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Hydrogen-air deflagrations in open atmosphere: Large eddy simulation analysis of experimental data

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Abstract

The largest known experiment on hydrogen-air deflagration in the open atmosphere has been analysed by means of the large eddy simulation (LES). The combustion model is based on the progress variable equation to simulate a premixed flame front propagation and the gradient method to decouple the physical combustion rate from numerical peculiarities. The hydrodynamic instability has been partially resolved by LES and unresolved effects have been modelled by Yakhot's turbulent premixed combustion model. The main contributor to high flame propagation velocity is the additional turbulence generated by the flame front itself. It has been modelled based on the maximum flame wrinkling factor predicted by Karlovitz et al. theory and the transitional distance reported by Gostintsev with colleagues. Simulations are in a good agreement with experimental data on flame propagation dynamics, flame shape, and outgoing pressure wave peaks and structure. The model is built from the first principles and no adjustable parameters were applied to get agreement with the experiment.

Keywords: Hydrogen; Deflagration; Open atmosphere; Large eddy simulation

1. Introduction

One of the likely accidental scenarios for hydrogen applications is a deflagration of hydrogen–air mixture in the open atmosphere at large scales. The understanding of underlying physical phenomena is essential to develop reliable predictive tools for risk assessment and hydrogen safety engineering. A relatively high burning velocity makes hydrogen–air explosions potentially more dangerous in comparison with most of hydrocarbons. The theory suggests that various instabilities can strongly affect flame front propagation velocity [1].

Accidental combustion of initially quiescent premixture commences usually from laminar flame propagation, then flame cracking and cell formation, cellular flame propagation, and finally self-turbulising flame propagation [2]. The onset of the cellular structure for propane–air deflagration occurs at a flame Reynolds number about $Re = 10^4$ [3]. If the same critical value is adopted for stoichiometric hydrogen–air flame at normal conditions ($\mu_u = 2.3 \times 10^{-5}$ Pa s, $\rho_u = 0.88$ kg/m^3, $S_u = 1.91$ m/s) then the flame front becomes cellular (non-laminar) already at size of 0.14 m.

The study performed by Karlovitz et al. [4] using burner premixed flames led to the conclusion that a flame front itself generates additional turbulence. The maximum theoretical value of the flame front wrinkling due to self-induced turbulence may be estimated as

$$\Xi_{\max} = \frac{E_i - 1}{\sqrt{3}}, \tag{1}$$

where E_i is the combustion product expansion coefficient.

Gostintsev et al. analysed about 20 experiments on large-scale unconfined deflagrations and concluded that after mixture ignition by a point source the flame front instabilities lead to acceleration of initially laminar flame, and after an initial stage the self-similar regime of fully developed turbulent flame propagation is established at some distance from the ignition source [5]. According to their analysis, the flame front surface obeys the fractal theory after the self-similar regime is established. The authors found that the transition to the self-similar

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Nomenclature

CFL	Courant–Friedrichs–Lewy number
c	progress variable (normalised product mass fraction)
E_i	expansion coefficient, $E_i = \rho_u/\rho_b$
g	gravity acceleration, m/s^2
M	molecular mass, kg/kmol, $M = \sum_m V_m M_m$
p	pressure, Pa
R	radius, m
R_0	radius of polyethylene hemisphere filled with hydrogen–air mixture, m
R^*	radius for onset self-turbulised flame propagation regime, m
R_μ	universal gas constant, $R_\mu = 8314$ J/kmol K
Re	Reynolds number, $Re = S_u R_{ff} \rho_u/\mu_u$
S_c	source term in the conservation equation for the progress variable, kg/m^3 s
Sc	Schmidt number
S_{u0}	burning velocity at initial conditions, m/s
S_u	burning velocity, m/s
T	temperature, K
t	time, s
$u_{i,j,k}$	velocity components, m/s
u'	sub-grid scale unresolved fluctuation velocity, m/s
$x_{i,j,k}$	spatial coordinates, m
Y_a	mass fraction of air

Greek

Δ_{CV}	control volume characteristic size, m
Δt	time step, s
μ	dynamic viscosity, Pa s
ρ	density, kg/m^3, $\rho = (pM)/(R_\mu T)$
Ξ	flame front wrinkling factor

Subscripts

b	burned mixture
CV	control volume
cell	cellular structure
eff	effective value
i, j, k	spatial coordinate indexes
t	turbulent
u	unburned mixture
0	initial conditions

Bars

–	LES filtered quantity
LES	mass-weighted filtered quantity

turbulent regime of flame propagation occurs after the critical value of the flame front radius R^* is achieved, which was found to be $R^* = 1.0$–1.2 m for near stoichiometric premixed hydrogen–air flames. This result suggests that characteristic features of large-scale hydrogen–air deflagrations may be quite different from those obtained in small-scale experiments. This is in line with a recent critical review [6], where it was concluded that "large scale research has shown that explosions may be more severe than was previously recognised". Accordingly, there is a need to demonstrate that the models and tools used for risk assessment and hydrogen safety engineering are valid at scales typical for real accident scenarios.

2. Overview of experimental data

The series of experiments on hydrogen–air explosions in the open atmosphere was conducted in 1983 in Germany [7]. The general objective was a study of the dependence of a flame propagation velocity on the size of a flammable mixture. Near stoichiometric hydrogen–air mixtures were prepared in hemispherical ground-based polyethylene (PE) balloons with radii of $R = 1.53, 2.88, 5.0$ and 10.0 m. The balloon envelope consisted of several PE segments, similar to the surface of individual orange slices, which were welded together (see Fig. 1). Ignition was initiated by an exploding wire with energy between 10 and 1000 J, or, by pyrotechnical charges. The ignition device for the exploding wire contained a condenser battery with a capacitance of 320 μF, which can be loaded by a high voltage device operating between 250 and 2500 V, so that the available energy is adjustable between 10 and 1000 J. It was found that the flame propagation velocity was independent of the ignition energy within the investigated energy range. There was no dependence of the turbulence factor, i.e. the ratio of maximum flame propagation velocity to initial flame propagation velocity, on ignition energy: from tests GHT 20–26 with 3.06-m diameter hemisphere the turbulence factor was found to be 2.55 ± 0.10 and 2.71 ± 0.15 for ignition energies of 10 and 1000 J, respectively. The experimental data included the dependence of the flame front radius with time, flame front contours

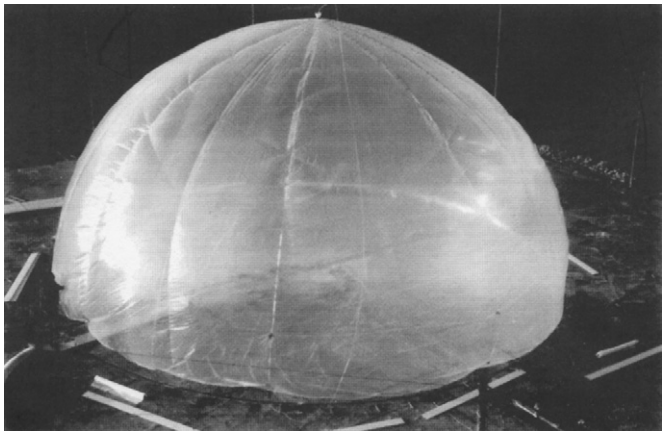

Fig. 1. The hemispherical balloon with hydrogen–air mixture, $R_0 = 10$ m.