

**Figure S1.** The quantile-quantile (Q-Q) plot for the transformed (a) NO<sub>2</sub>, (b) SO<sub>2</sub>, (c) CO, (d) HCHO, (e) precipitation and (f) wind speed. The red line is 1:1 line between theoretical quantiles and ordered values.



**Figure S2.** Boxplots for monthly averaged  $PM_{2.5}$ . The brown color in the box indicates the dry season in Thailand, and the blue does for the wet season.



**Figure S3.** Model comparison across various thresholds of high  $PM_{2.5}$  concentrations: (a)  $R^2$ , (b) RMSE, (c) MAPE and (d) the slope coefficient. (e) visualizes number of samples above each of the threshold.



**Figure S4.** Spatial distributions of validating results: (a) R<sup>2</sup>, (b) RMSE, (c) MAPE and (d) the slope coefficient of regression between observation and estimated concentrations. The bounding box zooms up area nearby the capital Bangkok (100.2-101.4°E, 12.5-14.0°N).



**Figure S5.** Timeseries for the north region of Thailand during January to April 2021: FRP (red),  $PM_{2.5}$  concentrations (observed: grey, estimated: blue), CO (brown), AAI (dark yellow), HCHO (green), NO<sub>2</sub> (blue), SO<sub>2</sub> (purple) and O<sub>3</sub> (light blue). The correlation coefficient with FRP is shown in the topleft of each panel. Red columns are marked for the period when sudden increase of fire radiative power (FRP) is detected for all the sub-regions from February 25<sup>th</sup> to March 2<sup>nd</sup> 2021 (Figure S5-9).



**Figure S6.** Timeseries for the northeast region of Thailand during January to April 2021: FRP (red),  $PM_{2.5}$  concentrations (observed: grey, estimated: blue), CO (brown), AAI (dark yellow), HCHO (green), NO<sub>2</sub> (blue), SO<sub>2</sub> (purple) and O<sub>3</sub> (light blue). The correlation coefficient with FRP is shown in the topleft of each panel. Red columns are marked for the period when sudden increase of fire radiative power (FRP) is detected for all the sub-regions from February 25<sup>th</sup> to March 2<sup>nd</sup> 2021 (Figure S5-9).



**Figure S7.** Timeseries for the central region of Thailand during January to April 2021: FRP (red),  $PM_{2.5}$  concentrations (observed: grey, estimated: blue), CO (brown), AAI (dark yellow), HCHO (green), NO<sub>2</sub> (blue), SO<sub>2</sub> (purple) and O<sub>3</sub> (light blue). The correlation coefficient with FRP is shown in the topleft of each panel. Red columns are marked for the period when sudden increase of fire radiative power (FRP) is detected for all the sub-regions from February 25<sup>th</sup> to March 2<sup>nd</sup> 2021 (Figure S5-9).



**Figure S8.** Timeseries for the east region of Thailand during January to April 2021: FRP (red),  $PM_{2.5}$  concentrations (observed: grey, estimated: blue), CO (brown), AAI (dark yellow), HCHO (green), NO<sub>2</sub> (blue), SO<sub>2</sub> (purple) and O<sub>3</sub> (light blue). The correlation coefficient with FRP is shown in the topleft of each panel. Red columns are marked for the period when sudden increase of fire radiative power (FRP) is detected for all the sub-regions from February 25<sup>th</sup> to March 2<sup>nd</sup> 2021 (Figure S5-9).



**Figure S9.** Timeseries for the south region of Thailand during January to April 2021: FRP (red),  $PM_{2.5}$  concentrations (observed: grey, estimated: blue), CO (brown), AAI (dark yellow), HCHO (green), NO<sub>2</sub> (blue), SO<sub>2</sub> (purple) and O<sub>3</sub> (light blue). The correlation coefficient with FRP is shown in the topleft of each panel. Red columns are marked for the period when sudden increase of fire radiative power (FRP) is detected for all the sub-regions from February 25<sup>th</sup> to March 2<sup>nd</sup> 2021 (Figure S5-9).



**Figure S10.** Density scatterplots of  $PM_{2.5}$  estimation ( $\mu g/m^3$ ) including aerosol optical depth (AOD) for (a) all regions in Thailand and the five divided regions in Figure 1: (b) north, (c) northeast, (d) central, (e) east and (f) south. The black solid diagonal line is the best-fit line from linear regression. The red line is estimated regression line shown in the topleft of each panel.



**Figure S11.** Density scatterplots of  $PM_{2.5}$  estimation ( $\mu g/m^3$ ) including aerosol index for (a) all regions in Thailand and the five divided regions in Figure 1: (b) north, (c) northeast, (d) central, (e) east and (f) south. The black solid diagonal line is the best-fit line from linear regression. The red line is estimated regression line shown in the topleft of each panel.



Figure S12. Monthly missing days count per grid.

month embedding dimension	4, 6, 9, 12				
land cover embedding dimension	ension 3, <b>17</b> , 32				
N <sub>d</sub> , N <sub>a</sub>	8, 16, <b>24</b> , 32				
Nsteps	3, 4, 5, 6				
γ	1.3				
$\lambda_{\mathrm{sparse}}$	0.001				
mask type	entmax, sparsemax				
learning rate	0.005, <b>0.01</b> , 0.02				
batch size	32, <b>64</b> , 128, 256				

**Table S1.** TabNet parameters optimized by grid search method. The bold numbers indicate selected parameters in each of search space.

	Random Forest		
number of estimator	1000, <b>2000</b> , 5000		
maximum depth	3, 7, <b>9</b> , 11, 15		
minimum number of samples to split	0.01, 0.1, <b>2</b> , 5, 10		
minimum number of samples for a leaf node	0.01, 0.1, 1, 2, 5		
	CatBoost		
maximum depth	3, 7, <b>11</b> , 13		
L2 regularization term	<b>0</b> , 0.01, 0.1		
maximum size of one-hot encoding	4, 8, <b>16</b>		
learning rate	0.002, 0.005, <b>0.01</b> , 0.02		
	XGBoost		
maximum depth	3, 7, <b>11</b> , 13		
minimum sum of instance weight for a child	1, 2, 5		
subsample ratio of training instances	0.5, <b>0.7</b> , 1.0		
subsample ratio of columns for a tree	0.5, <b>0.7</b> , 1.0		
minimum loss reduction for a leaf partition	<b>0</b> , 0.01, 0.1		
L1 regularization term	0, <b>0.01</b> , 0.1		
learning rate	0.001, 0.005, <b>0.01</b>		
	LightGBM		
maximum depth	3, 7, 11, 13		
minimum sum hessian in a leaf	0.0001, <b>0.001</b> , 0.01		
bagging fraction	0.5, 0.7, <b>1.0</b>		
feature fraction	<b>0.5</b> , 0.7, 1.0		
L1 regularization term	0.0, 0.01, <b>0.1</b> , 0.2		
L2 regularization term	0.0, 0.01, <b>0.1</b> , 0.2		
learning rate	0.001, 0.005, <b>0.01</b>		

**Table S2.** ML model parameters optimized by grid search method. The bold numbers indicate selected parameters in each of search space.

		regional					
		north	northeast	central	east	south	
CO	0.52	0.69	0.55	0.39	0.48	0.12	
$NO_2$	0.09	0.19	0.28	0.13	0.06	0.05	
НСНО	0.16	0.23	0.13	0.08	0.10	0.03	
$SO_2$	0.0	0.0	0.0	0.01	0.04	0.0	
O <sub>3</sub>	0.14	0.05	0.11	0.31	0.35	0.01	

Table S3.  $R^2$  score between transformed  $PM_{2.5}$  and chemical predictors.