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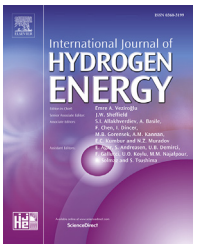

Turbulent mixing and molecular transport in highly under-expanded hydrogen jets

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ABSTRACT

Highly under-expanded hydrogen jets releasing in quiescent air atmosphere are studied using highly resolved numerical simulations accounting for complex multicomponent molecular transport phenomena. In a first step of the analysis, the main overall features of the hydrogen jet structure are described and compared to those of the classical under-expanded air jet at the same nozzle pressure ratio (NPR). Even if the global flow topology remains quite similar in both cases (i.e., hydrogen and air discharges), the modification of both mean density and mean velocity gradients leads to different relative energy levels for each velocity component. The corresponding change of fluid properties mainly leads to an enhanced mixing at the jet periphery. In comparison to the air case, the turbulence development within the internal part of the under-expanded hydrogen jet surrounding the subsonic core also yields a different structure. While a significantly higher peak of streamwise turbulent stress is observed downstream of the reflected shock, the vorticity dynamics is dampened by viscous diffusion and velocity divergence (i.e., volumetric expansion) contributions. Then, the performance of the simplified Hirschfelder and Curtiss approximation of the multicomponent molecular diffusion phenomena is evaluated with respect to the detailed multicomponent transport representation, as deduced from the EGLIB library. The detailed representation of molecular phenomena is shown to have a significant influence on the estimated local levels of hydrogen mass flux, leading to a non-negligible alteration of the global jet structure.

Introduction

The sonic discharge of a highly under-expanded hydrogen jet in quiescent surrounding atmosphere is investigated. The understanding of the mixing features in such jets is essential in many applications related to both the design of hydrogen-based combustion systems and the elaboration of consistent safety standards relevant to hydrogen storage. For instance, it still remains a prerequisite before considering a wider deployment of hydrogen solutions in the world's automotive fleet [1]. Such high-pressure hydrogen jets also constitute a key element in combustion chambers of space launchers [2] or air-breathing high-speed scramjet propulsion technologies for which they may be generated through high-pressure release in transverse supersonic vitiated air flow [3]. The improvement of the design of injectors in internal combustion engines [4] also heavily depends on our ability to understand and

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predict the transient development of such jets. In this context of road transport, the possible use of hydrogen as an alternative fuel indeed gives rise to specific safety issues related to possible unexpected accidental release through pressure relief valve or small cracks of high-pressure storage vessels walls. In such a case, it is critical to prevent any occurence of jet fire which would result from the under-expanded hydrogen jet release in the surrounding oxidizing medium. For all these applications, among others, some great efforts are still required to characterize both large- and small-scale features of hydrogen/air mixing processes and to develop reliable reduced-order modeling tools.

An abundant literature has been already dedicated to the characterization of either the global evolution of the upstream shock structure or the far-field axial evolution of mean properties. The case of moderately under-expanded air jet flows has probably received more attention in order to study screech noise generation associated to the interaction of instability waves with the diamond-like shock cell structures embedded within the supersonic jet core [5]. A detailed description of the evolution of large-scale coherent motions and turbulence properties of such jets at higher NPRs is however still lacking even for the most simple case of air jet. The case of high-pressure hydrogen jet release leads to consider even more challenging issues. Due to their far different molecular weights, thermochemical, and transport properties, high-pressure air and hydrogen jets are likely to yield significantly different behaviors both from a macroscopic point of view (transition mechanisms, stability properties, coherent structure topology, etc.) and at the smallest scales of the turbulent flow, where molecular diffusion processes play the essential role. As far as the objective would be to optimize any industrial process, replicating a full scale direct numerical simulation of all these interrelated physical phenomena would naturally require unreachable computational efforts. Great simplifications are thus often introduced to model multicomponent transport and possible combustion. In particular, the unity Lewis number assumption ($\mathscr{L}e_\alpha = 1$) is often retained as a simplifying assumption. In this case, the composition of the unburned mixture may be quite efficiently described through the use of a single variable, i.e., the mixture fraction ξ, and the mass fractions Y_α of any species α can be related to this quantity [6]. In practice, this also requires the local mixture to be issued from two inlets only, but a possible extension of this formalism to multiple inlets has been recently discussed in Ref. [7]. In any case, it is still needed to assess how far such simplifying assumptions can lead to a sufficiently accurate description of complex flowfields such as the one considered herein. The unity Lewis number assumption indeed implies that the values of molecular diffusivities are similar for all chemical species, an approximation that may become critical for mixtures containing hydrogen. Hydrogen molecules are indeed very light compared to other species like oxygen and nitrogen. According to the Graham's law [8], molecular diffusivity scales like the square root of the molecular weight in such a manner that the ratio of hydrogen to oxygen diffusivities significantly differs from unity and is of the order of four. In this respect, the influence of complex molecular transport on either hydrogen-air or hydrogen-oxygen flames has been illustrated in a wealth of studies, see for instance references [9–12]. Questioning the relevance of molecular transport approximations seems all the more legitimate (i.e., relevant) for highly under-expanded hydrogen jets since they generate very high gradient levels of all the physical variables, i.e., not only those of species concentrations but also temperature and pressure gradients, which are at play in the molecular diffusion processes.

This study focuses on the case of highly under-expanded hydrogen jets representative of high-pressure hydrogen release into quiescent atmosphere. Its objective is twofold. It aims first at characterizing the main differences that exist between the near-field structure of high-pressure releases of air and hydrogen. This could be of interest in the perspective to rescale *adhoc* reduced-order models for hydrogen jet release, based on databases that are more widely available for air jet conditions. This will also complement recent comparisons performed between nitrogen and hydrogen jets at smaller NPR [13]. Then, it aims at evaluating more precisely the influence of molecular diffusion effects and their representation on the global properties of mixing with the surrounding air. In order to isolate such small-scale effects from both (i) large-scale instabilities and (ii) heat release influence due to ignition and development of jet flame, surrounding wall boundaries and potential chemical sources are neglected. A high temperature jet is yet considered. This allows both (i) a drastic reduction of the Reynolds number value, so that high-fidelity simulations can be conducted at a reduced computational cost, and (ii) a significant increase of molecular activity up to levels comparable to those encountered in the presence of heat release induced by chemical reactions.

The presentation of the results is divided into two distinct parts: the first is devoted to comparisons between the dynamics of air and hydrogen highly under-expanded jets. This topic is especially relevant for practical purposes. Indeed, since conducting experiments with hydrogen in highly under-expanded conditions raise severe difficulties, air is often used so as to perform experimental investigations. The second part of the manuscript aims at assessing the possible influence of the molecular transport description. The choice of this description may indeed alter some of the conclusions drawn in the first part of the manuscript. The detailed organization of the paper is as follows: the main expected features of highly under-expanded jets are first briefly reviewed in Section Background and literature review. Then, the representation of molecular transport is discussed in Section Representation of molecular transport, while the numerical solver and the computational setup are presented in Section Numerical set-up. The global characterization of the hydrogen jet structure is reported in Section Comparison between air and hydrogen jets where its topology is compared to the more classical air jet structure. Finally, differential diffusion and complex multicomponent transport effects are investigated in Section Influence of the molecular transport description. The manuscript ends with a last section where the main conclusions are summarized.

Background and literature review

A typical sketch of the near-field structure of an under-expanded jet obtained for NPR values larger than ten is

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