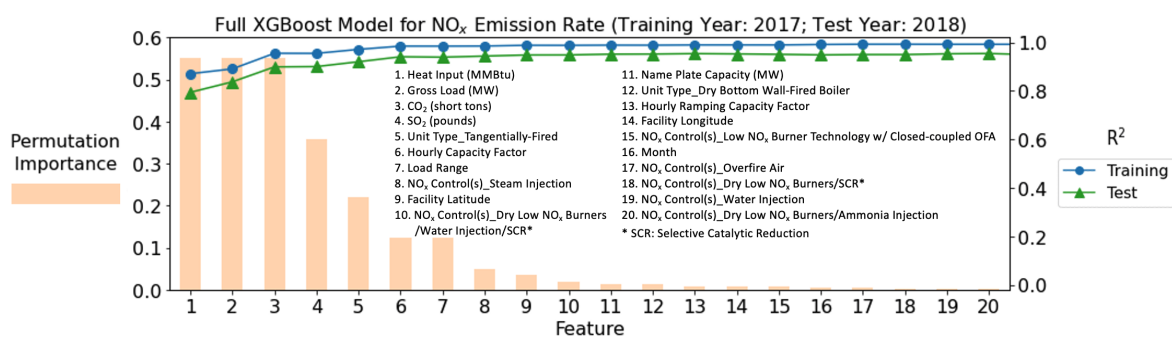
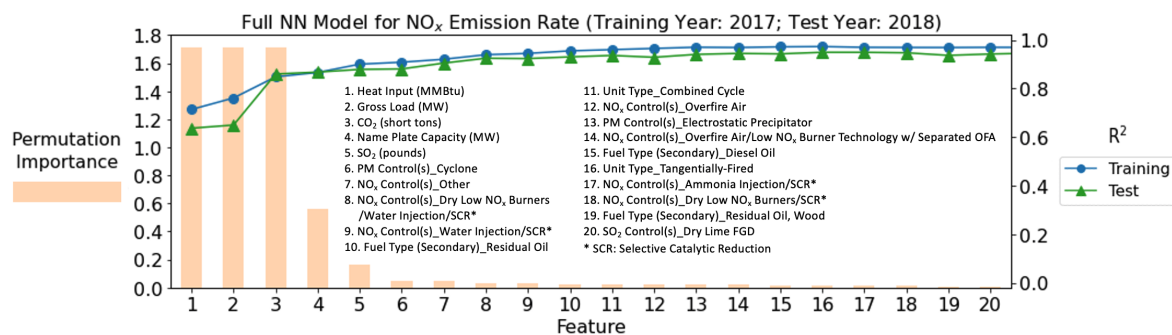


## Supplementary Information

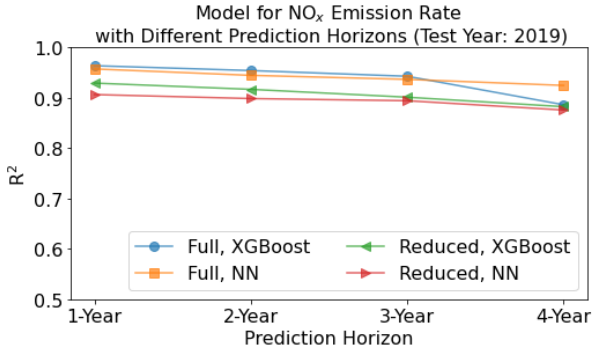


(a)

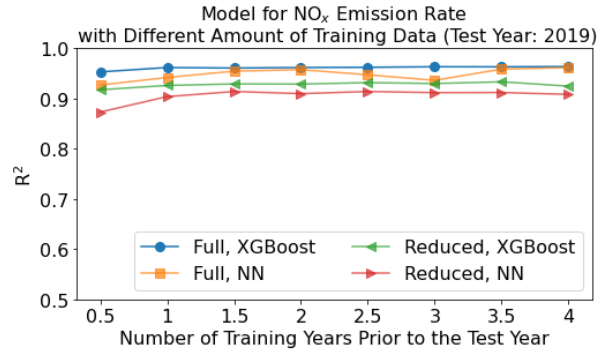


(b)

Figure S1: The permutation importance of the features ranked from the most important to the least (bars, left axis), together with the corresponding training R<sup>2</sup> (blue dots) and test R<sup>2</sup> (green triangles) by adding features to the model one at a time (lines with markers, right axis), of the (a) full XGBoost model; (b) full NN model for NO<sub>x</sub> emission rate (trained on 2017 data, tested on 2018 data).



(a)



(b)

Figure S2: The model performance on 2019 data in terms of  $R^2$  with respect to (a) different prediction horizons increasing from 1 (trained with the data from 2015 to 2018) to 4 years (trained with the data from 2015); (b) different amount of training data, starting with half-year data of 2018, and ending with 4-year data from year 2015 to year 2018.