stoichiometrically with the oxidant mixture.
- SL_i is the percent volume of the fuel species i in its flammability limit.
- $T_{f,SL,i}$ is the adiabatic temperature of the stoichiometric limit mixture for fuel species i, expressed in K.
- T_o is the temperature of the stoichiometric mixture prior to reaction, also expressed in K.
- $\Delta H_{c,i}$ is the heat of combustion of the fuel species i.
- n_p is the number of moles of combustion products per mole of reactant (stoichiometric mixture of the fuel and oxidant streams).
- C_p is the specific heat of the combustion products; for convenience, constant average specific heats will be used in the calculations.

This number calculated on the left hand side of Equation (2) is referred in this article as Le Chatelier's number. If, for a given mixture, Le Chatelier's number is higher than 1.0 the mixture might become flammable and therefore, backdraft can occur if a hot element comes into contact with the flammable region along the gravity current interface; on the contrary, if this number is lower than 1.0 the mixture cannot become flammable and backdraft cannot occur even with a new supply of fresh air.

In Table 1 [8], the adiabatic flame temperature of the stoichiometric limit mixture and the heat of combustion for some common fuel species is given. Table 2 shows the specific heat at 1000 K of typical combustion products [8].

Table 1. Adiabatic flame temperature and heat of combustion for selected fuels.

Fuel species		$T_{f,SL,i}$ (K)	ΔH_c (kJ/mol)
Carbon monoxide	CO	1450	283
Methane	CH_4	1720	800
Hydrogen	H_2	1080	242
Ethane	C_2H_6	1620	1423
Propane	C_3H_8	1730	2044
n-Butane	$n\text{-}C_4H_{10}$	1830	2650
n-Pentane	$n\text{-}C_5H_{12}$	1810	3259
Methanol	CH_3OH	1690	635
Ethanol	C_2H_5OH	1700	1232

Table 2. Specific heat of typical combustion products at 1000 K.

Gas species		C_{pi} (1000 K)
Carbon dioxide	CO_2	54.3
Water (gas)	H_2O	41.2
Oxygen	O_2	34.9
Nitrogen	N_2	32.7

VALIDATION OF THE DIFFUSION CRITERION

The validity of the diffusion flame limit criterion is checked with the backdraft experiments carried out by Weng et al. [3] and Fleischmann et al. [1]. A brief description of the experiments is given below.

The dimensions of the experimental apparatus used by Weng and Fleischmann are, respectively, 1.2 m × 0.6 m × 0.6 m, and 2.4 m × 1.2 m × 1.2 m (length, height, depth). A methane burner was placed against the wall opposite to the wall with the opening. Figure 1 shows a schematic view of the apparatus with the side panel removed to show the gas burner and the thermocouple tree in the compartment. To ignite the combustible mixture in the compartment, an electrical heated metal wire provided an ignition source.

Three different positions of the opening were studied in Weng's experiments: upper slot opening, middle slot opening, and lower slot opening (Figure 2), and only one position in Fleischmann's experiments: middle slot opening. All of these openings were placed against the wall opposite the gas burner.

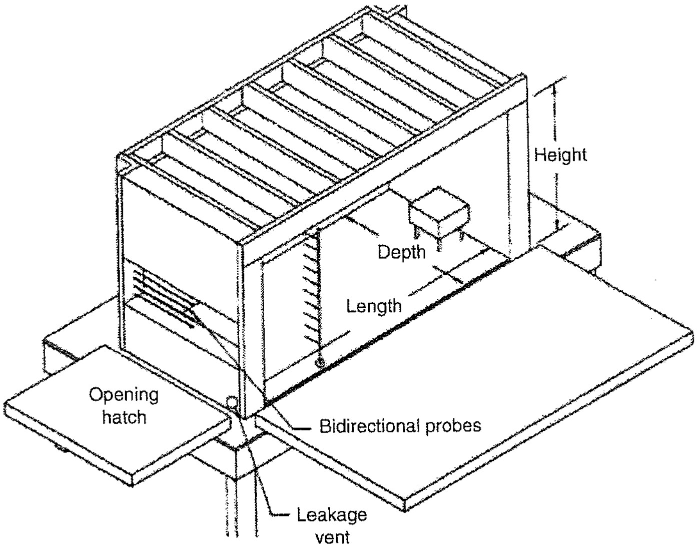

Figure 1. Schematic backdraft apparatus used in Fleischmann and Weng's experiments.

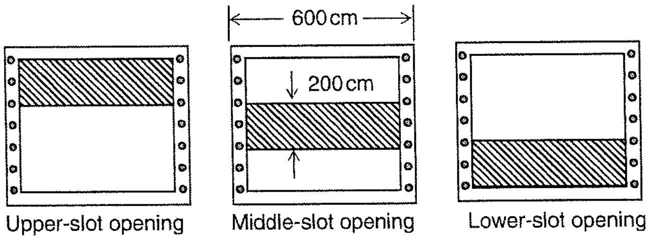

Figure 2. Different openings used in Weng's backdraft experiments.

In their experiments, they recorded the species concentration of hydrocarbon (HC), carbon dioxide (CO_2), carbon monoxide (CO), and oxygen (O_2) just before opening the window that would create the gravity current of fresh air. The concentration of nitrogen (N_2) and water (H_2O) were calculated based on the equation for oxidation of methane. The upper and lower temperatures were also recorded.

Tables 3 [11] and 4 [11] summarize Fleischmann and Weng's backdraft experiments. Columns 1 and 2 give the experimental case number and ambient temperature, T_a. Columns 3 and 4 describe the burner characteristics, i.e., the burner flow rate and the amount of time during

Table 3. Summary of backdraft experiments in the reduced-scale compartment: Weng's experiments.

				Species concentration					Compart. temp. (K)		Backdraft occurrence	
Case	T_a (K)	Flow (10^{-3} kg/s)	Burner time (s)	HC (%)	CO (%)	Fuel (%)	CO_2 (%)	O_2 (%)	T_U (K)	T_L (K)	Test	Equation (2)
Upper-slot opening												
1	297	0.2549	260	11.2	0.5	11.7	0.3	14.0	396	357	Yes	1.11
2	297	0.2549	240	10.4	0.55	10.99	0.2	15.0	381	343	Yes	1.12
3	296	0.1609	300	8.40	0.18	8.65	0.4	14.5	391	353	Yes	1.04
4	297	0.2529	180	7.80	0.48	8.36	0.3	16.0	396	352	Yes	1.09
5	294	0.1603	280	7.60	0.23	7.89	1.0	14.8	373	332	Yes	1.01
6	297	0.2549	160	7.10	0.51	7.65	0.1	16.8	399	352	Yes	1.10
7	295	0.1543	260	7.10	0.32	7.42	0.2	14.6	388	348	No	0.99
8	294	0.1589	240	6.80	0.20	7.03	0.2	14.6	384	343	No	0.97
Middle-slot opening												
9	300	0.1603	780	19.0	0.08	19.11	2.1	12.5	374	339	Yes	1.19
10	299	0.1609	540	13.4	0.13	13.59	3.1	13.0	374	339	Yes	1.12
11	298	0.3210	210	10.5	0.75	11.33	2.1	12.0	377	337	Yes	1.03
12	300	0.1597	360	9.0	0.25	9.31	2.8	13.0	391	347	Yes	1.01
13	298	0.3156	180	8.7	0.9	9.69	2.2	11.0	399	344	Yes	0.96
14	299	0.3196	160	8.2	1.1	9.3	1.0	12.5	382	335	No	0.97
15	297	0.3206	120	5.7	1.0	6.75	2.1	12.5	407	343	No	0.87
16	298	0.1583	210	5.3	0.18	5.49	2.1	13.5	388	338	No	0.84
Lower-slot opening												
17	298	0.3146	260	12.67	0.21	12.88	3.1	12	378	341	Yes	1.08
18	298	0.3226	240	12.13	0.70	12.83	2.1	11.9	380	337	Yes	1.07
19	300	0.2399	300	11.45	0.63	12.08	1.8	14.5	381	345	Yes	1.13
20	300	0.2389	240	9.31	0.58	9.89	1.5	13.8	382	344	Yes	1.05
21	296	0.3206	180	9.14	0.80	9.94	1.8	12.0	369	327	Yes	0.98
22	299	0.2310	210	8.22	0.50	8.72	0.7	14.6	384	342	No	1.04
23	297	0.3246	160	8.06	1.0	9.06	1.9	11.0	380	333	No	0.92
24	298	0.2569	180	7.36	0.6	8.16	0.5	14.6	400	335	No	0.99

which the burner gas flowed. Columns 5–9 give the compartment species concentration at the opening for hydrocarbon, HC, carbon monoxide, CO, carbon dioxide, CO_2, and oxygen, O_2. Column 7 is the sum of Columns 5 and 6. Columns 10 and 11 are the results calculated from the thermocouple tree data for the upper layer temperature, T_U, and lower layer temperature, T_L. Column 12 indicates whether backdraft occurred or not during the test. Column 13 shows Le Chatelier's number, Equation (2), for each case.

Table 4. Summary of backdraft experiments in the reduced-scale compartment: Fleischmann's experiments.

				Species concentration					Compart. temp. (K)		Backdraft occurrence	
Case	T_a (K)	Flow (10^{-3} kg/s)	Burner time (s)	HC (%)	CO (%)	Fuel (%)	CO_2 (%)	O_2 (%)	T_U (K)	T_L (K)	Test	Equation (2)
Middle-slot opening (70 kW)												
P3EXP38	297	72	295	10	0.5	10.5	7	9	417	378	No	1.08
P3EXP36	297	72	355	12	0.4	12.4	6	11	390	361	Yes	1.15
P3EXP35	297	72	415	14	0.4	14.4	6	11	379	353	Yes	1.19
P3EXP34	297	72	475	16	0.3	16.3	5	11	362	339	Yes	1.19
P3EXP33	297	69	535	16	0.3	16.3	5	11	377	356	Yes	1.20
P3EXP45	297	77	535	20	0.3	20.3	5	11	363	344	Yes	1.24
P3EXP32	297	69	555	19	0.3	19.3	5	11	359	340	Yes	1.22
P3EXP42	297	69	595	19	0.3	19.3	4	12	363	346	Yes	1.24
P3EXP39	297	73	655	21	0.3	21.3	4	12	350	331	Yes	1.24
P3EXP40	297	71	715	20	0.3	20.3	4	11	348	332	Yes	1.21
P3EXP43	297	68	715	22	0.3	22.3	4	12	347	332	Yes	1.25
P3EXP41	297	70	775	22	0.2	22.2	4	12	344	330	Yes	1.25
Middle-slot opening (200 kW)												
P3EXP26	297	200	115	13	1.2	14.2	9	4	517	445	No	1.13
P3EXP30	297	200	145	10	1.2	11.2	10	4	570	475	Yes	1.10
P3EXP27	297	200	175	24	0.9	24.9	7	5	474	427	Yes	1.27
P3EXP28	297	200	205	29	0.8	29.8	6	6	447	408	No	1.30
P3EXP29	297	200	235	29	0.7	29.7	6	6	433	400	Yes	1.29

The results of the last column have been obtained by assuming a heat of combustion for methane of 800 kJ/mol and an efficiency of 0.8.

When applying Equation (2) to these experiments, the mole fraction of each gas species is needed. However, the data given in Tables 3 and 4 are expressed in mass fraction and, in addition, the concentration of water H_2O and nitrogen N_2 are not given. Therefore, the mole fraction cannot be obtained directly. Consequently, the methodology described below is used.

The following overall reaction for the methane is assumed to occur in the compartment:

$$a \cdot CH_4 + b \cdot (O_2 + 3.76 \cdot N_2) \rightarrow c \cdot CO_2 + d \cdot CO + e \cdot N_2 + f \cdot H_2O + g \cdot O_2 + h \cdot CH_4 \tag{3}$$

where a, b, c, d, e, f, g, and h represent the moles of each gas species.

The sum of the mass fractions of the combustion products must fulfill Equation (4):

$$1 - Y_{CO_2} + Y_{CO} + Y_{CH_4} + Y_{O_2} = Y_{H_2O} + Y_{N_2} \tag{4}$$

Considering that the total mass of the mixture is 1 kg, Equation (4) can be expressed as Equation (5) where m_i represents the mass of gas species i.

$$1 - m_{CO_2} + m_{CO} + m_{CH_4} + m_{O_2} = m_{H_2O} + m_{N_2} \tag{5}$$

The moles of each gas species such as carbon dioxide, carbon monoxide, methane, and oxygen can be obtained easily by dividing with their molecular weight, MW_i, respectively. Thus, it remains to calculate the moles of nitrogen, water and, consequently, the total quantity of moles in the mixture.

The moles of nitrogen can be obtained approximately using Equation (7). This Equation is obtained by simple oxygen balance Fleischmann [9] using the stoichiometric reaction defined by combustion to CO_2, see Equation (6)

$$CH_4 + 2 \cdot (O_2 + 3.76 \cdot N_2) \rightarrow CO_2 + 2 \cdot H_2O + 2 \times 3.76N_2 \tag{6}$$

It can be observed in Equation (6) that one mole of oxygen must be accompanied with 3.76 moles of nitrogen and one mole of CO_2 is formed when 2 moles of oxygen reacts with methane; therefore one mole of CO_2 must be accompanied with 3.76 × 2 moles of nitrogen.

That is, knowing the number of moles of oxygen accumulated in the container at the moment of opening, the number of moles of nitrogen that accompany it is obtained. In a similar manner, the number of moles of nitrogen that accompany the number of moles of CO_2 can be obtained, see Equation (7).

$$\mathrm{mol}_{N_2} = 3.76 \cdot \left(\mathrm{mol}_{O_2} + 2 \cdot \mathrm{mol}_{CO_2}\right) \tag{7}$$

Then, mol_{H_2O} can be obtained by Equation (4) and MW_{H_2O}. Once mol_{N_2}, and mol_{H_2O} have been obtained, the molar fraction of each gas species in the mixture can be obtained and Equation (2) can be used to predict the occurrence of backdraft.

Comparing on Figure 3 the experimental results against those of Equation (2), one may observe a rather good correspondence, especially for the tests of Weng (cases 1–24). It is clearly seen that for Le Chaterlier's numbers higher than 1.0, the risk of backdraft is possible but it does not mean that backdraft is going to occur (e.g., P3EXP38).

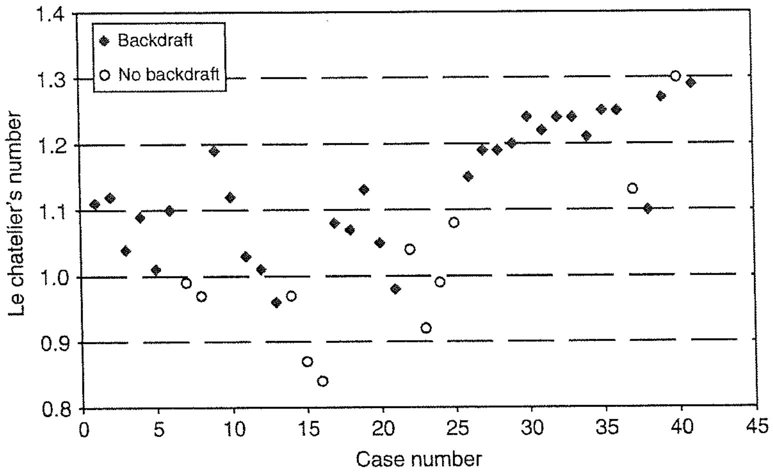

Figure 3. Critical value for a safety Le Chatelier's number criterion.

There are a few cases (e.g., case 13 and 21) which have a Le Chatelier's number less than 1.0 backdraft nevertheless occurred. The lowest value of Le Chatelier's number in which this phenomenon occurred is 0.96. A variation from 1.0 to 0.96 corresponds to a decrease in the volume concentration of the hydrocarbon (methane) of only 8%.

One may also note that P3EXP28 and P3EXP29 show two similar backdraft conditions with two different outcomes. The first one does not reach backdraft, whereas the second one does. Similar cases have been found in the literature. That indicates that backdraft may be a stochastic phenomenon, assuming that the experimental measurements and results are reasonably accurate.

The average value of the Le Chatelier's number for the cases when backdraft occurred is 1.14, whereas it is 1.01 when no backdraft occurred.

PARAMETRIC STUDY: INFLUENCE OF GAS SPECIES ON BACKDRAFT PROBABILITY

In this section the risk of backdraft is established according to the type of gas species accumulated in the compartment. For that purpose, a general mixture is considered which consists of C–H–O constituent fuel, carbon dioxide, oxygen, nitrogen, and water, Equation (8), at opening is evaluated using Le Chatelier's rule, Equation (2).

$$a \cdot \mathrm{CxHyOz} + b \cdot \mathrm{CO_2} + c \cdot \mathrm{O_2} + d \cdot \mathrm{N_2} + e \cdot \mathrm{H_2O} \qquad (8)$$

Table 5. Reference mixture inside the compartment just before ignition.

Fuel	Molecular W (g/mol)	Moles in mixture	Molar fraction (%)
$C_xH_yO_z$; (x: 1; y: 4; z: 0)	16.0	1.7	0.146
CO_2	44.0	1.0	0.086
O_2	32.0	0.4	0.034
N_2	28.0	8.0	0.689
H_2O	18.0	0.5	0.043

The studied parameters examine the influence of varying:

- The moles of fuel.
- The number of atoms of carbon (C) of fuel.
- The number of atoms of hydrogen (H) of fuel.
- The number of atoms of oxygen (O) of fuel.
- The moles of H_2O of the mixture.
- The moles of N_2 of the mixture.
- The moles of O_2 of the mixture.
- The moles of CO_2 of the mixture.

The reference case in which methane is used as fuel is defined in Table 5. A single parameter is modified at a time, whereas the other parameters remain unchanged.

Figure 4 shows the results obtained concerning the influence on the risk of backdraft of increasing the moles of fuel, carbon dioxide, oxygen, nitrogen, and water. The horizontal axis represents the moles of gas species and the vertical axis represents the Le Chatelier's number. The four X marked on the figure at the level 0.90 represent the reference case. According to the proposed model, the mixtures with a Le Chatelier's number above 1 could be flammable and lead to backdraft, whereas a mixture below this value is not flammable and backdraft can not occur.

It can be observed that increasing the amount of moles of oxygen and/or fuel increases the risk of having a flammable mixture (more heat is available for reaching the temperature that ignites the mixture). The opposite effect is observed for water, nitrogen, and carbon dioxide. With these gases, a higher amount means a lower risk of having a flammable mixture since a great part of the available heat is used to heat these inert species.

According to this figure, to become inert a flammable mixture should use CO_2 or H_2O as the inert species since a lower quantity of moles

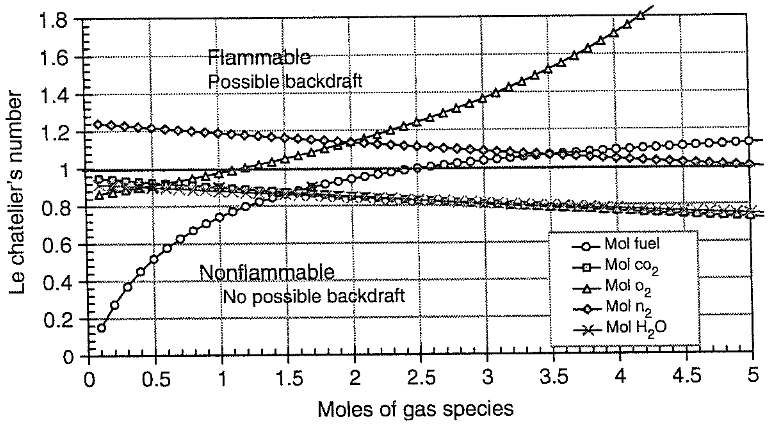

Figure 4. Effect of increasing the gas species on flammability.

is needed than in the case when N_2 is used. The reason lies in the specific heat, see Table 2.

$$Cp_{CO_2} > Cp_{H_2O} > Cp_{N_2} \tag{9}$$

The same kind of study is carried out about the number of atoms of C, H and O in the fuel. Note that changing the number of C, H, or O also entails a change in the combustion heat of the fuel examined (Equation (10)).

Figure 5 shows the obtained results. The horizontal axis represents the number of atoms and the vertical axis represents the Le Chatelier's number.

Increasing the number of C and H increase the Le Chatelier's number and therefore, the risk of having a flammable mixture. The opposite effect is obtained with atoms of O.

The effect of oxygen contained in the fuel on Le Chatelier's number is justified as follows; since in the parametric study Equation (11) has been used for obtaining the combustion heat of the fuel, when increasing oxygen content in the fuel, the amount of oxygen needed for the stoichiometric combustion decreases until the moment it becomes zero or less than zero.

$$C_xH_yO_z + \left(\frac{2x + (y/2) - z}{2}\right)O_2 \rightarrow xCO_2 + \left(\frac{y}{2}\right)H_2O \tag{10}$$

$$\Delta H_{c,\text{fuel}} = \left(\frac{2x + (y/2) - z}{2}\right) \cdot MW_{O_2} \cdot 12.5 \tag{11}$$

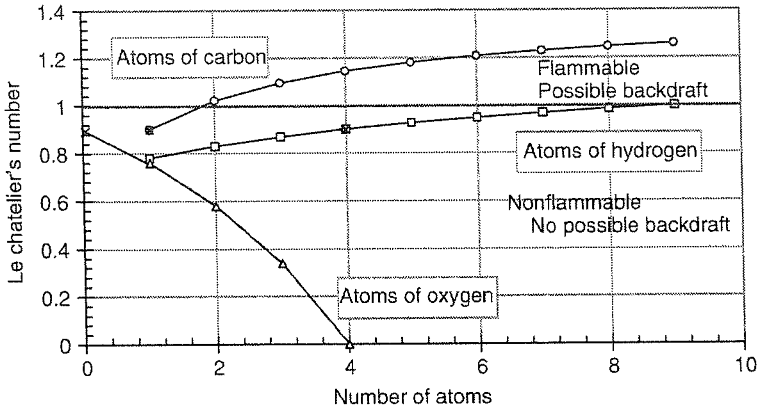

Figure 5. Effect of the number of atoms of C, H, and O on the possibility of having backdraft.

Note that Equation (11) is obtained by assuming that the heat released per gram of O_2 consumed is independent of the fuel that reacts and has an approximate value of 12.5 kJ/g(O_2) [10].

The physical representation of this idea could be explained by one of the following:

- The fuel does not exist in reality.
- The fuel is not combustible.

According to Figure 5, having a fuel with higher number of atoms of C is more dangerous than having a fuel with a higher number of atoms of H. In terms of risk, nine atoms of H (hydrogen) are equivalent to two atoms of C (carbon).

CONCLUSIONS

A diffusion flame criterion is used to evaluate the risk of having backdraft in a compartment. This criterion has been validated with 41 backdraft tests, which have provided good predictions.

Among these backdraft tests, several cases have been found with similar conditions just before the opening time but resulting in different outcomes: occurrence of backdraft or not. If the experimental measurements can be assumed to be reasonably accurate, this indicates that backdraft may be a stochastic phenomenon.

A parametric study for establishing the influence of the composition of the flammable mixture on the risk of backdraft has been carried out.

It reveals that an increase in the quantity of gas species that participate in the combustion such as hydrocarbon or oxygen increases the risk of backdraft. The same conclusion is obtained when increasing the number of atoms of carbon and hydrogen of the fuel. On the contrary, an increase in the quantity of gas species such as nitrogen, carbon dioxide, and water which do not participate in combustion as well as in the number of atoms of oxygen of the fuel reduces the risk of backdraft.

The results provide us with knowledge on the backdraft phenomenon that can be used for fire fighting. The knowledge can also be useful for building design; for example, knowing that fuels with a higher number of carbons increase the risk of backdraft, the materials of the partitions can be taken into consideration in view of this effect.

It would be of interest to carry out experiments with gases other than methane in order to further investigate the criterion for backdraft occurrence proposed in this work.

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BIOGRAPHIES

Christian Pérez Jiménez

Christian Pérez-Jiménez graduated as a industrial engineer from the University of Basque Country (Spain) in 2002. He got his Ph. D. in 2006 in the University of Liege (Belgium). He worked as the person in charge of the department of instalation in an international company of construction from 2006 to 2007. Currently he is working in the deparmento of fire safety of LABEIN TECNALIA a technological center located in Bilbao.

Jean-Marc Franssen

Jean-Marc Franssen graduated as a civil engineer from the University of Liege in 1992. He made all his career in research on structural fire behaviour and on the development of compartment fires. He got his Ph. D. in 1987 and his habilitation thesis in 1997. Most of his career was with the National Fund for Scientific Research Belgium. Since October first 2008, he is a professor at the University of Liege.

Bjorn Karlsson

Dr. Bjorn Karlsson is the Fire Marshal and Director General of the state run Iceland Fire Authority and is in charge of reglulations to do with buildings and fire brigades in Iceland. He worked as Associate Professor at the department of Fire Safety Engineering at Lund University, Sweden, from 1992 to 2001 and is currently Associate Professor at the Department of Environmental and Civil Engineering at the University of Iceland.