Molecular diffusion as rate-controlling process in premixed hydrogen flames: implications for power generation, propulsion and safety

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ABSTRACT

In the context of the ongoing energy transition to a modern low-carbon and low-pollution society many power-generation, propulsion and high-temperature heat applications must become able to operate on novel and unconventional carbon-free fuels and energy vectors for large-scale energy storage [1]. This applies to a range of technologies based on thermal energy conversion and exploiting the conversion rates enabled by high-pressure turbulent combustion. Although fuel-flexible in principle, gas turbines and reciprocating piston engines can encounter serious operational issues related to flame stability and emissions because of the vastly different combustion properties of relevant carbon-free fuels, as hydrogen and ammonia, compared with conventional hydrocarbon fossil fuels [2]. Hydrogen is highly diffusive, extremely reactive, and its turbulent burning rate exhibits a strong pressure dependence yet to be fully explained [3]. Furthermore, accidental release of hydrogen from large-scale high-pressure storage can result in strongly turbulent non-premixed jet flames or, if ignition is delayed until enough hydrogen fuel has mixed with an oxidizer (air), the resulting deflagration can rapidly transition from a laminar to a turbulent premixed flame, and even to a detonation, in the presence of obstacles [4]. In all these scenarios, accurate knowledge and predictive capabilities about the propagation characteristics of turbulent premixed hydrogen-air flames is of crucial importance. However, experimental evidence and numerical studies suggest that the fundamental understanding of the physical process controlling the burning rate response of hydrogen flames to varying pressure and turbulence conditions remains elusive [5].

Hydrogen's fast molecular diffusion velocity was indicated (by Zel'dovich & co-workers in the 1980s) as the root cause of a peculiar global behaviour observed in hydrogen premixed flames, due to a so-called thermo-diffusive instability that, at fuel-lean conditions, greatly accelerates thri propagation [6]. In the present work, based on 2-D and 3-D Direct Numerical Simulation (DNS) data, we propose a novel scaling approach for the turbulent burning rate in turbulent premixed hydrogen-air flames at (globally) fuel lean conditions. The new scaling relates the *stretch factor* $\mathbf{I_0}$, proposed by Bray & Cant [7], to a parameter consisting of the ratio between the *Zeldovich* (**Ze**) and *Peclet* (**Pe**) numbers defined for each specific reactants mixture. Crucially, the quantity $\mathbf{I_0}$, selected here to provide a more accurate quantification of the effect of thermo-diffusive

instabilities on hydrogen-enriched flame, represents the ratio between the (actual) global fuel consumption rate and the (hypothetical) fuel consumption rate of an idealized laminar flame that has undergone the same flame area increase as the turbulent one. In the conventional case (methane-air mixtures) of turbulent flames where the burning rate is controlled by the flame surface area generation, the stretch factor $I_0 \cong 1$. However, in the case of thermo-diffusively unstable flames (i.e., hydrogen-air flames at fuel lean conditions) the stretch factor I_0 can increase well beyond unity. This implies that I_0, scaled by the Ze/Pe parameter, can be potentially exploited in models to quantify the extent to which increments of the turbulent burning rate are controlled by changes to the local flame structure, through localized enrichment and enhanced burning for positively curved portions of the flame front, relative to the "conventional" acceleration mechanism, governed by flame surface area generation.

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