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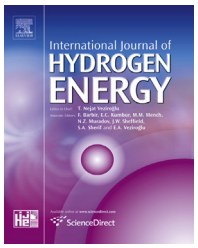

Hydrogen non-premixed combustion in enclosure with one vent and sustained release: Numerical experiments

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ABSTRACT

Numerical experiments are performed to understand different regimes of hydrogen non-premixed combustion in an enclosure with passive ventilation through one horizontal or vertical vent located at the top of a wall. The Reynolds averaged Navier–Stokes (RANS) computational fluid dynamics (CFD) model with a reduced chemical reaction mechanism is described in detail. The model is based on the renormalization group (RNG) k-ε turbulence model, the eddy dissipation concept (EDC) model for simulation of combustion coupled with the 18-step reduced chemical mechanism (8 species), and the in-situ adaptive tabulation (ISAT) algorithm that accelerates the reacting flow calculations by two to three orders of magnitude. The analysis of temperature and species (hydroxyl, hydrogen, oxygen, water) concentrations in time, as well as the velocity through the vent, shed a light on regimes and dynamics of indoor hydrogen fires. A well-ventilated fire is simulated in the enclosure at a lower release flow rate and complete combustion of hydrogen within the enclosure. Fire becomes under-ventilated at higher release flow rates with two different modes observed. The first mode is the external flame stabilised at the enclosure vent at moderate release rates, and the second mode is the self-extinction of combustion inside and outside the enclosure at higher hydrogen release rates. The simulations demonstrated a complex reacting flow dynamics in the enclosure that leads to formation of the external flame or the self-extinction. The air intake into the enclosure at later stages of the process through the whole vent area is a characteristic feature of the self-extinction regime. This air intake is due to faster cooling of hot combustion products by sustained colder hydrogen leak compared to the generation of hot products by the ceasing chemical reactions inside the enclosure and hydrogen supply. In general, an increase of hydrogen sustained release flow rate will change fire regime from the well-ventilated combustion within the enclosure, through the external flame stabilised at the vent, and finally to the self-extinction of combustion throughout the domain.

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Nomenclature

A	vent area, m^2
A_r	pre-exponent, consistent units
a	speed of sound, m/s
$C_{j,r}$	molar concentration of species j in reaction r, $kmol/m^3$
c	specific heat, J/kg-K
D	molecular diffusivity, m^2/s, diameter, m
E	total energy, J/kg
E_r	activation energy, J/kmol
H	vent height, m
h	enthalpy, J/kg
G_k	generation of kinetic energy due to mean velocity gradients, kg/ms^{-3}
G_b	generation of kinetic energy due to buoyancy, kg/ms^{-3}
g	gravity acceleration, m/s^2
K_r	equilibrium constant for the reaction r, –
k	turbulent kinetic energy, m^2/s^2; thermal conductivity, W/m/K
$k_{f,r}$	forward rate constant for reaction r, consistent units
$k_{b,r}$	backward rate constant for reaction r, consistent units
M	Mach number, –
N	number of chemical species in the system, –
Pr	Prandtl number, –
p	pressure, Pa
R_m	source term, $kg/m^3/s$
$R_{m,r}$	rate of species m production/destruction in reaction r, consistent units
Sc	Schmidt number, –
S	source term, –
S_m	entropy, –
S_{ij}	rate-of-strain tensor, s^{-1}
T	temperature, K
t	time, s
$u_{i,j,k}$	velocity components, m/s
$x_{i,j,k}$	spatial coordinates, m
Y	mass fraction, –

Greek

α	inverse effective Prandtl number
β	coefficient of expansion, –
β_r	temperature exponent, –
Γ	net effect of third bodies on the reaction rate
γ	specific heat ratio, –
$\gamma_{i,r}$	third-body efficiency of specie j in reaction r, –
δ_{ij}	Kronecker symbol
ε	energy dissipation rate, m^2/s^3
λ	thermal conductivity, W/m/K
μ	dynamic viscosity, Pa s
υ	kinematic viscosity, m^2/s
$\nu'_{m,r}$	stoichiometric coefficient for reactant m in reaction r, –
$\nu''_{m,r}$	stoichiometric coefficient for product m in reaction r, –
ξ	length fraction of turbulent structures, –
ρ	density, kg/m^3
τ	time scale, s
ω	component of the flow velocity parallel to the gravitational vector, m/s

Subscripts

atm	atmospheric
E	energy
eff	effective
i,j,k	spatial coordinate indexes
m	index of chemical species
p	pressure
t	turbulent
r	reaction index

Bars

$\overline{}$	Reynolds averaged parameters, –
$\sim$	Favre averaged parameters, –
*	fine scale quantities, –
^	Arrhenius reaction, –

Constants and model parameters

$C_{1\varepsilon}$	1.42
$C_{2\varepsilon}$	1.68
$C_{3\varepsilon}$	$\tanh\lvert\omega/u\rvert$
C_μ	0.0845
C_ξ	volume fraction constant $C_\xi = 2.1277$
C_τ	time-scale constant $C_\tau = 0.4082$
R	universal gas constant

Introduction

Unscheduled release of hydrogen followed by a jet fire in an enclosure with one vent is a possible incident/accident scenario for hydrogen and fuel cell systems and infrastructure. To the best authors' knowledge there are no experimental or numerical studies on indoor hydrogen fires published up to date. There are publications on under-ventilated compartment fires with "regular" combustion materials. For example, Sugawa et al. [1] investigated behaviour of a methyl alcohol pool fire, including so-called ghosting flames, in a poorly ventilated compartment of size $W \times L \times H = 2 \times 3 \times 0.6$ m. Bertin et al. [2] performed experiments with wall fires simulated by porous vertical burner fed with propane in a semi-confined room to understand temperature distribution, chemical composition of products and radiation from ghosting flames in vitiated atmosphere. Utiskul et al. [3] studied heptane pool fires behaviour in a compartment under limited ventilation, and observed three distinct regimes of indoor combustion: extinction, blow off (separation of fire from the pan with fuel) and ghosting flames, and sustained steady oscillations. In two last regimes burning was observed at the vent area too. Under-ventilated enclosure fires of natural gas and other combustibles without extinction were carried out by Lock et al. [4] to measure room temperature, heat fluxes, and composition of combustion products depending on fuel type and ventilation rate. Coppalle et al. [5]