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# A simple and effective approach for evaluating unconfined hydrogen/air cloud explosions

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## ABSTRACT

The topic of hydrogen safety assessment has been focused by many researchers. The overpressure evaluation of vapor cloud explosion (VCE), is an important issue for both designing and evaluating on chemical plants, as well as buildings. Unknown flame radius history limits the original acoustic approximation model's application. The objective of this work is to develop an achievable model for hydrogen/air deflagration assessment in engineering applications, and the model should have high computational efficiency. A tentative scheme that starts from flame/piston speed history solving was adopted, and the flame/piston radius and acceleration history will be obtained subsequently. Thus, the overpressure history for far field could be gotten based on the acoustic approximation model. A simplified scheme was employed for the region inside the flame cloud. The model proposed in this paper could be solved in several seconds, because there are no differential equations but only algebraic equations. The model was verified by hydrogen/air deflagration tests from small scale to large scale. Compared with the experimental data, the model appeared well agreements in the medium and large scale cases. In the small scale cases, the model obtained acceptable solutions.

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## Introduction

Hydrogen is a promising energy carrier. Because of the flammability of hydrogen, its safety utilization has always been a key concern [1–4]. Not only hydrogen, the leakage of combustible gas or liquefied combustible gas (with a low boiling point at ambient temperature), like methane, ethylene, propane etc., will form flammable cloud in the atmosphere [5]. Once the flammable cloud meets ignition source, the VCE (Vapor Cloud Explosions) accident may be occurs, which is a main hazardous issue in energy and chemical industries [6]. It is reported that approximately 174 VCE accidents occurred

during 1940–2010 in the world [7,8], which resulted in huge personal and property losses. The large overpressure load created by the flammable cloud explosion, could cause serious damage. Thus, it is necessary to investigate the pressure wave of potential accidents, for the safety assessment of existing and designed chemical plants and buildings [9]. And this topic has attracted much attention by researchers for several decades.

There are three categories models to predict the overpressure of VCE accidents [10–12]: empirical models (TNT equivalence model [13], TNO Multi-Energy model [14,15], Baker-Strehlow model [16], CAM [17], etc.), phenomenological models (CLICHE model [18] and SCOPE model [19]) and CFD

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**Nomenclatures**

$a_f$	flame/piston acceleration (m/s <sup>2</sup> )
$a_i$	empirical parameter in Eq. (5)
$c_0$	sonic speed (m/s)
$C$	molecular fraction (%)
$D$	flame/piston speed in Eqs. (4) and (5) (m/s)
$D_2$	maximum flame speed in Eq. (4) (m/s)
$M$	molecular weight
$p$	pressure (Pa)
$R$	distance from ignition center (m)
$\bar{R}_a$	affected distance from ignition center (m)
$R_0$	initial radius of hemispherical unburnt mixture cloud (m)
$S'$	average flame speed in Eqs. (5), (20) and (23) (m/s)
$S_L$	laminar flame speed in Eq.(18)–(21), (23) (m/s)
$t$	time (s)
$T$	temperature (°C)
$u$	flame speed in Eq.18 and 19 (m/s)
$V$	volume of unburnt mixture (m <sup>3</sup> )
$x$	distance between obstacles in Eq. (18) (m)
$y$	characteristic size in Eq. (18) (m)

**Greek symbols**

$\alpha$	reciprocal of $\beta$
$\beta$	expansion coefficient in Eq. (7)
$\delta$	flame thickness in Eq. (21) (m)
$\mu$	dynamic viscosity (Pa·s)
$\rho$	density (kg/m <sup>3</sup> )
$\tau$	shifted time (s)
$\varphi$	equivalence ratio
$\chi$	thermal diffusivity in Eq. (19) (m <sup>2</sup> /s)

**Subscripts**

0	initial
ex	external
f	flame or final
i	inflexion
in	internal
k	index of component
max	maximum
s	start

models. Compared with the first two models, an appropriate CFD model can obtain much accurate overpressure time history and more details of the flow field. However, the great demand for time and computer resource of CFD models makes it impractical for engineering applications, especially for complex geometries [10,20–23]. At this aspect, the empirical models and phenomenological models have their advantages, but these models also have their weaknesses. For empirical models, the weaknesses includes: the drawbacks of weak accuracy (TNT, Baker-Strehlow), only positive phase peak pressure can be solved (TNT, Multi-Energy), and not good realizability (Multi-Energy, CAM), etc. The sophistication of phenomenological models is between empirical models and complex CFD models, but few information of the flow field

could be provided in phenomenological models [10,11]. The detailed comments of the previous models can be seen in Ref. [10] and Ref. [12].

In addition, Deshaies [24] proposed an acoustic approximation model, in which the flow field outside the flame was divided into two zones, incompressible source flow (near the flame front) and acoustic approximation of source flow (far from the flame front). The overpressure time history at a distance of  $R$  from the ignition center was given as follows:- near the flame front:

$$p(R, t) - p_0 = \frac{\rho_0}{R} (1 - \alpha) \left\{ 2R_f(t) \left( \frac{dR_f(t)}{dt} \right)^2 + R_f^2(t) \left( \frac{d^2R_f(t)}{dt^2} \right) - \frac{1 - \alpha}{2} \frac{R_f^4(t)}{R^3} \left( \frac{dR_f(t)}{dt} \right)^2 \right\} \quad (1)$$

and far from the flame front:

$$p(R, \tau) - p_0 = \frac{\rho_0}{R} (1 - \alpha) \left\{ 2R_f(\tau) \left( \frac{dR_f(\tau)}{d\tau} \right)^2 + R_f^2(\tau) \left( \frac{d^2R_f(\tau)}{d\tau^2} \right) \right\} \quad (2)$$

$$\tau = t - \frac{r}{c_0} \quad (3)$$

The acoustic approximation model can provide the pressure-time history with a varied distance  $R$ , and it has been checked by several deflagration experiments [25,26]. As can be seen in Eqs. (1) and (2), the flame radius history  $R_f(t)$  is necessary for overpressure calculation, but it is unknown before the experiment. Thus, this drawback restricts the practical use of the acoustic approximation model. Moreover, the acoustic approximation model can't obtain the pressure wave inside the flame sphere. However, the length of the flame may be hundreds of meters to several kilometers, and the affected zone is very broad in large scale VCE accidents.

Based on the discussions mentioned previously, the weaknesses of the models motivate the authors to develop a simple and effective model for engineering application of safety assessment. In the present study, a model on the basis of the acoustic approximation model is proposed, in which an independent flame history function improves the availability of the original model. In Section **Theory hypothesis**, the pressure wave shapes are classified with findings from hydrogen/air deflagration tests. The calculation model of overpressure is presented in Section **Method**, and in Section **Result and discussion** it will be validated.

## Theory hypothesis

### Findings in gas deflagration experiments

In 1983, the Fraunhofer Institute for Propellants and Explosives (Germany) conducted a series of large scale unconfined vapor cloud explosion (UVCE) tests in open area, with H<sub>2</sub>/Air mixtures [27]. This program was part of the Prototype Plant Nuclear Process Heat project (PNP). Table 1 lists the experimental details of some tests in the series. The unconfined flammable clouds were considered as hemispherical shape,

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