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A comparison on predictive models of gas explosions

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Abstract−A comparison on existing models of gas explosion predictions has been done. The advantages and drawbacks, and the possibilities and limitations of the different empirical, phenomenological, and computational fluid dynamics assessment models of gas explosions were discussed. Particular attention was paid to CFD models.

Key words: Gas Explosions, Empirical Models, Phenomenological Model, CFD Models

INTRODUCTION

Large accidental gases or vapour cloud explosions represent a considerable hazard in some industries such as gas utilities, petrochemical, and coal mining. Predicting the possible consequences of gases explosions occurring in these industries is important to ensure the safe design of existing and new installations, and the risk assessment must be considered in the development of its design and installation. The predictions through the assessment of such explosions are improved by carrying out experiments and by using theoretical models [1].

However, there are limitations to the experimental data available for making such predictions because large-scale explosion experiments are prohibitively expensive to perform [2]. Therefore, various theoretical models are increasingly employed to assess explosion hazards and to design safer structures.

Presently, different models are available for predicting the behaviour of gas explosions. The models are grouped into three categories such as correlation models, phenomenological models, and numerical models. These types of models in this study are discussed based on the critical advantages and disadvantages of the different models used for the quantification of explosion hazards, in terms of the fundamental assumptions employed and their predictive accuracy. Particular attention has been paid to computational fluid dynamics models.

CORRELATION MODELS

Correlation models are known as empirical models, and are based on correlations obtained from analysis of experimental results. This type of models includes the venting guidelines, TNT equivalence model, TNO model, Multi-Energy (ME) model, Baker-Strehlow (BS) model and Congestion Assessment (CA) model.

1. Venting Guidelines

Explosion venting is a widely applied technique to mitigate the adverse impact of accidental explosions in equipment and building. The crucial problem in venting is the appropriate design of the vent area necessary for an effective release of the material. An understanding of the physical phenomenon by which pressure is generated in vented explosions is important for safe venting design, and such knowledge gives the basis for the development of prediction models [3].

There are a number of empirical and semi-empirical methods that can be used for the sizing of explosion venting [4-9]. Most of these methods have been derived from experimental data measured in small- and medium-sized vessels. These formulas are valid only within the validity ranges covered by the experiments. Application of the commonly used vent sizing methods for enclosures where the length to width or diameter ratio is greater than about 3 : 5 could lead to a serious underestimate of the vent area required.

Bradley and Mitcheson [4,5] have reported previous extensive compilations of the existing empirical equations and experimental data for a large range of conditions. Bradley and Mitcheson [4,5] suggested that the vent area should be related to the surface area of the vessel. Many investigators have used the ratio to A/V to specify vent area requirements, but have used the dimensionless vent ratio, $A_v/V^{2/3}$, to scale data obtained from experiments. This was found to be a satisfactory empirical scaling parameter for small- and medium-size vessels. The main benefit of the relationship term for practical use is that the necessary vent area, A_v, may be directly derived from it, provided the maximum allowed pressure and the enclosure volume are given. Solberg et al. [10] has pointed out that this scaling law is no longer valid for large and very large enclosures ($V>30\ m^3$). The ratio $A_v/V^{2/3}$ is similar to the ratio $\overline{A}$ suggested by Bradley and Mitcheson [4].

Bradley and Mitcheson [4] have presented an alternative venting parameter, $\overline{A}/\overline{S_o}$ for combustion venting for explosions in a spherical vessel with central ignition. The dimensionless parameter $\overline{S_o}$, which is the ratio of the gas velocity ahead of the initial flame front and the acoustic velocity in the unburned gas, depends on the initial composition and state of explosive mixture, while $\overline{A}$ is the ratio of the vent area to the total vessel surface area, multiplied by the discharge coefficient. The two dimensionless parameters are defined below:

$$\overline{A}=\frac{C_d A_v}{A_s} \tag{1}$$

$$\overline{S_o}=\frac{S_{uo}}{c_o}\left(\frac{\rho_{uo}}{\rho_{bo}}-1\right)=\frac{S_{uo}}{c_o}(E_o-1) \tag{2}$$

with

$$c_o=(\gamma_u P_o/\rho_{uo})^{0.5} \tag{3}$$

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where c_o is the velocity of sound, $\overline{A}$ is the vent area ratio, A_s is the surface area of the spherical vessel, A_v is the vent area, C_d is the coefficient of discharge, E_o is the expansion ratio, P is the pressure, S is the burning velocity, ρ is the gas density, the subscripts b, o and u denote burnt, initial and unburnt, respectively, and an overbar denotes a dimensionless parameter.

As indicated by Bradley and Mitcheson [4], in most cases one can assume that vents of smaller dimensions compared to the cross-section of the vessel have sharp edges and use a constant value of C_d=0.6. However, for vent diameters close to that of the vessel diameter, the discharge coefficient does not have a constant value. Yao [11] suggested C_d=1.0 should be considered when the entire wall is used as a vent opening and C_d=0.98 when the vent is a well rounded nozzle. From the numerical solutions of the two models mentioned above, Bradley and Mitcheson [4] have derived the following equations:

$$p_{red}=p_{stat}=2.43(\overline{A}/\overline{S}_o)^{-0.6993} \qquad \text{for } p_{stat}\geq 1 \text{ bar g} \tag{4}$$

$$p_{red}=p_{stat}=12.46(\overline{A}/\overline{S}_o)^{-2} \qquad \text{for } p_{stat}\leq 1 \text{ bar g} \tag{5}$$

and are valid for explosions in a spherical vessel with central ignition. Also, Eqs. (4) and (5) are valid for cases when a single pressure peak is observed in the vented vessel. This reflects a venting scenario when the static activation pressure of the vent is not exceeded after the opening of the vent. Such a scenario may be expected if the vent ratio $A_v/V^{2/3}$ is sufficiently high and the static activation pressure is low. Thus, an effective release of the vessel contents is achieved and the enhancement of the reaction by venting-induced turbulence does not produce a significant overpressure.

$$p_{red}=4.82p_{stat}^{0.375}(\overline{A}/\overline{S}_o)^{-1.25} \tag{6}$$

The same scaling dimensionless ratio $\overline{A}/\overline{S}_o$ was used by Bradley and Micheson [4] in the Eq. (6) for vented explosions where the pressure exhibits two peaks. The equation includes explicitly the dependence of p_{red} on p_{stat}.

In order to correlate p_{red} on the same dimensionless ratio $\overline{A}/\overline{S}_o$ Bradley and Mitcheson [4] have cited some correlations previously derived, such as Eq. (7) of Cubbage and Simmonds [12] and Eq. (8) of Yao [11]. Yao [11] introduced the dependence of the flame velocity on an empirical turbulence factor, χ, which can be defined as the ratio of turbulent to laminar flame surface. For smoothly opening vents, Yao [11] recommended the use of χ=3 and for bursting diaphragms, χ=4. Bradley and Mitcheson [4] recommended χ=4 in all cases.

$$p_{red}=0.365(\overline{A}/\overline{S}_o)^{-1} \tag{7}$$

$$p_{red}=\left[\frac{0.375\chi^{0.675}E_o^{7/6}}{E_o-1}\right]^{2}(\overline{A}/\overline{S}_o)^{-2} \tag{8}$$

Further critical examinations of various existing formulas and especially, of their extrapolation within and beyond their recommended validity range, have been represented by Molkov et al. [8,9]. Molkov et al. [9] presented "a new correlation" based on two new dimensionless numbers, Br and χ/μ, which include all important parameters of a vented deflagration. The deflagration-outflow-interaction number χ/μ was derived by fitting the calculated pressure-time curves to the experimental data. The Bradley number Br is closely related to the dimensionless number $\overline{A}/\overline{S}_o$ introduced by Bradley and Mitcheson [4]. Eq. (12) is valid for unobstructed enclosures [9], however, Razus and Krause [13] mentioned that it is also available for obstructed enclosures.

$$Br=\frac{A_v}{V^{2/3}}\frac{c_o}{S_{uo}\left(E_o-\dfrac{1-1/\gamma_b}{1-1/\gamma_u}\right)} \tag{9}$$

$$\frac{\chi}{\mu}=0.9\left[\frac{(1+10V^{1/3})(1+0.5Br)}{1+\pi_v}\right]^{0.37} \tag{10}$$

$$\pi_v=\frac{p_{stat}(\text{bar\_abs})}{p_o} \tag{11}$$

$$\pi_{red}=9.8\left[\frac{Br(E_o-1)}{(36\pi_o)^{1/3}\sqrt{\gamma_u}}\frac{\mu}{\chi}\right]^{-2.4} \tag{12}$$

where Br is the Bradley number, χ is the turbulence factor, describing the flame stretch by turbulence, μ is generalised discharge coefficient, γ is an adiabatic coefficient, π is a dimensionless pressure, and the subscript, v, denotes vented or referring to a vent.

For the venting of low strength structures, but without restrictions due to vessel shape, and provided L/D does not exceed a value of 3, the NFPA [7] recommends the following equation:

$$p_{red}=(C\,A_s)^2 A_v^{-2} \qquad p_{stat}\leq 0.1 \qquad \text{bar g} \tag{13}$$

where A_s is the internal surface area of the structure (m^2), A_v is the vent area (m^2), p_{red} is the maximum internal overpressure which can be withstood by the weakest structural element and C is a venting constant. The value of the constant for methane is C=0.037 bar$^{0.5}$.

2. TNT Equivalency Model

The TNT equivalence model is the traditional model used for gas explosion effects. In this model, the available combustion energy in the gas cloud is assumed to convert into an equivalent charge weight of TNT [14] according to Eq. (14). If the equivalent charge weight is known, the explosion characteristics and the possible damage are derived from the large amount of data available from TNT explosions.

$$W_{TNT}=\alpha_e\frac{W_f H_f}{H_{TNT}}=\alpha_m W_f \tag{14}$$

Where α_e (based on energy), α_m (based on mass) is known as the efficiency factor, W_{TNT} the equivalent weight of TNT, W_f the total weight of fuel in cloud, H_f the heat of combustion of fuel, and, H_{TNT} the heat of explosion of TNT.

3. TNO Model

The TNO model developed by Wiekema [15] assumes that all the combustion energy present in the flammable part of the cloud contributes to the explosion. If the characteristic explosion length is calculated, the blast parameters, such as peak pressure and the duration of the positive pressure phase at a certain distance from the centre of the hemisphere are derived from the blast chart. Unlike the TNT equivalence model, the blast chart accounts for the effect of fuel reactivity on the blast characteristics by distinguishing fuel reactivity into three regions, such as low reactivity, average reactivity and high reactivity.

4. MULTI-ENERGY (ME) Model

The Multi-Energy concept [16-19] assumes that only the part of the combustion energy present in the flammable cloud which is confined or obstructed contributes to pressure generation in the explosion. In this way, the multi-energy model takes account of the positive feedback mechanism of a gas explosion.

This positive mechanism [20] assumes that flame acceleration occurs in regions with a turbulence level in the flow field due to the presence of obstacles prior to the arrival of the flame. The expansion of unburned gases ahead of the propagating flame during the combustion process will create turbulence due to the interaction of the flame with distortions and turbulence in the flow field. The flame propagation will be accelerated to high speeds with an accompanying increase in overpressure.

The model is based on a flux-corrected transport code to numerically simulate the explosion of a centrally ignited hemispherical, homogeneous, stoichiometric cloud, with constant flame speed. If the volume of the flammable cloud trapped in a congested region is known, the combustion energy participating in the explosion can be estimated. The blast charts that determine peak overpressure and the duration of the positive phase form a family of curves relating the dimensionless overpressure to the combustion energy scaled distance. The source strength index that is an overpressure level expected to occur in the obstructed region, varying from 1 for weak explosion in an unobstructed and unconfined region to 10 for detonation, is assigned a value to determine the curves to use. The source strength depends on number, type and orientation of the obstacles present in obstructed region as well as the fuel reactivity. More detailed description of this source strength can be found in some publications [20,21].

5. BAKER-STREHLOW (BS) Model

The Baker-Strehlow model was first developed by Baker et al. [22] and the model was further improved by Baker et al. [23]. This model is based on dimensionless overpressure and positive impulse as a function of energy-scaled distance from the gas blast centre, the maximum flame speed is selected using the method based on the fuel reactivity, degree of confinement, and obstacle density [22].

The BS model for spherical air explosions has similarities to the ME model for hemispherical explosions. In both the BS and the ME models, the source energy is defined by a stoichiometric flammable cloud that is in a congested or partially confined region [14]. The flame speed for the BS model or initial explosion strength for ME model is determined by empirical approaches based on the degree of confinement and obstruction with the source region as well as the distance available for flame acceleration [14,22,23].

The major difference between the ME model and the BS model is the method used to construct the graphical relationship between dimensionless overpressure and combustion energy-scaled distance. The curves used in the BS model are based on numerical modelling of constant flame velocities and accelerating flames spreading through spherical vapour clouds. With this method, the strength of blast wave is proportional to the maximum flame speed, which is presented in the form of a Mach number, achieved with the cloud.

6. Congestion Assessment (CA) Model

The Congestion Assessment model developed by Cates and Samuels [24] has much in common with the ME model. As originally developed, the source strength of an explosion was derived from a decision tree and the decay of blast wave was obtained from a simple formula. Since the initial development, the CA model was modified to include the estimation of pulse duration and shape by Puttock [25,26], and it is now capable of making more detailed prediction of explosion in an obstructed situation. Furthermore, it can also account for the reactivity of different fuels.

PHENOMENOLOGICAL MODELS

Phenomenological models are simplified physical models, which attempt to model the dominant physical processes of an explosion based on idealized geometry and empirical correlation. The major idea of simplification is that the actual geometry is converted to the modelled geometry. The physics of combustion processes may be described both empirically in conjunction with experimental data and theoretically. The models can give reasonable results when the actual geometry has a structure with repeated rows of similar obstacles, while may not be adequate for more complex geometries. Representatives of this type of models are the CLICHÉ and SCOPE.

1. CLICHÉ

The CLICHÉ (Confined Linked Chamber Explosion) model developed by British Gas and is incorporated into the CHAOS software package [27]. It was initially used study gas explosions in buildings involving flame propagation from one room to another and has now been widely extended to modelling in offshore and onshore areas. The conservation laws for the unburnt and burnt gas volumes in each chamber are applied in the CLICHÉ model, and the model assumes that the properties within each chamber are uniform and that any momentum changes occur only at the perimeter of these volumes. A wrinkled laminar and turbulent combustion model is also included in the CLICHÉ model. The wrinkled laminar combustion model calibrated against balloon experiments performed by British Gas uses the average burning velocity as a function of travel distance from the ignition point. The turbulent combustion model considers the turbulence effects caused by obstacles and includes the root mean square turbulence velocity and the turbulent integral length scale which enable a turbulent burning velocity to be derived from a combustion model devised by Bray et al. [28].

2. SCOPE

The earlier SCOPE1 (Shell Code for Overpressure Prediction in Gas Explosions) model, based on the underlying physical processes proposed by Cates and Samuels [24] was designed for modelling explosions generated by the accidental release and ignition of a gas cloud in congested regions like offshore modules. SCOPE1 was validated against the experimental data obtained from a 35 m^3 volume with obstacle grids performed by Det Norske Veritas and, a reasonable agreement between the predictions and experimental data was found. The root mean square deviation was of 28.5%. SCOPE2 based on the SCOPE1 model was further improved by Shell TRC in 1994 to model gas explosions by representing the dominant physics in simplified geometries like a cuboid shape and single compartments containing a series of obstacle grids. The main improvement in SCOPE2 was to enable the amount of burnt and unburnt gas in the box to be tracked as a function of time, pressure time histories, the position of the flame front with time, etc. by introducing a differential equation formulation, and has the ability to handle mixed scale objects. The model was validated against extensive experimental data, including 425 m^3 DNV tests, 91.6 m^3 (1/6 of the SOLVEX scale) experiments and 550 m^3 SOLVEX experiments

[29]. The current SCOPE3 model produced by Puttock [1] is an enhanced model of the SCOPE2 program and has been in use since in 1997. The SCOPE3 model has been validated against more than 300 experiments including 35 m^3 box, 91.6 m^3 (1/6 of the SOLVEX scale) rig, 550 m^3 SOLVEX and BFETS Phase 2.

CFD MODELS

Computational Fluid Dynamics (CFD) models are based on the fundamental partial differential formulations governing the explosion process. These models start with the basic conservation equations for mass, momentum, energy as formulated in the Navier-Stokes equations which govern fluid flow, and use physical submodels to treat turbulence and combustion [30]. The control domain is discretised into a grid of computational cells. The conservation equations are integrated over control volumes surrounding the relevant grid points in both space and time.

A number of CFD-codes are available for gas explosion modeling. A review of most existing models for gas explosion modeling can be found in some literatures [30-37]. According to Lea and Ledin [31], the CFD codes can be classified into simple and advanced groups. The simple CFD-models such as EXSIM, FLACS and AutoReaGas are based on the PDR method for representation of the geometry. However, the advanced models such as CFX-4, COBRA, NEWT and McNEWT use more complicated numerical schemes to improve the representation of the geometry.

1. EXSIM

The EXSIM (EXplosion SIMulator) code was developed at the Telemark technology R&D Centre (Tel-Tek) in Norway. EXSIM uses a finite volume code based on a structured Cartesian grid to solve the time averaged conservation equations of fluid flow and chemical reactions. The first or second order upwind differencing schemes are used for all variables. The geometry for the representation of small-scale objects is modelled by the Porosity Distributed Resistance (PDR) method. EXSIM updates pressure and corrects velocities by the SIMPLE algorithm and uses simplified wall boundary conditions. Turbulent combustion rate is modelled with the eddy dissipation combustion model proposed by Magnussen and Hjertager [38] and with the ignition/extinction criterion modifications introduced by Hjertager [39].

The EXSIM code based on the model of Hjertager [39] has been validated against the experimental data obtained from the tube geometry of Moen and Lee [40] and the vented channel of Chan et al. [41]. The agreement reported by Hjertager [39] between the predictions and the experiments for over-pressures at both the enclosures was reasonable. However, it was stressed that the computation model (EXSIM) must be further developed and validated against large-scale experiments in a variety of geometries.

Hjertager [42] has presented a computation procedure capable of dealing with transient compressible turbulent flows. The major flow parameters used in the model were the velocity components and pressure. All conservation equations are discretised by integration over control volumes. The integration is performed by application of upwind differencing in a staggered grid system and extension of the SIMPLE-algorithm [43] is adopted for solution procedure. The analytical solution and computed prediction by EXSIM have both been applied to the shock tube, and results were very similar. However, the computation method needs to be tested through various geometrical configurations to examine the ability of the model to predict explosion effects in practical situations.

The predictions of gas explosions in complex congested geometries were performed by Hjertager et al. [44]. The good agreement between the predictions with the EXSIM coded and the measurements of relevant for offshore situations was reported, however, no results of any realistic uncertainly were provided. It is needed to develop the PDR model for explosion propagation in more highly congested obstacle fields and a model for deflagration to detonation transition, and improve the turbulent combustion model.

Hjertager [32] reported the results of modelling turbulent explosions using the EXSIM in a variety of geometries such as tube, vented channel, empty volumes, module geometries, and geometrical layout of Piper Alpha accident. The comparisons between predictions and measurements were founded to be in good agreement, but, no information of the statistical uncertainty was given. However, it was also pointed out that the improvement of the turbulence combustion model and the model of DDT (Deflagration to Detonation Transition), and more experimental data for validation of the model in high density geometries were needed. In addition, Hjertager et al. [32] demonstrated a scenario analysis of gas explosions on realistic process plant using 3D EXSIM code. The three ignition positions chosen were (1) outside the process line area: (2) inside the process line area: (3) under the compressor building. The results from the calculations showed that the overpressures for the three cases ranged from about 0.2 bars and up to 9 bars. The ignition under the compressor building caused the highest pressure while the lowest one was found outside the process line area.

The 3D EXSIM-94 code has been extensively validated against several experimental data from relevant offshore module tests for quantification of uncertainly between experiments and simulations [45]. The module experiments were the DNV module, the Shell SOLVEX modules, CMR compressor (M24) and separator modules (M25), and Shell troll process module. Their results showed that there is a 95% confidence that the mean maximum overpressure lines within ±46% of the predicted value.

Hjertager et al. [33] reviewed computer models for detailed analysis of gas explosions. The predictions of four computer codes using EXSIM, FLACS, REAGAS and COBRA codes were compared with the experimental data of Type E and C* of MERGE (Model Evaluation Group for Gas Explosions) geometries. The EXIM code showed an average underprediction of 15% and the predictions indicated that there was a 95% confidence.

Sæter [46] has validated the code against 40 realistic gas explosion experiments. The main results reported are that the code is founded to be relatively grid-independent in terms of predicting explosion pressure in different offshore geometries. The code also shows that it has abilities capable of simulating the effects such as ignition point location, vent arrangements, different geometries, scaling effects and gas reactivity. However, it is recommended that other explosion parameters involving pressure rise time, pressure pulse duration, flame speed and dynamic pressure, and other geometries, other scales, degree of confinement and congestion should be further validated in the code.

Høiset et al. [47] have performed the simulations with the EXSIM code of the Flixborough plant accident. The comparison showed that the explosion pressure estimates in the literature based on visual inspection are much lower than the values from the simulation while the results of the simulations results agree well with estimates in the literature based on calculations.

2. FLACS

The FLACS (FLame ACceleration Simulator) code was initially developed by the Christian Miichelsen Research (CMR) Institute in Norway for the purpose of the simulation of gas explosions in offshore modules. It has been extended to cover a wide range of plant geometry and fuels encountered onshore. The versions of FLACS code have been improved over the last decade, and the code is continuously developing under CMR-GEXCON. FLACS uses a finite volume code based on a structured Cartesian grid. The code also uses the PDR approach to model sub-grid obstacles. A weighted upwind/central differencing scheme that is first order accurate are used for all variables, however, the second-order Van Leer scheme is for the reaction progress variable. The turbulence is modelled by the k-ε turbulence model and the combustion is modelled with a model, called β flame model based on correlations of turbulent burning velocities with turbulence parameters [48].

The FLACS has been extensively validated against a wide range of explosion experiments such as simple idealized geometries and realistic geometries. The representative simple geometries are a 10 m tube, 1 m and 10 m wedge-shaped vessels, 3 m cuboid vessel, scale 1 : 33 and 1 : 5 offshore modules, TNO geometry, MERGE geometries, Mobil/British Gas geometry and Shell SOLVEX geometries. The realistic geometries are the CMR Compressor Module (M24) and SCI module. The description of explosion experiments and results in a range of the geometries can be found in Arntzen [48] and Bjerketvedt et al. [49].

The 2D FLACS-ICE code proposed by Bakke and Hjertager [50] has been applied to the three different tests (0.0036 m^3 vessel, 35 m^3 vessel and 425 m^3 vessel). The comparisons were examined in terms of the influence of size of vent area and location of ignition source on gas explosion overpressure. The results of the comparison between predicted and measured variation of the explosion pressure as a function of the scaled vent area were in reasonable agreement with measurements for all three volumes. The model also gave reasonable agreement as long as the ignition point is some distance from the vent whereas it did not meet with any success for ignition near the vent opening.

Van den Berg et al. [51] have simulated the vapour cloud explosion accident which happened at Beek with the FLACS code. A comparison between the damage that occurred in the accident and the simulation with idealized gas clouds shows similar trends in pressure distributions. The result were dependent on the properties of the flammable cloud such as composition and cloud height. The simulations have also shown that the FLACS code can also be used to estimate the effects of vapour cloud explosions in large land based installations and complex geometries.

Tam et al. [52] have undertaken a numerical simulation with FLACS code for the design of the BP Andrew platform for gas explosion mitigation. The simulation results reported on the lower process area showed that as the propagating flame traversed the deck area it resulted in increasing over-pressure. The high pressures were generated near the east stair tower and near the ESD valve enclosure. These were due to locally high over-pressures caused by the higher turbulence between the flame and obstacles locally.

Van Wingerden et al. [53] have compared 3-D FLACS code simulations with the two traditional prediction models such as the TNT-equivalency and the Multi-Energy model for a practical case. The results showed that due to the simplifications in the two traditional models the effects of vapour cloud explosions in the near filed can be both overestimated and underestimated The results for the blast pressures predicted in four directions using the code also showed that the blast decay away from the facility was stronger than predicted by the ME model. The blast decay appeared to be stronger in the near field but the FLACS and the TNT-equivalency model were found to become closer in the far field.

3. AUTOREAGAS

AutoReaGas code has been jointly developed by TNO and Century Dynamics. The code integrates solvers of the REAGAS and BLAST codes developed by TNO Prins Maurits laboratory (PML) in Netherlands. The gas explosion (NavierStokes) solver used in the REAGAS code is used for the analysis of gas explosions, including flame propagation, turbulence and the effects of obstacles in the flow. The blast solver used in the BLAST code is used for accurate, efficient capture of shock phenomena and blast waves.

The gas explosion simulator in the AutoReaGas contains a finite volume code based on a structured Cartesian grid. Numerical solution of the set of equations is accomplished by use of the first order accurate Power Law scheme applied within a finite volume approach, with the SIMPLE algorithm implemented for pressure correction. Large objects are resolved by the grid whereas the presence of a subgrid object is modelled as a source of turbulence and drag. Turbulent combustion is modelled by an expression which relates the combustion rate to turbulence. Turbulent combustion rate can be modelled with the eddy break up model [54] the eddy dissipation model [38] and experimental correlations for flame speed [55].

AutoReaGas has been extensively validated against many experiments on several key projects, involving MERGE [56,57], EMERGE [16] and Fire and Blast Joint Industry (JIP) Phase 2 that involved full scale tests as described in the report by Selby and Burgan [58]. The code has been also applied to case studies such as real offshore platforms [59,60] and real process plants [61,62].

Van den Berg et al. [51] have performed a case study using AutoReaGas code on gas explosions in practical process plants. The case study showed that the equipment present in the process area of chemical plants provides the turbulence generative conditions for gas explosions to develop damaging overpressures and blast. Higher overpressures were generated in the direction of flame propagation than in the opposite direction. The blast effects from violent vapour cloud explosions have a high degree of directionality. The simulated results also showed that the blast loading on a building was shown to be greatly influenced by the presence of other structures in its vicinity.

Gas explosion and subsequent blast analyses in an actual offshore platform complex were performed with the AutoReaGas by Mercx et al. [63]. In comparison with the AutoReaGas results for the overpressures inside the cloud entrapped in the platform, the Multi-Energy results are considerably higher. Despite the lower explosion overpressures, the numerical calculation resulted in higher peak blast overpressures than the simplified approach.

4. COBRA

The general purpose COBRA code has been developed by Mantis Numerics Ltd. for industrial applications. COBRA is based on solutions of the fluid flow equations using a second-order accurate, finite-volume integration scheme coupled with an adaptive grid algorithm. The code uses solutions of the ensemble-averaged, density-weighted forms of the transport equations for mass, momentum, total energy, and a reaction progress variable. Diffusion and source terms are approximated using central differencing and the convective and pressure fluxes are obtained using a second order accurate variant of Godunov's method. The code models large obstacle exactly, while small obstacles are represented at sub-grid level. COBRA uses the PDR approach for modelling sub-grid scale obstacles. Turbulence formed ahead of a propagating flame is modelled using a k-ε turbulence model. The premixed combustion process is modelled using a semi-empirical approach which admits both chemical kinetic and flow field influences on the burning velocity of a flame, while maintaining realistic flame thicknesses throughout the course of a flame's propagation.

COBRA code has been validated against experimental data of explosion tubes [64,65]. Catlin et al. [65] have presented a mathematical model capable of predicting turbulent, premixed flame propagation and the consequent overpressures, and validated predictions of the model against experimental data gained in a large-scale cylindrical vessel containing turbulence-inducing rings [40]. Comparison of predictions made using COBRA code which includes the mathematical models mentioned above and measurements showed that the model appears to yield reasonable predictions of propagating turbulent premixed flames which interact with obstacles, and the resulting generation of damaging overpressures. However, the model needs to be validated against a wider range of experimental data at a variety of scales, including flow field measurements.

Fairweather et al. [64] have presented an experimental and computational study of premixed flame propagation in small-scale, cylindrical vessels. The experimental data obtained have been used to further assess the accuracy of a mathematical model described by Catlin et al. [65]. Overall, the comparisons between experimental results and predictions have demonstrated that the model provided a reasonable simulation of combustion within cylindrical vessels that contain turbulence-inducing obstacles like baffles, however, the data of the realistic uncertainty were not reported. Comparisons have also demonstrated that provided obstacle-generated turbulence occurs sufficiently early in the computations, this modelling approach allows the transition from laminar to turbulent flame propagation which occurs in explosion situations to be accommodated. However, the model needs to be validated against detailed experimental data in the highly turbulent shear layers and recirculation zones of the flow to allow a more quantitative assessment of the turbulent premixed combustion model.

5. Other Codes

Green et al. [66] have applied the EXPLODE2 code to the baffled ignition tube which has a 10 metre by 2.4 metre diameter published by Moen and Lee [40] for massively parallel systems. The code employed a Total Variation Diminishing (TVD) scheme based on finite volume discretization with a fourth order Runge-Kutta algorithm. The physical and chemical modelling uses a k-ε turbulence model with the eddy break-up model for turbulent premixed combustion as modified by Magnusson and Hjertager [38]. The results showed that highest over-pressures are generated at the exit region, which is in agreement with the experimental data. The results also revealed the importance of flame acceleration due to turbulent generation and acoustic coupling within the flow and the role played by the geometry of the simulated system in generating these effects.

The modified combustion model which was based on eddy break-up, turbulent length scale and flame stretch factor proposed by Green and Nehzat [67] was encoded in the EXPLODE 2 code. The predictions were performed for validation with experimental data presented by Freeman [68]. The results showed that the deviation between prediction and measurement for the peak pressure, peak pressure time and rate of pressure rise was 1.5%, 4% and 10% respectively. However, the code does not include a fine grid and detailed chemical reaction model.

Lea and Freeman [69] have reported FLOW3D code predictions of stoichiometric methane/air explosions in vented enclosure containing baffles of varying widths. The code used was "SIMPLER" a variant of the SIMPLE pressure solution algorithm. The numerical modelling of convection uses the high-order accuracy "QUICK" scheme in all equations except those for k and ε. Fully-implicit differencing is used for time-stepping. The physical models used for turbulence and combustion are a k-ε turbulence and eddy break-up models [38]. Comparison between predictions and experimental data for the box with 3-baffles fitted and for three different widths of baffles showed that the peak pressures and the rates of pressure rise generated by the model are over-predicted by about an order of magnitude. The reason for this discrepancy seems to be due to the eddy break-up combustion model which contains no chemical kinetics or turbulent strain-related limit to the combustion rate, and infinitesimally small ignition energy.

Freeman [68] has also validated the FLOW3D code against experimental data obtained by gas explosion experiments of both confined empty vessel and semi-confined enclosure including three and five different widths of baffles. For fully confined explosions, the predicted overpressures and rate of pressure rise were higher than those observed experimentally due to the underestimation of heat loss to the walls of the enclosure. Model predictions for the pressure in the vented enclosure were significantly lower than the experimental values due to the inaccuracies of k-ε turbulence model used for turbulence. In order to improve the accuracy of CFD models for gas explosions, the physical sub-model for turbulence needs to be improved or replaced with one developed specifically for the highly turbulent recirculating flows associated with the progress of an explosion around obstacles.

Pritchard et al. [70] applied the CFDs-FLOW3D (now known as CFX) code for vented enclosures to predict explosion pressures and flame speeds. The model uses a multi block, body-fitted grid of hexahedral volumes, and the governing equations are solved implicitly using the standard method of iteration on the segregated, linearized equation set. The SIMPLE, or a variant SIMPLEC is used to solve for mass and momentum, the solvers are robust and a variety of bounded second-order differencing schemes are available for explosion modelling. The turbulence model is the two-equation k-ε and the combustion model is the eddy break-up model [38]. The results from the validation of the model against experimental data have led to significant improvements for both pressure values and behaviour of the propagation of the flame front. Guilbert and Jones

[71] have applied the CFX-4 (formerly CFDs-FLOW3D) code to linked vessels performed by Phylaktou and Andrews [72]. All flow variables in the model are stored in collocated grid, and the model uses implicit solvers, CONDIF which is based on a central differencing scheme and the standard law of the wall. The comparisons between experiment and simulation for the pressure histories were found to be good agreement, but there were no data for the standard deviation between the prediction and the experimental data. However, the greatest limitations on the modelling arise out of the use of the standard k-ε model for turbulence. It is important to include additional terms in the equations to account for the acceleration of the hot gases.

Huld et al. [73] have presented a computer code named REACFLOW for simulating the behaviour of compressible and incompressible gas flows with chemical reactions in a two-dimensional area. The code contains a finite-volume scheme based on an approximate Riemann solver, an unstructured triangular grid. Chemical reactions are calculated fully implicitly. The REACFLOW also includes adaptation grid capability, which automatically detects locations of refinement and coarsement based on local gradients of flow variables. The code uses two methods for the calculation of the chemical source terms, the first is based on finite rate chemistry and the other is based on the eddy dissipation concept. The two-dimensional calculations of a hydrogen/air explosion in a container and tulip flame in a closed vessel showed the capabilities of the code.

Wilkening and Huld [74] have simulated large-scale hydrogen explosions using the grid adaptation system implemented in the REACFLOW code. The use of adaptation mesh refinement was found to be good effect. The predicted results were a reasonable agreement with the experiments in terms of peak pressure, pressure time history and detonation velocity.

Clutter and Luckritz [75] based on the CFD model named CEBAM (Computational Explosion and Blast Assessment Model) has carried out CFD simulations of explosions compared to experimental results obtained from EMERGE and BFETs projects. CEBAM uses a finite volume formulation within a curvilinear framework for solution of the equations. A flux-vector splitting scheme with variable extrapolation is used along with a predictor-corrector method to achieve 2nd order in time and space. The model also includes a reduced combustion model which uses a characteristic flame speed to set the reaction rate with in various congested regions and the porosity model that represents the vast amounts of small objects. There is no explicit equation for turbulence. The rate of reaction is based on empirical data but the combustion process is represented by a single-step chemical reaction. The comparisons to the data from the small and medium tests of the EMERGE project, as with BFETs results show the reduced combustion model provides useful predictions within the risk assessment process.

Naamansen et al. [37] have performed two dimensional numerical simulations with the McNEWT code of the experimental work of Ibrahim and Masri [76]. The code, a modified combustion version of the code NEWT, solves the reacting flow field with a laminar flamelet model on an unstructured tetrahedral grid with adaptive mesh refinement. A total of 12 cases were investigated involving different obstacles such as cylinders, triangles, squares, triangles and flat plates with blockage ratios (from 10 to 75%). The shape of the flame agrees well with the high speed video images from the experiment of Masri et al. [77]. The statistical analysis showed that the averaged differences between predicted and experimental overpressures were about +12.4% and the standard deviation of the relative errors was 38%. It indicated that more levels of grid refinement in the adaptive mesh refinement were required to improve the accuracy further.

Patel et al. [78] have performed an experimental and computational study to investigate the deflagration of a turbulent premixed flame inside a semi-confined explosion chamber. Three consecutive solid obstacles of rectangular configuration were mounted inside the chamber to examine the interaction of the propagating flame. The simulation calculations were carried out with a two-dimensional finite difference code, named TRF2D which solves the Favre averaged conservation equations for momentum, turbulence and energy. A modified flame surface density (FSD) combustion model has been applied to simulate to predict the flame propagation past multiple obstacles. The simulated results showed that the turbulence stretch is dominant in regions behind the obstacle wakes due to the presence of highly recirculating zones while the mean flamelet stretch dominates in the flow jetting regions around the obstacles. The predicted results using modified combustion model applied were in good agreement with the experimental observations in terms of flame structure, pressure time history and flame speed.

Industrial facilities were pipes, machines, tanks etc. form obstacles for the flow. The flow develops turbulent structures. The turbulence interacts with the flame and accelerates it. This process is unsteady and dominated by the large turbulent structures. For this reason large eddy simulation (LES) should be well suited for the prediction of this process. The drawback of the common LES approach appears in near wall regions. In the near wall region turbulent structures are very small. As a consequence a very high grid resolution would be necessary for LES in the near wall region. This is computationally much more time-consuming than Reynolds averaged Navier Stokes (RANS) methods. Although the LES approach has its difficulties in the wall region, it is recently gaining acceptance as a visible tool for simulating turbulent premixed flame [79]. Masri et al. [79] have performed an experimental and large eddy simulation of a freely propagating flame around obstacles within a chamber. The predictions were implemented in the PUFFIN code [80]. The dynamic Germano model and a flamelet combustion model were employed in a sub-grid scale. LES simulations were found to be in good agreement with the experiments in terms of flame structure and overpressure, however, no data of the statistical uncertainty between the calculations and measurements were presented. The application of the LES model for experimental data obtained from large-scale empty 547 m^3 SOLVEX enclosure reported by Puttock et al. [29] was made by Molkov and Makarov [81]. The initial flame propagation stages and pressure development up to first peak pressure of the simulation was in good agreement with the experimental data without introduction of any adjustable parameter. However, the experimental pressure dynamics inside and outside the enclosure as well as the shape of the external deflagration were accurately reproduced in large eddy simulations using a modified LES model.

DISCUSSION AND RECOMMENDATIONS

1. Correlation Models

The venting guidelines are to calculate the maximum pressure inside a vessel, however, its does not contain information on the duration and shape of the pressure time history associated with an explosion, which may be required for structural analysis of an enclosure. The TNT, TNO models and etc. are to calculate the maximum free-range explosion pressure and hence assess likely damage. It is normal to equate the maximum internal pressure in explosions to Youngs modulus and to the ultimate yield stress of the enclosure. The former is used when an explosion is fairly frequently expected and requires the vessel to not be deformed by the explosion. The latter is to ensure that if an explosion occurs the vessel will not disintegrate. The reasoning behind this is that the loading in the vessel is over a relatively long timescale so the shape and impulse are not really an issue unlike in detonations. The other models are used to calculate damage away from the centre of the explosion.

TNT equivalence model is easy to use and has a wide range of applications, and satisfactory for far distances [82], while this model has some limitations when applied to gas explosions: (1) It is difficult to select a yield (efficiency factor) that is appropriate for a given situation; (2) The yield factor is only associated with the amount of fuel involved and not the combustion mode; (3) At short distances this model over predicts the overpressure by a gas cloud explosion; (4) Some of the important influencing factors in a vapour cloud explosion such as the degree of mixing, and ignition strength, ignition positions, obstacles positions, degree of confinement, turbulence, etc. are not considered; The use of the TNT equivalence model is not recommended for near field predictions. Despite these deficiencies, the TNT equivalency model is still being widely used because it is ease and it requires only limited assumptions for determining the initial release size and yield factor [83]. This model is used for the assessment of far field effects when considering impact on people for emergency management, and for design purposes.

The TNO model also allows for the flame acceleration by obstacles placed in a congested region by simply relating the boundary of the reactive region to the obstacle density. However, the clear separation of the fuel reactivity and obstacle obstruction on the blast charts in the TNO model causes limitations to determining the maximum and minimum source overpressure.

A considerable improvement in prediction of explosion pressure was achieved with ME model The ME model is an alternative model to the TNT-equivalence model. However, the ME model still has some limitations for gas explosions: (1) The hemispherical shape, stoichiometric concentration throughout the cloud and constant flame speed assumed in the model concept are unrealistic and are not likely to occur in practice; (2) The important parameters such as confinement level, turbulence level, fuel reactivity, ignition strength and ignition positions, etc. influencing explosion strength are not considered in the model; (3) The choice for the source strength while depending on the nature of the obstructed region may be difficult in practice. This difficulty is a similar problem to selecting the efficiency factor in the TNT equivalence model. The available guidance to choose the explosion strength of the ME model was proposed by CCPS [20], Baker et al. [22] and Kinsella [84].

The BS model with one dimensional numerical curves like the ME model takes into account some geometrical details, with regards to confinement and can handle multi-ignition points, and provides a better representation of vapour cloud explosions blast parameters than the TNT-Equivalence model. However, this model cannot describe the impact of non symmetric vapour cloud shapes and ignores the location of obstacles or the ignition location. The CA model is calibrated against the results of the MERGE project that includes small scale, medium scale and large scale experiments, and it can deal with non-symmetrical congestion [31]. However, the assessment for level of congestion and the level of confinement for complex geometries is difficult.

2. Phenomenological Models

The main advantage of the CLICHÉ model is that it has similar capabilities to the numerical models, and its computing time is fast because of the simplified modelling approach. However, the model does not provide the detailed information about the flow field like CFD models. The major improvement in the SCOPE3 model is consideration of the effects of obstacle complexity, and the model includes rear venting as well as side and main vents included in the SCOPE2 model, treatment of gas mixtures and variations in stoichiometry and revised turbulent burning velocity equations. The major limitations of the model are that it can only treat a single enclosure, it contains less geometrical detail than CFD models due to idealised processes relative to real geometries and it does not provide the detailed information about the flow field like CFD models.

3. CFD Models

The CFD models provide a great wealth of information and can predict more detailed and accurate results of an explosion than correlation models and phenomenological models over a wide range of conditions and geometrical arrangements. The information obtained through each computation about the flow field consists of velocities, pressure, temperature, density, turbulence, species concentration, etc.

The principle difficulty associated with the use of CFD models is that solving the governing equations numerically by an iterative method for all control volumes and repeating these for each successive time is computationally expensive and can take a very long time to compute. This problem often limits the application in predicting gas explosion behaviour in complex geometries that consist of a large number of different process equipment. The alternative method is to use the physical models of turbulence and combustion validated against experiment data.

The CFD models investigated in terms of physical sub-models such as turbulence and combustion models can be summarized as follows: All the models use finite-domain approximations to the governing equations including the effect of turbulence and the rate of combustion. Turbulence effects are considered by the k-ε model. EXSIM code uses the eddy dissipation combustion model. FLACS code uses burning velocity controlled flame model, where the burning velocity is expressed empirically from the experimental data presented by Abdel-Grayed et al. [85] and the Bray correlation [55]. Turbulent combustion rate in AutoReaGas is modelled with the eddy break up model, the eddy dissipation model and experimental correlations for flame speed [55]. The COBRA code uses a semi-empirical approach which admits both chemical kinetic and flow field influences on the burning velocity of a flame and the correlations of Bray [55] are used to derive the turbulent burning velocity. The REACT-FLOW code uses an eddy break-up model. The CFX-4 code offers a number of turbulence models, including Reynolds stress transport models, and the eddy break-up and thin flame model. The combustion in the NEWT code is modelled using the eddy break-up model or a laminar flamelet model. The McNEWT code uses a laminar flamelet model. The EXPLODE 2 employs combustion model combined based on eddy break-up and an integral length scale. CEBAM code includes a reduced combustion model which uses a characteristic flame speed to set the reaction rate within various congested. TRF2D uses a modified flame surface density (FSD) combustion model.

The majority of CFD models investigated use the eddy break-up combustion model. If the flame front cannot be properly resolved, the use of eddy break-up combustion model should be reconsidered. Laminar flamelet methods are applicable to only specific regions of the regime of turbulent combustion. Incorporation of detailed or reduced chemical kinetics with a probability density function (PDF) transport approach is emerging and holds great promise for the future. However, it is unlikely to be feasible for real complex arrangements in the near future due to the heavy demand on computer resources in terms of both processor speed and computer memory.

4. Recommendations

Presently, different models are available for predicting the consequences due to gas explosions. These models have their own advantages and disadvantages. In order to improve the reliability in model predictions, further improvements in terms of the physics and the numerics are needed, particularly for the CFD-based models such EXSIM, FLACS, AUTOREAGAS, COBRA, and etc. Verificaiton is a necessary step in the development of physical sub-models of CFD codes, and this must be done against experimental data relevant to the final application. Recent developments [86,87] in experimental techniques have allowed measurement of flame position and probablility density functions (PDF) of flame speed and burning velocity in premixed gas systems including small scale explosion experiments. However, the use of these data in modelling explosion has been limited and at the present does not seem to have been applied to assessment of vulnerability for risk studies.

To develop Computation Fluid Dynamics explosion model based on PDF methods that can accurately predict, further investigation are required to quantify statistically the turbulent flow fields generating during flame/obstacle interaction, it would be advantageous to use the laser system to measure chemical species pdf's and their covariance with other quantities such as concentration, temperature and pressure directly. The advantage of using a PDF formulation for simulation is the ability to use fundamental chemical kinetic schemes to generate the required PDFs that can then be tested against the experimental results. Once developed this will provide a flexible tool for assessment of a wide variety of geometries and not be as restrictibve as current simulation techniques.

CONCLUSIONS

Theoretical models of explosion hazard assessment currently available fall into three different categories. This study has presented a comparison of these three correlation models, physical models and computational fluid dynamics models for gas explosions.

Correlation models such as venting guidelines, TNT equivalence model, TNO, Multi-Energy model, Baker-Streholw model, and etc. are based on correlations gained from analysis of experimental studies. Phenomenological models such as SCOPE and CLICHE are simplified physical models, which take account of only the dominant physical processes of explosion process with the individual sub-models calibrated against a wide range of experimental data. The physical processes may be used in conjunction with both correlation and CFD models.

Among the different models it seems that the most effective method to assess the explosion hazard was provided by the computational fluid dynamics approach. There have been very few published reviews on comparisons of different codes on the same geometric problem. The published studies show wide variations in results from significant under-prediction to over-prediction. The CFD models should be properly validated against extensive experimental data. These CFD models currently available have been tested against limited experimental data. As a result, different models give widely differing answers for the same geometry. Validation and development of physical sub-models like turbulence and combustion used in the CFD models has been a great interest for hazardous industries. Therefore, the CFD models must be validated against extensive experimental data prior to becoming a reliable predictive tool. For practical purposes, the detailed modelling of vented explosions based on CFD codes can be excessively sophisticated and time consuming and even not feasible for large and complex geometries. Simpler models used in venting guidelines are often used to predict the overpressures generated in such situations, with validity restricted to certain limits of parameters characteristics for the vessel, the vent and explosive mixture. Some models were in a good agreement with results within their validity ranges. The practical application of venting techniques will be based on relatively simple models in the near future.

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