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Comparison of two-layer model for hydrogen and helium jets with notional nozzle model predictions and experimental data for pressures up to 35 MPa

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ABSTRACT

A two-layer, reduced order model of high pressure hydrogen jets was developed which includes partitioning of the flow between the central core jet region leading to the Mach disk and the supersonic slip region around the core. The flow after the Mach disk is subsonic while the flow around the Mach disk is supersonic with a significant amount of entrained air. This flow structure significantly affects the hydrogen concentration profiles downstream. The predictions of this model are compared to previous experimental data for high pressure hydrogen jets up to 20 MPa and to notional nozzle models and CFD models for pressures up to 35 MPa using ideal gas properties. The results show that this reduced order model gives better predictions of the mole fraction distributions than previous models for highly underexpanded jets. The predicted locations of the 4% lower flammability limit also show that the two-layer model much more accurately predicts the measured locations than the notional nozzle models. The comparisons also show that the CFD model always underpredicts the measured mole fraction concentrations.

Introduction

Hydrogen fueled cars are being developed in many countries to address the pollution problems caused by fossil-fueled cars and to provide viable alternatives for when fossil fuels are no longer available. Thus, hydrogen will be an important part of the energy mix of future low carbon societies [1,2]. One fueling option for hydrogen fueled vehicles is to have on-board hydrogen storage tanks at pressures up to 70 MPa that hold about 5 kg of hydrogen, giving vehicles a range that is comparable to current fossil-fueled cars. The fueling stations store the hydrogen at about 35 MPa and then further compress the hydrogen to fuel the vehicles. The vehicles and fueling stations should be designed so that their safety levels are equal to or better than for current fossil-fueled vehicles and stations. Thus, the safety issues of leaks from these high pressure systems must be addressed when designing these systems.

Hydrogen leaks can be classified as low pressure leaks, where the exit flow is not choked, or high pressure leaks, where the flow is choked at the orifice, forming an underexpanded jet. The flow fields and gas distributions from low pressure leaks can be modeled using an integral similarity

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Nomenclature

Roman

A	area, m^2
B	slip region width, m
c_p	specific heat, W/kg·K
d	diameter, m
$\dot{m}$	mass flow rate, kg/s
M	Mach number
P	pressure, Pa
T	temperature, K
u	velocity, m/s
V	voltage, v
X	mole fraction
x	axial location, m
y^+	y plus along the wall

Greek

γ	specific heat ratio
ρ	density, kg/m^3
ω	mass fraction

Subscripts

0	stagnation
1, 2a, 2b, 3	state points
∞	ambient
air	air
exit	nozzle exit
H_2, He	hydrogen, helium
Mach	Mach disk
slip	slip region

model [3–5]. Most experimental studies of jet flows have used relatively small Froude numbers due to experimental size and cost limitations, with only four studies having pressures above 10 MPa [6–9] with most of their measurements at hydrogen mole concentrations below 10% where all the models agree within the measurement accuracy.

Hydrogen releases from high pressure tanks result in high pressure jets with very complex shockwave structures [10,11] until the flow expands to a subsonic jet that disperses the hydrogen into the air. The central part of the jet accelerates up to the Mach disk where the flow becomes subsonic. However, a slip region forms outside this central core with numerous expansion waves. The supersonic flow in the slip region interacts with the flow through the Mach disk downstream of the Mach disk, where the hydrogen and air continue to mix. The current study presents experimental and numerical studies of the release and dispersion of hydrogen into air with a two-region reduced order model that partitions the flows in the core region and in the slip region unlike current models that only have one flow region. This model can be used to rapidly and more accurately model high pressure, under-expanded jet flows.

One key goal is to identify the flammability limit when hydrogen accidently leaks from a system. The lower flammability limit for hydrogen in air is a 4% mole fraction; thus, designers need to be able to quickly identify the location of the 4% hydrogen mole fraction contour. The flammability of a hydrogen-air cloud is not only a function of the hydrogen concentration at the lower flammability limit, but is also a function of the hydrogen distribution within the cloud, the flow field and the turbulence within the cloud. Thus, ignition will be strongly affected by the external flow conditions around the jet and the confinement of the hydrogen-air cloud. Therefore, computational models are needed that can accurately predict the flow, temperature, concentration and turbulence fields during the release and dispersion of the hydrogen [12] and these models must be verified against experimental data.

There are few numerical studies of high pressure highly under-expanded hydrogen jets into the atmosphere because the hydrogen properties make the numerical calculations very unstable and slow [13]. Chin et al. [14] modeled the flow from a 353 kPa tank and found higher spreading ratios than seen experimentally. Papanikolaou and Baraldi [15] predicted the hydrogen jet flow and dispersion for a 9.8 MPa tank pressure. Xu et al. [13] divided the analysis for a 20 MPa tank pressure into two problems with large eddy simulations (LES) near the exit and a second finite-difference analysis downstream. They noted that there is a lack of good experimental data available at high pressures to validate the numerical results. Angers et al. [16] numerical simulated hydrogen releases from a 70 MPa tank for very short times and also noted the lack of high pressure experimental data for validation. Others have presented limited results for flow fields very near the nozzle or for short times due to stability and time limitations for high Mach number flows [16–18]. The accuracy of CFD model predictions is also limited by the ability of the turbulence model to predict these flows [15,19]. Many studies have used the standard k-ε turbulence models, while others have used more advanced models [20] or LES [18]. More comparisons with experimental data are needed to verify the accuracy of the turbulent models.

The difficulties and computational expense of CFD simulations of the near-orifice region has led to a simplified approach based on the notional nozzle concept using an effective nozzle diameter [4,21–26]. This method does not model the complex shock structure, but rather the release is assumed to start with a jet flow from a pseudo nozzle orifice [21] assuming that all of the flow passes through this notional nozzle with uniform velocity and concentration profiles. This nozzle approach has been widely used even though the assumptions, such as neglecting air entrainment into the jet and uncertainties about the temperatures downstream [13], affect prediction accuracy [18]. These models also do not account for the very nonuniform jet velocity profile due to the partitioning of the flow between the central core that passes through the Mach disk and the flow in the supersonic slip region [27]. HySafe [28] recommended that such approaches be further validated for a wide range of stagnation pressures. Li and Christopher [27] and Li et al. [29] presented results for jet flows for pressures up to 70 MPa that showed that much more than half of the hydrogen flows into the supersonic slip region with significant air entrainment, so the notional nozzle model cannot accurately represent the flow fields. Tchouvelev [30] compared CFD predictions to notional nozzle results for a hydrogen release from a 43 MPa tank to show that the notional nozzle results were significantly different from the CFD model

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