Supplementary material: Influence of mesh size and transport model on the training database

1 Influence of mesh size

A study of the influence of mesh size is performed to ensure that the generated database is not sensitive to mesh refinement. For this purpose, new computations of the slot burner have been done on a homogeneous 80 μm mesh for all cases, and on a homogeneous 50 μm mesh for the cases with the lowest flame thickness $\phi_g = 0.6$ and 0.7.

The flame structure statistics are represented by the conditional mean and standard deviation of the H_2 source term $\dot{\omega}_{\mathrm{H_2}}$ related to the progress variable c in Figs S10, S11 and S12. The progress variable c is defined as

$$c = c_{\mathrm{H_2}} = \frac{Y^u_{\mathrm{H_2}}(\xi) - Y_{\mathrm{H_2}}}{Y^u_{\mathrm{H_2}}(\xi) - Y^b_{\mathrm{H_2}}(\xi)} \text{ with } Y^u_{\mathrm{H_2}}(\xi) = \xi \text{ and } Y^b_{\mathrm{H_2}}(\xi) = \begin{cases} 0 & \text{if } \xi \leq \xi_s \\ \frac{\xi - \xi_s}{1-\xi_s} & \text{otherwise} \end{cases}. \tag{S1}$$

The statistics are not affected by successive refinements, demonstrating that the 100 μm mesh size database can be used for training purposes.

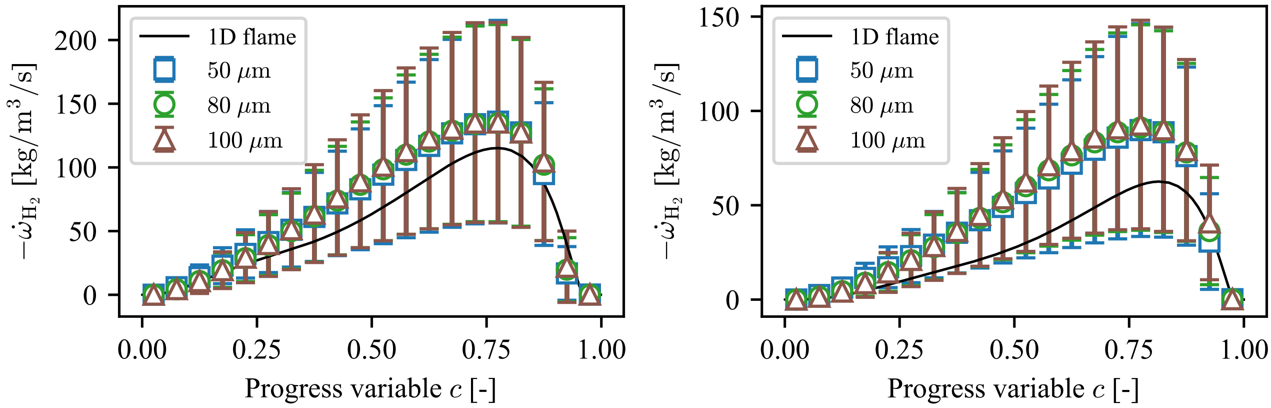

Figure S10: Conditional mean and standard deviation of the H_2 source term $\dot{\omega}_{\mathrm{H_2}}$ related to the progress variable c for three different mesh sizes (100, 80 and 50 μm) in the 3D slot burner used to generated the training database. The profile of a 1D laminar flame at the same global equivalence ratio is superimposed for reference. Left: global equivalence ratio $\phi_g = 0.7$, right: global equivalence ratio $\phi_g = 0.6$.

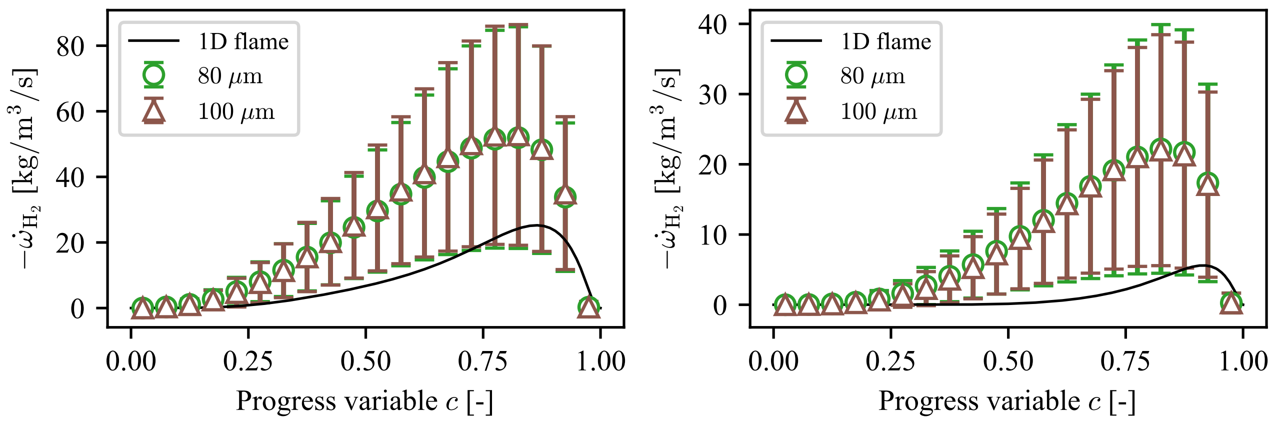

Figure S11: Conditional mean and standard deviation of the H_2 source term $\dot{\omega}_{\mathrm{H_2}}$ related to the progress variable c for two different mesh sizes (100 and 80 μm) in the 3D slot burner used to generated the training database. The profile of a 1D laminar flame at the same global equivalence ratio is superimposed for reference. Left: global equivalence ratio $\phi_g = 0.5$, right: global equivalence ratio $\phi_g = 0.4$.

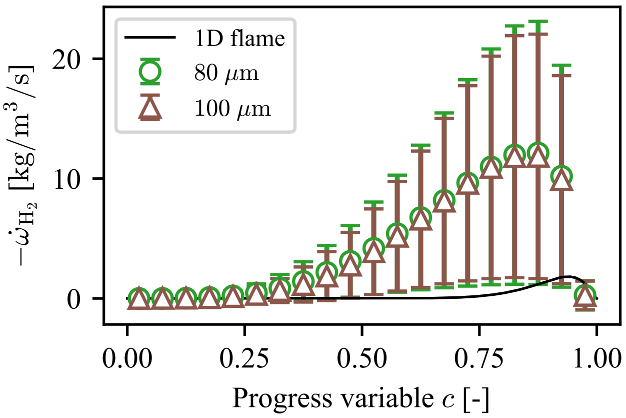

Figure S12: Conditional mean and standard deviation of the H_2 source term $\dot{\omega}_{H_2}$ related to the progress variable c for two different mesh sizes (100 and 80 μm) in the 3D slot burner used to generated the training database. The profile of a 1D laminar flame at the same global equivalence ratio is superimposed for reference. Global equivalence ratio $\phi_g = 0.35$.

2 Influence of the transport model

A study of the influence of transport model is performed to ensure that the assumption of a constant Schmidt number per species does not affect flame statistics. In the computations performed to generate the training database, the dynamic viscosity μ follows a power law function of temperature. The diffusion coefficients D_k are then calculated with constant but species-dependent Schmidt numbers Sc_k

$$D_k = \frac{\mu}{\rho \mathrm{Sc}_k} \text{ for species } k, \tag{S2}$$

where ρ is the gas density. The thermal conductivity λ is based on a constant Prandtl number Pr and the specific heat capacity of the mixture C_p

$$\lambda = \frac{C_p \mu}{\mathrm{Pr}} \, . \tag{S3}$$

The values of Sc_k and Pr are computed to correspond to the detailed transport coefficients in the burnt gases of a 1D laminar flame of reference.

To check that these simplifications do not bias the database, we have performed two computations at $\phi_g = 0.7$ and 0.35 with a more precise description of the transport via the mixture averaged approach, involving composition dependent contributions of each species in the mixture. The dynamic viscosity is computed via Wilke's mixing law. The Hirschfelder and Curtiss's mixing law is used for diffusivities

$$D_k = \frac{1 - Y_k}{\sum_{j \neq k}^{n} X_j / \mathcal{D}_{jk}} \, , \tag{S4}$$

where $\mathcal{D}_{jk}$ is the binary mass diffusion coefficient of species j into species k, X_k and Y_k are the mole and mass fraction of the species k. The thermal conductivity λ is computed as

$$\lambda = \frac{1}{2} \left(\sum_{i=1}^{n} X_i \lambda_i^s + \frac{1}{\sum_{i=1}^{n} X_i / \lambda_i^s} \right) \, , \tag{S5}$$

where λ_k^s is the conductivity of the species k.

The flame structure statistics are represented by the conditional mean and standard deviation of the H_2 source term $\dot{\omega}_{H_2}$ related to the progress variable c (Eq. (S1)) in Fig. S13. The statistics are not affected by the transport model, demonstrating that constant Schmidt number per species and constant Lewis number can be assumed to model diffusivities and generate the training database at a lower computational cost.

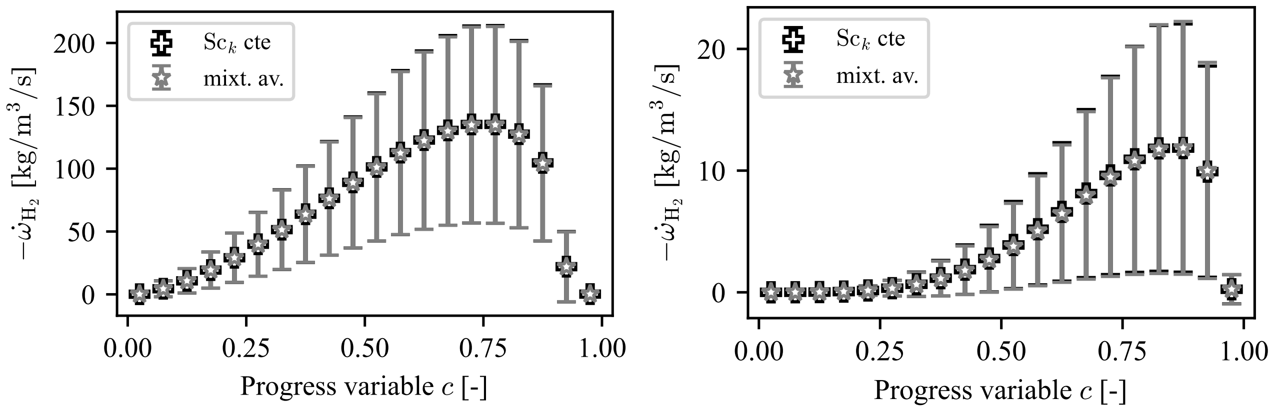

Figure S13: Conditional mean and standard deviation of the H_2 source term $\dot{\omega}_{\mathrm{H}_2}$ related to the progress variable c for two different transport models in the 3D slot burner used to generated the training database. Simplified transport model (Le and and Sc_k constant) and mixture-averaged transport model. Left: global equivalence ratio $\phi_g = 0.7$, right: global equivalence ratio $\phi_g = 0.35$.