

Quantification of uncertainty in CFD simulation of accidental gas release for O&G quantitative risk assessment

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Abstract

Quantitative Risk Assessment (QRA) of Oil&Gas installations implies modeling accidents evolution. Computational Fluid Dynamics (CFD) is one way to do this, and off-the-shelf tools are available, such as FLACS developed by Gexcon US and KFX developed by DNV-GL. A recent model based on ANSYS Fluent, named SBAM (Source Box Accident Model) has been proposed by the SEADOG lab at Politecnico di Torino. In this work, we address one major concern related to the use of CFD tools for accident simulation, that is the relevant computational demand that limits the number of simulations that can be performed. This brings with it the challenge of quantifying the uncertainty of the results obtained, which requires performing a large number of simulations. Here we propose a procedure for the Uncertainty Quantification (UQ) of FLACX, KFX and SBAM, and show its performance considering an accidental high-pressure methane release scenario in a realistic offshore Oil&Gas (O&G) platform deck. The UQ of the CFD models is originally propagated to a set of risk measures that can be used to support the decision-making process to prevent/mitigate accidental scenarios.

Keywords: *Quantitative Risk Assessment (QRA), Computational Fluid Dynamics (CFD), Uncertainty Quantification, impinging jet, gas release.*

1. Introduction

The Oil&Gas (O&G) industry is hazardous to the environment and the people, due to the presence of dangerous fluids that may be toxic, flammable and pressurized (Ogwu, 2015). To ensure O&G plants safety, national and international regulations impose that risk assessment is mandatory (Vinnem, 2014). Modeling and simulation of accidental scenarios are essential for Quantitative Risk Assessment (QRA) (Casal, 2007 and Vinnem, 2019), to evaluate the consequences of accidents in O&G facilities. For offshore plants characterized by complex congested geometries, the state of practice is to use semi-empirical models (Carpignano, 2017), which lead to a large overestimation of damages and a consequent oversizing of the safety systems with waste of economical and material resources.

Computational Fluid Dynamics (CFD) for accident simulation can guarantee more accurate results, even for complex phenomena and geometries (Davids, 2013). Different tools and models, based on numerical techniques, are available: FLACS developed by Gexcon US and KFX developed by DNV-GL, but also innovative CFD approaches, such as the Source Box Accident Model (SBAM), developed by the SEADOG Lab Group of Politecnico di Torino.

However, the input parameters, numerical methods, and physical models used in CFD are affected by uncertainties, typically classified as: *physical modeling uncertainties* (e.g., boundary conditions, initial conditions, geometry, fluid properties, turbulence modeling uncertainties) and *numerical uncertainties* (e.g., discretization mesh size, round-off and iterative convergence uncertainties) (Hanna, 2018). These uncertainties need to be propagated through, for quantifying the uncertainty of the CFD output, in order to know the confidence on the results, used for decision-making on protective measures of the O&G facilities.

Physical modeling uncertainties include boundary and initial conditions uncertainties, turbulence model uncertainties, uncertainties due to the insufficient knowledge of the flow properties, uncertainties due to the approximation of the constitutive laws. They are due to assumptions in the formulation of the model and deliberate simplifications in the governing equations for the purpose of their solutions. Investigating physical modeling uncertainties is challenging due to the strong non-linearity of the models (Gorle, 2019). For this reason, appropriate probabilistic and non-probabilistic approaches are being developed (Gorle, 2013), but still far from being adopted and implemented (Heng Xiao, 2018).

Numerical uncertainties include discretization uncertainties and uncertainties in the numerical schemes adopted. In particular, they are caused, for example by: i) discretization of the mesh size, ii) discretization of the Navier-Stokes (N-S) equations that require iterative procedures to be solved, and iii) computing machine errors, which give an upper bound on the relative error due to rounding in

floating points (KeWen-Chyan, 2019). To minimize the discretization uncertainty, we may adopt two different strategies: either increase the order of the discretization scheme or adapt the mesh to improve the size/quality (François Frayss, 2019), with, in both cases, a dramatic increase of the computational burden.

In this work, we aim at structuring an Uncertainty Quantification (UQ) approach for CFD calculation that is computationally feasible, provides insights on the confidence of the results of the simulation, and supports decision-making, enabling robust design/reliability analysis and safety margins quantification for risk analysis (E. Colombo, 2012 and A. Cutrono, 2018). We limit the scope of the UQ to the discretization source of uncertainty, related with the mesh size used to represent the governing (N-S) flow equations and other physical models, such as algebraic expressions in a discrete domain of space (finite-difference, finite-volume, finite-element). To ensure that the solution of the discretized equations closely approximates that of the original equations (George Em Karniadakis, 2002), and quantify the spatial discretization uncertainty, we will rely on the Grid Convergence Index (*GCI*) method and a generalization of the Richardson's extrapolation (Richardson, 1911) ((Roache, 1998) and (F.Stern 1999), respectively).

Without loss of generality, in this paper, we present the UQ approach due to the discretization mesh size of the FLACS, KFX and SBAM models on a case study regarding a typical accidental high-pressure methane release in an offshore O&G platform. The effects of the propagation of these uncertainties to a set of risk measures are considered. In this regard, it is worth mentioning that in the O&G fields the state of practice is using the plume length of the flammable gas cloud as risk measure (Lloyd's Register, 2012); however, in a congested environment, as it usually is in O&G facilities, due to the presence of the obstacles, the gas cloud shape may differ from the typical "plume" and the severity of the accident might be underestimated. For a more realistic and risk-oriented analysis, the severity of the accident, e.g., the ratio between flammable volume and total volume (σ_{Damage}), the external perimeter of the platform reached by the flammable cloud (σ_{target}), and the flammable volume developed under 1.5 m ($\sigma_{d1.5}$), is considered in the risk measures used to support decision-making (for example, to decide the location of safety systems (e.g., fire-fighting system, fire doors, etc.) and setting of the control systems (e.g., sensors, gas detectors, etc.)):

- *Ratio between flammable volume and total volume (σ_{Damage}):*

$$\sigma_{Damage} = \frac{V_{Flammable}}{V_{TOT}} \sim [0,1] \quad (1)$$

where $V_{Flammable}$ is the volume occupied by an air-methane mixture within the flammability limits and V_{TOT} is the total volume of the domain. The larger σ_{Damage} , the worse the damage; in particular, if $\sigma_{Damage} = 0$, no accident has occurred, if $\sigma_{Damage} = 1$, the worst-case scenario has

occurred, i.e., the entire platform deck is enveloped within the flammable cloud.

- *External perimeter of the platform reached by the flammable cloud (σ_{target})* can be seen as a measure of possible damage to specific targets (e.g. escape routes) that in the offshore platform are commonly located on the external perimeter:

$$\sigma_{target} = \frac{P_{danger}}{P_{TOT}} \sim [0,1] \quad (2)$$

where P_{TOT} is the total perimeter of the deck and P_{danger} is the perimeter of the deck reached by the flammable cloud. The larger σ_{target} , the worse the damage; in particular, if $\sigma_{target} = 0$, the flammable cloud does not reach the target; if $\sigma_{target} = 1$ the whole target is enveloped within the flammable cloud.

- *Flammable volume developed under 1.5 m ($\sigma_{d1.5}$)* can be considered an important measure of the damage because the main electrical and mechanical components are placed on the floor; these can generate friction triggers and electrical triggers, which may ignite the flammable gas cloud, whereas, at higher elevation, the probability of having ignition sources is quite low:

$$\sigma_{d1.5} = \frac{V_{fla|u1.5}}{V_{Flammable}} \sim [0,1] \quad (3)$$

where $V_{fla|u1.5}$ is the volume of flammable gas under 1.5 m height and $V_{Flammable}$ is the total flammable volume on the platform. The scenarios with large $\sigma_{d1.5}$ are the most critical, because for such cases the volume of flammable gas is concentrated at low elevation, that increases the ignition probability.

The remainder of the paper is as follows: in Section 2, the CFD tools considered are briefly described. In Section 3, the validation of the FLACS, KFX and Fluent with respect to experimental data is presented, considering both the case of free-jet and of jet impinging a cylindrical obstacle. In Section 4, the realistic case study is described, and the qualitative and quantitative results presented. In Section 5, conclusions are drawn.

2. CFD Tools

In this Section, the CFD tools here used to carry out the release accident analysis are presented. In section 2.1, the CFD modelling approach based on ANSYS FLUENT, named SBAM (Source Box Accident Model) and developed by the research group of the SEADOG lab at Politecnico di Torino, is presented. In Section 2.2 FLACS, developed by Gexcon US, and KFX, developed by DNV-GL, are also introduced briefly. The interested reader may refer to (Pappalardo et al., 2020), for further details. For the sake of the CFD tools comparison and the description of the proposed UQ approach, without loss of generality, we will consider the simulation of a typical accidental high-pressure methane release

in an offshore O&G platform, that results in the build-up of a flammable cloud. The accidental scenario is widely known and consists in a gas release at high-pressure from a hole section in the form of an under-expanded jet (Franquet et al., 2015), that leads to the formation of a Mach disk (Franquet et al., 2015), with a compressible and supersonic flow (i.e., *release* phase). Moving away from the release point, the flow becomes slower, until the gas reaches the ambient pressure and starts to disperse at low velocities (~ 10 m/s), and can be treated as incompressible (i.e., *dispersion* phase). As we shall see in what follows, the FLACS, KFX and SBAM differ in the way this phenomenon is modelled.

2.1 SBAM

The basic idea behind SBAM is to model the release and the dispersion phases separately, using different assumptions and models. In fact, two CFD simulations are realized using ANSYS FLUENT, which solves the N-S equations by a finite volume approach: one simulation for the release phase and the other for the dispersion phase.

The former accounts for the initial jet expansion and its interaction with the nearby obstacle, and is performed in a dedicated and limited domain called Source-Box (SB) (Moscatello et al., 2021), in which the flow can be assumed and modeled as compressible. The domain is defined large enough to contain all the compressibility effects. The mesh is refined enough to fully resolve the Mach cell and the boundary layer arising from the interaction with the nearby obstacle; therefore, all the geometric details are considered, while the gravitational forces are neglected due to the high inertia of the flow which reaches a supersonic regime. The results of the release simulation are, then, used as input of the dispersion simulation, in which the flow is assumed incompressible and gravitational forces become relevant, as the velocities are in a subsonic regime (Moscatello et al., 2021).

In SBAM, an unstructured tetrahedral mesh is created in ANSYS FLUENT for both the release and the dispersion simulations, as it permits to save setup-time and limit mesh skewness; in fact, as complex geometries are involved both in the release and dispersion phases, the creation of a structured mesh can be extremely time-consuming or not possible or it could decrease the mesh quality. In addition, the unstructured mesh has a high-efficiency mesh distribution, which permits to create fewer cells than structured one (ANSYS FLUENT, 2018).

2.2 FLACS and KFX

The idea behind FLACS and KFX models is similar to SBAM, i.e., separating the analysis of the two phases (release and dispersion) in two different models. In FLACS and KFX, the supersonic jet behavior is described according to the semi-empirical Birch model, valid in a pressure range between

2 and 70 bars (Birch et al., 1984). The main idea of the model is to calculate characteristic values for the jet description after it has reached environmental conditions; in particular, (Birch et al., 1984) defines the concept of *pseudo-diameter* (d_{ps}), which is the value of the jet diameter when it reaches the ambient conditions, and, in an analogous way, a *pseudo-velocity* is introduced in correspondence of the pseudo-diameter. These *pseudo-values* are imposed on the cell surface corresponding to the new pseudo release point, from where the subsonic dispersion starts. In FLACS and KFX, the governing equations that describe the dispersion phase of the phenomenon are characterized by the fact that geometries are represented as a porous media. This new formulation of the transport equation is popularly called PDR method (Porosity Distributed Resistance) (Patankar & Spalding (1974)). The model is a generalization of the N-S equations for fluid flow and Darcy's law commonly used for flows in porous regions (Miguel et al., 2001). Geometries are represented as porous regions and the presence of obstructions modifies the governing equations in two ways: firstly, the volume of the obstruction is represented in the control volume in such a way that only the non-blocked areas are available for fluid flow; secondly, obstacles give additional flow resistance, which must be modeled. In FLACS and KFX, only a Cartesian structured mesh can be created, and a mesh refinement is applied near the release point to observe the gradients that develop. It is important to say that different levels of mesh refinement correspond to different geometric representations of the domain as a porous object. Among the Reynolds-averaged Navier–Stokes (RANS) equations, the most common is the Standard k- ϵ model (Launder and Spalding, 1974; Jones and Launder, 1972), and it is the only model that is implemented in both KFX and FLACS.

3. CFD Validation

The presented CFD tools are here compared with respect to experimental data of commonly adopted benchmark cases (i.e. free-jet and jet impinging on a cylinder) (Eggins and Jackson, 1974 and R.P. Cleaver, 1991). In Section 3.1, the free-jet validation case is presented, whereas in Section 3.2 the validation of the case of jet impinging on a cylindrical obstacle is summarized. It is worth to note that in this paragraph the considered tools are FLACS, KFX and a generic 2D Fluent approach: since SBAM is a 3-D model, useful for large, congested domains, in these validation cases a simpler and computationally manageable model has been considered sufficient. SBAM is, instead, used in Section 4, where the realistic case of the O&G offshore platform is analyzed.

3.1 Free jet validation

3.1.1 Benchmark description

The benchmark consists in a free jet, high-pressure CH_4 release in open environment. The scenario

considered refers to that presented in (Eggins and Jackson, 1974) and (Novembre, 2006); the characteristic parameters are summarized in the following:

- Hole diameter: $d_e = 0.5 \text{ m}$;
- Upstream pressure and temperature: $p_{rel} = 11 \text{ bar}$ $T_{rel} = 293 \text{ K}$;
- Environmental pressure and temperature: $p_{amb} = 1 \text{ bar}$ $T_{amb} = 293 \text{ K}$;
- Dimension of the simulated domain: 120 m (X-direction), 40 m (Y-direction), 8 m (Z-direction).

A schematic view of the simulated domain is presented in Figure 1.

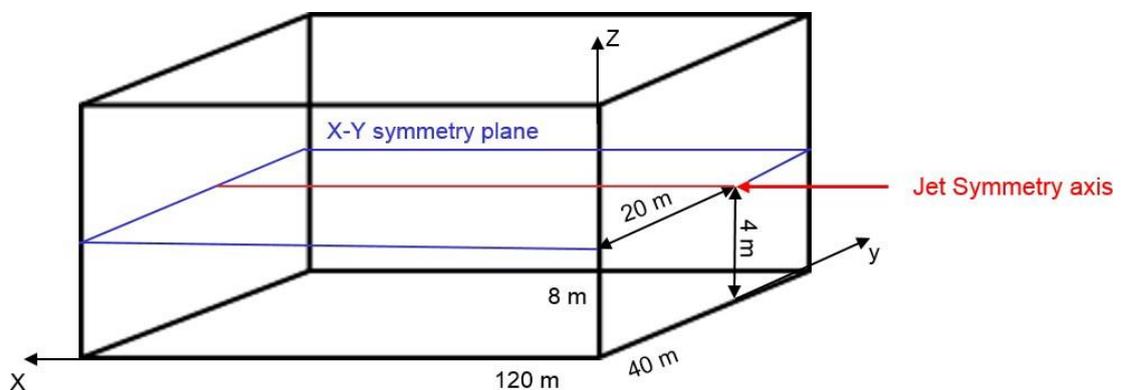


Figure 1 Simulation domain for the 'free jet validation' benchmark case

The boundary conditions, on the external faces of the domain are:

- FLACS
 - A mass flow is imposed on all the boundaries
 - semi-empirical Birch model is used for the release phase
- KFX
 - A static pressure (atmospheric) is imposed on all the boundaries
 - semi-empirical Birch model is used for the release phase
- Fluent
 - A static pressure (atmospheric) is imposed on all the boundaries
 - CH_4 concentration equal to 1, and pressure equal to 11 bars are imposed on the release hole.

3.1.2 Results

In FLACS and KFX, the following simulation conditions are set: a 3-D transient solver is used to solve the Reynolds-Averaged N-S equations (in fact KFX allows modeling 3-D processes) and the Standard k -

ε model is employed to model the turbulence of the flow (in fact the $k-\varepsilon$ turbulence model is the only turbulence model implemented both in FLACS and KFX).

In Fluent, the following simulation conditions are set: 2-D steady simulations using Standard $k-\varepsilon$ model as the turbulence closure equation, in order to be consistent with the simulations implemented in FLACS and KFX. The analysis is carried out on the $X-Y$ symmetry plane (see Fig. 2).

The obtained results are compared with the experimental data of (Eggins and Jackson, 1974), in relation to the CH_4 mass fraction decay along the jet symmetry axis. In Figure 2, the results are shown: it is possible to notice that, qualitatively, all the tools are capable of well describing the diffusion phenomenon, especially in the far-field region where all the tools trends converge. Fluent, however, is more accurate than the others in following the trend, and KFX is the worst.

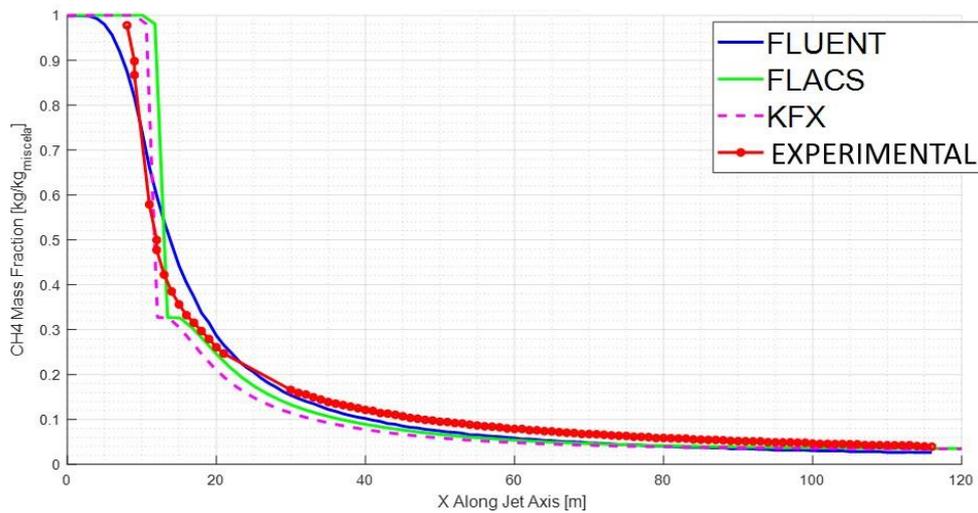


Figure 2 Mass fraction decay on the jet symmetry axis

From a quantitative point of view, the relative error (Err) between the curves can be calculated through (Eq.4) (Abramowitz, 1972):

$$Err = \frac{\|Z_{exp} - Z_{simul}\|}{\|Z_{exp}\|} \quad (4)$$

where $\|Z_{exp} - Z_{simul}\|$ is the norm of the difference between the experimental data and the FLACS, KFX, Fluent results, and $\|Z_{exp}\|$ is the norm of the experimental curve. In Table 1, the errors are listed, for each considered tool: Fluent commits the smallest error and KFX the largest.

<i>Err</i>	FLACS	KFX	Fluent
	5,0 %	12,2 %	1,46 %

Table 1 Error of the tools with respect to experimental data

3.2 Jet impinging on a cylinder

3.2.1 Benchmark description

This benchmark regards the impact of a subsonic CH_4 jet on a cylindrical obstacle. The scenario considered refers to that presented in (R.P. Cleaver, 1991), whose experimental data refer to the *dispersion* phase of a subsonic jet of CH_4 horizontally released to impact on a single cylindrical obstacle, whose length is longer than the diameter of the jet, and it is positioned perpendicularly to the jet. The phenomenon was studied for two different distances between the release point and the obstacle: 157 mm and 683 mm. A schematic view of the simulated domain is presented in Figure 3. The characteristic parameters are summarized in the following:

- Hole diameter: 0.0107 m
- Mass flow rate from the hole: $\dot{m} = 0.011$ kg/s
- Obstacle diameter: $d_{cyl} = 0.150$ m
- Distance, along the axis of symmetry, between the release point and the obstacle: $l = 683$ mm or 157 mm
- Dimensions of the simulated domain: 26 m (X-direction), 4 m (Y-direction), 24 m (Z-direction).

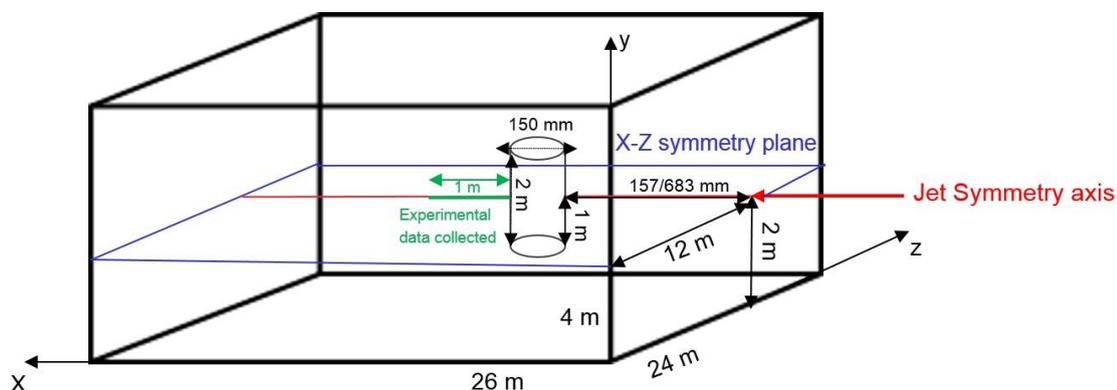


Figure 3 Simulation domain for the 'jet impinging on a cylindrical obstacle' benchmark case

The boundary conditions on the external faces of the domain are:

- FLACS
 - A mass flow is imposed on all the boundaries
- KFX
 - A static pressure (atmospheric) is imposed on all the boundaries
- Fluent
 - A static pressure (atmospheric) is imposed on all the boundaries
 - CH_4 concentration equal to 1 and mass flow rate of 0.0107 kg/s are imposed on the release hole.

3.2.2 Results

Since FLACS and KFX do not model the release phase by numerical techniques (DNV-GL, 2019), the following simulation conditions are set: a 3-D transient solver to solve the N-S equations and the Standard k- ϵ turbulence model.

In Fluent, the following simulation conditions are set: 2-D steady simulations using Standard k- ϵ model (to be consistent with the settings in FLACS and KFX) and SST k- ω as the turbulence closure equation. The analysis is carried out in the X-Z symmetry plane (see Fig. 3).

The obtained results are compared with the experimental data of (R.P. Cleaver, 1991), where CH_4 volume concentration is measured using aspirating probes, along a segment of the jet symmetry axis located behind the obstacle (see Figure 3). In Figures 4 and 5 (for the obstacle positioned at 157 mm and 683 mm from the release point, respectively), it is shown that, qualitatively, Fluent best reproduces the experimental data, whereas KFX is the worst. Also, this result is exacerbated by the smaller distance from the release point. In general term, we can conclude that the off-the-shelf tools (i.e., FLACS and KFX), also in this case, seem to be less capable of catching the physics of the phenomenon, but more conservative; in fact, they overestimate the CH_4 volume concentration. This might be due to the fact that, with respect to the case of a release point far from the obstacle, the CH_4 concentration naturally decreases along the X-axis and a lower concentration gradient develops around the object: in other words, FLACS and KFX manage small gradients better than large ones. On the other hand, Fluent results are more consistent with the experimental data thanks to its better flexibility, allowing the implementation of appropriate types of mesh and turbulence models for the analyzed scenario.

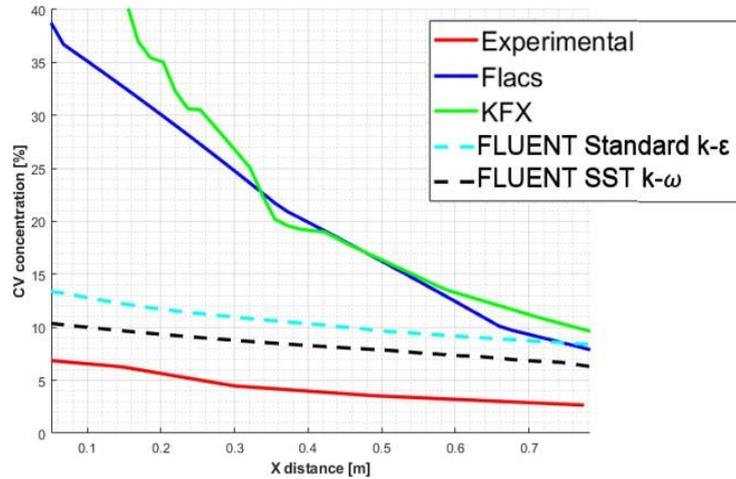


Figure 4 Results for the case of jet and obstacle distance equal to 157 mm

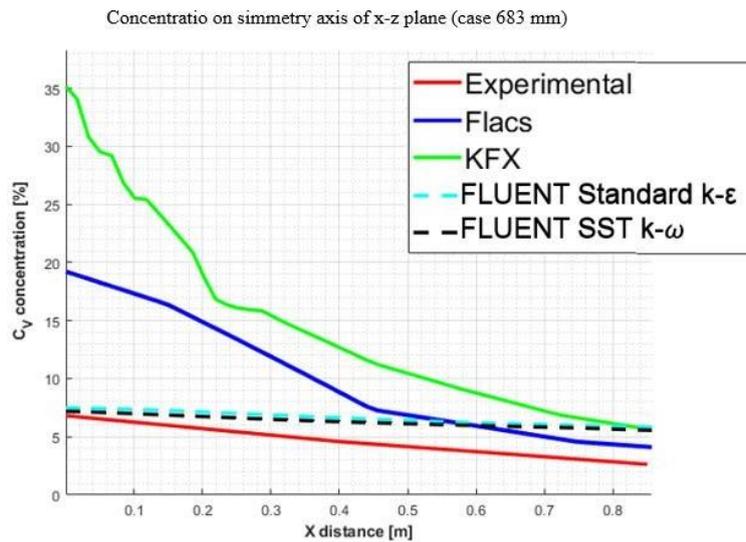


Figure 5 Results for the case of jet and obstacle distance equal to 683 mm

From a quantitative point of view, the *Err* between the results obtained and the data is calculated with Eq. (4) and reported in Tables 2 and 3. It is worth noting that FLACS and KFX, being based on the Porosity Distributed Resistance (PDR) approach, are not suitable to model the interactions between the CH_4 and the obstacle (in these cases, $Err \sim 200\%$, with respect to the experimental data).

Case 157 mm	FLACS	KFX	Fluent (Standard k-ε)	Fluent (SST k-ω)
<i>Err</i>	223 %	230 %	55,9 %	42,3 %

Table 2 Error of the tools with respect to experimental data (157 mm)

Case 683 mm	FLACS	KFX	Fluent (Standard k-ε)	Fluent (SST k-ω)
<i>Err</i>	42,8 %	98,2 %	22,4 %	18,2 %

Table 3 Error of the tools with respect to experimental data (683 mm)

4. The realistic case study

The realistic case study concerns a “major accident” scenario, according to (Directive 2013/30EU, 2013), that consists in an accidental high-pressure CH_4 release in a realistic offshore platform deck. In particular, the supersonic jet impinges on a cylindrical near-obstacle with $d_{cyl} = 30$ cm at $l = 45$ cm from the release point. This event is likely to occur in congested offshore installations, where a free-jet release is, on the other hand, improbable.

The simulation domain is shown in Figure 6 (i.e., a simplified 3D CAD version of an existing Italian natural gas extraction platform placed in Ravenna Punta Marina).

The representative parameters for simulating the scenario are chosen according to (Vivalda et al., 2018) and are summarized in the following:

- Release pressure: $p_{rel} = 50$ bar;
- Release hole diameter: $d_e = 3$ cm;
- Domain dimensions: 5 m height (Z), 30 m lengths (X), 20 m width (Y);
- Release point and direction: $X=3$ m, $Y=2$ m, $Z=1.5$ m along the X direction;
- Wind direction: $0.5X+0.5Y$;
- Wind intensity: $u = 6$ m/s.

It is worth to note that, in this case, the used tools are FLACS, KFX and SBAM (based on Fluent).

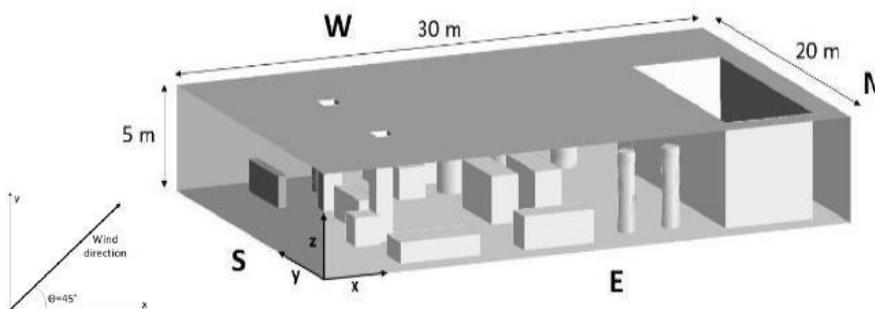


Figure 6. CAD of the production deck

4.1 Simulation setup

In SBAM, the following boundary conditions are implemented for the release phase:

- CH_4 concentration equal to 1 and a pressure of 50 bar are imposed on the release hole;
- The cylindrical nearby obstacle is modeled as a wall with no-slip conditions;
- Ambient pressure is imposed on the external faces of the source box (SB).

In SBAM, the following boundary conditions are implemented for the dispersion phase:

- Wind velocity with a magnitude of $u=6$ m/s with a direction of $0.5X+0.5Y$ is imposed on S and E sides;
- Atmospheric pressure is imposed on N and W faces;
- All the interactions with obstacle surfaces are modeled with walls with no-slip conditions.

SBAM simulations use a 3D solver for RANS equations and the SST $k-\omega$ model as turbulence closure equation, as suggested in (Wilcox, 2013) for the simulation of under-expanded jets, and validated in (Li et al., 2016). Simulations are performed in steady state with an unstructured tetrahedral mesh. The “Species Transport” model is used in order to solve a transport equation without chemical reactions and the ideal gas law is used to evaluate the density field (Pappalardo et al., 2020).

In FLACS and KFX the following boundary conditions are implemented:

- Uniform wind profile is imposed on S and E sides (analogous to SBAM).
- Ambient pressure is imposed in KFX on W and N sides (analogous to SBAM).
- Mass flow outlet is used in FLACS, as suggested in (Gexcon, 2019), to obtain a convergent solution.

Both FLACS and KFX use a 3D solver to solve RANS equations and the Standard $k-\epsilon$ model (Launder and Spalding, 1974; Jones and Launder, 1972) as turbulence closure equation. The analysis was conducted with a steady solver in FLACS, while KFX only allows for transient simulations.

4.2 Results

4.2.1 Simulation results

In this Section, the differences between the spatial distributions of the gaseous cloud release provided by FLACS, KFX and SBAM are analyzed. The comparative analysis is conducted considering the results on the plane at a height (z) of 0.5 m, since at this elevation, the ignition probability is larger than at higher elevations and, therefore, the comparison is conservative in the hypotheses adopted (i.e., large presence of mechanical and electrical equipment, and of personnel). The related contour maps are

shown in Figures 7-9 for SBAM, FLACS and KFX, respectively.

The flammable clouds obtained using FLACS and KFX (Figures 8 and 9) are similar, whereas both deeply differ from the flammable cloud obtained with SBAM (Figure 7). On one hand, FLACS and KFX flammable clouds appear like a stretched free-jet plume, which is curved due to the wind effect and barely influenced by the congested environment. On the other hand, in SBAM map (Figure 7), the jet impacts the obstacle “A” causing a deformation of the plume; this interaction influences the evolution of the cloud, generating a highly “irregular” shape of the area involved by accidental scenario, as it should be realistically. The difference is mostly due to the use of the PDR approach by FLACS and KFX, because the boundary layer near the obstacles is not solved and, therefore, the separation phenomenon of a flow impacting on an object is not correctly addressed: the PDR approach, used by FLACS and KFX, seems inappropriate to model the flow-obstacle interactions in a proper way, since it neglects or badly approximates many geometrical features. On the other hand, it should be acknowledged that the computational costs of FLACS and KFX are much smaller than those of SBAM.

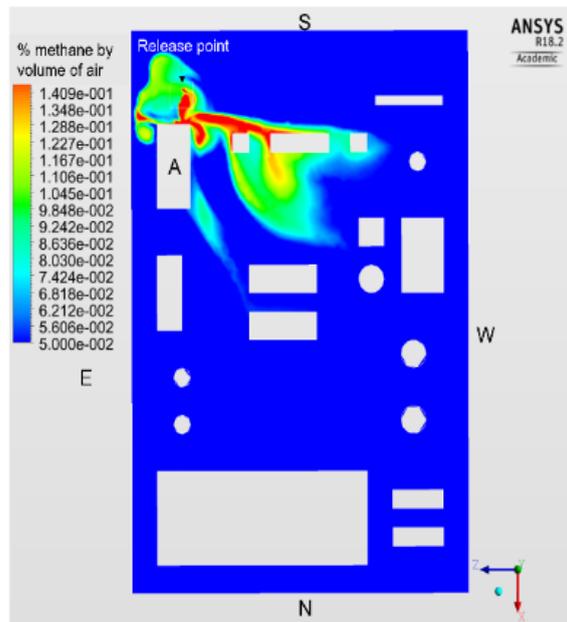


Figure 7 SBAM flammable area at $z=0.5$ m

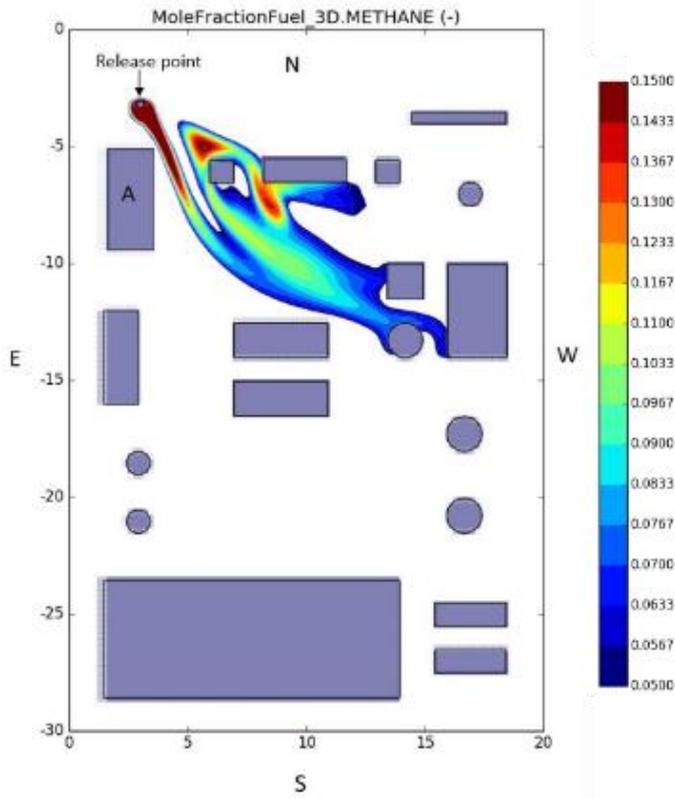


Figure 8 FLACS flammable area at $z=0.5\text{ m}$

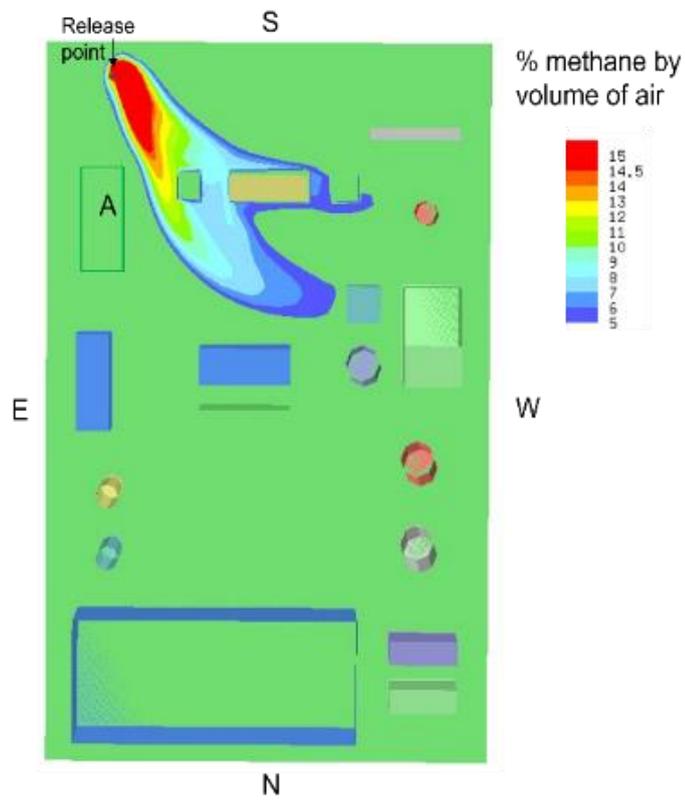


Figure 9 KFX flammable area at $z=0.5\text{ m}$

4.2.2 Uncertainty Quantification for risk-informed decision-making

We here present an approach for UQ that considers the effects of the discretization source of uncertainty on the volume of the flammable cloud, and, ultimately, on the risk indicators σ_{Damage} , σ_{target} and $\sigma_{d1.5}$ (Eqs. 1-3). The discretization source of uncertainty is unequivocally related to the mesh size used to represent the governing (N-S) flow equations. To ensure that the solution of the discretized equations closely approximates the solution of the original equations (George Em Karniadakis, 2002), and quantify the spatial discretization uncertainty, we rely on the Grid Convergence Index (*GCI*) method and the identification of the *exact* value f_0 .

The calculation of f_0 (F.Stern 1999) and GCI (Roache, 1998) proceeds as follows:

- Assume a discrete solution f as a function of the characteristic size of the grid h

$$f = f_0 + g_1 h + g_2 h^2 + g_3 h^3 + \dots (5)$$

where f_0 represents the *exact* value for the continuum case with the size of the grid $h = 0$.

- According to the method of order p , the equation (5) becomes:

$$f = f_0 + g_p h^p + O(h^{p+1}) \quad g_i = 0 \text{ with } i = 1, 2, \dots, p-1 (6)$$

and two solutions f_1 and f_2 of order p can be found (referring to the characteristic lengths of the grid h_1 and h_2 (with $h_1 < h_2$ and grid refinement ratio equal to $r = h_1/h_2$ in the equation (6)):

$$f_1 = f_0 + g_p h^p + O(h^{p+1}) (7)$$

$$f_2 = f_0 + g_p (rh)^p + O((rh)^{p+1}) (8)$$

- Linearly combining f_1 and f_2 , the general Richardson's extrapolation is defined:

$$f^* = \frac{f_1 r^p}{r^p - 1} - \frac{f_2}{r^p - 1} = f_1 + \frac{f_1 - f_2}{r^p - 1} (9)$$

$$f^* = f_0 + O(h^{p+1})$$

where f^* approximates f_0 with order $p + 1$.

- If order p is unknown (i.e., the order of the solution is influenced by numerical schemes, boundary conditions...), three solutions f_1, f_2, f_3 with constant grid refinement ratio and $h_1 < h_2 < h_3$ can be used to estimate:

$$p = \frac{\ln\left(\frac{f_3 - f_2}{f_2 - f_1}\right)}{\ln(r)} (11)$$

the relative error ε of the solution f_1 :

$$\varepsilon = \frac{f_2 - f_1}{f_1} (12)$$

and an estimation E_1 of order $p + 1$ of the solution f_1 :

$$E_1 = \frac{\varepsilon}{r^{p-1}} (13)$$

In order to define an index of the spatial discretization error, Roache (1994, 1995) further developed the Richardson's extrapolation method, defining the Grid Convergence Index (GCI) as:

$$GCI_1 = F_s \frac{|\varepsilon|}{r^p - 1}$$

where GCI_1 is the index for the grid h_1 (the finest one) and F_s has a value of 3 (i.e., the ratio between E_1 and ε for grids with grid refinement ratio r and order p equal to 2). Repeating the same procedure for the grid with size h_2 , it is possible to define the ratio between GCI_1 and GCI_2 , verifying the asymptotic trend of the solutions f_1 and f_2 through the relation:

$$GCI_2 = r^p GCI_1 \quad (14)$$

For performing the required simulations with the different mesh refinements, the same simulations features adopted in Section 4 have been kept, to avoid adding in the solutions bias not due to the spatial discretization of the mesh. It is worth mentioning that the results obtained with SBAM are only due to the mesh discretization for the dispersion simulations, whereas the SB module is considered as a 'black-source'; instead, as customary in FLACS and KFX the whole release-dispersion CFD simulation is performed. Results are:

- FLACS: $GCI = 7.8 \%$, $f_0 = 163 \text{ m}^3$
- KFX: $GCI = 10.6 \%$, $f_0 = 199 \text{ m}^3$
- SBAM: $GCI = 1.2 \%$, $f_0 = 83 \text{ m}^3$

With respect to f_0 , it is interesting to notice that FLACS and KFX provide more conservative results with respect to SBAM, to cover the simplifying modelling assumption adopted (and overcome by SBAM): f_0 estimated by KFX is >100% larger than for SBAM, whereas f_0 estimated by FLACS is ~100% larger than for SBAM, which means that the energies and damage towards which countermeasures and barriers are to be designed for are much larger than what they actually should be. The propagation of the results for GCI on the risk indicators is summarized in Table 6.

	FLACS	KFX	SBAM
σ_{Damage}	(5,43±0,45) %	(6,63±0,7) %	(2,7±0,01) %
σ_{target}	0 %	0%	0%
$\sigma_{d1,5}$	(39 ± 4,82) %	(41± 5,6) %	(29 ± 0,5) %

Table 6 Risk indexes with uncertainty

It is important to notice the important role played by the mesh size in the assessment of the risk indicators: for example, the uncertainty brought by the mesh size (0.7% of σ_{Damage} for KFX) accounts for ~10.5% of the nominal value (6.63%). In general terms, it can also be observed that the estimated

risk measures are similar for FLACS, KFX, whereas the estimated risk measures with SBAM deeply differ: SBAM, indeed, being more realistic than the other CFD approaches (as widely analyzed in Section 2), provides less conservative estimation of the risk measures, whereas KFX is the most conservative (mainly due to the adopted PDR approach, which does not solve the boundary layer to reproduce the separation of a flow impacting an object): the flow-obstacle interactions are hardly approximated (see Figure 9), and, therefore, the jet seems to be insensitive (i.e., does not changes direction) to the interaction with the obstacle, leading to larger values of $\sigma_{d1,5}$. Conversely, in Figure 8, we can also note, for SBAM, that the jet gets trapped near to the release point, because of the interaction with the obstacle: this, realistically, increases the dispersion and mixing of CH_4 with the air, diminishing the flammable volume and generating a highly “irregular” shape of the area involved by the accident. Therefore, the calculated $\sigma_{d1,5}$ for SBAM is due to the slow-down of CH_4 jet motion, caused by the collision with the obstacle, that moves the gas to elevation higher than 0.5m, since CH_4 density is lower than air density. Another interpretation can be imputed to a jet soaring along the axis of the obstacle, once the interaction fluid-solid occurs. As a last remark, we point out that σ_{target} is not significant whatever CFD approach is adopted, because, for all the simulated cases, the CH_4 does not reach the perimeter of the domain.

Conclusions

In this work, a novel approach for the UQ of CFD calculations such as FLACS, KFX and SBAM and its propagation to a set of novel risk indices is proposed and tested on a realistic case study regarding an accidental high-pressure methane release scenario in a realistic offshore O&G platform deck. Among the sources of uncertainty affecting CFD calculations, such as modeling (boundary conditions, initial conditions, geometry, fluid properties, turbulence modeling errors) and numerical (discretization, round-off and iterative convergence errors) errors, in this work we have only considered the effects of mesh discretization on the uncertainty of the calculation results. The uncertainty due to the mesh size is quantified by means of the metrics GCI and f_0 and, then, propagated to the novel risk measures for a realistic and risk-oriented analysis. Results show that FLACS and KFX provide more conservative results with respect to SBAM, to cover the simplifying modelling assumptions adopted, that may lead to oversizing of preventive/mitigative oversizing of the safety systems with waste of economical and material resources.

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