CFD modelling of pressurized gas releases: sensitivity analysis of driving parameters

CFD modelling of pressurized gas releases: sensitivity analysis of driving parameters

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The consequences analysis is a crucial aspect of the Risk Assessment, especially for Oil & Gas structures, where hundreds of accidental scenarios must be simulated. This work investigates the accidental release of high-pressure flammable gas in a congested offshore environment considering multi-physics and multi-scale nature of the phenomenon. Initially, the flow results supersonic with compressible effects and then it evolves in a subsonic dispersion. To handle this change of physics, a Computational Fluid Dynamics (CFD) two steps approach is developed at the SEADOG laboratory in Politecnico di Torino. This approach imposes two simulations: the first one considers the compressible phenomena in a small domain called Source Box (SB), the second one considers the gas dispersion in the platform. The advantage is to use the results of the first simulation as an input for several dispersion simulations. The aim is to compile a library of plausible SB and to evaluate the consequences of an accidental scenario selecting the proper SB for the dispersion simulation, allowing a timesaving. This work is focused on the optimization of the number of SB to construct a SB library. The objective of this work is to achieve a sensitivity analysis on the input parameters (release pressure, hole diameter, distance and dimension of an obstacle inside the SB) in order to optimize the number of SB to be simulated reducing the computational effort.

Keywords: Risk Assessment, safety, Oil & Gas, gas release, high-pressure, CFD, ANSYS Fluent.

1. Introduction

Risk Assessment procedures are in continuous development, especially for complex industrial installations involving the presence of hazardous substances; a Quantitative Risk Assessment (QRA) is mandatory according to laws and needs to be always optimized as the technology and safety requirements are growing rapidly. In particular, QRA needs the simulation of hundreds of accidental scenarios; the state of practice for all the onshore installations is based on the use of empirical methods, whose simplicity and fast response permit their utilization during the plant design phase. The limits of these methods regard their incapability to model complex geometries and physical phenomena: if a hazardous high-pressure gas leakage happens in a congested plant, these models fail in modeling the interaction with the surrounding structures, which strongly influences its flow pattern, and the compressibility effects typically characterizing high-pressure jets. Empirical methods neglect the jet-obstacles interaction, leading to an overestimation of the damage area extension, hence to an excessively conservative design which main consequences are the waste of resources and money, and nonetheless, the mechanical overloading of the plant structures. The necessity of more realistic consequences evaluations suggests the use of more accurate methods for the accidents simulation, like the Computational fluid-dynamics (CFD). This approach seems the most appropriate, but its implementation in the risk assessment procedure is nowadays infeasible due to the high computational time required, which results incompatible with the design phase schedule. The SEADOG lab researchers at Politecnico di Torino have been working on an optimized CFD approach aiming at guaranteeing a suitable cost-accuracy trade-off for the simulation of accidental pressurized gas releases in congested industrial environments.

In the present work, a high-pressure methane leakage from a small hole in a congested environment is considered. The phenomenon is complex and for simplicity it will be split in two parts: *release* and *dispersion*. Near the rupture, the released gas is under-expanded and tends to adjust to the ambient conditions through some expansion and compression waves (shock waves). The resulting flow is supersonic and highly compressible with strong discontinuities of the flow field variables, clearly represented by the presence of a Mach disk: this is the "*release*" phase. Once the gas adjusts to the ambient conditions, the flow becomes subsonic and incompressible: this is the "*dispersion*" phase.

1.1 *Literature review and motivation of the work*

Several studies were performed on accidental high-pressure gas leakages modeling. In Wilkening and Baraldi (2007), the authors

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simulated both the release and the dispersion of pressurized hydrogen through a single CFD simulation. The resulting computational cost was considerable, in fact, High-Performance Computing was employed to make the calculations; the motivation is that the release poses some strict constraints in order to resolve appropriately the initial expansion of the jet: dense mesh and very small time-step. To avoid this time-consuming simulation, (Venetsanos et al. (2008); Choi et al. (2013); Liu et al. (2014, 2015); Deng et al. (2018)) proposed to split the calculation of the release and dispersion phases. In (Deng et al. (2018); Liu et al. (2015)), the high-pressure natural gas and CO_2 pipeline ruptures are considered, respectively. In both cases, the release is treated through the *Birch model:* a *pseudo-source* is calculated and used as input of the dispersion. The initial expansion of the gas is accounted in this pseudo-source, which is assumed to be positioned in correspondence of the first Mach disk. All the variables of the source (pressure, temperature and velocity) are calculated by the model and an equivalent diameter is found. In (Choi et al. (2013); Venetsanos et al. (2008)), a similar approach is used for the simulation of a high-pressure H_2 leakage; in particular in Choi et al. (2013), an equivalent flow rate at the end of the initial expansion is calculated hypothesizing the *blockage effect*, i.e. the supersonic velocity of the gaseous jet can be neglected since the gas is rapidly slowed down by the presence of the adjacent components. In Venetsanos et al. (2008), the source term is evaluated, instead, with the alternative *Fanno flow* model. In Liu et al. (2014), the high-pressure CO_2 leakage from a pipeline is studied. The release is modeled via CFD, the flow is fully resolved, and the expansion of the jet is accurately reproduced in order to find the input values for the dispersion. It is important to underline that in the release simulation a free jet is considered, i.e. no interaction between the supersonic jet and an obstacle is modeled. The approaches proposed by (Wilkening and Baraldi (2007); Venetsanos et al. (2008); Choi et al. (2013); Liu et al. (2015); Deng et al. (2018)) are very cheap from the computational point of view but too coarse for our purposes, in fact if an object is placed near the release hole, the interaction must be accounted, and this means that the flow-field must be resolved. The approach presented in Liu et al. (2014) seems to be the best solution also for our purposes, but there still is a missing point: the jet-obstacle interaction. In fact, a cylinder or a flat plate in front of the release point can change dramatically the jet behavior, and this can't be neglected in complex geometries.

In the two-steps approach adopted in this paper, the supersonic release phase is computed in a small domain, called Source Box (SB), where also the interaction with a near-obstacle is considered. The results of the release are then used as input of the dispersion simulation. Furthermore, it is proposed to collect the results of a set of relevant release simulations (different SB) in a catalog: when a particular accidental scenario is needed, the release results are ready to be used as input for the successive dispersion phase. Therefore, only the dispersion phase will be simulated, which has a very low computational cost since the flow can be assumed incompressible and the flow-field variable gradients are very low. This approach permits a drastic reduction of the overall computational time.

Each release, and consequently each SB, is characterized by several parameters (pressure, type of gas, hole size, etc.); it is fundamental to perform a sensitivity analysis in order to optimize the catalog and avoid "redundant" or "non-relevant" combination of parameters.

The specific outcome of the research presented here is the preliminary result of the sensitivity analysis on the SB; therefore, for this work only the release phase is considered.

A literature review on the high-pressure gas releases was performed in order to understand the physics of the problem and its computational issues. The high-pressure gaseous releases were studied in the past from an experimental (Birch et al. (1987); Lovreglio et al. (2016)) and numerical (Birkby and Page (2001); Fairweather and Ranson (2006)) point of view and their behavior is well known. Nonetheless, it must be underlined that in the works analyzed a free jet is always considered; instead, the proposed approach considers the obstacle presence near the release point, i.e. the supersonic jet-near obstacle interaction is also modeled.

2. Methods

2.1 *Description of the problem*

The two-steps model adopted in this work is conceived to provide a valid CFD simulation method for safety analysis of plants involving toxic and/or flammable pressurized gases; in particular, in this work the supersonic phase of a high-pressure methane release in a congested environment is analyzed: the supersonic jet impinging on a near cylindrical obstacle is modeled.

The phenomenon is characterized by several parameters, identified according to the method proposed by Vivalda et al. (2018), in which the identification of a sufficient set of representative release scenarios for CFD simulations aiming at consequences estimation is discussed. Starting from the study of literature, statistics and investigation reports on offshore Oil & Gas platforms loss of containments, a set of representative scenarios is selected, and consequently a set of characteristic parameters with their own ranges are defined. In this work, only the parameters related to the release phase are considered:

- p_0: release pressure (10-80 bar);
- d_e: hole diameter (1-5 cm);
- d_{cyl}: diameter of the cylindrical obstacle (9-17 cm);
- l: distance between the release point and the center of cylinder (d_{cyl} - $2d_{cyl}$).

2.2 *Source Box definition*

The Source Box (SB) is a small portion of the domain modelling the supersonic jet and its impingement with the near cylindrical obstacle. In the SB the compressibility effects are considered and must be exhausted in its volume; for this reason, an appropriate dimensioning rule for this domain is essential.

Crist et al. (1966) suggested an experimental correlation according to which the compressibility effects are not anymore relevant when the distance from the release hole becomes bigger than ten times the first Mach disk distance from the release hole (X_M). Different authors, e.g. Franquet et al. (2015), defined the first Mach disk position as:

$$X_M = 0.645 \cdot d_e \cdot \sqrt{p_0/p_a} \qquad (1)$$

where p_a is the ambient pressure.

According to Eq. (1), the resulting source box side length is:

$$L_{SB} = 10 \cdot\ 0.645 \cdot d_e \cdot \sqrt{p_0/p_a} \qquad (2)$$

where L_{SB} represents the length of the sides of a cube, the most conservative shape in order to ensure that all the compressibility effects are exhausted in the SB in all the directions (Carpignano et al. (2017)).

The SB includes also the obstacle and it is characterized by the parameters discussed in section 2.1 (Fig. 1).

As each parameter has its own range of plausible values, if all the combinations are considered, the catalog composed by the potential SB becomes very large and its construction becomes hugely expensive. In order to avoid this time-consuming process and reduce the number of SB to be simulated, it is necessary to perform a sensitivity study on the characteristic parameters.

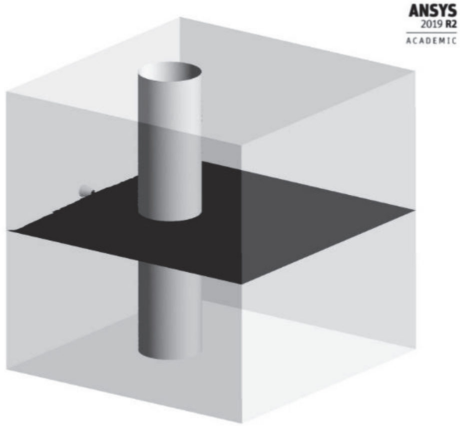

Fig. 1. 3D SB and reference 2D plane.

3. Sensitivity study

The sensitivity study regards a geometric ratio, involving the parameters l and d_{cyl}, and the release pressure. The former was investigated in order to reduce the number of representative geometric configurations and the latter to see if some useful relations between input and output variables could be extrapolated. Since a large number of simulations are necessary for the sensitivity analysis, it was chosen to perform a 2D analysis on a significant SB plane (Fig. 1), which is the midplane transversal to the obstacle and contains the jet axis. This plane is the most representative since it involves all the useful geometrical parameters (l, d_{cyl}) and since it contains the maximum jet separation due to the impingement with the obstacle.

3.1 *Geometric ratio l/d_{cyl}*

For this study, some parameters were fixed: d_e = 1 cm and p_0 = 10 bar. A set of cylinder diameters is selected, and the distance l is varied in such a way to define 5 different values of the ratio l/d_{cyl} for each d_{cyl} value:

- d_{cyl} = 9-10-12-15-17 cm;
- l/d_{cyl} = 1-1.25-1.5-1.75-2.

In this way 25 different geometric configurations are analyzed. The results are discussed in section 4 paying attention to the gas velocity and CH_4 mass fraction (CH_4 m. f.) on the SB outer boundaries, since they represent the input for the dispersion simulation, i.e. they influence the final pollutant dispersion and consequently the damage area.

3.2 *Release pressure p_0*

For this sensitivity study the geometric configuration was fixed, and characterized by these parameters: d_e=1 cm, d_{cyl}=10 cm, l/d_{cyl}=1.5 and L_{SB}=0.57 m.

The release pressure p_0 is varied from 10 to 80 bar with a step of 5 bar. It can be noticed that the SB dimension is fixed, while in theory it should change according to the different pressures (see Eq. (2)). To simplify the study, we choose to size the SB according to the maximum pressure (80 bar); in this way it is assured that the compressibility effects are always exhausted in its volume and there is no need to re-mesh each domain. Finally, also in this case, the gas velocity and mass fraction on the SB outer boundaries are analyzed.

3.3 *CFD simulation settings*

Since the problem involves some symmetries in the geometry and boundary conditions, the computational domain was reduced by half: in particular, the plane considered for the 2D analysis can be divided along the jet axis direction, which becomes a symmetry axis. Another important feature of the domain is the presence of a convergent nozzle in correspondence of the release point useful to properly model the fluid-dynamic jet behavior, i.e. to guarantee a choked flow condition. In the following paragraphs more details about the simulation's implementation are given: some terminologies come from the adopted software, ANSYS Fluent 18.2.

3.3.1 *Mesh generation*

Due to the high exit velocity, the resulting flow is highly directional, therefore a structured mesh is adopted, as it is suggested for this kind of flows (Jiyuan et al. (2018)). A non-uniform mesh is generated, in order to optimally model the high flow field variations in the Mach disk region (shock wave), and the jet-obstacle interaction. The "inflation layer" algorithm has been adopted to model the boundary layer arising at the jet-wall interaction, i.e. jet-nozzle wall and jet-obstacle wall. A convergence study has been performed in order to ensure the solution independence from the computational grid. The resulting mesh is shown in Fig. 2, it consists of ~ 27 000 elements which sizes vary from 5e-4 to 8e-3 m passing from the finest region to the coarsest one; the inflation layers were optimized for the different wall regions considering a y+ value lower than 5 (Munson et al. (2009)).

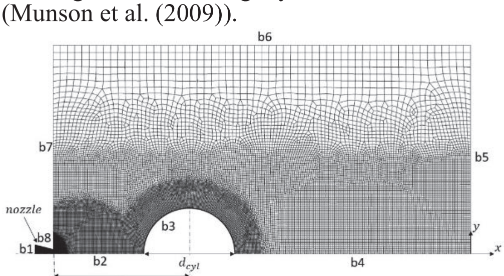

Fig. 2. Computational domain mesh and boundary names.

3.3.2 *Boundary conditions and numerical models*

To explain the boundary condition settings the Fig. 2 can be considered. The boundary conditions are set in this way: pressure inlet on b1, pressure outlet at b5-b6-b7, wall at b3-b8 and symmetry at b2-b4.

In the different simulations of the sensitivity analysis the pressure inlet is set according to a case study definition, on the wall boundaries a no-slip condition is set and for the pressure outlet the ambient pressure is imposed.

All the simulations were performed in steady state since the final configuration of the jet is of interest for the purpose of this analysis. The chosen turbulence model is the SST k-ω; the viscous dissipation term is included in the energy equation, as it becomes relevant for high velocity compressible flows (ANSYS Fluent user's guide (2018)). The "Species Transport" model is used in order to solve a transport equation modelling the CH_4-air interaction. As a compressible flow is involved, the energy equation is solved in addition to the momentum equation in order to evaluate the temperature flow field needed by ideal gas law for the calculation of the density.

4. Results

4.1 *CFD results consistency*

Before discussing the sensitivity analysis results, it is important to ensure that the fluid-dynamic behavior of the jet is correctly reproduced in all the simulations.

Since gas releases with $p_0 \geq 10$ bar discharging in ambient pressure are considered, the ratio p_0/p_a is always larger than 10, therefore, the resulting jet is always highly under-expanded (Franquet et al (2015)). In Fig. 3 a 10 bar CH_4 release from a circular hole with d_e = 1 cm is shown. As expected, the rapid expansion of the methane in the air generates compression waves leading to the formation of a Mach cell: a typical fluid-dynamic structure of highly under-expanded jets. Furthermore, a Coanda effect is visible in the jet-

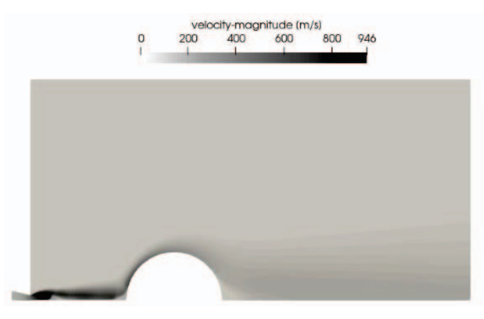

Fig. 3. Velocity contours.

cylinder interaction as expected from jet theory. The physics seems very well reproduced in the simulation, and in agreement with most of the available literature, therefore the next step is the analysis of the sensitivity study.

4.2 *Sensitivity analysis results*

4.2.1 *Geometric ratio l/d_{cyl}*

In Fig. 4 and Fig. 5, the average velocity and CH_4 m. f. behaviors at the SB outlet b5 are shown in function of the different d_{cyl} values; considering the curves with a fixed value l/d_{cyl}, no matter the value of the ratio, the velocity or CH_4 m. f. tends to decrease as the diameter of the cylinder grows and it is further away. It seems that the effect of the obstacle tends to decelerate the flow and permits a higher mixing between the CH_4 and the surrounding air as it is bigger and distant. A general comment can be proposed: the obstacle presence influences the jet and in this case it causes a reduction of the velocity about ~10 m/s as d_{cyl} goes from 9 to 17 cm. Looking at this difference in terms of percentage on the maximum velocity value, a reduction of about 30% is noted, which is a relevant reduction with respect to the subsequent dispersion, happening at very low flow speeds. Starting from the previous point, it can be deduced how considering a free-jet for the release (as done in the works reviewed in the introduction), can induce very large overestimation of the flow speed and CH_4 concentration, leading to larger dangerous zones in terms of flammable areas.

The most significant result which can be appreciated from Fig. 4 and Fig. 5, is the slight difference occurring in the velocities and CH_4 m. f. for a fixed value of d_{cyl} no matter the ratio l/d_{cyl}, the velocity or mass fraction values are inside a small range defined by an error bar of 3 % around the mean value; this result suggests that a lot of geometrical configurations with a l/d_{cyl} ranging between one and two can be neglected in the SB catalog compilation, because the difference in the output values is negligible.

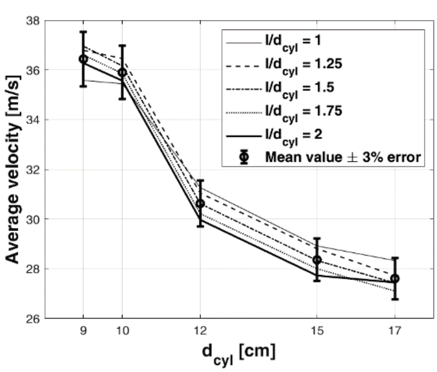

Fig. 4. Average velocity on b5 boundary, in function of d_{cyl} for different l/d_{cyl}.

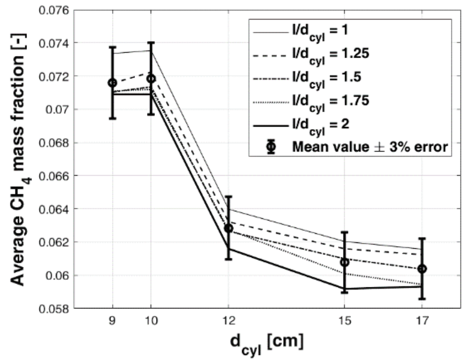

Fig. 5. Average CH_4 m.f. on b5 boundary, in function of d_{cyl} for different l/d_{cyl}.

From a general point of view, the results show that if a release impinging a nearby cylinder is under consideration, a set of different geometrical configurations can be represented only by one, with a certain l/d_{cyl} ratio. For any application which needs the simulation of a large set of scenarios this result can simplify considerably the work reducing the computational time.

This last consideration is valid for the average value of the output variables, but since the subsequent dispersion of the pollutant is of interest for this study, also the spatial description of the phenomena becomes relevant. For this reason, the spatial distributions of the velocity and CH_4 m. f. are analyzed on the output b5. Considering the case with d_{cyl}=10 cm, the velocity and mass fraction profiles for the different l/d_{cyl} ratios are represented respectively in Fig. 6 and

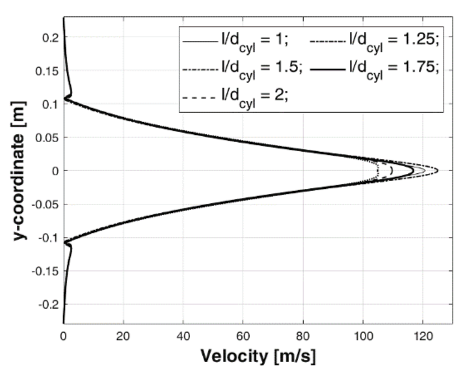

Fig. 6. Velocity profiles for different l/d_{cyl}.

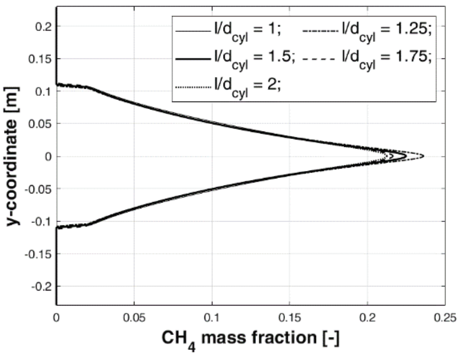

Fig. 7. CH_4 m. f. profiles for different l/d_{cyl}.

Fig. 7 in function of the y-coordinate along the boundary b5.

As it can be seen, for both quantities a simil-gaussian distribution is obtained no matter the geometric ratio, and the profiles are all nearly coincident except for a narrow region around the peak. The study in terms of space distribution confirms the result obtained looking at the average values: if a cylinder diameter is defined, the distance *l* does not have a relevant effect in the selected range.

This result has a strong impact on the SB catalog construction; if, for example, the parameters ranges defined in section 2.1 are considered, using these discretizations: 14 pressure levels (p_0 varied with a 5 bar step), 3 diameters (d_e varied with a 2 cm step), 8 cylinder diameters (d_{cyl} varied with a 1 cm step) and 10 distances values (l), the resulting SB total number for the catalog will be ~3360, but, since it has been proven that the factor *l* has no relevant effect on the interest output results, the initial SB number can be drastically reduced; in fact, by neglecting the 10 possible geometrical configurations defined by the *l* variation, the resulting useful SB number could be ~336: a strong improvement in terms of computational cost saving is achieved.

4.2.2 *Release pressure*

First of all, to check that the physical phenomena are correctly reproduced in each simulation, i.e. a highly under-expanded jet is reproduced, the Mach disk position obtained numerically can be compared with the theoretical one obtained using Eq. (1). In Table 1 the results are summarized.

Table 1. Mach disk positions: theoretical vs numerical estimation and relative errors.

p_0 (bar)	X_M (theory) (cm)	X_M (CFD) (cm)	Rel. err. (-)
10	2.0397	2.0172	1.1
15	2.4981	2.5222	0.97
20	2.8845	2.9262	1.4
25	3.2250	3.2293	0.13
30	3.5328	3.5323	0.02
35	3.8159	3.8353	0.51
40	4.0793	4.0373	1.03
45	4.3268	4.2394	2.02
50	4.5608	4.7394	3.91
55	4.7834	4.8404	1.19
60	4.9961	4.9414	1.1
65	5.2002	5.0404	3.07
70	5.3965	5.3434	0.98
75	5.5859	5.5474	0.69
80	5.7691	5.6484	2.1

The percentage error is quite small for all the simulations since it is always below 3.91 %, therefore the Mach disk position is acceptably well reproduced.

In Fig. 8 and Fig. 9 the average velocity and CH_4 m. f. on b5 are plotted in function of the pressure. For both quantities a linear behavior can be observed, in fact as shown in the same figures a linear fit can be derived for each of them with an

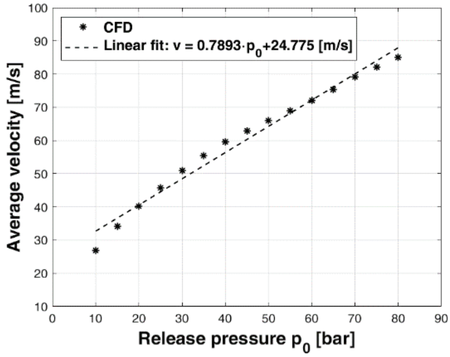

Fig. 8. Average velocity in function of the release pressure and linear fit of the numerical results.

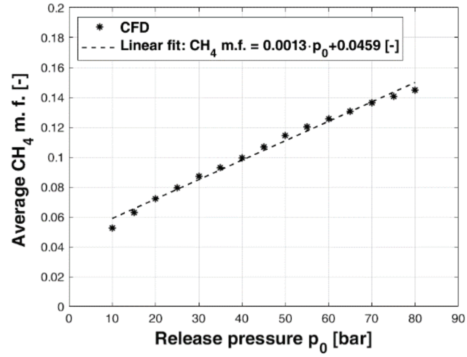

Fig. 9. Average CH_4 m. f. in function of the release pressure and linear fit of the numerical results.

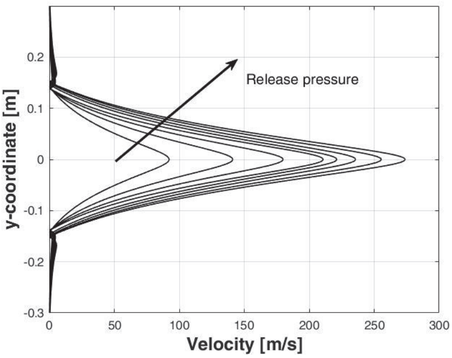

Fig. 10. Velocity profiles for increasing release pressure.

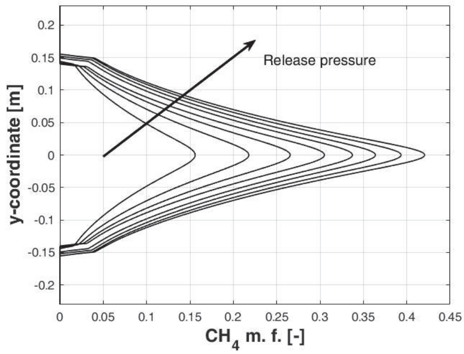

Fig. 11. CH_4 m. f. profiles for increasing release pressure.

accuracy, as the relative Pearson coefficient R is 0.9897 and 0.9949 respectively.

These last relations can be used to obtain velocities and mass fractions for a certain pressure in the range, without performing the simulation, therefore saving computational time; obviously, this is true only if average quantities are needed. In case a higher accuracy in the dispersion phase simulation is requested, spatial distributions of the input velocity and mass fraction must be used, and therefore it is crucial to see how the profiles evolve with the increasing pressure.

In Fig. 10 and Fig. 11 these results are presented. It can be appreciated that the distributions, in both cases, maintain a similar "shape" no matter the pressure; they resemble a Gaussian distribution (typical of the gas jets) with an increasing peak for increasing pressures. This result gives another important information: the spatial distribution of the quantities is similar for all the simulations with different pressures, as the geometry is fixed. This 2D study gives an important hint: a certain "regular" and "reproducible" behavior of the jet can be observed in function of the pressure, also looking at the spatial distributions.

This 2D study was instrumental to proving the feasibility of a possible algorithm development to reproduce the jet behavior in the SB. An analogous 3D study can now be performed in order to further develop the methodology, and ideally build a metamodel to reproduce the SB behavior avoiding the simulation of all the SB cases.

5. Conclusions

This work is part of a bigger project, which aims at developing a CFD tool for a fast and accurate simulation of toxic and/or flammable high-pressure gas leakages consequences in congested industrial environments. In particular, the CFD modeling adopted at the SEADOG lab in Politecnico di Torino is based on splitting the phenomenon in two steps: the *release* and the *dispersion*. The first one (the release phase) is simulated in a small domain, the source box (SB); the velocity and mass fraction profiles on its outer faces are used as input boundary conditions for the dispersion. In addition, the SB results are stored in a catalog in order to be used as input for a specific dispersion simulation, without repeating the release simulation and consequently assuring a relevant timesaving.

In the present work, a reference case study is chosen: the high-pressure methane release from a small hole in congested spaces. Starting from this study case, a sensitivity analysis on some parameters characterizing the SB is performed in order to optimize the construction of the SB catalog. At first, the physical consistency of the CFD solution is studied by comparing the fluid-dynamic jet structure with the correspondent theoretical references: this comparison shows a good agreement between computational results and theoretical expectations, suggesting that the simulations are well posed.

Successively, the sensitivity analysis involves two different parameters: a geometrical one, a relationship between the obstacle characteristic length (e.g. cylinder diameter d_{cyl}) and its distance from the release point (l), and the release pressure (p_0). The effect of different ratios l/d_{cyl} for a set of different d_{cyl} values is investigated.

The main outcomes follow:

- As the cylindrical obstacle is bigger and further away from the release hole, the flow is more slowed down and the methane air mixing is enhanced, therefore, the jet-obstacle interaction is more significant;
- For a fixed diameter (d_{cyl}), the effect of the distance l is negligible; in fact, the variations of the average velocity and CH_4 m. f. on the outlet faces are both negligible;
- The previous result can be extended to the spatial distributions of the output

velocity and mass fraction, since similar profiles are obtained varying l for a fixed d_{cyl}.

These results suggest that many geometrical configurations can be neglected, as their influence on the output values is negligible.
The main outcome is that the representative set of releases can be drastically reduced, and the SB catalog construction can be optimized.
In the end, a sensitivity analysis on the release pressure is carried out. It results that the average outlet velocity and mass fraction linearly increase as the pressure increases, and in both cases, a linear trend can be found with high accuracy. Furthermore, the spatial distribution of the velocity and mass fraction are analyzed, showing a regular behavior: as the pressure increases, maintain a similar shape no matter the pressure level. This result, obtained with a 2D analysis, shows that a certain regular behavior of the SB can be found, and it suggests that a method aiming at reproducing the SB behavior without making the simulation can be developed.
A future step will be an analogous 3D analysis to further develop the methodology and study the feasibility of a meta-model to reproduce the SB behavior, aiming at a faster SB catalog construction.

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