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# Deflagrations of localised homogeneous and inhomogeneous hydrogen-air mixtures in enclosures

D. Makarov <sup>a,\*</sup>, P. Hooker <sup>b</sup>, M. Kuznetsov <sup>c</sup>, V. Molkov <sup>a</sup>

<sup>a</sup> Hydrogen Safety Engineering and Research Centre (HySAFER), Ulster University, Newtownabbey, BT37 0QB, UK

<sup>b</sup> Health and Safety Executive, Harpur Hill, Buxton, SK17 9JN, UK

<sup>c</sup> Karlsruhe Institute of Technology, 76344, Eggenstein-Leopoldshafen, Germany

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## ABSTRACT

Two original models for use as novel tools for the design of hydrogen-air deflagration mitigation systems for equipment and enclosures are presented. The first model describes deflagrations of localised hydrogen-air mixtures in a closed space such as a pressure vessel or a well-sealed building while the second model defines safety requirements for vented deflagrations of localised mixtures in an enclosure. Examples of localised mixtures include ‘pockets’ of gas within an enclosure as well as stratified gas distributions which are especially relevant to hydrogen releases. The thermodynamic model for closed spaces is validated against experiments available from the literature. This model is used to estimate the maximum hydrogen inventory in a closed space assuming the closed space can withstand a maximum overpressure of 10 kPa without damage (this is typical of many civil structures). The upper limit for hydrogen inventory in a confined space to prevent damage is found to be equivalent to 7.9% of the closed space being filled with 4% hydrogen. If the hydrogen inventory in a closed space is above this upper limit then the explosion has to be mitigated by the venting technique. For the first time an engineering correlation is presented that accounts for the phenomena affecting the overpressure from localised vented deflagrations, i.e. the turbulence generated by the flame front itself, the preferential diffusion in stretched flames, the fractal behaviour of the turbulent flame front surface, the initial flow turbulence in unburnt mixture, and the increase of the flame surface area due to the shape of an enclosure. Validation of the new vented deflagration model developed at Ulster has been carried out against 25 experiments with lean stratified hydrogen-air mixtures performed by the Health and Safety Executive (UK) and Karlsruhe Institute of Technology (Germany).

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## Introduction

Deflagration of inhomogeneous, e.g. stratified, fuel-air mixtures in an enclosure, where fuel concentration varies

mainly in vertical direction, is a realistic accident scenario for both industrial environment and domestic premises [1,2]. This scenario may result from a slow release of heavier or lighter than air flammable gas, or a spill of

\* Corresponding author.

E-mail address: [dv.makarov@ulster.ac.uk](mailto:dv.makarov@ulster.ac.uk) (D. Makarov).

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Nomenclature			
A	fraction of vent area occupied by combustion products, or coefficient in equation (49)	$\Phi^*$	volumetric fraction of the fastest burning fuel-air mixture in enclosure
B	coefficient in equation (49)	$\gamma$	adiabatic index, $\gamma = c_p/c_v$
$Br_t$	turbulent Bradley number, $Br_t = (\sqrt{E_i/\gamma} \mu F c_{ui}) / ((36\pi_0)^{1/3} \Xi V^{2/3} S_{ui} (E_i - 1))$	$\varphi$	volumetric fraction of fuel in localised fuel-air mixture, and number of moles in equations (9)–(11)
$Br_t^*$	parameter for scaling overpressure in equation (60)	$\mu$	discharge coefficient
$c_p$	specific heat at constant pressure in equations (8) and (12) (J/kg/K)	$\pi$	non-dimensional pressure $\pi = p/p_i$
$c_v$	specific heat at constant volume in equation (20) (J/mol/K)	$\pi_0$	“Pi” number, 3.14159
$c_{ui}$	speed of sound in unburnt mixture (m/s), $c_{ui} = \sqrt{\gamma RT/M}$	$\Xi/\mu$	deflagration-outflow interaction (DOI) number, $\Xi/\mu = \Xi_K \Xi_{LP} \Xi_{FR} \Xi_u \Xi_{AR} \Xi_O$
D	fractal dimension	$\Psi$	empirical coefficient
e	energy per unit mass (J/kg)	$\Xi_K$	wrinkling factor to account for the turbulence generated by the flame front itself
$E_i$	combustion products expansion coefficient, $E_i = M_{ui} T_{bi} / M_{bi} T_{ui}$	$\Xi_{LP}$	wrinkling factor to account for the leading point flame acceleration mechanism
F	vent area (m <sup>2</sup> )	$\Xi_{FR}$	wrinkling factor to account for the fractal increase of the flame surface area
G	mass flow rate (kg/s)	$\Xi_u$	wrinkling factor to account for the initial flow turbulence in unburnt mixture
H	height (m), or enthalpy (J)	$\Xi_{AR}$	wrinkling factor to account for the aspect ratio of the enclosure
$\Delta H_c$	heat of combustion (J/mol)	$\Xi_O$	wrinkling factor to account for the presence of obstacles
$\Delta h_c$	heat of combustion (J/kg)	$\rho$	density (kg/m <sup>3</sup> ), $\rho = pM/(RT)$
h	enthalpy per unit mass (J/kg)	$\sigma$	relative density, $\sigma = \rho/\rho_i$
L	length (m)	$\tau$	non-dimensional time, $\tau = t S_{ui} / c_{ui}$
M	molecular mass (g/mol)	$\omega$	volume fraction in enclosure
m	mass (kg), or burning velocity temperature index (Table 7)		
n	mass fraction, or burning velocity baric index (Table 7)		
p	pressure (Pa abs)	<b>Subscripts</b>	
q	heat per unit mass (J/kg)	air	air
R	flame radius (m), or universal gas constant, $R = 8314$ (J/K/kmol)	b	burnt mixture
$R^\#$	non-dimensional venting parameter, $R^\# = \{ (2\gamma)/(\gamma - 1) \pi \sigma [(1/\pi)^{2/\gamma} - (1/\pi)^{1+1/\gamma}] \}^{1/2}$	corr	correlation value
$R_0$	critical radius for transition from laminar to fully turbulent flame propagation regime (m)	exp	experimental value
$S_t$	turbulent burning velocity (m/s)	f	fuel
$S_u$	laminar burning velocity (m/s)	H <sub>2</sub>	hydrogen
T	temperature (K)	i	initial conditions
t	time (s)	MAX	maximum
u	internal energy per unit mass (J/kg)	MIN	minimum
V	volume (m <sup>3</sup> )	m	flammable mixture
v	specific volume (m <sup>3</sup> /kg)	t	turbulent
W	width (m), or non-dimensional venting parameter, $W = \mu F c_{ui} / [(36\pi_0)^{1/3} \sqrt{\gamma_u} V^{2/3} S_{ui}]$	u	unburnt mixture
w	mechanical work of gas per unit mass (J/kg)	0	initial thermodynamic state (before combustion)
$x_{H_2}$	volumetric fraction of hydrogen in entire enclosure, $x_{H_2} = \phi \cdot \Phi$	1	thermodynamic state 1 (on completion of adiabatic isochoric combustion)
Z	non-dimensional number, $Z = \gamma_b [E_i - (\gamma_u/\gamma_b)(\gamma_b - 1)/(\gamma_u - 1)] \pi^{(1-\gamma_u)/\gamma_u} + (\gamma_u - \gamma_b)/(\gamma_u - 1)$	2	thermodynamic state 2 (on completion of adiabatic expansion)
<b>Greek</b>		<b>Superscripts</b>	
$\Phi$	volumetric fraction of localised flammable fuel-air mixture in enclosure	'	value in flammable mixture
		<b>Acronyms</b>	
		BOS	Background Oriented Schlieren
		CFD	Computational Fluid Dynamics
		DOI	Deflagration-Outflow Interaction
		LES	Large Eddy Simulation
		RHS	Right-Hand Side
		SGS	Sub-Grid Scale

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