Available online at www.sciencedirect.com

SciVerse ScienceDirect

journal homepage: www.elsevier.com/locate/he

A study of numerical hazard prediction method of gas explosion

Takayuki Tomizuka [a,*], Kazunori Kuwana [b], Toshio Mogi [a], Ritsu Dobashi [a], Mitsuo Koshi [c]

[a] Faculty of Engineering, The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8565, Japan
[b] Faculty of Engineering, Yamagata University, 4-3-16 Jonan, Yonezawa-shi, Yamagata 992-8510, Japan
[c] Rocket Engine Modeling Laboratory, The University of Tokyo, 2-11-16 Yayoi, Bunkyo-ku, Tokyo 113-8565, Japan

ARTICLE INFO

Article history:
Received 13 August 2012
Received in revised form
5 January 2013
Accepted 6 February 2013
Available online 13 March 2013

Keywords:
Hydrogen
Hydrodynamic instability
Burning velocity
Fractal theory
Premixed combustion
Premixed gaseous explosion

ABSTRACT

A 3-dimensional computational fluid dynamics (CFD) simulation of a premixed hydrogen/air explosion in a large-scale domain is performed. The main feature of the numerical model is the solution of a transport equation for the reaction progress variable using a function for turbulent burning velocity that characterizes the turbulent regime of propagation of free flames derived by introducing the fractal theory. The model enables the calculation of premixed gaseous explosion without using fine mesh of the order of micrometer, which would be necessary to resolve the details of all instability mechanisms. The value of the empirical constant contained in the function for turbulent burning velocity is evaluated by analyzing the experimental data of hydrogen/air premixed explosion. The comparison of flame behavior between the experimental result and numerical simulation shows good agreement. The effect of mesh size on simulated flame propagation velocity is also tested, showing that the numerical result agrees reasonably well with experiment when the mesh size is less than about 20 cm.

1. Introduction

Hydrogen is regarded as a new clean fuel for the next generation due to its lower overall pollutant emission and more excellent fuel economy. However, hydrogen safety engineering requires estimating the consequences of a gaseous explosion caused by the leakage and diffusion of hydrogen. Difficulties in calculating flame propagation in premixed gas are associated in part with the nature of the intrinsic instabilities of propagating flame, which may result in flame wrinkling and acceleration of burning velocity [1–3]. The acceleration of burning velocity generates higher blast pressure and pressure rise rate which cause serious damages; therefore the prediction of the flame velocity is very important in the point of view of safety engineering. Dobashi et al. [4] developed new prediction methods to estimate the blast-wave intensity of gas deflagrations considering the intrinsic instabilities.

In premixed combustion, the deformation of flame surfaces plays a key role in the total burning rate. Its complicated behaviors, characterized by multiple scales of flame wrinkles that fluctuate both in time and space renders it difficult for quantitative analysis and prediction. Gostintsev et al. [5] reported the survey of experimental studies on outwardly propagating spherical flames in the regime of well-developed hydrodynamic instability (Darrieus–Landau instability [6]). The available data indicate that freely expanding wrinkled flames undergo a noticeable acceleration.

* *Corresponding author*. Tel.: +81 3 5841 1799; fax: +81 5841 7313.
E-mail addresses: gzz00134@nifty.com, t1965maverick@gmail.com (T. Tomizuka).
0360-3199/$ – see front matter
http://dx.doi.org/10.1016/j.ijhydene.2013.02.029

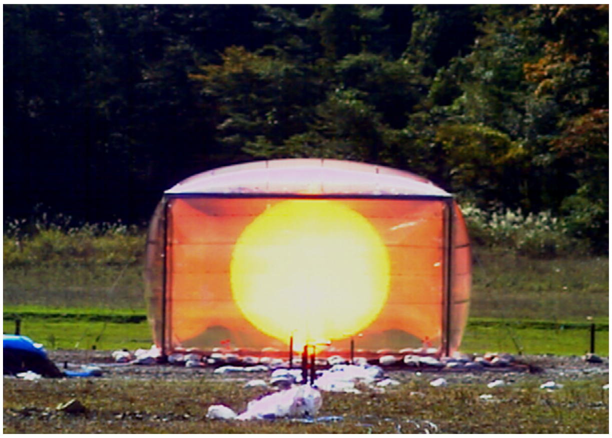

Fig. 1 – An image of a hydrogen/air explosion experiment: sodium is added to the hydrogen/air mixture for visualizing the flame. The photograph is provided by National Institute of Advanced Industrial Science and Technology.

Our group previously reported the construction of a numerical model and the calculation of premixed DME/air explosion [7]. In the present research, the model is applied to hydrogen/air mixture, and 3-dimensional computational fluid dynamics (CFD) calculations of premixed hydrogen/air explosion within a large-scale domain are conducted. Though a spherical flame can be treated as 1-dimensional calculation, 3-dimesional CFD is necessary if we considered applying this prediction method to various gas explosion accidents. The main feature of the numerical model is the solution of a transport equation for the reaction progress variable using a function for turbulent burning velocity. The function characterizes the turbulent regime of propagation of free flames derived by introducing the fractal theory [5,8,9]. Though the calculation of premixed combustion by CFD requires a fine mesh size of micrometer order in order to provide enough

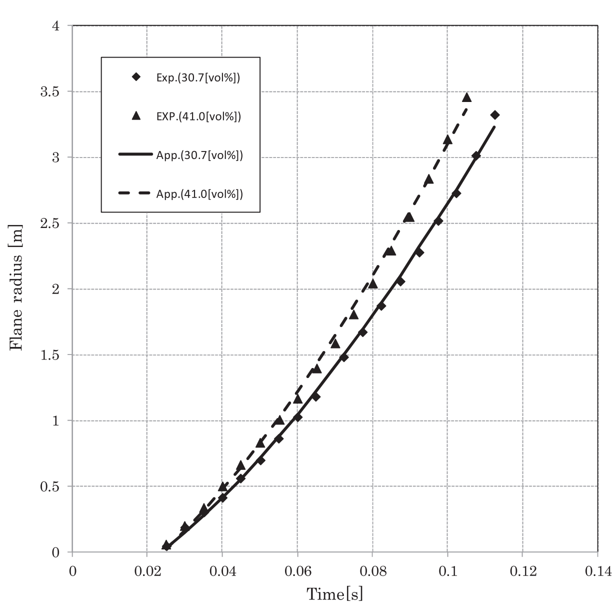

Fig. 2 – The approximate curves of flame radius.

Table 1 – The value of c_g.

Gas concentration	Φ	ρ_b/ρ_u	κ [m^2/s]	S_L [m/s]	c_g
30.7	1.1	6.9	3.2×10^{-5}	2.6	1.7×10^{-3}
41.0	1.7	6.4	3.8×10^{-5}	3.2	1.6×10^{-3}
Mean value					1.6×10^{-3}

resolution to solve flame behavior, the new model enables to solve it with a mesh size of centimeter order. The empirical constant which is contained in the function for turbulent burning velocity was evaluated by analyzing the experimental data of hydrogen/air premixed explosions.

2. Flame instability and fractal theory

Williams [10] indicated the following three types of spontaneous instability mechanisms which initiate and dominate flame wrinkles:

- Hydrodynamic instability,
- Diffusive-thermal instability, and
- Body-force instability.

It is known that the effect of hydrodynamic instability is significant when the scale of flame becomes large [3]. Further, the diffusive-thermal instability is supposed to be not so effective for stoichiometric hydrogen mixture according to consideration of the Lewis number. Also the body-force instability is usually not effective, because it becomes active only when the flame is significantly accelerated (if the buoyancy force is not important as in the case of fast flame propagation during explosion). The characteristic size of turbulent flames is taken to be that of the smallest coherent structure generated by the flow, i.e., the Kolmogorov micro scale [11,12]. However, flame wrinkles may also be initiated and dominated by the hydrodynamic instability on the order of the critical wavelength associated with the maximum growth rate [13] indicated by linear stability analysis. Indeed, this possibility was demonstrated by Cambray and Joulin [14]

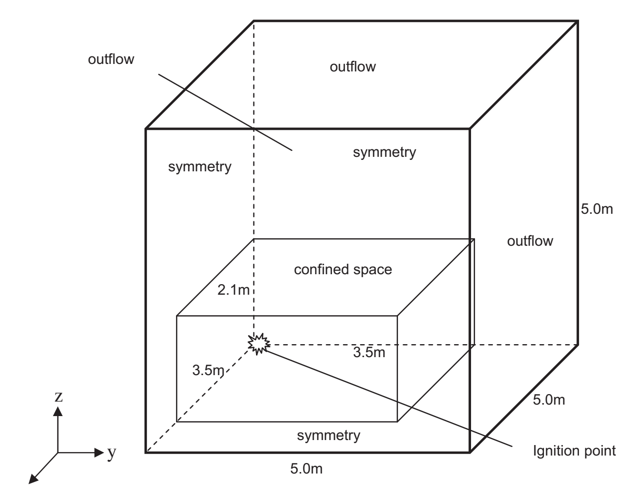

Fig. 3 – The scheme of computational domain.