

A closer look to some aspects of the methodology of hazardous area classification using CFD

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Hazardous area classification is normally carried out based on the approach described in the Explosive Atmospheres Hazardous Area Classification Standard IEC 60079-10-1. This allows the classification of hazardous areas into zone 0, zone 1, or zone 2, based on the likelihood of the presence of flammable/explosive gas atmosphere. The extent of the zone depends on the estimated or calculated distance over which an explosive atmosphere exists before it disperses to a concentration in air below its lower flammability limit LFL – with an appropriate safety factor. The Standard includes a methodology for its calculation.

However, critical formulae given in the Standard IEC 60079-10-1 to calculate the expected gas cloud volume that is used to determine area classification do not have any scientific justification. Previous work by HSL (e.g. Webber at al, 2011) has found that the predicted volume of the gas cloud from CFD models can be several orders of magnitude smaller than that given by the formulae in question, thus having a very significant effect on the zoning requirements. This observation is confirmed in the present study: CFD-simulations show that both the 2008 (STD08) and the 2015 (STD15) versions demand ventilation velocities to obtain non-hazardous conditions in an enclosure which are over-conservative.

The current work also shows that there is a trend of flammable volume increase with increased extension of the room along the ventilation direction. This trend is accounted for in the definition of degree of ventilation in STD08 but not in the definition of degree of dilution in STD15. This seems to be a limitation of the newer methodology.

Analysing the CFD-simulations performed using the concept of local age of air shows that the air circulation has a relatively homogenous distribution inside the modelled room. In general, the great spread of resulting flammable volumes depending on the selected scenarios demonstrates the advantages of air flow and dispersion modelling by CFD simulation in addition to the application of simplified methodologies, as recognised by STD08 and to a larger extent by STD15. CFD modelling is proposed for hazardous area classification in critical areas.

Keywords: hazardous area classification, ventilation, dispersion

Scope of the analysis

The formation of flammable atmospheres in and around a process unit will depend on the geometrical configuration of structures and equipment, whether the unit is located indoor or in the open and on the physical characteristics of the flammable flow including phase state, flow buoyancy and velocity.

The scope of the present analysis is limited to enclosed spaces, with ventilation provided mechanically, and gaseous releases at ambient temperature having neutral buoyancy and zero momentum. The goal is to study how the ventilation and air flow determines the formation of a flammable cloud. We do not analyse the role of other factors that are usually part of the hazardous area classification procedure such as the likelihood of releases or the reliability of the ventilation system. Specifically, in the application of the hazardous area classification methodologies, we consider the case where:

- the ventilation is present continuously; defined in the Standard IEC 60079-10-1 as "good availability of ventilation";
- the release occurs frequently or continuously in time; defined in the Standard IEC 60079-10-1 as "continuous grade of release".

In addition, we set:

- the efficiency of ventilation to 1 (corresponding to "ideal ventilation", no impeded flow);
- the maximum allowable flammable concentration equal to the lower flammability limit (*LFL*) with no safety factor;

so that no additional conservativism is added in the methodology proposed by the Standard.

The following paragraphs summarize and compare the calculation procedures that are used to classify zones depending on the hazard level, as defined by the Standard IEC 60079-10-1 in the two versions released in 2008 (IEC 60079-10-1, 2008) and 2015 (60079-10-1, 2015). We analyse in particular the threshold between "medium" and "high" ventilation that, for continuous grade releases and good ventilation availability defines the boundary between non-hazardous zones and zone 0. Subsequently we present the results of CFD-simulations and use the information derived from the model to compare two versions of the Standard.

Definition of the non-hazardous zone limit in the 2008 Standard

The Standard IEC 60079-10-1 2008 (in the following referred to as STD08) provides an equation to calculate the volume V_z over which the mean concentration of flammable gas or vapour is above a "safe" concentration level. Fixing the safe concentration level to *LFL*, we calculate V_z , following the given equation, as the ratio between the rate at which the flammable cloud is generated by the volumetric release W_r and the number of air changes F_a generated by the room ventilation:

$$V_z = \left(\frac{W_r}{LFL}\right) / F_a \tag{1}$$

 V_{z} , referred to as the "hypothetical volume", is a representation of the potential extent of the flammable cloud. A hypothetical volume less than 0.1 m³ indicates a "high degree of ventilation" and a non-hazardous zone.

The limits of the aforementioned approach have already been highlighted by Webber et al. (D.M. Webber, 2011): the calculation leads to an over-estimation of the assessed flammable volume and over-conservativism in the hazard evaluation. It can be easily seen that equation (1) is based on the steady state solution of the following ordinary differential equation describing the accumulation of flammable mixture into the room space:

$$\frac{dV_z}{dt} = \frac{W_r}{LFL} - W_{out} \tag{2}$$

where W_r / LFL represent the rate of generation of flammable volume, assuming a homogenous mixing of air and fuel at the lower flammability limit; W_{out} represents the outflow rate of flammable volume. The latter is calculated, assuming homogeneous outflow transport in the room, from the ventilation volumetric rate W_a and the ratio V_z / V_{room} representing the fraction of flammable volume in the room:

$$W_{out} = \frac{V_z}{V_{room}} \cdot W_a = V_z \cdot F_a \tag{3}$$

 V_z represents the volume occupied by the mixture of fuel and air as a homogeneous cloud, while in reality most of the fuel forms concentrations above the *LFL* and the actual flammable volume is one or two order of magnitude below V_z . Equation (1) describes the accumulation process of released fuel in the room but ends up with an overestimated flammable volume.

Definition of the non-hazardous zone limit in the 2015 Standard

The new Standard released on 2015 (in the following referred to as STD15) introduces revised criteria for the assessment of adequate levels of ventilation associated with potential hazardous releases. The novel regulation recognises the effect of the ventilation velocity in determining the fuel-air mixing efficiency more than, or in addition to, the number of air changes. The notion of "degree of ventilation" is revisited and renamed as "degree of dilution". The degree of dilution substitutes in fact the degree of ventilation in the definition of the zone type and, in STD15, a flammable volume less than 0.1 m³, indicating a non-hazardous zone, corresponds to "high dilution" conditions.

The degree of dilution depends on the ventilation velocity U_w and the "release characteristic". The latter is the volumetric rate of released flammable volume, already defined in the previous paragraph as W_r / LFL . Following the suggested methodology for indoor configurations, the ventilation velocity is calculated dividing the ventilation volumetric rate by the room area perpendicular to the ventilation flow:

$$U_w = W_a / A_{room} \tag{4}$$

The release characteristic and ventilation velocity are combined in a chart that is used to identify the degree of dilution. The chart, reproducing figure C.1 of STD15, is shown in Figure 1 highlighting the non-hazardous zone boundary.



Figure 1 Boundary between medium dilution and high dilution and non-hazardous zone (green area) in STD15.

Since the degree of dilution in STD15 is related to the ventilation velocity while the degree of ventilation in STD08 is based on the air changes, there is a dimensional difference between the two approaches. The degree of dilution does not depend on the room size parallel to the ventilation flow while the degree of ventilation does (via the number of air changes generated by the ventilation rate).

Graphical comparison between the current and former versions of the Standard

Relations (1) and (4) can be combined to obtain the ventilation velocity for a given release characteristic, hypothetical volume and room size (volume V_{room} and area A_{room}) according to STD08:

$$U_{w} = \frac{\left(\frac{W_{r}}{LFL}\right)}{V_{z}} \cdot \left(\frac{V_{room}}{A_{room}}\right)$$
(5)

Using equation (5) and parametrising the enclosure size it is possible, to plot the ventilation velocity required for nonhazardous conditions defined in STD08 as a function of the release characteristic obtaining a graphical comparison with STD15. The chart (Figure 2) is generated considering cubical enclosures and varying room volumes between 10 and 1000 m^3 , a range that is chosen to represent typical sizes of enclosed spaces of industrial units.



Figure 2 Non-hazardous zone boundary in STD15 (blue line) and in STD08 (green area) parametrized with the volume of the enclosed space.

The comparison shows that STD08 is more conservative than STD15, with an increasing degree of conservativism for larger volumes. In the range of volumes considered, the required ventilation velocity is up to one order of magnitude higher in STD08 compared to STD15. The ratio increases further when changing the shape factor of the room considering a larger extension along the ventilation inlet-outlet direction compared to the extension in the cross-wise direction. This is illustrated in Figure 3 for a room size of 100 m³ and aspect ratios from 1 to 10.



Figure 3 Non-hazardous zone boundary dilution in STD15 (blue line) and in STD08 (green area) for an enclosed size of 100 m³ parametrized with the enclosure aspect ratio.

Comparison of the Standard IEC 60079-10-1 with CFD simulations

We perform CFD simulations to verify whether the required ventilation rates defined by STD08 and STD15 correspond to realistic values and what is the dependency of the ventilation rates on the room size.

The simulated scenario represents an empty cubic room of 4 m side, with ventilation generated by a fan extracting air from the room combined with a free opening on the opposite wall, as shown in Figure 4. The ventilation velocity of 2 m/s through the $0.4x0.4 \text{ m}^2$ inlet and outlet openings generates a volumetric flow of 0.32 m^3 /s that, divided by the room cross section area of $4x4 \text{ m}^2$, corresponds to a ventilation velocity of 0.02 m/s or 18 air changes per hour. A 1 g/s rate of neutrally buoyant flammable gas is released in the centre of the room at floor level.

This scenario is simulated with the Reynolds averaged Navier Stokes equations solver FLACS 10.5r2, using the $k \cdot \varepsilon$ model for turbulence closure and defining an initial ambient pressure of 10000 Pa and temperature of 293 K. The room is covered with a uniform computational grid of 0.1 m and the velocity-pressure fields are solved iteratively until a relative mass residual less than 10⁻⁶ is achieved. The air flow is simulated for 600 seconds before starting the release and the simulation is continued for 1200 seconds after the release start time outputting time series of velocity and fuel concentrations.

The velocity field and gas cloud never reach a steady state, showing irregular oscillations perpendicular to the inlet-outlet direction (Figure 5).



Figure 4 Representation of the simulated room showing the location of inflow and outflow openings (left) and bidimensional section along the X-Z plane of the simulated velocity vectors at a particular time (right).



Figure 5 Simulated contour areas of the flammable volume at two different moments (top and bottom) in a horizontal section X-Y (left) and in a vertical section X-Z (right) illustrating the non-steady character of the simulated scenario.

The simulated time-averaged fuel concentrations are postprocessed to determine the concentration level exceeded by 0.1 cubic metres of fuel-air mixture. Such value, taken as *LFL*, defines the release characteristic, W_r / LFL , that is used to calculate the ventilation velocity leading non-hazardous zone ($V_z = 0.1 \text{ m}^3$) according to equation (5) for STD08 and according to the chart in Figure 1 for STD15. The two calculated ventilation velocities are compared with the simulated value of 0.02 m/s in Table 1. For the present scenario, the methodology adopted by the Standard is highly conservative prescribing 116 and 38 times higher velocities according to STD08 and STD15 respectively.

	STD08	STD15	simulation
U _w [m/s]	2.32	0.753	0.0200

Table 1 Comparison of simulated ventilation velocity in the air-extraction scenario and ventilation velocity determined according to STD08 and STD15 to reach a non-hazardous zone in the room.

It is possible that the large conservativism of the Standard in this particular scenario is a consequence of the ventilation pattern and the release location in the room that induced a very effective dilution and reduction of the simulated flammable volume. Indeed, the simulated velocity field (Figure 4) shows a stream of fresh air passing through the fuel release area.

To confirm the results presented above an additional simulation is performed replacing the fan extracting air from the room by a blower pushing air into the room. In the new configuration, the opening on the left side of Figure 6 is an outlet and the main flow direction is reversed compared to the previous simulation case: now the region of higher velocities is located on the top of the room. Results of the second simulation are postprocessed as in the previous simulation case, calculating *LFL* as concentration exceeded my 0.1 cubic metres of mixture, and the simulated ventilation velocity is compared to the ones calculated according to the two versions of the Standard (Table 2).

Since the calculated LFL is higher than in the previous simulation case, the ventilation velocity required to reach nonhazardous levels of flammable volume is now closer to the simulated one. Still, the ventilation velocity is over-predicted by a factor 70 and 23 applying STD08 and STD15 respectively.



Figure 6 Representation of the simulated room with air blower (left) and bi-dimensional section along the X-Z plane of the simulated velocity vectors at a particular time (right).

	STD08	STD15	simulation
Uw [m/s]	1.41	0.458	0.0200

Table 2 Comparison of simulated ventilation velocity in the air-supply scenario and ventilation velocity determined according to STD08 and STD15 to reach a non-hazardous zone in the room.

Effect of room size

We are interested in investigating the effect of the room size in the formation of flammable volumes since this quantity is accounted for in different ways in STD08 and STD15.

The transport model used for arriving at equations (2) and (3) and foundation of STD08, is based on the hypothesis that the flammable volume fraction in the out-flowing stream is proportional to the fraction of flammable volume in the room (equation (3)). The result is that, for a given release characteristic W_r / LFL , the required ventilation volumetric rate W_a is proportional to the room volume. On the other hand, as already stressed in the previous paragraphs, the required ventilation volumetric rate in STD15 is proportional to the room area perpendicular to the flow and does not depend on the room length in the parallel direction.

In practice, it is expected that increasing the distance between release position and ventilation outlet would reduce the concentration of flammable gas in the outflowing mixture leading to an accumulation of flammable volume. The equilibrium between generation (release) and removal (outflow) of flammable gas is restored by increased fuel concentrations and increased flammable volume.

To investigate this, the two simulation cases described above are repeated with a room size increased from 4 to 8 metres in the inlet-outlet direction. The same uniform grid resolution of 0.1 m is maintained in the new simulations; results, in terms of ventilation velocity required to dilute the flammable volume down to 0.1 m^3 (non-hazardous threshold), are presented in Table 3 and Table 4.

	STD08	STD15	simulation
U _w [m/s]	3.35	0.544	0.0200

Table 3 Comparison of simulated ventilation velocity in the air-extraction scenario and ventilation velocity determined according to STD08 and STD15 to reach a non-hazardous zone in the room. Room length of 8 m.

	STD08	STD15	simulation
U _w [m/s]	1.68	0.273	0.0200

Table 4 Comparison of simulated ventilation velocity in the air-supply scenario and ventilation velocity determined according to STD08 and STD15 to reach a non-hazardous zone in the room. Room length of 8 m.

As expected, the increased room volume diminishes the effectiveness of the ventilation in line with the transport model of STD08 and so that the fuel iso-concentration enclosing 0.1 m^3 of flammables increases by 38% and 68% in the air extraction and air supply scenario respectively. This is reflected in increased ventilation velocity according to STD08 and decreased ventilation velocity according to STD15 (Table 4 compared to Table 2 and Table 3 compared to Table 1)

These results are summarized in Figure 7 and Table 5. Table 5 reports the relative change of ventilation velocity to reach a non-hazardous zone in the room for the 4 m and the 8 m room length scenarios. The percentages illustrate how the relation between room size and ventilation effectiveness is accounted for in STD08 and STD15: a 0% variation means that the reduced ventilation effectiveness resulting from the increased room size is reproduced in accordance to the simulations; a positive value corresponds to over-estimation of the ventilation effectiveness reduction determined by the increased room size; a negative value corresponds to under-estimation of the ventilation effectiveness reduction determined by the increased room size. Figure 7 shows the ratio between prescribed and simulated ventilation velocity and the trend with room size variation.



Figure 7 Ratio between the ventilation velocity prescribed by the Standard IEC 60079-10-1, version 2008 and version 2015, and the simulated ventilation velocity in four scenarios representing the air-supply and the air-extraction configurations with 64 m^3 and 128 m^3 enclosure size.

STD08 air-supply	STD08 air-extraction	STD15 air-supply	STD15 air-extraction
19%	44%	-40%	-28%

Table 5 Relative variation of the ventilation velocity prescribed by STD08 and STD15 when the room x-length is changed from 4 metres to 8 metres with release characteristic determined by the simulation as the value corresponding to a 0.1 m³ of flammable volume.

Evaluation of the ventilation efficiency

The extension of the flammable cloud and the ventilation velocity required to reduce it down to 0.1 m^3 depend on the configuration of the air flow in relation to the position of the release. The possibility of modelling a non-homogenous ventilation flow and the identification of "dead" areas leading to possible formation of fuel pockets is, in general, an advantage of computational fluid dynamics compared to the simplified methodologies proposed in the Standard IEC 60079-10-1.

To assess the possible variation of the flammable volume extent dependent on the location of the release inside the room we use the notion of age of air. The age of air represents the average time required for a fresh air particle entering the room at time zero to clean a "polluted" location inside the room by replacing the pollutant in that position (Awbi, 2013). The age of air at a specific point Aa(x,y,z) in the room can be determined by filling the room with fuel, simulating the entrance of fresh air and calculating the following fuel molar fraction integral in time:

$$Aa(x, y, z) = \int_0^\infty F(x, y, z, t) dt$$
(4)

The age of air provides, for instance, information about the possibility of an explosive atmosphere to accumulate in a certain location in the room: in such case, if the fuel volume is indefinitely trapped by a vortex, the age of air is infinite.

The clear-out of fuel from the 64 m^3 and 128 m^3 rooms is simulated with the same setups already defined for the previous runs until complete cleaning of the room is reached. The age of air is calculated at 343 different positions regularly distributed inside the room, results are shown in Figure 9 as a function of the point location along the inlet-outlet direction.

Looking at the two plots on the top side of Figure 9, representing the 64 m^3 size case, it is observed that the range of variation of the age of air is similar in the air-extraction (left side of the figure) and air-supply (right side of the figure) configurations. There is a preferential stream, corresponding to the sequence of points with lower ordinate in the graphs, along which the age of air is considerably lower comparing to the other positions inside the room. Close to the inlet section along this stream the age of air approaches zero seconds while further into the room towards the outlet the low-air-age stream becomes less distinct. With the exception of the points along this air path, the range of variation of the age of air is rather limited with less than 15% variation from the average (approximately 200 seconds in both scenarios) meaning that there are no zones of fuel accumulation in the room. This may also be attributed to the unsteadiness of the velocity field generated by these particular ventilation scenarios.

We observe qualitatively similar results in the 128 m^3 case (two bottom sub-frames of Figure 8); surprisingly the age of air average among the points is approximately 200 seconds, as in the 64 m³ case. Again, no vortices trapping the fuel exist in simulated air flow.



Figure 9 Local age of air [s] vs position along the inlet-outlet direction at different points inside the enclosure. Top subfigures: 64 m³ room in the air-extractor (left) and air-supplier configuration (right). Bottom sub-figures: 128 m³ room in the air-extractor (left) and air-supplier configuration (right).

Conclusions

In this work we have studied the methodology for hazardous area classification in enclosed spaces focusing on the role of the ventilation velocity and the enclosure size.

The differences between the 2008 release (STD08) and the 2015 release (STD15) of the Standard IEC 60079-10-1 pose a question on the basis of the two procedures and on their ability to predict the ventilation rates required to achieve non-hazardous conditions. The two formulations are compared showing that STD15 is less conservative than STD08. At the same time, STD15 relies on the ventilation velocity as a driving force for the mixing that consumes the flammable volume only, ignoring the extent of the enclosure in the ventilation direction.

We have performed computer simulations of a passive flammable release in an un-obstructed ventilated room comparing the simulated ventilation velocity with the ventilation velocity prescribed by the Standard IEC 60079-10-1 and verifying that both the 2008 and the 2015 versions of the standard reproduce conservative conditions. The required ventilation velocity determined according to the Standard IEC 60079-10-1 may be regarded as over-conservative, considering that its magnitude has been found to be more than 70 and more than 13 times the simulated values respectively for STD08 and STD15. Moreover, additional conservativism is implied when taking into account safety factors for impeded ventilation and the lower flammability limit.

It has been observed that there is a trend of flammable volume increase with increased extension of the room along the ventilation direction. This trend is accounted for in the definition of degree of ventilation in STD08 but not in the definition of degree of dilution in STD15. This seems to be a limitation of the newer methodology.

The local age of air has been calculated in the simulated scenarios to evaluate the ventilation efficiency inside the room proving that the air circulation has a relatively homogenous distribution inside the room. This makes it possible to generalize the results of the simulated scenarios, independently form the specific location of the fuel release. In addition, it seems that the relative homogeneity of the ventilation in the simulated scenarios is promoted by the unsteadiness of the flow that creates oscillations contributing to the transport of fresh air in all parts of the room. This observation suggests that assuring conditions that trigger instability in the physical flow may be a practical way to the enhance the ventilation efficiency.

Additional effects introduced by obstructions like walls and any objects inside the room have not been investigated, clearly, they can largely affect the ventilation efficiency. Negative buoyancy of the release can also adversely affect the mixing efficiency. It is possible that the large conservativism of Standard IEC 60079-10-1 is, in a way, tailored to embrace those configurations of impeded flow and stratification of the fuel cloud, in combination with the existing safety factors for ventilation efficiency and *LEL* extent. In general, the great spread of resulting flammable volumes depending on the selected scenarios demonstrates the usefulness of air flow and dispersion modelling by CFD simulation in addition to the application of simplified methodologies, as recognised by STD08 and to a larger extent by STD15.

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