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Die Ausbreitung explosionsfähiger Atmosphären in einem Maschinenraum durch eine validierte CFD Simulation

The propagation of explosive atmospheres in a machine room by a validated CFD simulation

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Summary

Explosive atmospheres caused by escaping gases are a widespread topic in safety engineering. In recent years people died in gaseous accidents. In several accepted standards and directives, common procedures are determined to obtain an assessment of the hazard caused by explosive atmospheres. However, it is difficult to predict the shape, propagation and position of an explosive atmosphere in different spaces.

An experimentally validated computational fluid dynamic (CFD) Ansys Fluent simulation is used to evaluate the behavior of an explosive atmosphere, caused by escaping propane gas in a small machine room under supersonic conditions. The propane gas is released from a defined standard leakage (5 mm²) according to the European Standard EN 60079-10-1. For the experimental validation of the simulation, CO_2 gas is used due to safety reasons and its similarity (density) to propane.

CFD results legitimize the use of CO_2 gas instead of propane gas due to similar propagation behavior. The classification of an explosive atmosphere performed by the CFD simulation is compared to the classification according to standard regulations. A CFD simulation based classification of an explosive atmosphere leads to a smaller volume where an explosive atmosphere exists. Conclusions are drawn on the conservative assumptions of common regulations.

Introduction

For risk management a proper understanding of hazards caused by gas releases is crucial. The EN 60079-10-1 (Bozek 2017) shows an assessment for hazardous areas caused by gas releases. In the last couple of years, the importance of safety standards in industry has increased, so there is the need for a precise and cheap method to classify hazards in explosive atmospheres.
However, in the state of the art applied procedure there is no reference to local conditions (e.g. the geometry of the room or the installed equipment) and ventilation. In some studies the use

of a CFD simulation for the assessment of an explosive atmospheres is already discussed, see (Gant 2008; Gant et al. 2006; Santon et al. 2012; Tommasini 2013).

Explosive atmospheres and hazardous areas

Explosive atmospheres are specified in the EU directive 99/92/EC (Directive 1999). The exact wording is: “For the purposes of this Directive, 'explosive atmosphere' means a mixture with air, under atmospheric conditions, of flammable substances in the form of gases, vapors, mists or dusts in which, after ignition has occurred, combustion spreads to the entire unburned mixture”.

The EN 600079-10-1 (Bozek 2017) is a general guideline for explosive atmospheres. In general, a combustible medium and oxygen in a certain critical ratio are obligatory for an explosive atmosphere. The dangerous substances and explosive atmospheres regulation 2002 (DSEAR) defines hazardous areas as any place in which an explosive atmosphere may occur in quantities which require special precautions to protect the safety of people.

Classification

The EU directive 99/92/EC requires a classification of an area where a potential risk of explosions exists. Hazardous areas are caused by the presence of flammable substances in form of mist, vapors, gases or dusts. Those hazardous areas are classified into three zones depending on the frequency of occurrences and duration:

Zone 0: A place in which an explosive atmosphere consists of a mixture with air or flammable substances as gas, vapor or mist for long periods or frequently.

Zone 1: A place in which an explosive atmosphere consists of a mixture with air or flammable substances in the form of gas, vapor or mist is likely to occur in normal operation occasionally.

Zone 2: A place in which an explosive atmosphere consists of a mixture with air of flammable substances in the form of gas, vapor or mist is not likely to occur in normal operation but, if it does occur, will persist for a short period only.

Classification numbers and equations

Several conditions must be fulfilled before a hazardous area occurs, defined by classification numbers. The Lower Explosive Limit (LEL) is the minimum concentration of a vapor or a particular substance necessary for a combustion in air. Below the LEL the mixture of oxygen and the combustible medium is too "lean" so there is no explosive atmosphere.

The Upper Explosive Limit (UEL) defines the maximum concentration of a gas or vapor in air that creates an explosive atmosphere. For instance, the LEL and the UEL for methane is 5% and 15% at standard conditions.

The flashpoint is the lowest temperature at which the vapor of volatile material will ignite in the presence of an ignition source. The auto ignition temperature is the lowest temperature at which a medium spontaneously ignites in a normal atmosphere without an external source of ignition. The release rate W_g in kg/s for a supersonic gas release can be estimated by

$$W_g = C_d\, A_1\, p_0 \sqrt{\gamma \frac{M}{Z\, R\, T} \left(\frac{2}{\gamma + 1}\right)^{(\gamma+1)/(\gamma-1)}}\,.$$

C_d is a dimensionless outflow coefficient, which is a characteristic number of large vents, inlets or outlets. Furthermore, it takes the effect of turbulence and viscosity into account. A typical range is between 0.5 and 0.75. A_1 is the leak size in m^2. p_0 is the pressure in a pipeline or in

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a tank in Pa. M is the molecular weight of the gas in kg/kmol. R is the general gas constant in J/(kmol K). T is the absolute temperature in Kelvin of the medium. Z is the compressibility factor. γ is the poly-tropic index of adiabatic expansion or the ratio of specific heats. The release characteristic is defined by

$$W_g/(\rho_g \; k \; LEL),$$

where k is the instability factor of the LEL, a typical range is in between 0.5 - 1. ρ_g is the density of the gas in kg/m³.

In this study, a CFD simulation is used to classify an explosive atmosphere. A propane gas release in a small machine room with different process equipment is investigated. The classification of an explosive atmosphere by the validated CFD simulation is compared with a classification by EN 60079-10-1 (Santon et al. 2012).

Geometry and mesh

A model of the considered machine room is created, see Fig. 1. The dimension and the volume of the machine room are given in Tab. 1.

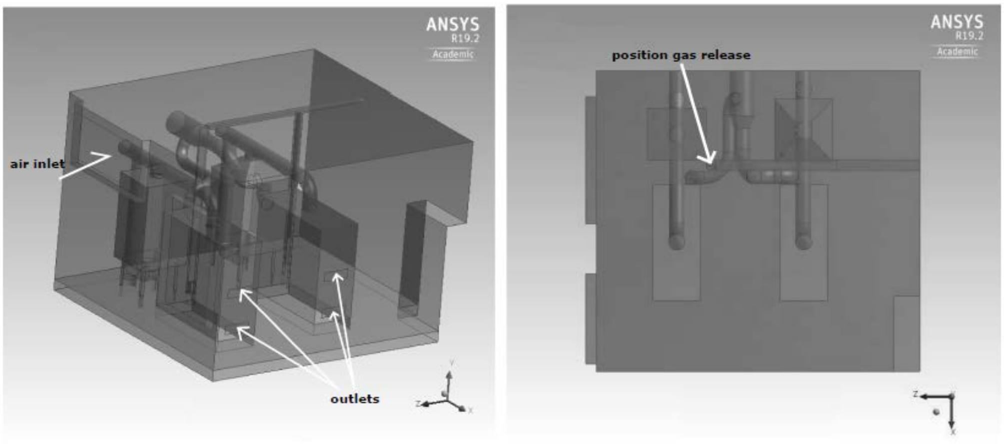
length l in m	**width b in m**	**height h in m**	**volume V in m³**
5.085	4.73	3.58	86.11

Tab. 1: Dimensions and the volume of the machine room.

The dimensions of the process equipment in the machine room are given in Tab. 2. The machine room has four exhaust air openings and one supply air opening. Two air exhaust openings are located 25 cm above the ground and two openings at approx. 1 m above the ground. The supply air opening is located close to the ceiling, see Fig. 1.

pos. nr	**units**	**dimensions l x b x h in cm³**
1.1	gas turbine	191.5 x 183.5 x 76
1.2	gas turbine	191.5 x 183.5 x 76
1.3	heat exchanger	81.5 x 93 x 153.5
1.4	heat exchanger	92 x 100.5 x 130
2.1	junction box	119 x 41 x 210

Tab. 2: Dimensions and the volume of the machine room.



(a) (b)

Fig. 1: (a): Top left view of the designed geometry. (b) Top view of the designed geometry. The in- and outlets are marked.

In order to perform a mesh independence study of the CFD simulation, three meshes with different refinement levels of the machine room are generated. The cell number of the three meshes are shown in Tab. 3.

refinement level	**normalized mesh size h_n**	**cell number**
Coarse	3	1 062 726
Medium	2	460 704
Fine	1	212 110

Tab. 3: Refinement level, the normalized mesh size h_n and the number of elements used for the mesh independence study.

The skewness of more than 90% of the cells is smaller than 0.5. The independence of the mesh is examined at the floor of the engine room and at one plane in 2.5 cm distance to the ground. The concentration in four cells on the floor and four cells on the plane parallel to the floor of the machine room are analyzed. The procedure corresponds to the suggested method from NPARC Alliance (Baker, Kelly, and O'Sullivan 2020).

CFD simulations

Simulations are performed with ANSYS Fluent (Fluent 2020) and the species transport model. Due to limited spatial resolution, the turbulence model realizable k - ε is selected to model unresolved eddies (Fluent 2020). The Birch 1984 approach (Birch et al. 1984) is used to define the gas propagation surface (diameter: $d = 4$ mm). The CO_2 or the propane-inlet is defined by a named selection and velocity inlet boundary condition which corresponds to the speed of sound (Landau and Lifshitz 1959). The air and gas outlets are defined as velocity inlets with negative speed. Openings are defined by pressure inlets. A pressure based solver (Fluent 2020) and an implicit transient solution method (Fluent 2020) are used. For the verification, two simulations are investigated: In one simulation the release of propane and in the other the release of CO_2 are simulated. For the validation of the CFD simulation the concentration is measured at 190 points in the machine room and compared with the simulation results.

Experimental set up

In the measurements CO_2 is released into the machine room through a standard hole according to EN 60079-10-1 (5 mm²). The measured mass flow is 5.90 ± 0.50 g/s. The room temperature is about 300 ± 3K and the pressure is about 92400 ± 100Pa. The air exchange rate is about 25 ± 3 1/h. Gas sensors are positioned parallel to the floor of the machine room. Furthermore, the concentration below the release source is investigated. The measuring device used is the X-am 7000 from the company Dräger. The measuring sensor used is the Smart IR CO2 HC. Errors for the measurements are shown in Tab. 4.

concentration error	< ±1Vol.-% (0Vol.-% - 20Vol.-%)
concentration error	< ±5%of the measured value (20 Vol.-% - 100 Vol.-%)
location error	between ±5.6 cm and ±6.8 cm
time-related error	negligible

Tab. 4: Defined errors for the concentration measurement.

Results

The simulated combustible gas cloud of propane is shown in Fig. 2 (a). It can be seen that the gas cloud is located at the floor area of the machine room. Fig. 2 (b) shows the gas cloud corresponding to 50% LEL. Considering the 50% LEL gas cloud the extent of the cloud extends into the ceiling area of the machine room. The simulated time corresponds to 3 minutes. This time-step is taken, since this is the critical time when a “quasi-stationary” flow field is found. There are areas in the machine room in which no explosive atmosphere is present. Furthermore, there are areas with small velocity in which the gas cloud is mainly located.

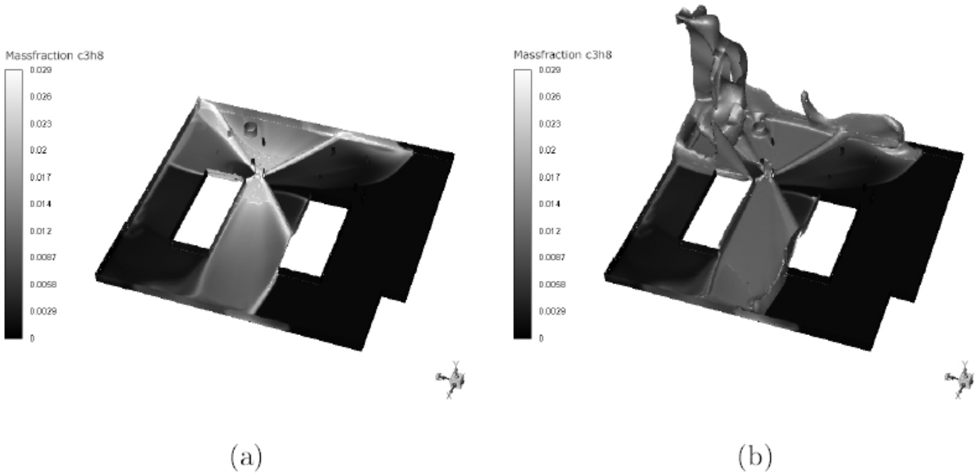


Fig. 2: (a) Representation of the explosive gas cloud. (b) Representation of the concentration cloud corresponding to the 50% LEL of propane.

In Fig. 3 the measurement results and the distribution of concentration can be seen in two of the five planes considered.

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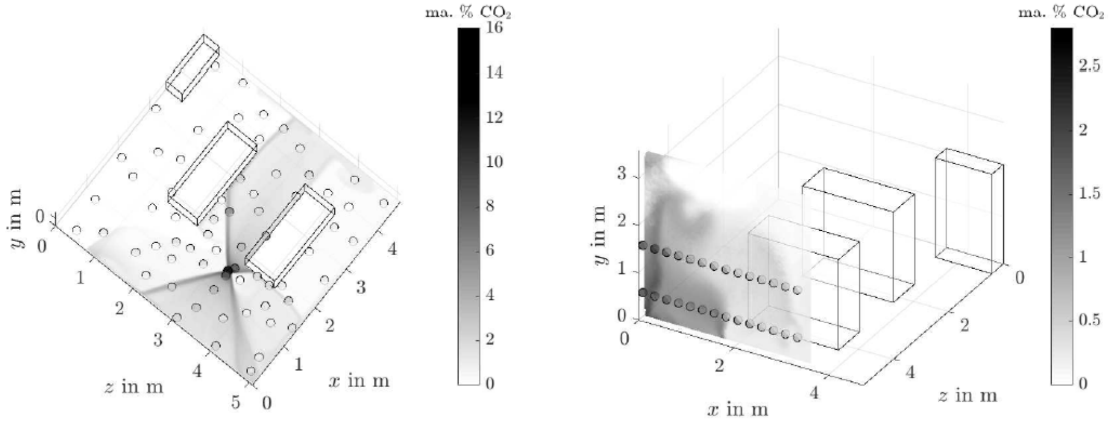
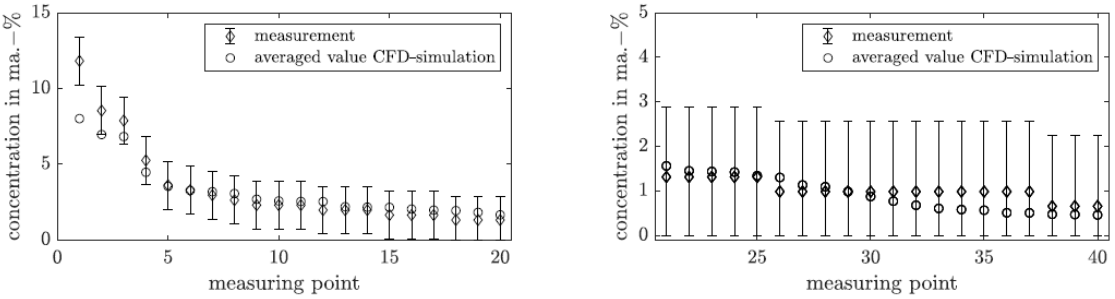


(a) (b)

Fig. 3: (a) Presentation of the measurement results on the floor and in one plane parallel to a wall of the machine room (b). Included is the concentration distribution calculated by the CFD simulation.

Fig. 4 shows the measured results and the temporally averaged CFD results on the ground of the machine room, see Fig. 3 (a). The temporally average results of the CFD simulation correspond to the mean concentration within the defined error. For this purpose, the cell values within the error sphere, which radius corresponds to the local error, are averaged. With the exception of one measured point, all other CFD results are within the considered errors of the experimental results. The deviation of one measured value results from the averaging of the results. High concentrations are more localized. In total, only 40 measurement results are shown, since the concentration of the other measurement values is close to zero and these also agree with the simulation results within the error range.



(a) (b)

Fig. 4: Representation of the measured concentration values and the averaged results of the CFD simulation for 40 points on the floor of the machine room.

Fig. 5 (a) shows the results of the CFD simulation along the first measured line (y = 0.5 m), see Fig. 3 (b). The measured values are symbolized by spheres. A tendential agreement between the measured values and the CFD simulation can be detected. A significant agreement between the measured values and the CFD simulation cannot be determined due to the large measuring error.

The release takes place towards the ground with a distance to the ground of 36 cm. In Fig. 5 (b) the concentration values of the CFD Simulation and the measured values along the center

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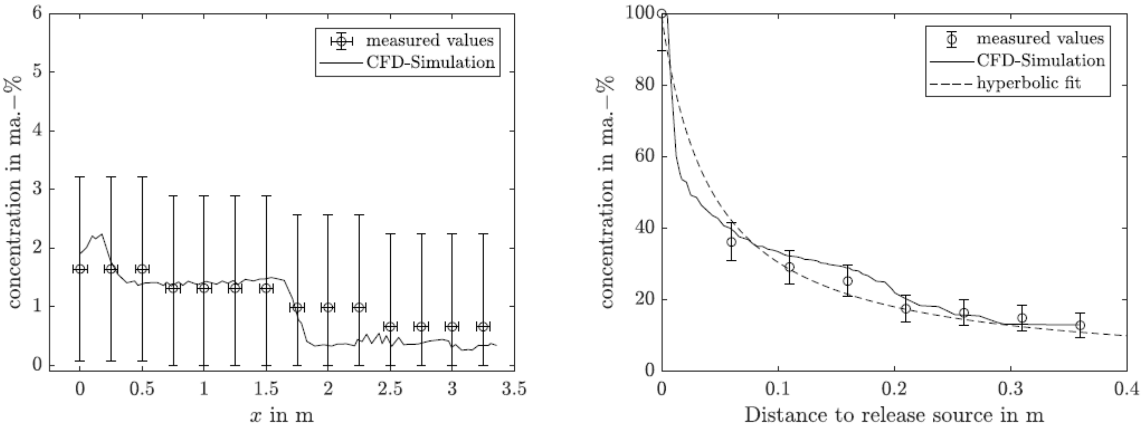
of the release cone are shown. In addition, the hyperbolic decrease is shown as a dashed line. For reasons of overview, the local error is not specified in Fig. 5 (b). The location error is shown in a Tab. 4. The measurement results agree with the CFD simulation in the defined error range.



(a) (b)

Fig. 5: (a) Representation of the measured values and the results of the CFD simulation of the lower measured concentration line in Fig. 3 (b). (b) Representation of the measured concentration values in the middle of the release cone. The continuous line describes the concentration values of the CFD simulation along this line. The dashed line symbolizes a hyperbolic decrease in concentration predicted in literature.

Two measurement planes are not considered explicitly, but the measurement results of these planes and the CFD simulation also agree within the defined error. In the case of large measurement errors, at least a tendency of agreement can be observed. At cells where no concentration was measured, no concentration is numerically calculated by the CFD simulation too. For the determination of the explosive distance, safety factors as well as the 50% LEL gas cloud are used. For this reason, the agreement between the measurement results and the CFD simulation is sufficient for the application under consideration.

Tab. 4 shows the results of the mesh independence study. Grid independence is valid for all investigation cells.

cell	**p**	**$GCI_{2,3}$**	**$GCI_{1,2}$**	**$\varepsilon_{1,2}$**	**$\varepsilon_{2,3}$**	**$f_{hn=0}$**	**κ**
1	1.82	2.91	10.92	0.06	0.22	0.49	1.06
2	0.83	14.97	29.43	0.09	0.18	1.60	1.10
3	1.48	5.17	15.55	0.07	0.22	8.04	1.08
4	2.57	2.25	14.66	0.09	0.58	1.90	1.10
5	2.86	6.47	23.30	0.11	0.41	3.33	1.13
6	2.20	8.39	22.62	0.10	0.26	2.21	1.11
7	4.47	80.34	114.60	-3.30	-4.70	0.01	0.23
8	4.32	0.33	1.95	0.01	0.08	9.27	1.01

Tab. 4: Results of the grid convergence study.p … order of convergence, GCI … grid convergence index, ε … relative errors, $f_{hn=0}$ …. extrapolation for a grid with 0 mm resolution, κ … asymptotic convergence. Point 1 to 4 are on the ground of the machine room. Point 5 to 8 are in the plane parallel to the ground.

Comparison of Classification Methods

Classification according to EN 60079-10-1 (Bozek 2017) leads to an explosive distance of approx. 6 m. The determined mass flow (5.99 g/s) corresponds to the measured mass flow within the defined error. The release characteristic can be determined from the mass flow using a safety factor (k = 0:5) and the LEL (1.7 VOl.-%) of propane (Oldenburg 1966). The calculated release characteristic is about 0.43 m³/s. Diagram D.1 according to EN 60079-10-1 is used to determine the explosive distance. In this case, this means that an explosive atmosphere is expected in the entire machine room. Using a CFD simulation as an alternative basis for assessment leads to the presence of an explosive atmosphere only near the ground. However, precise knowledge of the direction of release is assumed. In addition, the CFD simulation leads to a more differentiated view of explosive atmospheres and a more precise localization can be carried out. For instance, no explosive atmosphere is expected in certain areas. Furthermore, in individual areas an explosive atmosphere is unlikely to occur and the position of the ventilation openings plays a crucial role. E.g. the gas cloud shown in Fig. 2 shows an expansion up to the air-inlet. This is due to the absence of air flow in this area.

Conclusion

Explosion protection based on the EN 600079-10-1 1 is connected with many approximations and assumptions. In this contribution, a hazardous area classification based on EN 600079-10-1 is shown for a small machine room. But with this methodology not every case of gas releases and zone formations are described. With CFD simulations a hazardous area can be described more accurately. It is shown, that a CFD study of an explosive atmosphere can lead to a much smaller hazardous distance of the atmosphere. Certain areas can be observed in more detail and new knowledge can be gained. However, the evaluation according to EN 60079-10-1 does not lead to a dangerous misjudgment of an explosive atmosphere. The evaluation according to EN 60079-10-1 is quite permissible as a conservative estimation and evaluation. At the moment CFD simulations are not being used in small industry frequently. The main reason for that may be the high costs. Nevertheless, in the next years the number of useful CFD simulations for explosion protection will increase, because of its advantages described. So if the industry uses CFD simulations more frequently to gauge explosive atmospheres, more and more useful models will be available and the costs will decrease.

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