Supplementary material

"Hydrogen reaction rate modeling based on convolutional neural network for large eddy simulation", Data-Centric Engineering

1 Additional planar cuts

The results of CNN model on 3D test solutions are illustrated in Figs S1-S5 for all the global equivalence ratios considered in the companion paper i.e. $\phi_g = 0.35$, 0.4, 0.5, 0.6 and 0.7. The burning rate topology is accurately retrieved for all cases, even in the case of gas pockets detached from the main flame brush.

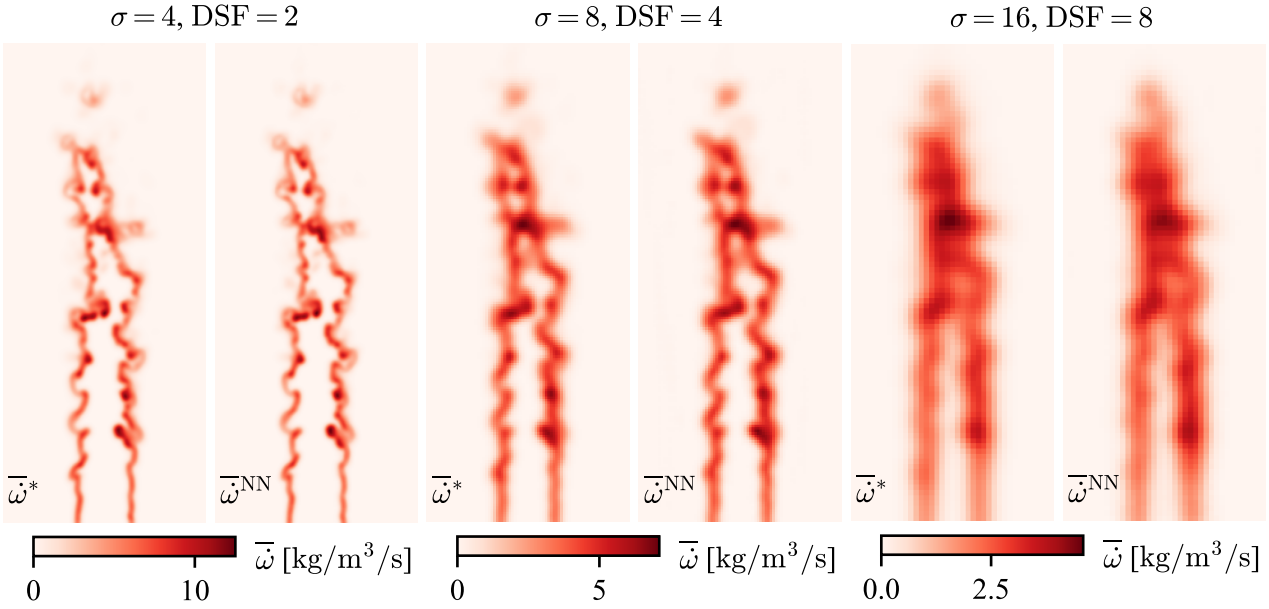

Figure S1: Planar cut normal to the z-axis, in the middle of the domain, colored by the ground-truth filtered burning rate $\overline{\dot{\omega}}^*$ and the CNN-modeled burning rate $\overline{\dot{\omega}}^{\mathrm{NN}}$ for three sets of LES parameters. The global equivalence ratio is $\phi_g = 0.35$.

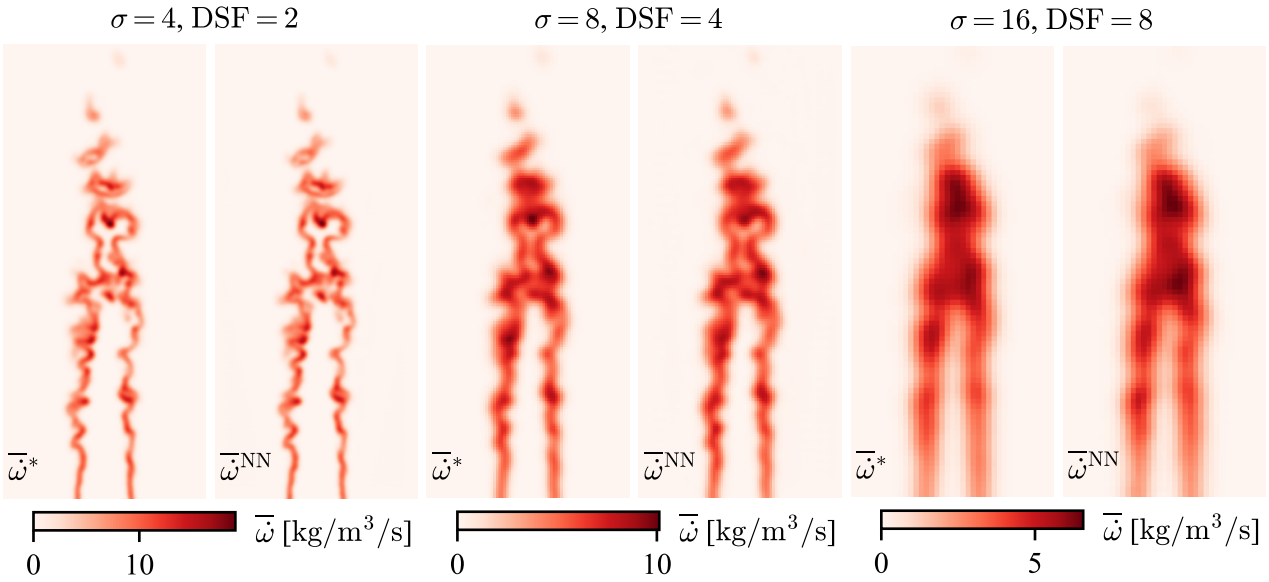

Figure S2: Planar cut normal to the z-axis, in the middle of the domain, colored by the ground-truth filtered burning rate $\overline{\dot{\omega}}^*$ and the CNN-modeled burning rate $\overline{\dot{\omega}}^{\mathrm{NN}}$ for three sets of LES parameters. The global equivalence ratio is $\phi_g = 0.4$.

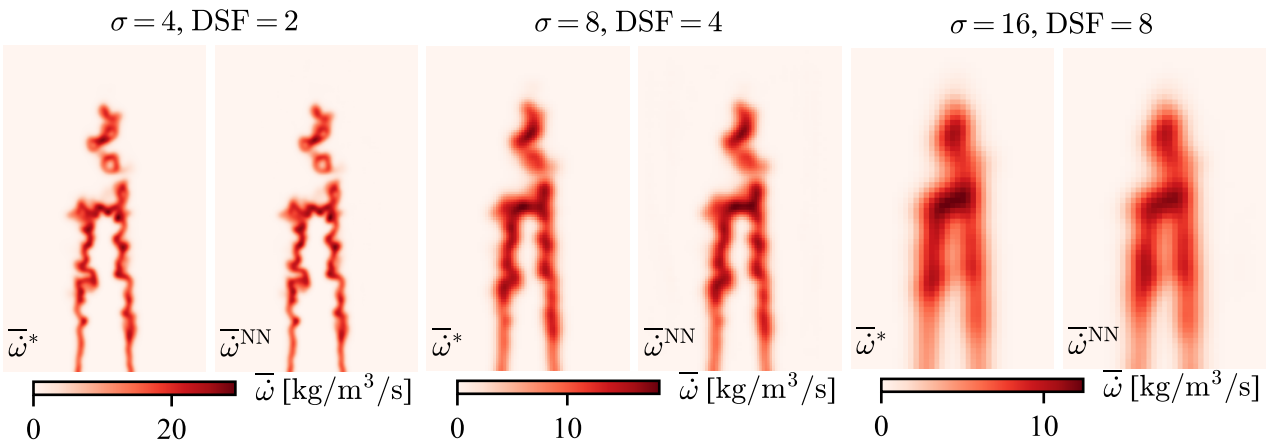

Figure S3: Planar cut normal to the z-axis, in the middle of the domain, colored by the ground-truth filtered burning rate $\overline{\dot{\omega}}^*$ and the CNN-modeled burning rate $\overline{\dot{\omega}}^{\mathrm{NN}}$ for three sets of LES parameters. The global equivalence ratio is $\phi_g = 0.5$.

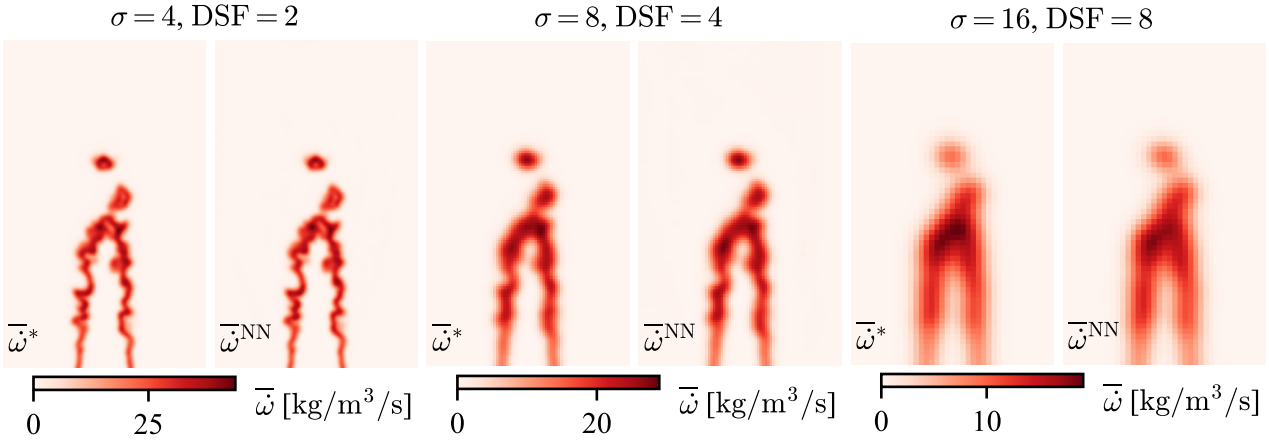

Figure S4: Planar cut normal to the z-axis, in the middle of the domain, colored by the ground-truth filtered burning rate $\overline{\dot{\omega}}^*$ and the CNN-modeled burning rate $\overline{\dot{\omega}}^{\mathrm{NN}}$ for three sets of LES parameters. The global equivalence ratio is $\phi_g = 0.6$.

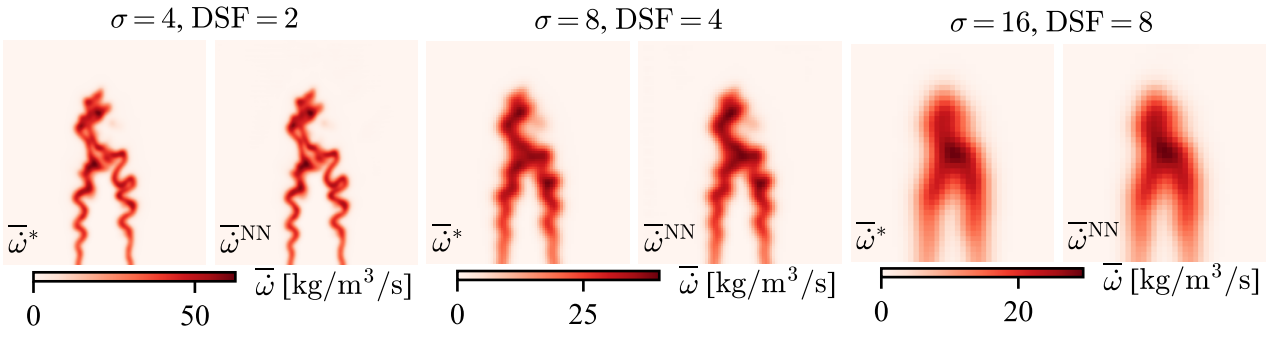

Figure S5: Planar cut normal to the z-axis, in the middle of the domain, colored by the ground-truth filtered burning rate $\overline{\dot{\omega}}^*$ and the CNN-modeled burning rate $\overline{\dot{\omega}}^{\mathrm{NN}}$ for three sets of LES parameters. The global equivalence ratio is $\phi_g = 0.7$.

2 Generalization, training without $\phi_g = 0.5$

The results of the CNN model trained without the case $\phi_g = 0.5$ are detailed in Figs S6 and S7. The model exhibits a significant bias at $\phi_g = 0.5$, showing the limitation of the interpolation ability that is achieved in the main paper only when enough cases are included during training.

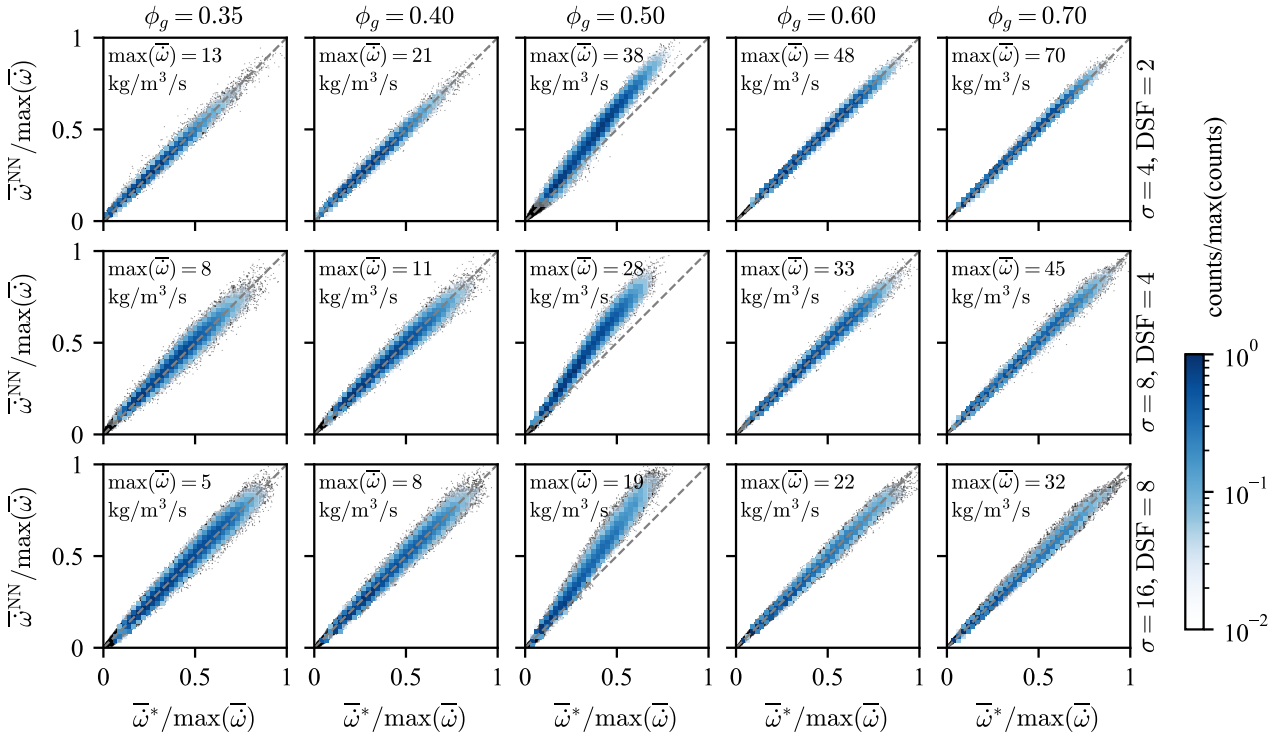

Figure S6: Scatter plots with 2D histograms: CNN-modeled burning rate $\overline{\dot{\omega}}^{\mathrm{NN}}$ versus ground-truth filtered burning rate $\overline{\dot{\omega}}^{*}$. Individual values are normalized by the maximum burning rate in the datasets. The points used for the histograms have 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. Result of training without taking into account the case $\phi_g = 0.5$. One can see a clear bias when inference is performed on test solutions for the $\phi_g = 0.5$ case (central column).

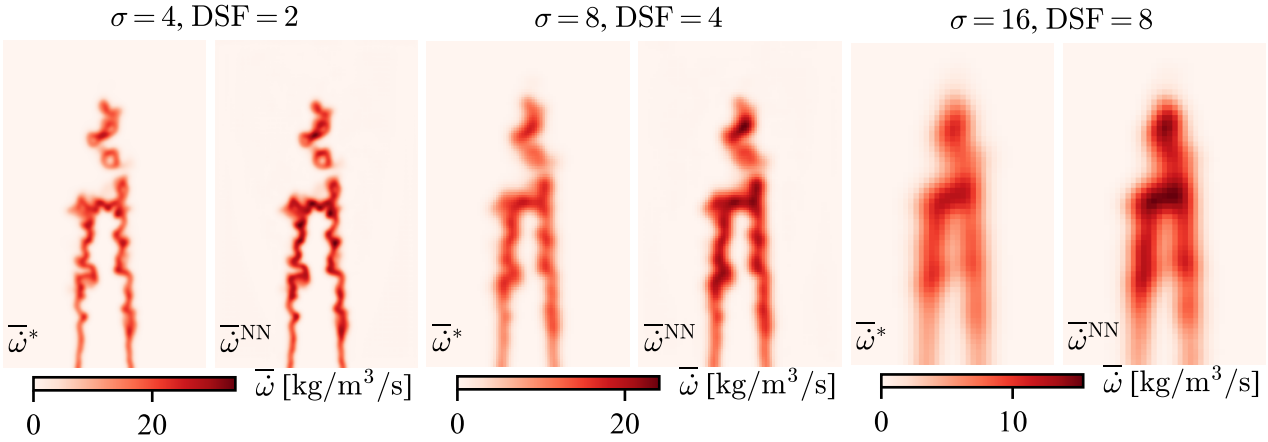

Figure S7: Planar cut normal to the z-axis, in the middle of the domain, colored by the ground-truth filtered burning rate $\overline{\dot{\omega}}^{*}$ and the CNN-modeled burning rate $\overline{\dot{\omega}}^{\mathrm{NN}}$ for three sets of LES parameters. The global equivalence ratio is $\phi_g = 0.5$. Result of training without taking into account the case $\phi_g = 0.5$. The flame morphology is well retrieved but the burning rates are overestimated.

3 Generalization, training without $\sigma = 8$, DSF $= 4$

The results of the CNN model trained without the case $\sigma = 8$, DSF $= 4$ are detailed in Figs S8 and S9. The model exhibits a significant bias at $\sigma = 8$, DSF $= 4$, showing the limitation of the interpolation ability that is achieved in the main paper only when enough cases are included during training.

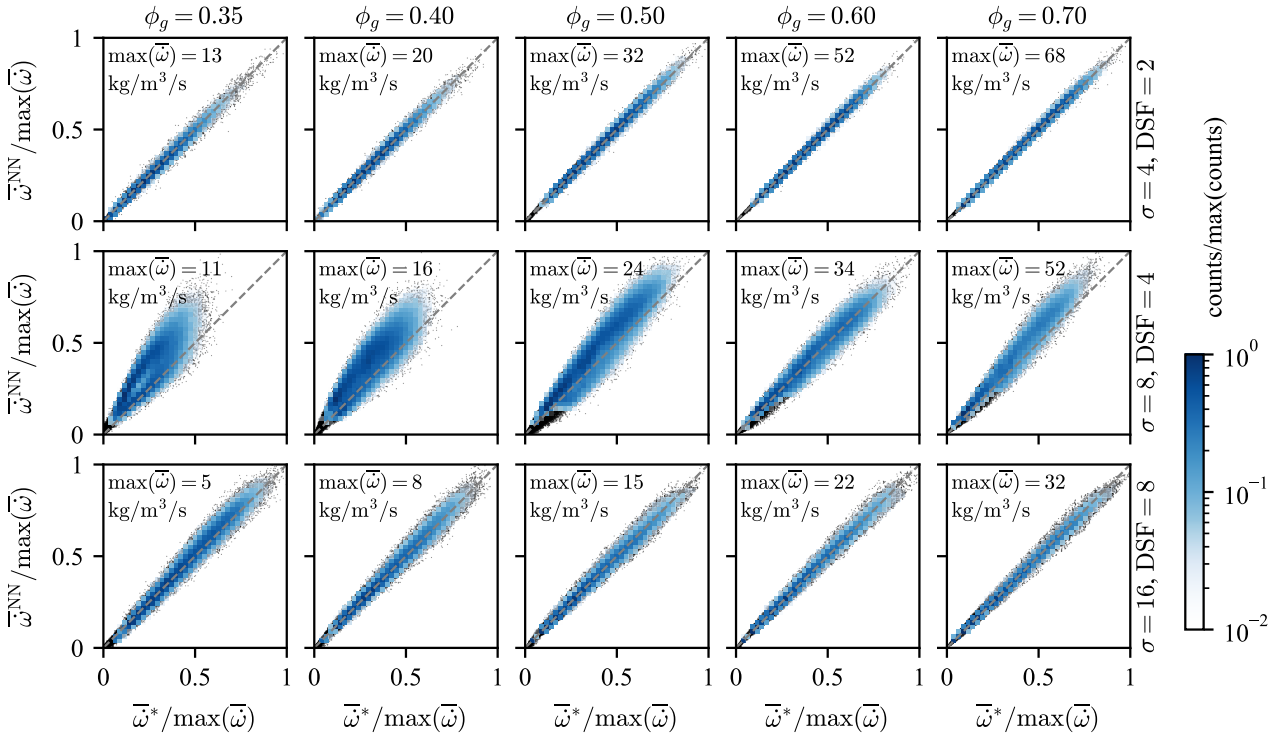

Figure S8: Scatter plots with 2D histograms: CNN-modeled burning rate $\overline{\dot{\omega}}^{NN}$ versus ground-truth filtered burning rate $\overline{\dot{\omega}}^{*}$. Individual values are normalized by the maximum burning rate in the datasets. The points used for the histograms have a progress 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. Result of training without taking into account the set of LES parameters $\sigma = 8$, DSF $= 4$. One can see a clear bias when inference is performed on test solutions for the set of LES parameters $\sigma = 8$, DSF $= 4$ (central row).

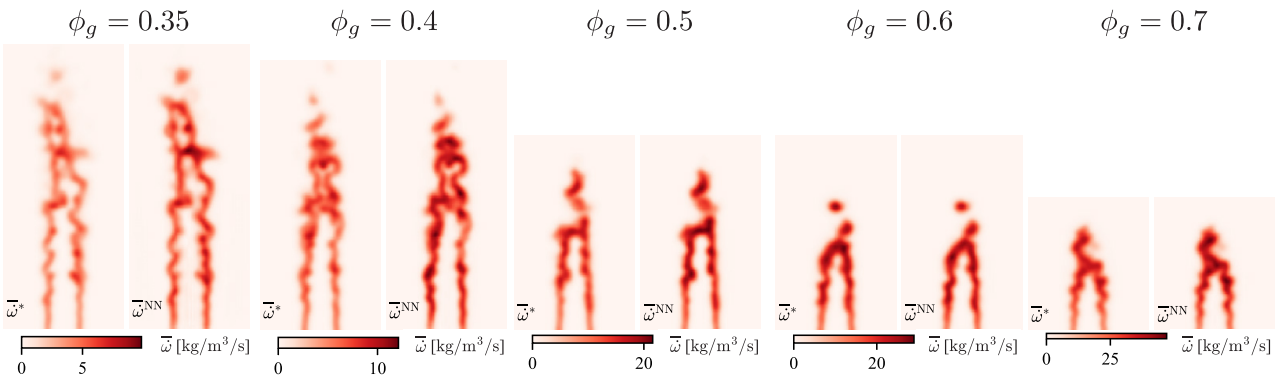

Figure S9: Planar cut normal to the z-axis, in the middle of the domain, colored by the ground-truth filtered burning rate $\overline{\dot{\omega}}^{*}$ and the CNN-modeled burning rate $\overline{\dot{\omega}}^{NN}$ for three global equivalence ratios. The set of LES parameters is $\sigma = 8$, DSF $= 4$. Result of training without taking into account the set of LES parameters $\sigma = 8$, DSF $= 4$. The flame morphology is well retrieved but the burning rate magnitudes are biased.