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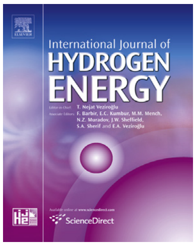

Numerical and physical requirements to simulation of gas release and dispersion in an enclosure with one vent

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ABSTRACT

Numerical and physical requirements to simulations of sub-sonic release and dispersion of light gas in an enclosure with one vent are described and discussed. Six validation experiments performed at CEA in a fuel cell-like enclosure of sizes $H \times W \times L = 126 \times 93 \times 93$ cm with one vent, either $W \times H = 90 \times 18$ cm (vent A) or 18×18 cm (B) or 1 cm in diameter (C), with a vertical upward helium release from a pipe of internal diameter either 5 mm or 20 mm located 21 cm above the floor centre, were used in a parametric study comprising 17 numerical simulations. Three CFD models were applied, i.e. laminar, standard k-ε, and dynamic LES Smagorinsky–Lilly, to clarify a range of their applicability and performance. The LES model consistently demonstrated the best performance in reproduction of measured concentrations throughout the whole range of experimental conditions, including laminar, transitional and turbulent releases even with large *CFL* numbers. The laminar and the standard k-ε models were under performing in the reproduction of turbulent and laminar releases respectively, as expected, as well as in simulation of transitional flows. The laminar model demonstrated high sensitivity to the *CFL* (Courant–Friedrichs–Lewy) number even below the best practices limit of 40. Three different computational domains and grids were used in order to clarify the influence of mesh quality on the capability of simulations to reproduce the experimental data. It is concluded that physically substantiated choice of CFD model, the control of the *CFL* number (and released gas mass balance where appropriate), and the mesh quality can have a strong effect on the capability of simulations to reproduce experiments and, in general, on the reliability of CFD tools for application in hydrogen safety engineering.

Introduction

Most accidents involving hydrogen would start from a leak and its dispersion in air and, if ignited, could be followed by a fire or deflagration with thermal and/or pressure effects that could be damaging to life and property. Indoor release and dispersion is potentially a worst case scenario due to effect of enclosure confinement on combustion. Hydrogen safety engineering [1,2], requires a ventilation system to keep the

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Nomenclature

A	area, m^2
C, C_s	Smagorinsky coefficient
c_p	specific heat at constant pressure, J/kg/K
D	molecular diffusivity, m^2/s
d	pipe diameter, m
E	total energy, J/kg
Fr	Froude number (–)
H	vent height, m
h	enthalpy, J/kg
I	turbulence intensity (–)
g	gravity acceleration, m/s^2
K	thermal conductivity, W/m/K
k	turbulent kinetic energy, m^2/s^2
L_S	mixing length for sub-grid scales, m
L	turbulent length scale, m
l	distance to the closest wall, m
M_0	momentum flux, $kg{\cdot}m/s^2$
m	mass, kg
m	mass flow rate, kg/s
Δm/m	relative mass difference (–)
Pr	Prandtl number (–)
p	pressure, Pa
R_m	rate of species generation source term, $kg/m^3/s$
Re	Reynolds number (–)
Sc	Schmidt number (–)
S	heat generation source term, $J/m^3/s$
S_{ij}	rate-of-strain tensor, s^{-1}
T	temperature, K
t	time, s
Δt	time step, s
U	release velocity, m/s
$u_{i,j,k}$	velocity components, m/s
V	volume, m^3
$\dot{V}$	volume flow rate, Nl/min
Δx, Δy, Δz	cell size, m
$x_{i,j,k}$	spatial coordinates, m
Y	mass fraction (–)

Greek

Δ	local grid scale, m
δ_{ij}	Kronecker symbol
ε	energy dissipation rate, m^2/s^3
μ	dynamic viscosity, Pa·s
ρ	density, kg/m^3
ν	kinematic viscosity, m^2/s

Subscripts

b	boundary
d	domain
E	energy
ent	entrainment
g	gas
i,j,k	spatial coordinate indexes
m	index of chemical species
mix	mixture
N	numerical
p	pressure
T	theoretical
t	turbulent

Bars

¯	Reynolds averaged parameters
~	Favre averaged parameters

Constants

$C_\mu = 0.09$, $C_{1-\varepsilon} = 1.44$ k-ε model constants

$\kappa = 0.4187$ von Kármán constant

$K_1 = 0.282$ constant in Ricou and Spalding equation [15]

Abbreviations

CEA	Commissariat à l'énergie atomique et aux énergies alternatives (France)
CFD	computational fluid dynamics
CFL	Courant–Friedrichs–Lewy number, $CFL = U\Delta t/\Delta x$
LES	large Eddy simulation
RANS	Reynolds averaged Navier Stokes
UC	uniformity criterion
Nl	normal litres (volume in liters at $T = 293.15$ K)
H × W × L	height, width, length

concentration of hydrogen below the lower flammability limit to exclude a possibility of ignition and flame propagation. Hydrogen can be dispersed in one vent enclosure with uniform or non-uniform concentration distribution over the enclosure height depending on conditions of the release, such as mass flow rate, leak diameter, direction, and the enclosure parameters, such as volume and vent sizes [3,4].

Cariteau and Tkatschenko of CEA [3,4], performed a series of tests on sustained helium release and dispersion in one vent enclosure with different conditions of release and ventilation. In the experiments helium was taken instead of hydrogen for safety reasons. Generally speaking releases could be in a form of expanded and under-expanded jets [2]. The experiments [3,4], were performed with expanded jets/plumes (term "jet" is usually applied to momentum-dominated flow regime and "plume" to buoyancy-controlled). Flow regimes studied include laminar through transitional to turbulent flows at an exit of helium from a release pipe.

The predictive capability of various CFD models to reproduce transient and steady state lighter than air gas concentrations in an enclosure with one vent with a sustained release is yet questionable and has to be clarified through the comparison of simulations with available experimental data. Numerical and physical requirements to predictive simulations have to be formulated to improve the credibility of CFD tools use in the hydrogen safety engineering.

Numerical simulation of a sub-sonic hydrogen release and dispersion in a large scale enclosure can require substantial to unaffordable calculation time. This could result in an attempt to increase a simulation time step (*CFL* number). Unfortunately, the predictability of simulations with large *CFL* number is usually poor. Probably, for the first time the problem was identified and dealt with during the inter-comparison exercise