Supplementary material: Influence of progress variable definition

1 One-dimensional flame structure

We chose to provide information on the evolution of combustion at the neural network by defining a progress variable c. This progress variable has been arbitrarily defined based on the H_2 mass fraction as

$$c_{\mathrm{H_2}} = \frac{Y^u_{\mathrm{H_2}}(\xi) - Y_{\mathrm{H_2}}}{Y^u_{\mathrm{H_2}}(\xi) - Y^b_{\mathrm{H_2}}(\xi)} \text{ with } Y^u_{\mathrm{H_2}}(\xi) = \xi \text{ and } Y^b_{\mathrm{H_2}}(\xi) = \begin{cases} 0 & \text{if } \xi \leq \xi_s \\ \frac{\xi - \xi_s}{1 - \xi_s} & \text{otherwise} \end{cases}, \tag{S2}$$

where ξ is the mixture fraction and ξ_s is the value of the mixture fraction at stoichiometry. Another option might have been to base the progress variable on H_2O as

$$c_{\mathrm{H_2O}} = \frac{Y_{\mathrm{H_2O}}}{Y^b_{\mathrm{H_2O}}(\xi)} \text{ with } Y^b_{\mathrm{H_2O}}(\xi) = \begin{cases} \frac{W_{\mathrm{H_2O}}}{W_{\mathrm{H_2O}} + 3.76/2 W_{\mathrm{N_2}}} \frac{\xi}{\xi_s} & \text{if } \xi \leq \xi_s \\ \frac{W_{\mathrm{H_2O}}}{W_{\mathrm{H_2O}} + 3.76/2 W_{\mathrm{N_2}}} \frac{1-\xi}{1-\xi_s} & \text{otherwise} \end{cases}, \tag{S3}$$

where $W_{\mathrm{H_2O}}$ and $W_{\mathrm{N_2}}$ are the molecular weights of H_2O and H_2 respectively.

Since the chemical kinetics of H_2 combustion is simple compared to hydrocarbon fuels, the definition of the progress variable on the H_2 reactant or the H_2O product has little effect on 1D laminar flame description (Figs S14, S15 and S16). We see no advantage or disadvantage in using either definition. Section 2 shows that training can be performed and the CNN model gives a very similar accuracy regardless of whether the progress variable is based on H_2 or H_2O.

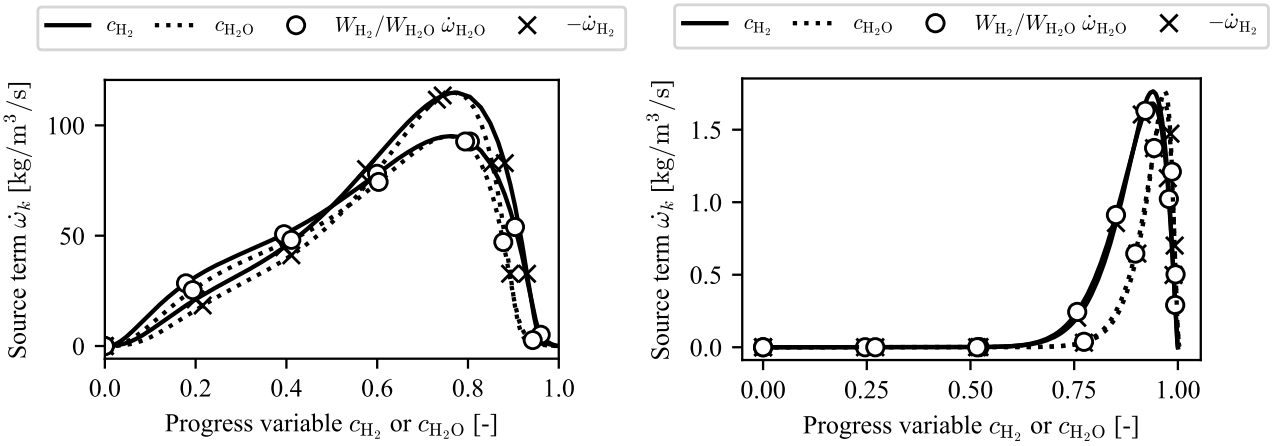

Figure S14: Evolution of the H_2 and H_2O species source terms as a function of a progress variable based on H_2 $c_{\mathrm{H_2}}$ (Eq. (S2)), solid line, and based on H_2O $c_{\mathrm{H_2O}}$ (Eq. (S3)), dashed line. Extracted from 1D laminar flame. Left: global equivalence ratio $\phi_g = 0.7$, right: global equivalence ratio $\phi_g = 0.35$.

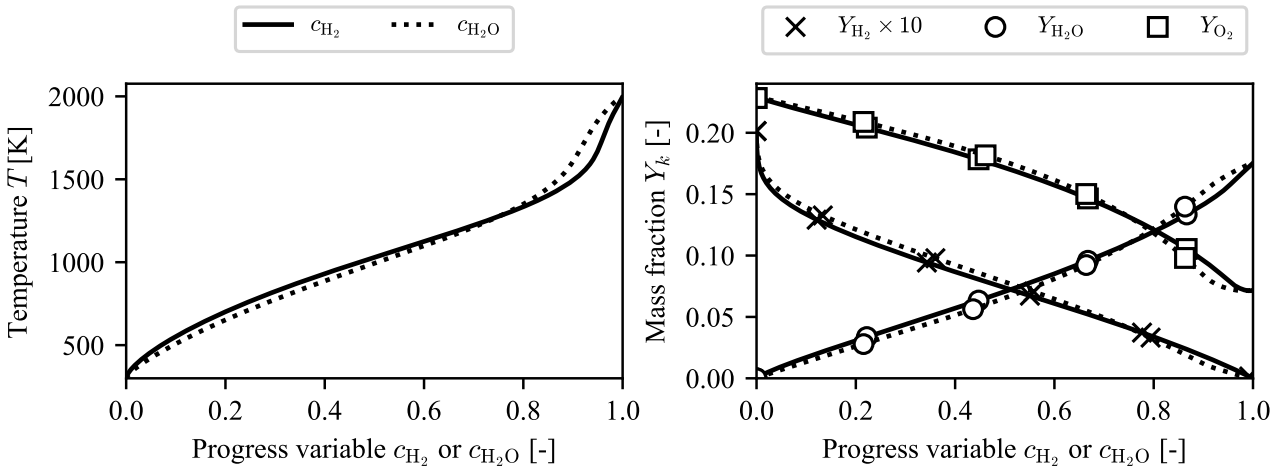

Figure S15: Evolution of the gas temperature and H_2, H_2O and O_2 species mass fraction as a function of a progress variable based on H_2 c_{H_2} (Eq. (S2)), solid line, and based on H_2O c_{H_2O} (Eq. (S3)), dashed line. Extracted from 1D laminar flame. Global equivalence ratio $\phi_g = 0.7$.

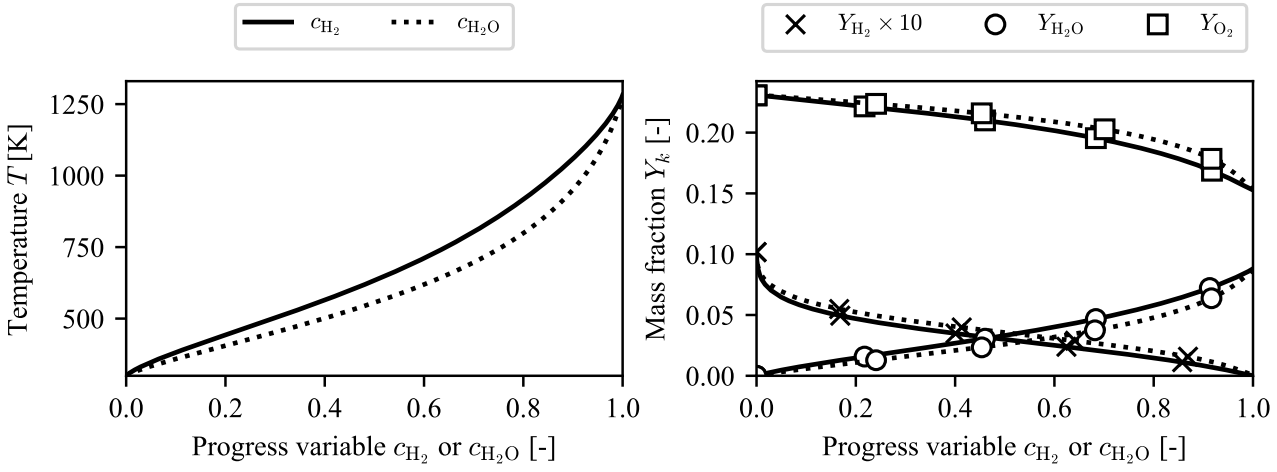

Figure S16: Evolution of the gas temperature and H_2, H_2O and O_2 species mass fraction as a function of a progress variable based on H_2 c_{H_2} (Eq. (S2)), solid line, and based on H_2O c_{H_2O} (Eq. (S3)), dashed line. Extracted from 1D laminar flame. Global equivalence ratio $\phi_g = 0.35$.

2 CNN training

To check that the choice of progress variable does not impact the CNN modeling abilities, a new training has been performed, basing the progress variable on H_2O c_{H_2O} (Eq. (S3)). The model conserves its very high accuracy with Normalized Mean Absolute Error (NMAE) very similar to the model trained using c_{H_2} (Eq. (S2)) introduced in the manuscript. This demonstrates that the proposed modeling framework is still valid with a change in definition of the progress variable based on H_2O.

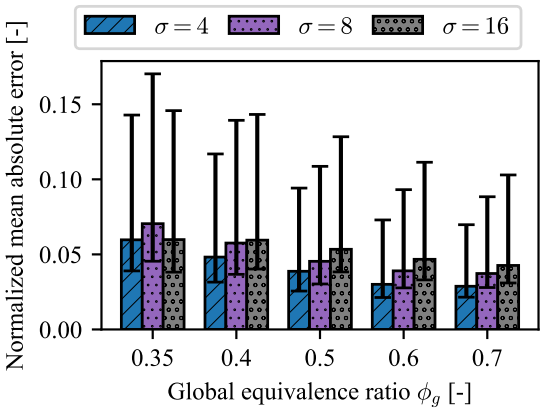

Figure S17: Normalized mean absolute error over the testing solutions (Eq. (3.1)) for the different equivalence ratios and LES parameters used for building the training dataset. Error bars show first and third quartiles of the data points. The progress variable is based on H_2O (Eq. (S3)).

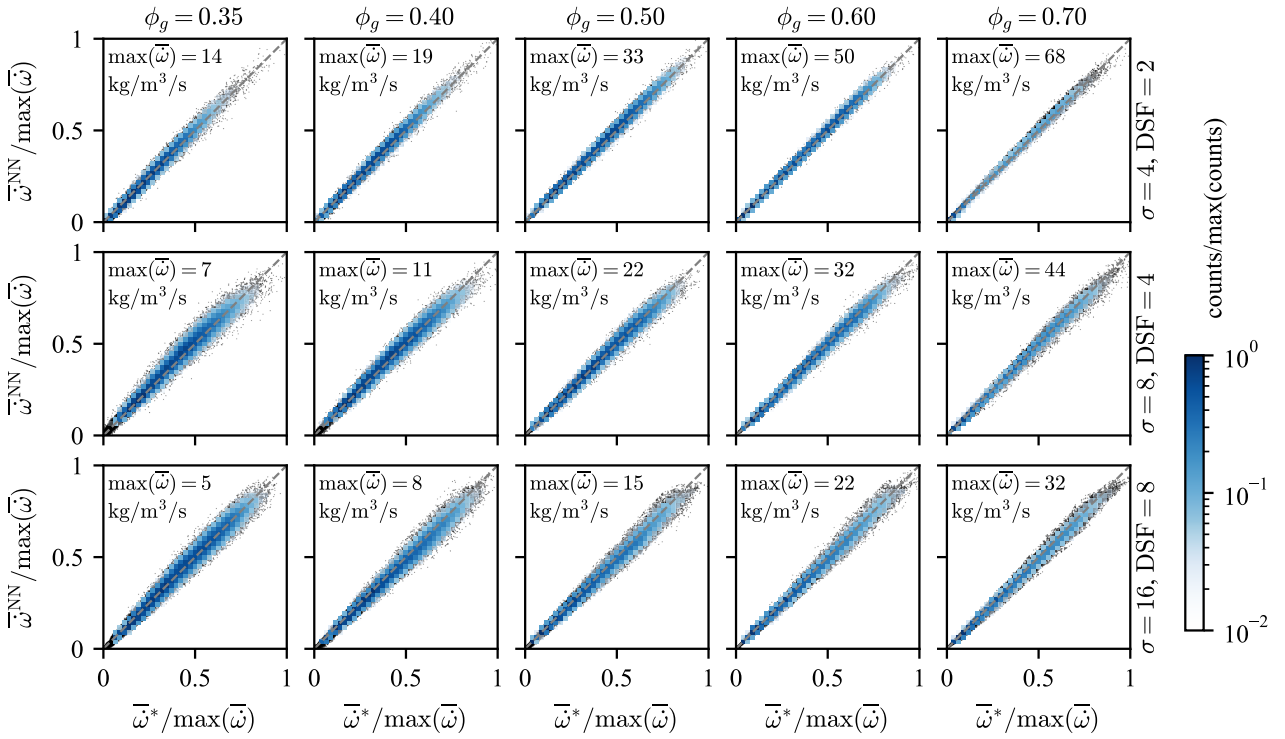

Figure S18: Scatter plots with 2D histograms: CNN-modeled burning rate $\overline{\dot{\omega}}^{NN}$ versus ground-truth filtered burning rate $\overline{\dot{\omega}}^{*}$. Individual values are normalized by the maximum burning rate in the datasets. The points used for the histograms have a progress variable c: $0.05 \leq c \leq 0.95$. Histogram values below the colour scale are transparent. Gray dashed line indicates $x = y$ (i.e. zero error). Each column corresponds to a global equivalence ratio. Each row corresponds to a set of LES parameters (filtering and downsampling). Data are collected from the testing solutions. The progress variable is based on H_2O (Eq. (S3)).