



A study on the scaling features for mixing and deflagration potential of stratified layer of hydrogen due to molecular diffusion[☆]



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ABSTRACT

Hydrogen deflagration in confined spaces is an important safety issue. The dispersion of a stratified layer of hydrogen due to molecular diffusion is studied. It represents an important class of problems related to long term behaviour of hydrogen release in confined spaces. Diffusion being a slow process, gives an upper bound on the time taken for the stratified layer to mix with air below. A method, based on four indices, namely, average mole fraction (of hydrogen), non-uniformity index, deflagration volume fraction and deflagration pressure ratio, developed recently by the authors, is used to provide vital temporal information on mixing of the stratified layer with air below and formation of flammable cloud in the enclosure. In the present paper, stratified layers of different thickness are considered and the temporal evolutions of the above indices are plotted against diffusion Fourier number. The results in non-dimensional form provide an upper bound of the time that would be required to form a uniform mixture and to attain a state with respect to deflagration potential for enclosures of different sizes. This estimate is an important input for planning mitigation measures before the accident and for post accident investigations.

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1. Introduction

Hydrogen is a prospective energy carrier for automotive and other applications and may be generated, transported and used in large quantity in the future. Hydrogen leakage from compressed gas cylinders into confined spaces such as garages, tunnels and parking bays is an important safety concern. Similarly, hydrogen leakage from hydrogen generation and storage facilities, battery banks and laboratories into unventilated confined space can pose safety concerns.

In thermal nuclear reactors (BWR, PWR, PHWR, etc.), hydrogen may be generated in large quantities during the progression of an accident leading to core degradation or meltdown. The hydrogen generated is due to metal water reaction (oxidation of zirconium fuel sheath), radiolysis and other mechanisms. The released gases cannot be vented out from the nuclear reactor containment because radioactive isotopes are present in the containment atmosphere.

A severe accident unfolds over several days. The time after the beginning of release can be divided into two important stages, namely, (a) the release phase and (b) the post release phase. The release phase

is usually of short duration, typically a few minutes, while the post release phase is of very long duration, typically days. In situations such as extended station blackout (SBO) there would be no power at site and all the building fans and coolers will be stopped. In such a situation, during the release phase, hydrogen is released as a jet or a plume and the spreading and mixing characteristics of the jet/plume play an important role in the distribution of gases in the enclosure. There are several studies [1–4] that have shown that stratified layers are formed some time after the end of release. During the post release phase, natural convection, steam condensation (in nuclear reactors), molecular diffusion, pressure differential between rooms, etc. have important roles.

The nuclear reactor containment is a large volume consisting of several compartments with vastly different sizes and thermal conditions. Natural convection and steam condensation are phenomena that occur near the walls and are important over short duration of time when thermal gradients are present. Depending on the gas and containment wall temperatures, natural convection and steam condensation may not be significant in some compartment. Due to this, natural convection and steam condensation have effect over a small region only. In the long term these mechanisms may become weak and it is seen that stratified layers are formed and maintained for a very long time in the reactor containment.

Thus, in the long term, molecular diffusion becomes the dominant mechanism that slowly causes the stratified layer to become homogeneous with time. Even if other mechanisms are present, the analysis of dispersion of a stratified layer by molecular diffusion gives an upper

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Nomenclature*English*

D	diffusion coefficient [m ² /s]
H	height of enclosure [m]
h	height of stratification in the enclosure [m]
M	molecular weight [kg/kmol]
p	pressure [Pa]
t	time [s]
X	mole fraction of a species
Y	mass fraction of a species
y	positions in co-ordinate direction [m]

Greek

λ	coefficient in transcendental equation no. 10.
ρ	density [kg/m ³]
σ	collision diameter [m]
Ω	collision integral for diffusion [dimensionless]

Symbol

X_{av}	average mole fraction [dimensionless]
χ	non-uniformity index [dimensionless]
P_{def}	deflagration pressure ratio [dimensionless]
V_{def}	deflagration volume fraction [dimensionless]
Ψ	volume [m ³]

Suffix

<i>Air</i>	referring to air
<i>i</i>	species index
<i>av</i>	average quantity
<i>CV</i>	control volume
<i>H₂</i>	referring to hydrogen
<i>s</i>	stoichiometric quantity
<i>total</i>	referring to total volume of the enclosure
<i>mix</i>	referring to mixture
<i>ref</i>	reference value

Abbreviations

AICC	Adiabatic Isochoric Complete Combustion
BWR	boiling water reactor
LFL	lower flammability limit
PWR	pressurized water reactor
PHWR	pressurized heavy water reactor
SBO	Station Black Out
UFL	Upper Flammability Limit

bound on the time required to uniformly mix a stratified layer of hydrogen with air below.

Diffusion model also provides an upper estimate of the critical time within which hydrogen combustion is possible, provided the conditions are conducive. Further, the time estimated by the diffusion model indicates the duration within which mitigative hydrogen combustion measures should be brought into service. Also, such estimates form an important input for post hydrogen combustion events in the containment buildings.

The study of hydrogen distribution in enclosures is a generic problem with special significance in nuclear industry. A given quantity of hydrogen release can form pockets of high concentration, stratified layer, or a uniform mixture. Detailed study of hydrogen distribution subsequent

to release is important to ascertain the mixing behaviour and combustion hazard associated with a given release situation. One important aspect of the hydrogen distribution and mitigation studies is the scalability of the results because the application of these predictions can range from hydrogen leak in a small laboratory to a huge nuclear reactor. The rate of mixing and change in deflagration potential need to be understood from the underlying physics rather than through enormously time consuming simulation of each specific case. There is a need to present the results in non-dimensional forms for ready reference. One important aspect of molecular diffusion of a stratified layer of hydrogen with air below is that it is amenable to one dimensional analysis [5]. Because of this, very important results with wide applications can be obtained using rather simple analyses.

A method to characterize mixing and deflagration potential of hydrogen–air mixtures in enclosed spaces was developed by the authors and presented in an earlier publication [6]. The method introduced four indices, namely, average mole fraction (X_{av}) of hydrogen, non-uniformity index (χ), deflagration volume fraction (V_{def}) and deflagration pressure ratio (P_{def}) to obtain quantitative information on hydrogen mixing and flammability without modelling combustion. The mathematical formulation of these indices has been presented in Appendix A for ready reference. A case study for dispersion of a stratified layer due to diffusion alone was considered in the publication [6]. However, the study of temporal evolution of these indices was specific to the fixed geometry considered there.

In the present study, an attempt has been made to understand the diffusion of a stratified layer of hydrogen from a fundamental mass transfer perspective and present the results in non-dimensional form so that a first hand information on hydrogen mixing and deflagration potential may be obtained for enclosures of any size without carrying out detailed numerical study of the specific enclosure geometry under consideration. In order to keep the analysis simple and general, distributions of hydrogen and air are considered and steam is ignored.

2. Mathematical model

The governing equation for diffusion of hydrogen in a gaseous medium of hydrogen and air is given by Eq. (1).

$$\frac{\partial(\rho_{mix} Y_{H_2})}{\partial t} = \frac{\partial}{\partial y} \left(D_{H_2, mix} \rho_{mix} \frac{\partial}{\partial y} Y_{H_2} \right) \quad (1)$$

The mole fraction of a species 'i' can be obtained from mass fraction using Eq. (2).

$$X_i = (Y_i/M_i) / \left(\sum_i (Y_i/M_i) \right) \quad (2)$$

The density of hydrogen ($\rho_{H_2, ref}$) and air ($\rho_{air, ref}$) at the ambient temperature and one atmosphere pressure are inputs in the analysis. The gas mixture density is obtained using Eq. (3). The diffusion coefficient is evaluated from Eqs. (4) to (5).

$$\rho_{mix} = X_{H_2} \rho_{H_2, ref} + X_{air} \rho_{air, ref} \quad (3)$$

$$D_{i, mix} = \frac{0.0018583 \sqrt{T^3 \left(\frac{1}{M_i} + \frac{1}{M_{mix}} \right)}}{\rho \sigma_{i, mix}^2 \Omega_{i, mix}} \quad (4)$$

$$M_{mix} = X_{H_2} M_{H_2} + X_{air} M_{air} \quad (5)$$

Numerical studies reported in the paper are carried out using Eqs. (1)–(5) through an in-house developed CFD code called Hydrogen Distribution Simulator (HDS). It is a multi-species flow, heat and mass transfer code with temperature and concentration dependent

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