Foreword

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Overview

Explosions involve complicated physical phenomena and they continue to be investigated due to their potential severity, as demonstrated by the major accidents that continue to occur world-wide.

While research continues to improve the accuracy and understanding of the mathematical modelling of Vapour Cloud Explosions (VCE), the numerical codes can be complicated and require significant computing power, time and expertise. As a result, simplified models and methods have been developed for use in quantified risk assessments, including those that make use of an equivalent cloud concept to represent the volume of flammable gas that is involved in the explosion.

As described by Tam *et al*. [1] “There is a number of ways this volume is defined. The three main methods are: i.) volume enclosed by the LFL contour surface, ii.) volume bounded by LFL and UFL contour surfaces, and iii.) burning velocity weighted volume (Q9)”. These methods give different flammable volumes and as such will normally result in different overpressure predictions. Unless great care is taken, significant under-predictions may occur, which could have serious safety implications and lead to excessive retrofit costs. In order to ensure adequate protection without excessive cost, a “cautious best estimate approach” is recommended for safety-related analyses. This equates to employing realistic estimates, rather than optimistic ones, where an appropriate level of sensitivity has been applied to account for the uncertainty that exists. It is also important that users of these methodologies are made aware of these issues and that suppliers/developers provide enough instruction and guidance to limit under-prediction, where such potential exists.

In this paper, one such approach (Q9) has been examined to evaluate its potential for under-prediction by users, within the limits provided in the explosion code user guide. It is intended that developers and users of such methodologies are made aware of the safety implications of hazard under-prediction and that they carefully consider how these inaccuracies are accounted for where overpressure assessments are conducted.

Wider Issues in Probabilistic Explosion Risk Assessments

As discussed in more detail in this paper, various studies have been published which have found a lack of consistency in explosion modelling results and a reliance upon expert judgement in the Explosion Risk Assessment (ERA) process, both of which present significant cause for concern. There appears to be a lack of clearly defined, unambiguous guidance that is consistently applied by different individuals undertaking ERA studies. The choice of Q9 over the alternative equivalent cloud methods is important. Other judgements are also significant, such as those concerning the use of pre-ignition turbulence, the choice of gas cloud positions and ignition locations, the ignition probabilities and other detailed choices made in the explosion model setup, such as the specified mesh resolution and modelling of time-varying releases. For example, Howell and Middha [2] demonstrated that a change in ignition model and the associated modelling assumptions within an

ERA could change the Design Accident Load (DAL) for a 1 in 10,000 year event by more than a factor of two. Changing the equivalent cloud method from using Q9 to using the total flammable volume was shown to have a similar overall effect.

The result of having such a large degree of flexibility and uncertainty when making modelling choices in the context of the current ERA process is a system which can be inconsistent and is open to abuse. Clearer guidance on how probabilistic ERA should be undertaken is needed, along with more rigorous documentation of the assumptions, and associated uncertainties, made when performing an ERA to determine an overpressure exceedance curve. With the present system, it is extremely difficult to have proper oversight (either by the client or regulator) when the ERA is based on so many expert judgement decisions. There is little value in undertaking ERA studies if the results cannot be trusted.

Recommendations

To address the issues raised above, it is recommended that a joint ERA inter-comparison exercise be undertaken to help: a.) identify the current scale of the issues, b.) share experience and c.) develop good practice guidelines. The exercise should ideally involve consultants, software developers, regulators and other experts within the industry. The aim of the good practice guidelines would be to provide more prescriptive conditions and/or limits on model input parameters within the ERA to help provide greater transparency in the ERA process and to harmonize results. An exercise along these lines was carried out nearly 20 years ago for consultants operating in the Norwegian offshore oil and gas sector, coordinated by Statoil [3], and it is timely to conduct a similar exercise again with consultants operating in the UK sector and internationally. One alternative to this option is for regulators to unilaterally adopt a more prescriptive approach to ERA.

Explosion modelling software developers are also strongly encouraged to improve their guidance on the use of their software for the purpose of ERA. This may benefit from having input from both software developers and users, i.e. consultants. This more detailed guidance should cover the use of Q9 and/or alternative equivalent cloud methods, and other modelling assumptions, such as specific guidance on the inputs needed to model pre-ignition turbulence (under a range of conditions). Software frameworks for risk assessments involving explosion models have recently been developed by Gexcon and DNV GL. Other consultants have also developed relevant tools. The proposed ERA inter-comparison exercise could provide an opportunity to test and compare these methods and work towards a more harmonized approach, based on good practice. This would help to provide reassurance to modellers that their approach for ERA is fit-for-purpose, and enable effective oversight by clients and regulators.

Current practitioners of probabilistic ERA should also be mindful of the issues raised in this review, concerning choices in the modelling process that can lead to non-conservative results. This includes, in particular, the choice of Q9 over alternative equivalent cloud methods and the use of pre-ignition turbulence in explosion simulations.

A Review of the Q9 Equivalent Cloud Method for Explosion Modelling

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Abstract

Equivalent cloud methods are used as a pragmatic means of reducing the computational cost associated with generating overpressure exceedance curves through an explosion modelling Quantitative Risk Assessment (QRA) using Computational Fluid Dynamics (CFD). Such methods are used to represent inhomogeneous, dispersed gas clouds with smaller homogeneous volumes of gas at, or near, their stoichiometric concentration. The most commonly used approach is the Q9 method, which is embedded in the widely-used CFD software package FLACS [4]. This paper seeks to review the available literature describing the various equivalent cloud methods and, where possible, to critically evaluate the justification and use of such approaches for industrial applications. The implications of the use of Q9 in QRA studies are also discussed. There are two published validation studies in which explosion overpressures predicted using Q9 have been compared to overpressures determined experimentally through the ignition of inhomogeneous gas clouds in offshore modules. The results of these two studies are inconsistent, making it difficult to draw any specific conclusions regarding the performance of Q9 for explosion modelling QRA. However, these validation studies do clearly demonstrate that the results of a QRA are strongly dependant on the modelling choices made by the model user and that the validity of the Q9 approach needs to be tested more thoroughly.

Keywords

CFD, equivalent stoichiometric cloud, Q9, explosion modelling, risk assessment, overpressure exceedance curve

Introduction

Probabilistic Explosion Risk Assessments (ERA) are used in the oil and gas industry to characterise the risks associated with the accidental ignition of unintended releases of flammable gases in onshore and offshore modules. The primary outputs of such studies are overpressure exceedance curves[1], which are used to inform design decisions relating to pressure loading on structures and safety critical plant. These studies are a requirement of the NORSOK Z-013 industry standard [5]. Due to the number of potential release scenarios, weather conditions, ignition locations, flammable cloud sizes etc., there are infinitely many scenarios that could be accounted for in such studies. Modelling all of these scenarios is not feasible. Of these simulations, the dispersion modelling has the largest contribution to the associated computational cost. As a result, industry has adopted the use of "equivalent cloud methods" as a pragmatic means of reducing the total number of

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[1] An overpressure exceedance curve presents overpressure plotted against the probability of exceeding that overpressure.

simulations required and lowering the overall duration and computational cost of performing such analyses. This is achieved by translating the predicted set of dispersed gas clouds into a subset of equivalent homogeneous gas volumes at, or near, stoichiometric concentration. These so-called equivalent stoichiometric clouds are then used in a matrix of explosion simulations using a range of cloud positions and ignition locations to produce a probabilistic representation of the expected overpressures.

Hansen *et al*. [6, 7] and Davis *et al*. [8] outline how probabilistic explosion studies can be performed, with the suggested methods broadly similar to those given in the NORSOK Z-013 [5] and Lloyds Register [9] guidance. More recently, extensions to the probabilistic ERA approach have been proposed by Gupta and Chan [10] and by Jin and Jang [11] to incorporate the effects of time-varying releases. All of the published probabilistic ERA methodologies rely upon the assumption that it is reasonable to represent an inhomogeneous cloud using an equivalent cloud approach, the most common of which is known as Q9. This paper seeks to evaluate the use and scientific justification of this approach and to consider the manner in which Q9 is used within the broader context of a probabilistic ERA.

Equivalent Cloud Methods

The equivalent cloud approach was originally introduced by Gexcon in the early 1990's via the introduction of the ERFAC parameter as an output of the FLACS model. This method assumes that equating the mass of gas within an inhomogeneous gas cloud to a smaller homogeneous volume of gas near stoichiometric concentration will result in similar overpressures, should the two clouds be ignited. In 1999, this method was refined by Gexcon to give the Q5 method, in which gas expansion effects are accounted for, in addition to differences in the concentration-dependent flame speed. The change was reportedly made due to the ERFAC approach exhibiting a bias towards fuel rich concentrations within a gas cloud. In 2005, a further adjustment was made to give the now widely-used Q9 approach. For certain gases, the maximum flame speed and the maximum volume expansion of combustion products do not occur at the same equivalence ratio, meaning that there are scenarios for which the flammable volume of an inhomogeneous cloud at the most reactive concentration would not be fully captured by the Q5 approach. The adjustment giving the Q9 method is intended to take account of this [7]. In certain circumstances, such as in the case of high levels of confinement, Gexcon recommend use of the more conservative equivalent cloud volume, Q8 [4].

Additional equivalent cloud metrics are suggested by others, such as the $> LFL$ and ΔFL (also known as FLAM in FLACS) volumes [1]. These volumes are calculated as the volume of gas within an inhomogeneous cloud with a concentration above the lower flammability limit (LFL) and the volume of gas with a concentration between the lower and upper flammability limits (UFL), respectively. These methods are considered to be more conservative alternatives to the Q9 approach.

Each of the equivalent cloud methods, and the equations on which they are based, are summarised in Table 1. For each metric, the summation is taken over all computational mesh cells $1 \leq i \leq n$, where n is the total number of cells used. The terms $fuel_{mass}$ and $fuel_{vol}$ represent the mass and volume of gas in a given cell, respectively, and C is the gas concentration in that cell. The parameters

S and E are the laminar burning velocity and combustion products volume expansion ratio, respectively.

When using equivalent cloud methods to calculate explosion loads, the volume of the equivalent cloud has a significant influence on the resulting explosion overpressure. The different methods used to determine the equivalent cloud volume give very different cloud sizes, with the ratio of volumes, $\Delta FL{:}\,Q8{:}\,Q9$, being approximately 3:2:1 [7]. The remainder of this paper will focus on the Q9 equivalent cloud approach, since this is the method currently in most widespread use by industry.

Table 1 Commonly-used equivalent cloud metrics from Tam *et al*. [1] and Hansen *et al*. [7] [2]

Equivalent Cloud Metric	Equation
ERFAC (kg) [7]	$M_{ERFAC} = \frac{1}{S_{max}} \sum_{i=1}^{n} (fuel_{mass} \times S)_i$
Q5 (m^3) [7]	$V_{Q5} = \frac{1}{S_{max} E_{max}} \sum_{i=1}^{n} (fuel_{vol} \times S \times E)_i$
Q9 (m^3) [7]	$V_{Q9} = \frac{1}{(SE)_{max}} \sum_{i=1}^{n} (fuel_{vol} \times S \times E)_i$
Q8 (m^3) [7]	$V_{Q8} = \frac{1}{E_{max}} \sum_{i=1}^{n} (fuel_{vol} \times E)_i$ where $LFL \leq C \leq UFL$
$> LFL$ (m^3) [1]	$V_{>LFL} = \sum_{i=1}^{n} (fuel_{vol})_i$ where $C \geq LFL$
ΔFL (m^3) [1]	$V_{\Delta FL} = \sum_{i=1}^{n} (fuel_{vol})_i$ where $LFL \leq C \leq UFL$

Basis of the Q9 Approach

As discussed above, the Q9 approach is one of a number of equivalent stoichiometric cloud methods incorporated in the widely-used CFD explosion model FLACS [4]. The method is essentially a correlation that has been adjusted over the years to give more consistent results when compared to

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[2] Where the gas concentration lies outside the flammable range, the laminar burning velocity, S, is zero. As such, non-flammable regions of an inhomogeneous gas cloud have no contribution to the ERFAC, Q5 or Q9 equivalent clouds.

experimental data. However, the Q9 approach is not expected to give good agreement with any one single experiment. Rather it has been developed to give a reasonable approximation of the overpressure based, importantly, on the assumption that it will be used as part of a probabilistic ERA, where there are a great number of variables and assumptions being made, and sensitivity tests will be performed to assess uncertainties. Using Q9 equivalent stoichiometric clouds is intended to offer a pragmatic means of performing probabilistic explosion analyses using CFD, though there are some limitations to the approach.

The Q9 approach is predicated on two key assumptions: firstly, that the explosion model being used will accurately predict explosion overpressures in uniform gas clouds and, secondly, that the scaling between an inhomogeneous gas cloud and the Q9 equivalent volume is such that ignition of the two gas clouds will result in similar explosion consequences. The evidence supporting each of these two assumptions is mixed.

Prediction of explosion overpressure for homogeneous gas clouds

Regarding the first assumption, Hansen *et al*. [7] presented FLACS predictions for nine test cases with homogeneous gas clouds in the Phase 3B Blast and Fire Engineering for Topside Structures (BFETS) experiments [12, 13]. These experiments involved full-scale tests using a geometry considered representative of an offshore module with natural gas concentrations close to stoichiometric. Hansen *et al*. [7] predicted the majority of the measured maximum overpressures within a factor of two. However, the results showed increasing under-prediction of the measured overpressures as the maximum recorded overpressure increased. For measured overpressures less than 0.5 barg, the model both under- and over-predicted the measured values within ±30%; for measured overpressures of roughly 2.5 barg, the model under-predicted by around 20%; and for measured overpressures greater than 5 barg, the model under-predicted by around 50%.

These results contrast with the recent blind-prediction study presented by Skjold *et al*. [14] for the HySEA[3] project on vented hydrogen deflagrations in uniform gas clouds. Modellers submitted a total of 11 predictions using seven different models for the comparison exercise. The results showed differences of a factor of 23 between the predicted maximum overpressures from the different modellers. The results from different FLACS users spanned the range from the highest to the lowest predicted overpressures. These results demonstrate the large uncertainties associated with predicting explosion overpressures in uniformly distributed clouds. It should be noted that the hydrogen gas concentration was below stoichiometric, the scale of the tests was relatively small and that development of the FLACS model has been focussed towards predictions of explosion overpressures in congested modules at scales relevant for the oil and gas industry (Skjold, private communication, December 12th 2018). Skjold *et al*. [15] presented evidence that the grid sensitivity of FLACS predictions of the BFETS Phase 3B tests is much smaller than the results presented in [14]. However, further work is needed to assess whether a similar user-effect to that seen in [14] would be obtained when modelling explosions in full-scale offshore modules.

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[3] Improving Hydrogen Safety for Energy Applications (HySEA) through pre-normative research on vented deflagrations, http://www.hysea.eu/, accessed 6 November 2018.

Prediction of explosion overpressure for inhomogeneous gas clouds and Q9 equivalent volumes

The second of the two key assumptions behind Q9 is that realistic releases can be reasonably represented by equivalent homogeneous clouds. This hypothesis was tested to a degree in the BFETS Phase 3B experiments, which involved both realistic releases (i.e. jets) and homogeneous gas clouds. Data from these experiments is presented in Figure 1 in terms of the equivalent Q9 volumes and measured maximum overpressures (taken from data using a 1.5 ms running average to minimise noise). There were two different confinement configurations in the Phase 3B experiments and the results in Figure1 all used Configuration 1. The jet releases used two different ignition locations (I1 and I2) and the data on homogeneous clouds in Figure 1 is taken from two series of tests, called the Partial Fill (PF) and Base Case (BC) tests. These used ignition locations I1 and I2 for the BC tests, and a third ignition location for the PF tests. The data on the Q9 volumes for the jet releases is based on the experimental measurements of gas concentration and is taken from the work of Hansen *et al*. [7]. The overpressures were taken from the Phase 3B summary report [12].

Figure 1 shows that there is a consistent trend in the data for overpressures in homogeneous clouds to increase with increasing Q9 cloud volume. In contrast, the jet releases show significant scatter, as might be expected from having non-uniform concentrations and varying degrees of pre-ignition turbulence. The majority of the overpressures from the jet release scenarios are higher than those for tests using homogeneous clouds with similar Q9 volumes, though there are a number of jet releases which give lower overpressures. This reduces confidence in the use of Q9, since the intention of the Q9 scaling is to produce an equivalent stoichiometric cloud that will give similar explosion consequences to the original cloud [4]. When a probabilistic ERA is conducted, simulations are performed with the homogeneous cloud in multiple different locations using a range of different ignition locations to find the maximum overpressure. This type of probabilistic approach was not taken in in the Phase 3B experiments (which would have required many more experiments to be conducted).

There is significant uncertainty in the calculation of the Q9 volumes from the BFETS Phase 3B experimental data, which involves estimating the concentration distribution in the dispersed cloud using a fairly sparse array of sensors. For these tests, 45 sensors were distributed in a gridded array within the 28 × 12 × 8 metre module to capture the concentration distribution within the inhomogeneous gas clouds resulting from the jet releases. This gave a sensor coverage of approximately one sensor per 60 m^3 (on average) within the module. Such a sparse sensor array is unlikely to adequately capture the non-uniform gas distribution resulting from a jet release issuing from an orifice with a 32.5 mm or 43 mm diameter, as was used in the BFETS Phase 3B tests [12]. As a consequence, the accuracy of the calculated Q9 volumes for these experiments is uncertain.

Data from the second confinement configuration of the BFETS tests is presented in Figure 2. Only one experiment was conducted in this geometry with a homogeneous cloud, which was for a stoichiometric cloud filling the entire module (Base Case 3). Figure 2 shows that one of the jet releases (Test 13) produced a 25% higher overpressure than this homogeneous stoichiometric cloud, despite the fact that the estimated Q9 volume for the jet release was less than half that of the homogeneous cloud. This suggests that pre-ignition turbulence in the jet release scenario has a strong effect. However, care is needed in interpreting these results, since there is natural (stochastic) variability in repeated explosion tests, which can give rise to higher or lower overpressures under nominally the same conditions [16]. There are also uncertainties in the calculated Q9 volume for the jet release. Further experiments would help to assess these uncertainties and enable firmer conclusions to be made.

Effect of pre-ignition turbulence

In the FLACS modelling study for an onshore facility presented by Hansen *et al*. [7], predicted overpressures from explosion simulations with realistic releases (i.e. with inhomogeneous gas clouds) were compared to predicted overpressures from equivalent homogeneous Q9 clouds, both with and without pre-ignition turbulence. The results of that comparison showed that the realistic clouds gave higher overpressures than the quiescent Q9 clouds and broadly similar overpressures to the highest overpressures obtained from the Q9 clouds with pre-ignition turbulence. This result, and the data from the BFETS experiments, highlights the importance of accounting for pre-ignition turbulence when modelling jet releases using Q9 equivalent stoichiometric clouds.

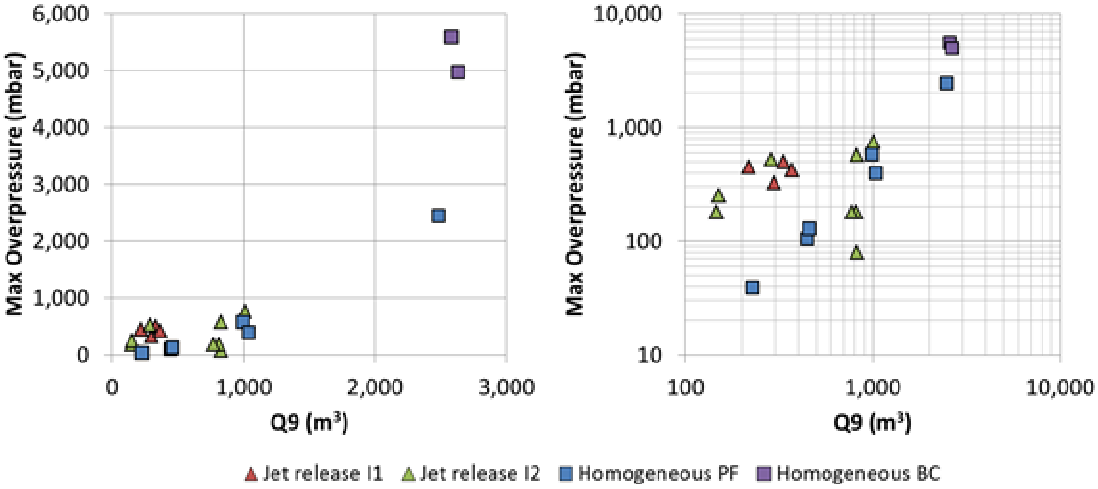

Figure 1 Maximum overpressures measured in the BFETS Phase 3B experiments for Confinement Configuration 1: comparison of jet release to homogeneous cloud results for ignition locations I1 and I2 and Partial Fill (PF) and Base Case (BC) tests. The left-hand plot uses a linear scale and the right-hand plot uses log-log axes.

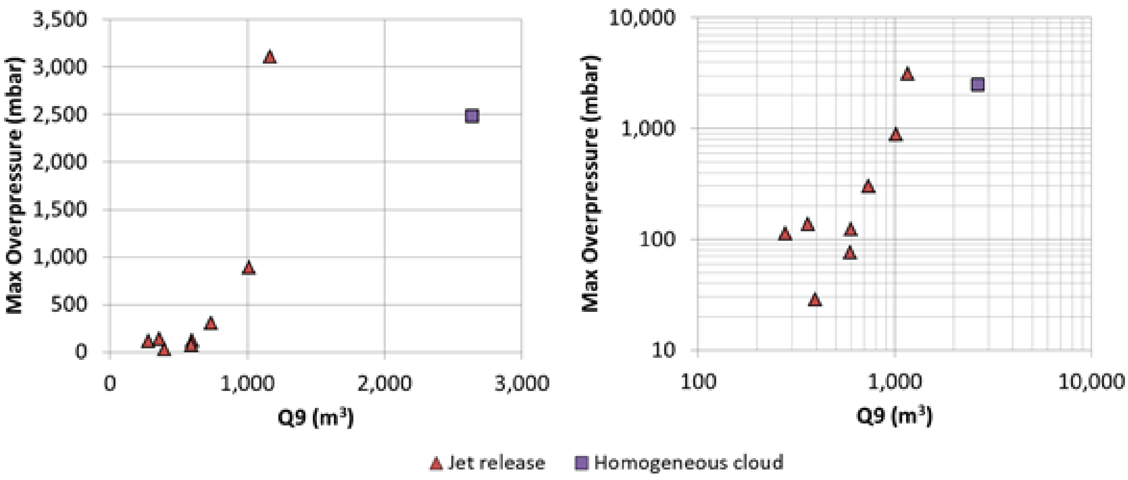

Figure 2 Maximum overpressures measured in the BFETS Phase 3B experiments for Confinement Configuration 2: comparison of jet release to homogeneous cloud results. The left-hand plot uses a linear scale and the right-hand plot uses log-log axes.

The FLACS user manual [4] suggests that initial turbulence should be taken into account for high-momentum jet releases when using Q9 by setting appropriate values for the Relative Turbulence Intensity (RTI) and Turbulence Length Scale (TLS). However, recommendations of what constitutes appropriate values for these quantities are not given, only a maximum upper limit for the TLS is provided. The Lloyds Register [9] guidance also recommends the inclusion of pre-ignition turbulence, at least for open geometries or those with low levels of congestion, but again it does not indicate how this should be implemented nor how the initial turbulence conditions should be determined. Hansen *et al*. [7] assumed values of the turbulent fluctuation velocity and the turbulent length scale for their FLACS simulations of the BFETS Phase 3B tests and stated that the chosen values represented typical conditions within the BFETS module from their dispersion modelling results for those tests. It is unclear if these values were intended as providing definitive general guidance on implementing pre-ignition turbulence in explosion modelling QRA studies.

Tolias *et al*. [17] showed that the initial turbulence length scale can have a significant impact on the predicted peak overpressure for explosions in a uniform hydrogen cloud. The FLACS modelling presented in that study showed that varying the turbulence length scale from 1-20% of the grid cell size gave peak overpressures differing by a factor of 2.5.

The recent review paper by Skjold *et al*. [18] acknowledged the limitations of existing guidelines on pre-ignition turbulence, and noted that “better guidelines are required to avoid arbitrary results depending on the settings defined by individual users of the CFD software”. The authors also noted that in some situations it may be better to run explosion simulations using initial conditions that are representative of a “real cloud”, with a spatially-varying concentration and turbulence fields, than running the explosion simulation using the Q9 equivalent cloud. They concluded that: “real cloud explosions tend to be more conservative for medium congestion, whereas Q9 tend to be more conservative for high congestion. These trends indicate that the Q9 equivalent method might be not sufficiently conservative for on-shore facilities, or for moderately congested off-shore modules. As such, the real cloud and initial flow field should be used when simulating worst-case scenarios”.

The issue of pre-ignition turbulence in realistic-scale jet releases into congested regions is currently being examined in Gexcon's ongoing AIRRE project (Skjold *et al.*, [18]). Their analysis of the experimental data, validation, improvements of the model and refinements to the QRA methodology are planned to continue until the end of the AIRRE project in December 2019.

Stratified clouds and the Q9 approach

Turbulence generated by flame propagation and the presence of congestion within a module is likely to lead to mixing of initially non-flammable pockets of gas (i.e. where the concentration is greater than the UFL) such that they reach flammable concentrations and are subsequently involved in an explosion, potentially contributing to higher overpressures. This phenomenon was noted in the BFETS Phase 3B tests with rich mixtures [12, 13]. However, the Q9 method does not include any contribution from volumes within an inhomogeneous cloud in which the concentration lies outside the flammable range. This has implications for a range of realistic release scenarios. For example, in jet releases, the core of the jet will be above the UFL concentration and thus non-flammable. Applied to such a scenario, using the Q9 approach would mean assuming that this portion of gas does not contribute at all to the explosion and the resulting overpressure. Another less likely but clear example is the case of a stratified gas layer in which the concentration in the upper layer is above the UFL and in the lower layer is below the LFL. In this case, the Q9 equivalent volume would be zero, suggesting that such a scenario poses no explosion hazard. However, it is possible for flames to propagate into such stratified layers, causing mixing of the initially non-flammable layers so that the gas composition passes into the flammable range and contributes to the explosion. This could potentially lead to the Q9 method giving non-conservative results.

Cloud reactivity

The equivalent cloud approaches presented in Table 1 are commonly referred to as *equivalent stoichiometric clouds*. However, the use of the term "stoichiometric" is potentially a source of confusion here, since in practice these equivalent clouds should comprise a uniform gas composition at the *most reactive* gas concentration, which is usually above the stoichiometric concentration. The most reactive mixture is that for which $SE/(SE)_{max}$ is maximised. To illustrate why the most reactive mixture should be used, consider the case of an 8 m^3 volume of methane at uniform concentration in air. Figure 3 shows a comparison of the Q5, Q8, Q9 and ΔFL volumes calculated for equivalence ratios, $\emptyset$, ranging from 0.6 to 1.5. All of the considered equivalent cloud metrics give the same volume (the actual cloud volume of 8 m^3) when $\emptyset = 1.08$, not when the concentration is stoichiometric (when $\emptyset = 1.0$). For the case where the methane concentration is stoichiometric, the Q9 volume is 96% of the actual gas cloud size, thus Q9 does not recover the full cloud size at stoichiometric concentration. This demonstrates that when using the Q9 approach, the stoichiometric gas concentration should not be used, unless the stoichiometric concentration coincides with the point at which the gas under consideration is at its most reactive. The confusion between the most reactive and the stoichiometric concentration is evident in several texts, including the FLACS user manual [4].

Whilst a 4% deviation in the computed cloud volume may not seem significant, when used in the context of a QRA study, this error will propagate through the process, potentially leading to much larger deviations in the predicted overpressures. The magnitude of such differences will depend on the levels of congestion, confinement and the ignition locations used in the analysis. Using the most reactive mixture as opposed to the stoichiometric concentration (where the two are different) presents a very simple correction to the simulation configuration that could have a significant impact on the output from a QRA study.

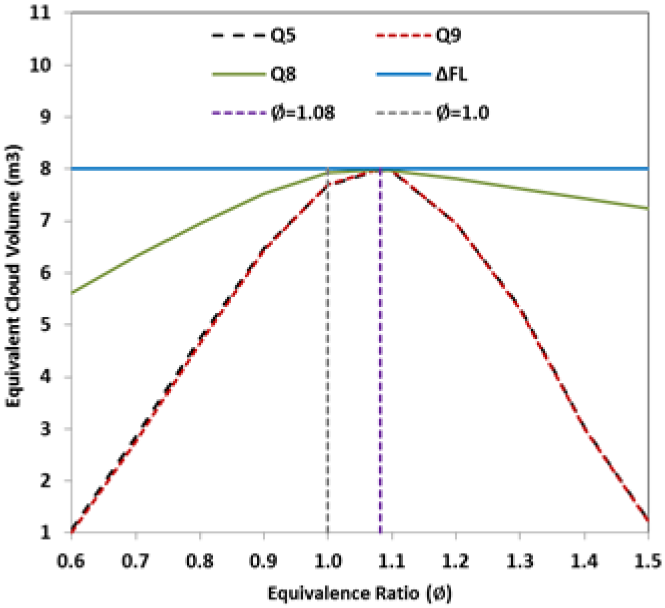

Figure 3 Comparison of calculated equivalent cloud volumes to represent an 8 m^3 volume of methane at a range of equivalence ratios

Validation of Q9

The two main validation studies of Q9 are the works of Tam *et al*. [1] and Hansen *et al*. [7]. Both studies modelled the BFETS Phase 3B experiments, although their findings appear to be contradictory.

Tam *et al*. [1] used three different equivalent cloud approaches ($> LFL$, ΔFL and Q9) in FLACS and compared predicted overpressures to the measured values from BFETS Phase 3B experiments. The gas cloud volumes used in their explosion modelling were estimated by processing the gas concentrations measured in the experiments, rather than from dispersion model predictions. For their explosion simulations, the cloud position and ignition location were varied in a manner similar to that which would be expected in an ERA study. The results of these simulations showed that for overpressures greater than 0.1 bar using the Q9 approach resulted in a negative bias, with FLACS under-predicting the measured overpressures. For the two other approaches used ($> LFL$ and ΔFL) the FLACS predictions were found to be conservative, with the measured overpressures over-predicted by the model. When using the Q9 approach, the degree of under-prediction was, on average, greater than a factor of two (a geometric mean of 0.4). The results also showed that using Q9 resulted in greater variance in the predicted overpressures than for the predictions made using either of the other two equivalent cloud approaches considered, i.e. the level of agreement between the model and the experimental data was less consistent when using Q9. As a result of these findings, Tam *et al*. [1] concluded that “This work does not support the use of Q9”.

The later study by Hansen *et al*. [7] first examined the performance of the FLACS dispersion model for predicting the size of the Q9 volume and then, independently of the dispersion simulations, examined the FLACS explosion model performance through comparison of predictions of maximum overpressure from a range of *assumed* cloud sizes (with Q9 volumes ranging from 2% to 100% fill of the BFETS module). Results were presented from explosion simulations both with and without pre-ignition turbulence. The results showed that FLACS simulations using Q9 clouds without pre-ignition turbulence gave overpressures comparable in magnitude to those measured in the BFETS Phase 3B tests. The results are therefore starkly different to those obtained by Tam *et al*. [1] for the same set of experiments. Hansen *et al*. [7] also showed that predicted overpressures were higher if the simulations used pre-ignition turbulence.

The main difference between these two studies appears to be that Hansen *et al.* [7] used a range of assumed cloud sizes, whereas Tam *et al*. [1] used cloud sizes estimated from the BFETS Phase 3B concentration measurements. This allowed Tam *et al*. [1] to calculate statistical performance measures directly from the predicted and measured explosion overpressures, whereas Hansen *et al*. [7] scaled both the experimental and predicted overpressures based on estimated Q9 cloud volumes before assessing the model performance by analysing the trends shown in the results. However, these differences are relatively minor and they do not explain the different conclusions.

There may have been other factors that affected the outcome of these two studies, such as the choice of grid resolution and the selection of cloud and ignition locations in the probabilistic explosion simulations, but without going through each study in detail it is impossible to reach firm conclusions. The two studies clearly illustrate that different experts, each with many years' experience in model validation studies, can produce different results using the same explosion model and equivalent stoichiometric cloud approach, even for a relatively well-defined case study such as BFETS Phase 3B. It would be useful for further analysis to be performed to understand the reasons why Tam *et al*. [1] and Hansen *et al*. [7] reached such different conclusions. However, this would probably require detailed examination of their input/output files and further modelling.

It should also be noted that a limitation of both the Tam *et al*. [1] and Hansen *et al*. [7] studies is that they relied upon estimating Q9 volumes from the experimental gas concentration data. As noted above, there is significant uncertainty associated with this, due to the relatively sparse array of concentration sensors. Furthermore, it is unclear whether the two groups used the same method to calculate Q9 volumes from the concentration measurements.

In an ERA study, clearly there are no measurements of gas concentrations that can be used to calculate Q9 cloud volumes. Instead, Q9 is calculated from dispersion simulation results. Neither Tam *et al*. [1] nor Hansen *et al*. [7] used this ERA approach of running dispersion simulations, calculating Q9 volumes from the predicted concentrations and then calculating explosion overpressures from simulations using the computed Q9 cloud sizes. In fact, there appears to be no published work that validates this type of approach. Whilst Hansen *et al*. [7] examined the performance of the dispersion and the explosion models independently, their work did not account for errors that could propagate through the modelling process from dispersion modelling into the calculation of Q9 cloud volumes and subsequent explosion modelling results.

One of the potential reasons why this approach has not been taken in any published studies may be that there are so many uncertainties. Skjold *et al*. [18] noted that "it is not straightforward to define a calculation procedure for equivalent stoichiometric clouds that consistently yields conservative predictions for all types of scenarios. Inherent uncertainties associated with initial and boundary conditions in large-scale experiments complicate the validation process”. To explain what this means with a practical example, in the BFETS Phase 3B experiments there was a degree of variability in the measured wind speed and direction during the tests. If the variable nature of these meteorological conditions was not included in the boundary conditions of the dispersion model, then the predicted gas clouds could be very different to the actual gas clouds seen in the experiments. If such dispersion model predictions were then used to define the inputs to a subsequent explosion model, it would be unreasonable to expect the explosion model to give sensible results (since incorrect inputs would lead to incorrect outputs), and thus the predicted overpressures may not be representative of those measured experimentally. However, the purpose of performing an ERA in a probabilistic manner is, in part, to compensate for propagating errors of the kind just described. The intention is for uncertainties in the calculated Q9 volumes to be minimised through the ERA process by performing multiple dispersion simulations, and by varying the position of the Q9 gas cloud and ignition locations used in the explosion model to determine worst-case overpressures. Given that such an approach is regularly used in offshore risk assessments and design, it is surprising that there is no publically-available literature comparing this methodology to experimental data.

Ultimately, further experiments are needed to test the validity of Q9 more thoroughly. It is unclear whether data from the ongoing AIRRE project will help to address this issue, or whether the data will be released publicly.

Conclusions

The Q9 equivalent cloud method is an engineering approach that is designed to be used within the framework of a probabilistic Explosion Risk Assessment (ERA). This review of Q9 has sought to examine the scientific basis of Q9 and summarise the findings of recent validation studies. Q9 is predicated on two key assumptions: that the explosion model accurately predicts explosion overpressures in uniform gas clouds, and that the scaling between an inhomogeneous gas cloud and the Q9 equivalent volume is such that ignition of the two gas clouds will result in similar overpressures. The evidence supporting the first of these assumptions is mixed, with one study reviewed here giving overpressure predictions within a factor of two of the measurements for homogeneous clouds, and another study showing a factor of 23 difference. The former study was for full-scale natural gas explosions in an offshore module (the BFETS Phase 3B tests) while the latter study was a blind model inter-comparison exercise that studied lean, small-scale hydrogen deflagrations. Further work is needed to investigate the cause of these differences, as the latter study reduces confidence in the ability of models (and modellers) to produce repeatable predictions of explosion overpressures.

The second key assumption on which Q9 is based (i.e. that inhomogeneous clouds can be represented by equivalent homogeneous clouds) was examined in part in the BFETS Phase 3B experiments. Results were presented that showed that higher overpressures were generated in the jet releases than the equivalent homogeneous clouds of the same Q9 volume. Whilst this reduces confidence in the use of Q9, there were insufficient experiments to reach definitive conclusions.

Hansen *et al*. [7] presented results from model predictions that indicated that pre-ignition turbulence needs to be used in conjunction with Q9 to avoid under-predicting overpressures in cases involving gas jets.

Two main studies have been published that have sought to assess the validity of using the Q9 equivalent stoichiometric cloud approach through comparison of model predictions to overpressure measurements from the BFETS Phase 3B tests. However, the authors of these studies came to quite different conclusions. The first study, by Tam *et al*. [1], concluded that using the Q9 approach lead to under-prediction of the measured overpressures by more than a factor of two, for overpressures in excess of 0.1 bar. The later study by Hansen *et al*. [7] found that Q9 gave overpressures that were in broad agreement with the data. The reasons for the different results are unclear. Both Tam *et al*. [1] and Hansen *et al*. [7] followed similar approaches and their analyses relied, in part, upon calculating "measured" Q9 volumes from a relatively sparse array of concentration sensors in the experiments (on average, there was one sensor per 60 m^3 within the module). These measured Q9 values therefore have inherent uncertainties. Neither of these two studies used the methodology that is generally used in an ERA for calculating Q9 volumes, which involves computing an equivalent stoichiometric cloud size from concentration predictions made using a dispersion model. It would be useful for further modelling and experiments to be conducted to test the validity of the Q9 approach more thoroughly.

What is clear from the review of relevant research on this topic is that inconsistent results can be produced in probabilistic ERA and there is currently a strong reliance upon expert judgement. Detailed modelling choices are made about equivalent cloud methods (Q9 versus the alternatives), the level of pre-ignition turbulence, the choice of optimum cloud locations, the choice of ignition locations, the ignition model and choices in the CFD model setup (particularly the choice of mesh resolution). It has been demonstrated that different experts can make different choices and get very different results for the same scenario.

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