

Analysis of preferential diffusion behavior in turbulent premixed hydrogen combustion

Citation for published version (APA):

Sanchez Bahoque, G., & van Oijen, J. (2021). *Analysis of preferential diffusion behavior in turbulent premixed hydrogen combustion*. Poster session presented at Combura 2021 Symposium, NVV 2021, Soesterberg, Netherlands.

Document status and date:

Published: 11/11/2021

Document Version:

Publisher's PDF, also known as Version of Record (includes final page, issue and volume numbers)

Please check the document version of this publication:

- A submitted manuscript is the version of the article upon submission and before peer-review. There can be important differences between the submitted version and the official published version of record. People interested in the research are advised to contact the author for the final version of the publication, or visit the DOI to the publisher's website.
- The final author version and the galley proof are versions of the publication after peer review.
- The final published version features the final layout of the paper including the volume, issue and page numbers.

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Analysis of preferential diffusion behavior in turbulent premixed hydrogen combustion

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Introduction

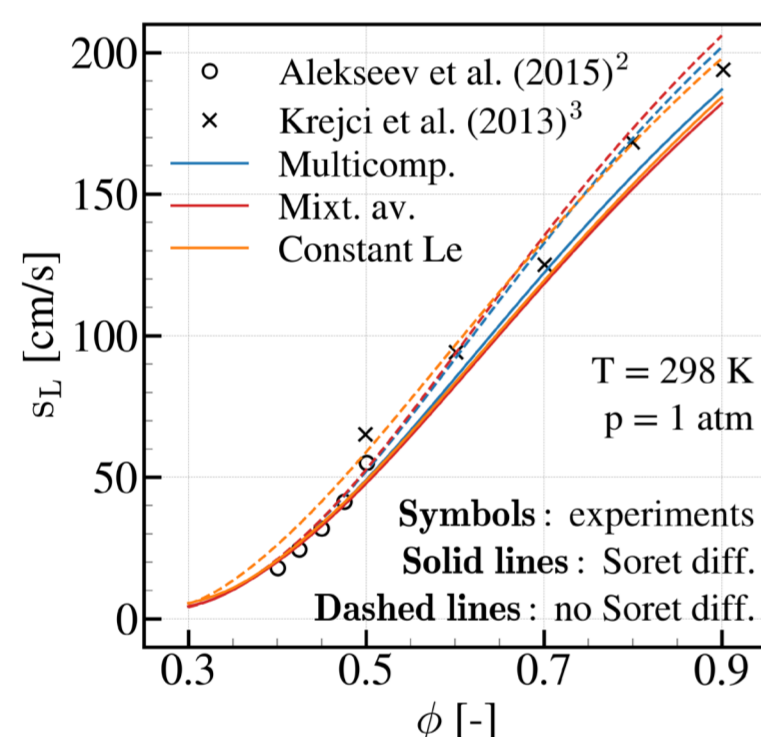
- The **Center of Excellence in Combustion (CoEC)** was created to develop advanced simulation software that support the decarbonization goals of the EU within the energy and transportation sectors¹.
- Hydrogen has become relevant as a cleaner fuel alternative.
- Combustion behaviors of H₂ are considerably different than those of hydrocarbon fuels and are still not fully understood.
- H₂ has a higher diffusivity than methane, leading to **preferential diffusion effects** and different flame dynamics.
- Objective: Investigate the interaction between H₂ premixed flames and turbulence.

Transport models

Due to the high diffusivity of H₂, it is important to choose a transport model that can predict the behavior of premixed H₂ flames accurately with a low computational cost.

The following models were studied with and without Soret diffusion: **multicomponent, mixture averaged** and **constant Lewis numbers**.

Flat flames



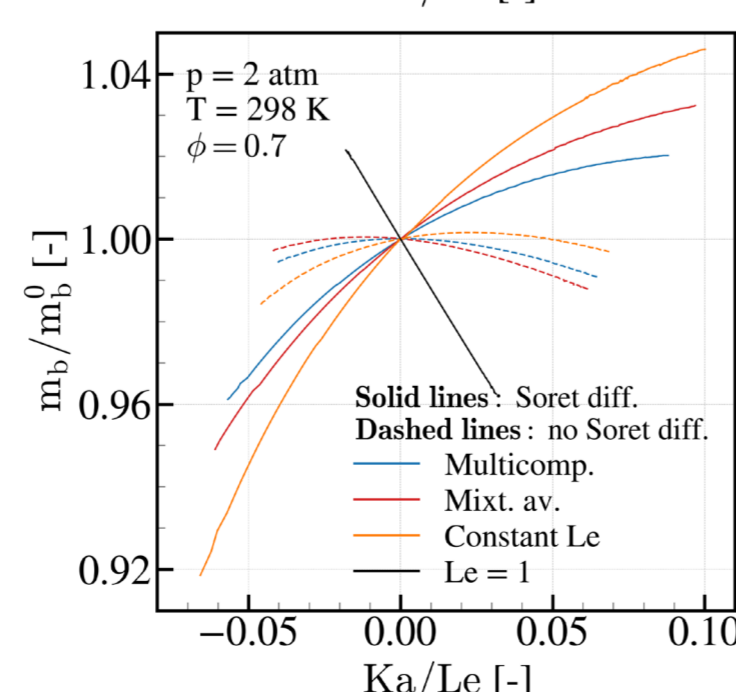
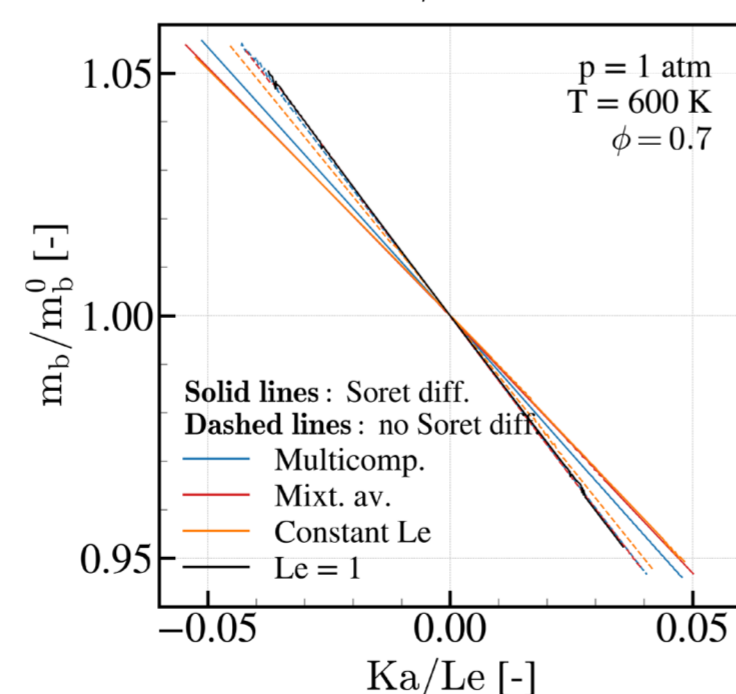
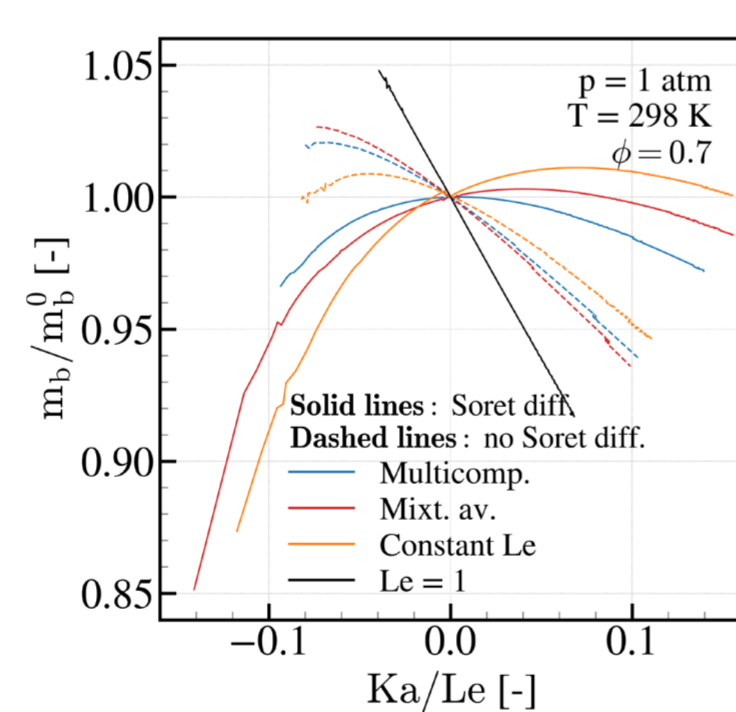
The figure at the left shows that the laminar flame speed of 1D premixed and lean H₂/air flames is well predicted by all the transport models and the reaction mechanism proposed by Burke et al. (2012)⁴ when Soret diffusion is taken into account.

Stretched flames

The mass burning rate of stretched H₂ flames is given by the sum of the **stretch effect** and **preferential diffusion effects**⁵.

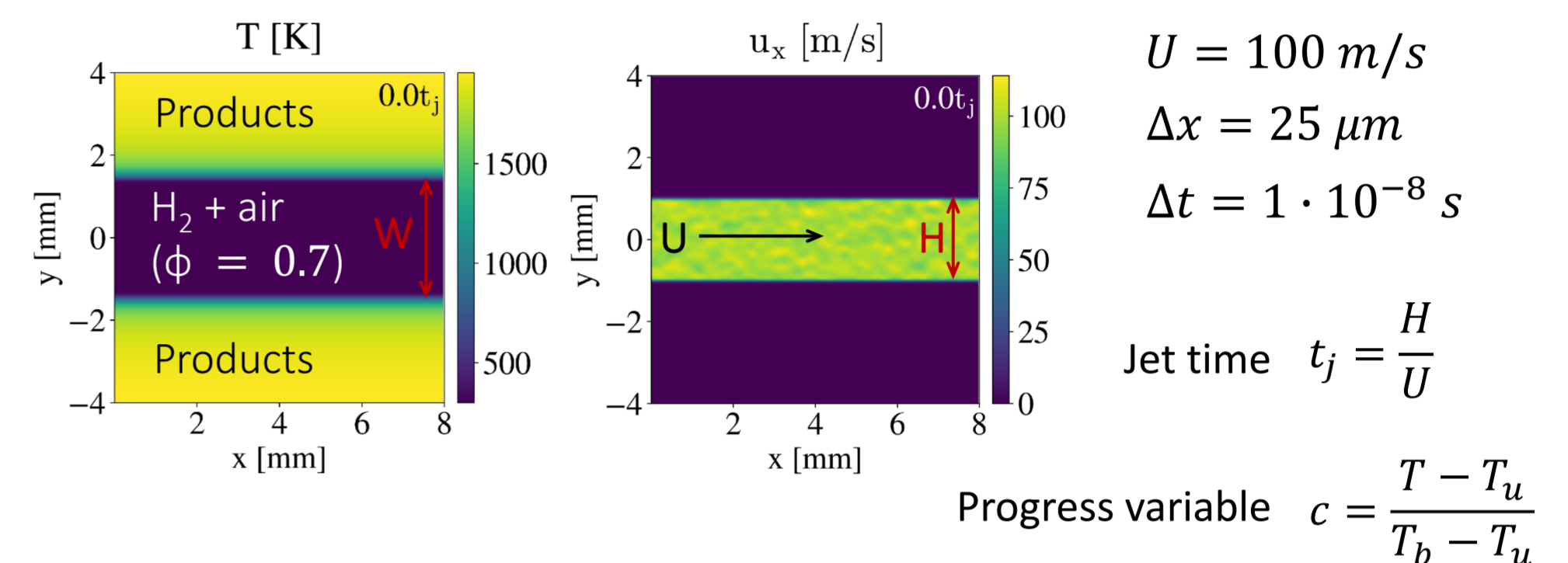
The figures at the right show the scaled mass burning rate of lean stretched H₂/air flames at different conditions vs. the Karlovitz number (dimensionless stretch rate).

- For $Le = 1$, the mass burning rate decreases with stretch, due to the direct stretch effect.
- For $Le \neq 1$, preferential diffusion effects take place and the mass burning rate increases.
- Preferential diffusion effects are diminished when increasing the inlet temperature and enhanced with pressure.

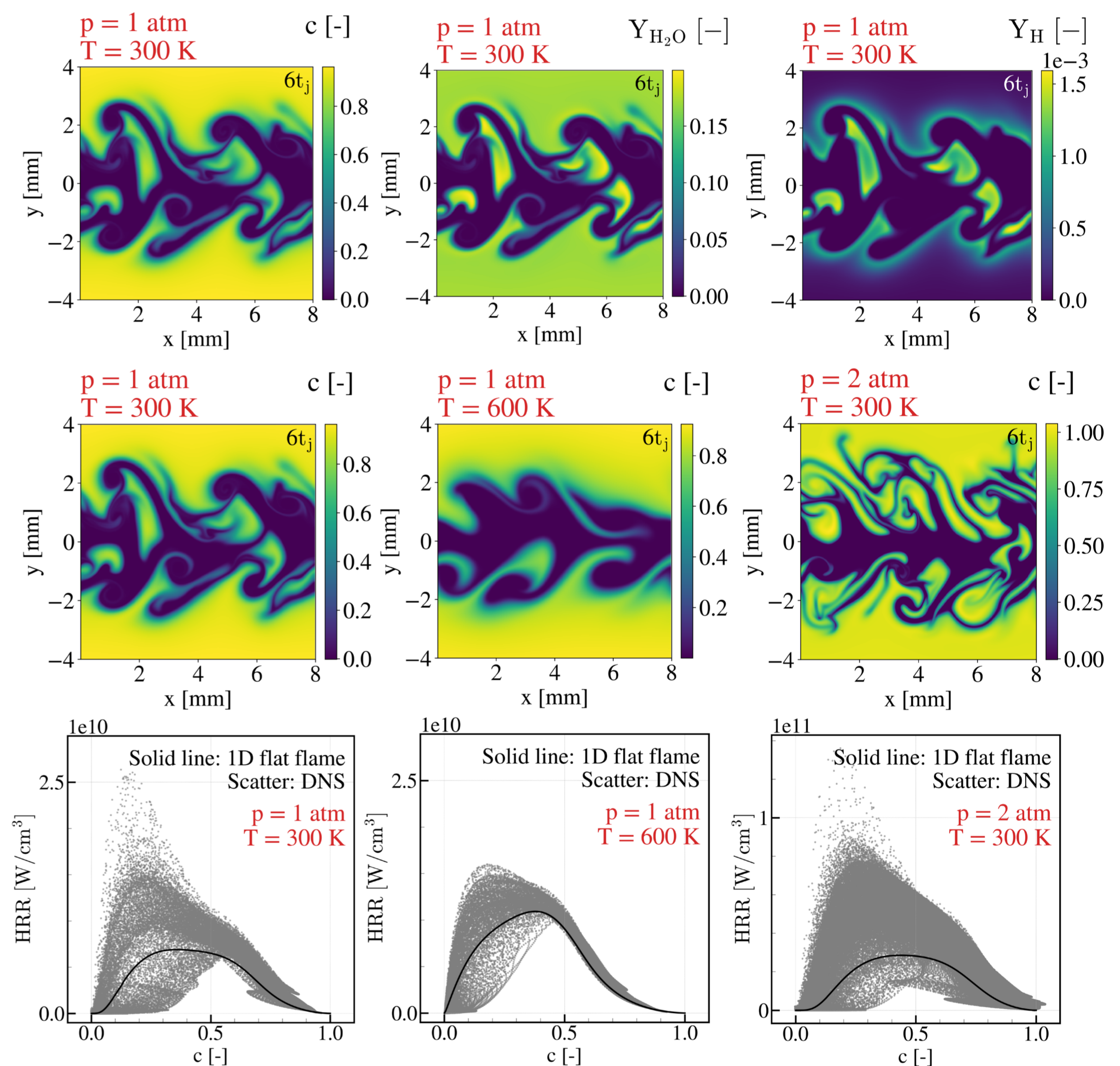


Direct Numerical Simulations

Setup: inspired by Hawkes et al. (2012)⁶



2D results



The contour plots of c , Y_{H_2O} and Y_H (first row) show the formation of flame islands where $c < 1$, and H₂O and H are accumulated, due to the higher diffusivity of hydrogen. The contour plots of c (second row) at different conditions show that preferential diffusion effects are reduced with increasing inlet temperature and intensified with pressure. The scatter plots of heat release rate (third row) show high heat release in regions with low c , due to exothermic reactions of radicals.

Conclusions

- Constant Lewis numbers with Soret diffusion is the most cost-effective transport model.
- Preferential diffusion effects take place in stretched H₂/air flames. This effects are reduced with increasing fresh gas temperature and enhanced with increasing pressure.
- Turbulence and high diffusivity of H₂ lead to the formation of flame pockets separated from the original flame front, that burn at an enhanced rate.

The research leading to these results has received funding from the European Union's Horizon 2020 research and innovation programme under the CoEC project, grant agreement No 952181.

¹ Center of Excellence in Combustion. <https://coec-project.eu/>.
² Alekseev et al. (2015). Combust. Flame, 162(10): 4063-4074.
³ Krejci et al. (2013). J. Eng. Gas Turbines Power, 135(2): 021503.
⁴ Burke et al. (2012). Int. J. Chem. Kinet., 44(7): 444-474.
⁵ van Oijen et al. (2016). Prog. Energy Combust. Sci., 57:30-74.
⁶ Hawkes et al. (2012). Combust. Flame, 159(8): 2690-2703.