



Letter

A new equivalent method to obtain the stoichiometric fuel-air cloud from the inhomogeneous cloud based on FLACS-dispersion



Yulong Zhang*, Yuxin Cao, Lizhi Ren, Xuesheng Liu

PowerChina railway construction Co., LTD, Beijing, 100044, China

HIGHLIGHTS

- The pseudo-component gas and its explanation.
- Deduction of new equivalent method.

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ABSTRACT

The fuel-air cloud resulting from an accidental discharge event is normally irregular in shape and varying in concentration. Performance of dispersion simulations using the computational fluid dynamics (CFD)-based tool FLACS can get an uneven and irregular cloud. For the performance of gas explosion study with FLACS, the equivalent stoichiometric fuel-air cloud concept is widely applied to get a representative distribution of explosion loads. The Q9 cloud model that is employed in FLACS is an equivalent fuel-air cloud representation, in which the laminar burning velocity with first order S_L and volume expansion ratio are taken into consideration. However, during an explosion in congested areas, the main part of the combustion involves turbulent flame propagation. Hence, to give a more reasonable equivalent fuel-air size, the turbulent burning velocity must be taken into consideration. The paper presents a new equivalent cloud method using the turbulent burning velocity, which is described as a function of $S_{L,t}$, deduced from the TNO multi-energy method.

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With the application of quantity risk analysis to the 18th sub-line of Chengdu, China, FLACS code, as a computational fluid dynamics (CFD) tool, plays a key role. It embedded Q4, Q5, Q8 and Q9 as the models for equivalent fuel-air cloud volume. The benefit of the equivalent approaches is ease to get a representative distribution of explosion loads with minimum number of simulations.

In these models, the laminar burning velocity and volume expansion ratio are taken into account in the Q5 and Q9 methods, only the laminar burning velocity is taken into account in Q4, the volume expansion ratio is only taken into account in the Q8 method. Detailed information about them can be found in

literature[1].

Q9, as the latest version, is widely used to assess the explosion loads as part of a risk or consequence analysis [2], and is described by Eq. (1) in FLACS:

$$Q9 = \frac{\sum_{i=1}^n V_i (V_e(ER_i) - 1) ERfac(ER_i)}{\max [(V_e(ER) - 1) ERfac(ER) : ER_{LFL} \leq ER \leq ER_{UFL}]}, \quad (1)$$

where ER is equivalence ratio, $ER = \frac{(F/O)}{(F/O)_{stoi}}$ (F/O is the ratio of fuel and oxygen); V_i is the i^{th} control volume of the numerical grid inside the fuel-air region where the fuel-air is in the range of lower flammability limit (LFL) and the upper flammability limit (UFL), that is $ER_{LFL} \leq ER \leq ER_{UFL}$; $V_e(ER_i)$ is volume

* Corresponding author.

E-mail address: jadedragon_zhang@163.com (Y.L. Zhang).

expansion ratio at constant pressure in the i^{th} control volume, its value depend on the ER_i ; $ERfac(ER_i)$ is shown with Eq. (2):

$$ERfac(ER_i) = \frac{S_L(ER_i)}{\max(S_L(ER) : ER_{LFL} \leq ER \leq ER_{UFL})}, \quad (2)$$

where S_L is the laminar burning velocity.

In Eqs. (1) and (2), the volume expansion ratio and laminar burning velocity are the two key factors for representing the inhomogeneous fuel-air cloud as a homogeneous fuel-air cloud in Q9 model.

The factor, volume expansion ratio, employed in Q9 denotes that the part of ignitable heated fuel-air is expelled out of the control volume in explosion process because the Q9 can be got in the dispersion simulation stage prior to explosion simulation stage, thus, the donation of the expelled fuel-air to explosion load is ignored and its effect may be underestimated. However, in most realistic cases, the computing domain will not be completely filled with an ignitable fuel-air cloud, the deemed expelled fuel-air is still in the computing domain and also plays an important role in the explosion process, its donation on the explosion load cannot be neglected. It seems inappropriate that the volume expansion ratio is introduced into the equivalent approaching.

On the other hand, Q9 only employs S_L with first order to describe the combustion process. Most of the realistic fuel-air explosion process, the fuel-air flow field turns into turbulent regime and the flame propagation is also in violent and turbulent status.

To give a more reasonable equivalent fuel-air cloud size, a turbulent burning velocity S_T is proposed. Many models, such as Zimont correlation, Peters Correlation and Mueller correlation[3], describe S_T as a function of S_L and turbulence quantities. So, it is also reasonable to describe S_T as the S_L with a non-one order based on TNO (abbreviation for the Netherlands Organization) multi-energy method (ME).

In the multi-energy method, an idealized fuel-air explosion scenario model is put forward, shown in Fig. 1. The explosion is based on a ground-level hemispherical fuel-air cloud which is filled with a fuel-air mixture at a stoichiometric concentration.

Figure 1 shows the main features of an idealized explosion scenario, a ground-level hemispherical fuel-air cloud is ignited in the center, the flame front will then propagate symmetrically from the centre. the initial peak overpressure in the hemispherical fuel-air cloud zone is assumed as a constant P_0 whereas the side-on overpressure and dynamic pressure will decay with dis-

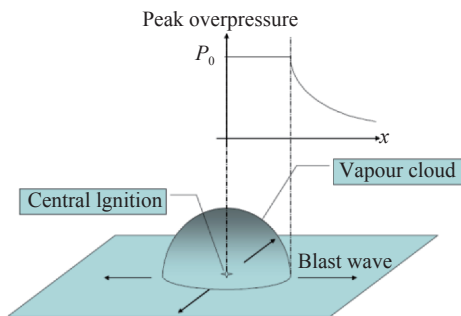


Fig. 1. Idealized fuel-air cloud explosion scenario model.

tance outside of the fuel-air zone.

The peak overpressure calculations in the fuel-air cloud zone are given with the Eqs. (3) and (4). Equation (3) shows the 2 dimensional (2D) explosion expansion, and Eq. (4) shows 3 dimensional (3D) explosion expansion.

2D expansion:

$$P_0 = 3.38 \left(\frac{VBR \cdot L_p}{D} \right)^{2.75} S_L^{2.7} D^{0.7}, \quad (3)$$

3D expansion

$$P_0 = 0.84 \left(\frac{VBR \cdot L_p}{D} \right)^{2.75} S_L^{2.7} D^{0.7}, \quad (4)$$

where P_0 is the peak overpressure; VBR is the volume blockage ratio of the obstructed region; L_p is the maximum flame path length; D is the typical diameter of the obstacles.

Here L_p is calculated as

$$L_p = \left(\frac{3V_{gr}}{2\pi} \right)^{1/3}, \quad (5)$$

where V_{gr} is the obstructed cloud volume in an obstructed region.

Detailed descriptions of the multi-energy method and the calculation of other variables in Eqs.(3) and (4) are found in the literatures [4-11].

It is practicable to assess the peak overpressure of a fuel-air mixture with any concentration by the introduction of stoichiometric concentration. that is, a certain concentration fuel-air mixture can be assumed as a kind of new pure flammable gas with a new S_{L1} when the flammable gas's ER value equals 1.0, the new flammable gas is called pseudo-component gas in literature [6, 12]. As Eq.(3) or Eq.(4) indicate the different peak overpressure value between stoichiometric fuel-air cloud and the other concentration fuel-air cloud depends only on $S_L^{2.7}$ if the other variables remain unchanged (that means the same obstructed region, the same ignition location and the same ignition energy), notably, $S_L^{2.7}$ also indicates that turbulent burning plays a key role during an explosion.

The new approach is trying to transform an inhomogeneous fuel-air cloud into a smaller stoichiometric fuel-air cloud where the explosion can generate similar peak overpressure as the inhomogeneous cloud.

The inhomogeneous fuel-air cloud gets the overpressure P_0 , and the stoichiometric fuel-air cloud gets the overpressure P_1 . Then, by setting $P_0=P_1$, the following Eq.(6) can be derived from the Eq. (3) or Eq. (4).

$$\frac{P_1}{P_0} = \left(\frac{L_{p1}}{L_{p0}} \right)^{2.75} \cdot \left(\frac{S_{L1}}{S_{L0}} \right)^{2.7} = 1, \quad (6)$$

$$\left(\frac{L_{p1}}{L_{p0}} \right)^{2.75} = \left(\frac{S_{L0}}{S_{L1}} \right)^{2.7}, \quad (7)$$

$$\frac{L_{p1}}{L_{p0}} = \left(\frac{S_{L0}}{S_{L1}} \right)^{\frac{2.7}{2.75}}. \quad (8)$$

Thus, the following Eq. (9) can be derived by the use of the Eq. (5)

$$\frac{L_{p1}}{L_{p0}} = \left(\frac{V_{gr1}}{V_{gr0}} \right)^{1/3} = \left(\frac{S_{L0}}{S_{L1}} \right)^{\frac{2.7}{2.75}}, \quad (9)$$

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