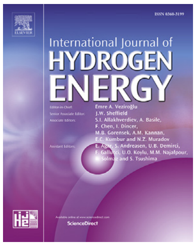
Available online at www.sciencedirect.com

ScienceDirect

journal homepage: www.elsevier.com/locate/he



Simplified partitioning model to simulate high pressure under-expanded jet flows impinging vertical obstacles

Jinghu Hu [a], *David M. Christopher* [a,*], *Xuefang Li* [b,**]

[a] *Key Laboratory for Thermal Science and Power Engineering of Ministry of Education, Department of Energy and Power Engineering, Tsinghua University, Beijing 100084, China*

[b] *Institute of Thermal Science and Technology, Shandong University, Jinan 250061, China*

ARTICLE INFO

Article history:
Received 10 February 2018
Received in revised form
5 May 2018
Accepted 7 May 2018
Available online xxx

Keywords:
Underexpanded jet
Two-layer partitioning model
Abel-Noble gas
Hydrogen safety

ABSTRACT

Various reduced-order models have been developed to quickly model high pressure underexpanded jets. One example is the two-layer partitioning model which was developed to model underexpanded jets, but it has not been evaluated for high pressure jets with obstacles in the jet flow region. This research describes an improved two-layer partitioning model based on the Abel-Noble equation of state that is applied here to model horizontal jet flows impacting a vertical obstacle with validations against high pressure gas experiments, full CFD simulations and a revised notional nozzle model based on the Abel-Noble equation of state. The improved two-layer partitioning model accurately predicts the gas concentrations on the obstacle for a 15 MPa underexpanded jet while consuming much less computational resources and time compared with the full CFD simulation.

Introduction

Hydrogen, with its low density and low volumetric energy density has to be stored at extremely high pressures for commercial use. A typical commercial hydrogen-fueled vehicle stores hydrogen at 70 MPa with the pressures in fueling station tanks typically reaching 35 MPa. Thus, risk assessments of the high pressure hydrogen storage tanks are necessary for safety evaluations. Protective walls are built around hydrogen storage tanks to prevent high pressure jets from leaks from extending far out into the surrounding area and extending the lower flammability region volume. Thus, detailed descriptions of the flow field for a high pressure, underexpanded jet impacting a vertical obstacle are needed to evaluate and design engineered safety solutions.

High pressure underexpanded jet flows will lead to complex nearfield shock structures. Different pressure ratios between the stagnation pressure and the atmospheric pressure lead to different underexpanded nearfield shock structures with four kinds of underexpanded jet flows categorized based on their pressure ratio and, hence, their underexpansion level. Relatively low pressure, underexpanded jets will form a weak shock outside the nozzle exit [1,2]. As the pressure increases, the jet flow becomes moderately underexpanded with diamond shaped oblique shocks [1–5]. The oblique shocks, also called the slip region or the barrel shock region, are reflected

---

* *Corresponding author.*
** *Corresponding author.*

E-mail addresses: hujh16@mails.tsinghua.edu.cn (J. Hu), dmc@tsinghua.edu.cn (D.M. Christopher), lixf@sdu.edu.cn (X. Li).

https://doi.org/10.1016/j.ijhydene.2018.05.036

Please cite this article in press as: Hu J, et al., Simplified partitioning model to simulate high pressure under-expanded jet flows impinging vertical obstacles, International Journal of Hydrogen Energy (2018), https://doi.org/10.1016/j.ijhydene.2018.05.036

to form the reflected oblique shock structure. The reflected oblique shock will regenerate new intersecting shocks when they reach the outer boundary of the jet core region. This cell structure in the slip region tends to repeat itself along the axial direction downstream until the jet reaches ambient pressure. Highly-underexpanded jet flows are characterized by the appearance of a Mach disk at the end of the supersonic jet core region inside the oblique shock structure slip region [6–8]. The Mach disk and the reflected shock intersect at a triple point and the Mach disk is not a perfect flat normal shock but has some curvature. The flow in the slip region continues at a much higher velocity than the flow in the core region after the Mach disk. The slip region can continue to be supersonic with more reflected shocks after the Mach disk location as the slip region expands into the slower core region until become one flow region. In very high pressure underexpanded jets, the slip region normally has a larger area than the potential core region [9,10]. Air is entrained into the slip region starting shortly after the flow leaves the nozzle with no air entrained into the core flow region. The total jet diameter decreases in very high pressure, underexpanded jets as ambient air is entrained into the flow [11].

Traditional CFD numerical simulations try to solve the Navier-Stokes equations plus other conservation equations throughout the whole simulation geometry, which is called the full CFD simulation model method in this paper. Full CFD simulations are intrinsically unstable when used to simulate supersonic flow shock structures. They require very long computational times and large computational resources for complete high pressure gas flow simulations [12]. Therefore, full CFD simulations are not practical for simulating the large flow fields of underexpanded jets.

In hydrogen safety risk analyses, however, the main interest is the gas concentration profiles in the far field of the underexpanded jet. The underexpanded jet flow profile can then be treated as a relatively simple subsonic compressible flow starting with an already expanded jet based on assumptions about the conservation of mass, momentum and energy [11]. That has given rise to the development of various reduced-order notional nozzle models. The key idea of the notional nozzle models is to predict simplified inlet boundary conditions for underexpanded jet flow simulations. Typical notional nozzle models replace the original high pressure boundary gas inlet condition with fully expanded low pressure velocity/mass inlet(s) boundary conditions which eliminates the nearfield shock structure region and avoids the complex numerical simulations of the shocks. The application of the notional nozzle models still require CFD simulations throughout the extended flow field model geometry. However, the simulations are much more efficient without the need to simulate the shock structures of the high pressure gas inlets. The objective of the simplified notional nozzles is then to predict reasonable gas flow profiles in the jet flow farfield with much faster calculations.

There have been many studies aimed at developing notional nozzle models that give more accurate predictions with more universally applicable simulation conditions. Thring [13] developed the first notional nozzle concept by assuming that the notional nozzle had the same momentum flux and velocity as the real gas nozzle with a gas density equal to that of the gas at ambient conditions. Their model and all other models also assumed an isentropic expansion between the stagnation conditions in the tank to the nozzle. Birch et al. [14] developed a notional nozzle model (Birch84 model) assuming mass conservation between the real nozzle and the notional nozzle without air entrainment. The notional nozzle pressure and temperature were assumed to be the ambient conditions and the gas velocity was assumed to be the local sonic velocity. Many other studies have been inspired by the Birch84 model. The basic assumptions of the Birch84 model, atmospheric pressure in the notional nozzle and the jet flow mass conservation with zero air entrainment, were used as the basic assumptions by many of the following models. Ewan et al. [10] slightly modified the Birch84 model by assuming that the notional nozzle temperature was equal to the real nozzle gas temperature with the other assumptions. Gore et al. [15] developed a modified notional nozzle model based on the momentum conservation assumption between the real nozzle and the notional nozzle. The notional nozzle diameter was assumed to be the same as the real nozzle but with the notional nozzle ambient pressure assumption. Birch et al. [16] gave an improved notional nozzle model (Birch87 model) by adding the momentum conservation assumption in addition to the original mass conservation assumption. The notional nozzle temperature was assumed to be equal to the stagnation temperature of the ideal gas. Several studies have shown that the Birch87 model gives more accurate predictions [16–18]. Yüceil et al. [19] used the atmospheric pressure assumption and the mass, momentum and energy conservation equations to derive a notional nozzle model. Harstad et al. [20] used real underexpanded jet shock structure observations and assumed that the notional nozzle was right after the Mach disk and shared the same diameter as the Mach disk. The flow between the real nozzle and the notional nozzle was assumed to be isentropic with the normal shock wave property relations between the flow before and after the Mach disk used to calculate the notional nozzle profiles. These notional nozzle models were all derived using the ideal gas equation of state (EOS), with later models using a real EOS like the Abel-Noble EOS [21–23].

These notional nozzle models give a simplified method to derive boundary conditions for the notional nozzle that are used as inputs to significantly simplified underexpanded jet flow numerical simulations. However, all these previous notional nozzle models assumed that the gas had uniform velocity and composition distributions at the notional nozzle which is not true in high pressure underexpanded jet flows. Observations have shown that real underexpanded jet flows have complex shock structures, Mach disks and flow stratification between the slip region and the core region with only some of the flow through the Mach disk and most of the high pressure jet flow flowing through the surrounding slip region with air entrainment [24,25].

Li et al. [17] developed a two-layer partitioning model that takes into account the gas partitioning between the core region and the slip region in real underexpanded jets. The two-layer partitioning model assumed that the gas flows into two separate regions upon exiting the orifice with part of the flow accelerating to very high Mach numbers before passing through the Mach disk where the flow becomes subsonic and

Please cite this article in press as: Hu J, et al., Simplified partitioning model to simulate high pressure under-expanded jet flows impinging vertical obstacles, International Journal of Hydrogen Energy (2018), https://doi.org/10.1016/j.ijhydene.2018.05.036