



Modeling of differential diffusion with virtual chemistry for ammonia/hydrogen blends

Natacha Galand^{1*}, Étienne Espada¹, Benoît Fiorina¹

*Lead presenter: natacha.galand@centralesupelec.fr

¹ Université Paris-Saclay, CNRS, CentraleSupélec, Laboratoire EM2C, 91190, Gif-sur-Yvette, France.

Among carbon-free fuel blends, the mixture of ammonia and hydrogen is particularly promising for decarbonizing combustion systems. However, simulating $\text{NH}_3/\text{H}_2/\text{air}$ flames presents significant modeling challenges due to the complexity of nitrogen chemistry [1], and the high diffusivity of hydrogen, which promotes thermodiffusive instabilities [2].

To reduce computational costs, detailed chemical mechanisms for ammonia-hydrogen-air combustion must be simplified before being implemented in industrial CFD codes [3]. Among existing simplification methods, the virtual chemistry approach offers an attractive balance between computational efficiency and accuracy in capturing complex chemical effects [4]. The originality of virtual chemistry consists in introducing virtual species and reactions whose thermodynamic and chemical properties are optimized by machine learning algorithms in order to retrieve properties of reference flames gathered in a learning base. This approach has been successfully applied to model key combustion characteristics such as flame propagation speed, auto-ignition, and pollutant formation [5].

However, in its original formulation, virtual chemistry assumes equal diffusivities for all virtual species, making it incapable of capturing intrinsic thermodiffusive instabilities. To address this limitation, we propose a new formalism in which the molecular diffusion properties of virtual species are also optimized. This new method is first validated on 1D freely propagating ammonia/hydrogen flames, where differential species diffusion is considered. Special attention is given to the method's ability to track demixing phenomena in the direction normal to the flame front. The approach is then applied to a 1D strained counter-flow flame configuration and to 2D laminar Bunsen flames.

References

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