Supplement of

Development of a deep neural network for predicting 6 h average PM$_{2.5}$ concentrations up to 2 subsequent days using various training data

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### Table S1. Statistical performance results according to the number of layers.

| Model       | Day | MSE  \((\mu\text{gm}^{-3})^2\) | RMSE \((\mu\text{gm}^{-3})\) | R  | IOA |
|-------------|-----|--------------------------------|----------------------------|----|-----|
| 2-layer     | D+0 | 59.3                           | 7.7                        | 0.91 | 0.94 |
|             | D+1 | 92.1                           | 9.6                        | 0.86 | 0.89 |
|             | D+2 | 156.3                          | 12.5                       | 0.75 | 0.80 |
| 4-layer     | D+0 | 54.7                           | 7.4                        | 0.91 | 0.95 |
|             | D+1 | 88.3                           | 9.4                        | 0.86 | 0.90 |
|             | D+2 | 134.5                          | 11.6                       | 0.77 | 0.84 |
| 5-layer     | D+0 | 53.3                           | 7.3                        | 0.91 | 0.95 |
| (DNN-ALL)   |     |                                 |                            |     |     |
|             | D+1 | 81.0                           | 9.0                        | 0.85 | 0.90 |
|             | D+2 | 112.4                          | 10.6                       | 0.79 | 0.86 |
| 6-layer     | D+0 | 174.2                          | 13.2                       | 0.81 | 0.66 |
|             | D+1 | 292.4                          | 17.1                       | 0    | 0.17 |
|             | D+2 | 292.4                          | 17.1                       | 0    | 0.17 |
| 8-layer     | D+0 | 302.7                          | 17.4                       | 0    | 0.15 |
|             | D+1 | 292.4                          | 17.1                       | 0    | 0.17 |
|             | D+2 | 292.4                          | 17.1                       | 0    | 0.17 |

### Table S2. AQI performance results according to the number of layers.

| Model       | Day | ACC (%) | POD (%) | FAR (%) | F1-score (%) |
|-------------|-----|---------|---------|---------|--------------|
| 2-layer     | D+0 | 70.0    | 63/90   | 81.8    | 18/22        | 28.0         | 7/25        | 77         |
|             | D+1 | 55.6    | 50/90   | 81.0    | 17/21        | 39.3         | 11/28       | 69         |
|             | D+2 | 51.1    | 46/90   | 81.0    | 17/21        | 50.0         | 17/34       | 61         |
| 4-layer     | D+0 | 71.1    | 64/90   | 81.8    | 18/22        | 28.0         | 7/25        | 76         |
|             | D+1 | 60.0    | 54/90   | 85.7    | 18/21        | 35.7         | 10/28       | 73         |
|             | D+2 | 60.0    | 54/90   | 81.0    | 17/21        | 45.2         | 14/31       | 65         |
| 5-layer     | D+0 | 77.8    | 70/90   | 72.7    | 16/22        | 11.1         | 2/18        | 80         |
| (DNN-ALL)   |     |         |         |         |              |              |             |            |
|             | D+1 | 64.4    | 58/90   | 71.4    | 15/21        | 31.8         | 7/22        | 70         |
|             | D+2 | 61.1    | 55/90   | 76.2    | 16/21        | 40.7         | 11/27       | 67         |
| 6-layer     | D+0 | 55.6    | 50/90   | 50      | 11/22        | 8.3          | 1/12        | 64         |
|             | D+1 | 47.8    | 43/90   | 0       | 0/21         | 0            | 0           | 0          |
|             | D+2 | 47.8    | 43/90   | 0       | 0/21         | 0            | 0           | 0          |
| 8-layer     | D+0 | 45.6    | 41/90   | 0       | 0/22         | 0            | 0           | 0          |
|             | D+1 | 47.8    | 43/90   | 0       | 0/21         | 0            | 0           | 0          |
|             | D+2 | 47.8    | 43/90   | 0       | 0/21         | 0            | 0           | 0          |
Recall about "good" category = \( \frac{a_1}{a_1 + b_1 + c_1 + d_1} \), \hspace{1cm} (S1)

Recall about "moderate" category = \( \frac{b_2}{a_2 + b_2 + c_2 + d_2} \), \hspace{1cm} (S2)

Recall about "bad" category = \( \frac{c_3}{a_3 + b_3 + c_3 + d_3} \), \hspace{1cm} (S3)

Recall about "very bad" category = \( \frac{d_4}{a_4 + b_4 + c_4 + d_4} \), \hspace{1cm} (S4)

Precision about "good" category = \( \frac{a_1}{a_1 + a_2 + a_3 + a} \), \hspace{1cm} (S5)

Precision about "moderate" category = \( \frac{b_2}{b_1 + b_2 + b_3 + b_4} \), \hspace{1cm} (S6)

Precision about "bad" category = \( \frac{c_3}{c_1 + c_2 + c_3 + c_4} \), \hspace{1cm} (S7)

Precision about "very bad" category = \( \frac{d_4}{d_1 + d_2 + d_3 + d_4} \), \hspace{1cm} (S8)
Table S3. Statistical evaluation results of CMAQ, DNN-OBS, DNN-OPM, and DNN-ALL models in the training set (2016 to 2018).

| Model     | Day | MSE ((μgm⁻³)²) | RMSE (μgm⁻³) | R   | IOA |
|-----------|-----|----------------|--------------|-----|-----|
| CMAQ      | D+0 | 136.9          | 11.7         | 0.76| 0.86|
|           | D+1 | 146.4          | 12.1         | 0.74| 0.84|
|           | D+2 | 185.0          | 13.6         | 0.67| 0.80|
| DNN-OBS   | D+0 | 79.2           | 8.9          | 0.78| 0.87|
|           | D+1 | 139.2          | 11.8         | 0.54| 0.65|
|           | D+2 | 158.8          | 12.6         | 0.43| 0.54|
| DNN-OPM   | D+0 | 53.3           | 7.3          | 0.86| 0.92|
|           | D+1 | 88.4           | 9.4          | 0.75| 0.83|
|           | D+2 | 108.2          | 10.4         | 0.68| 0.77|
| DNN-ALL   | D+0 | 39.7           | 6.3          | 0.90| 0.94|
|           | D+1 | 57.8           | 7.6          | 0.84| 0.90|
|           | D+2 | 72.3           | 8.5          | 0.80| 0.87|

Table S4. Statistical evaluation results of CMAQ, DNN-OBS, DNN-OPM, and DNN-ALL models in the validation set (2019).

| Model     | Day | MSE ((μgm⁻³)²) | RMSE (μgm⁻³) | R   | IOA |
|-----------|-----|----------------|--------------|-----|-----|
| CMAQ      | D+0 | 123.2          | 11.1         | 0.82| 0.90|
|           | D+1 | 132.3          | 11.5         | 0.80| 0.89|
|           | D+2 | 156.3          | 12.5         | 0.75| 0.86|
| DNN-OBS   | D+0 | 92.2           | 9.6          | 0.84| 0.88|
|           | D+1 | 182.3          | 13.5         | 0.63| 0.65|
|           | D+2 | 216.1          | 14.7         | 0.52| 0.52|
| DNN-OPM   | D+0 | 65.6           | 8.1          | 0.89| 0.92|
|           | D+1 | 123.2          | 11.1         | 0.78| 0.81|
|           | D+2 | 166.4          | 12.9         | 0.66| 0.72|
| DNN-ALL   | D+0 | 42.3           | 6.5          | 0.93| 0.95|
|           | D+1 | 77.4           | 8.8          | 0.88| 0.90|
|           | D+2 | 108.2          | 10.4         | 0.81| 0.84|
Table S5. Statistical performance of the DNN-ALL and Random Forest models.

| Model     | Day | MSE \((\mu gm^3)^2\) | RMSE \((\mu gm^3)\) | R   | IOA |
|-----------|-----|-----------------------|---------------------|-----|-----|
| DNN-ALL   | D+0 | 53.3                  | 7.3                 | 0.91| 0.95|
|           | D+1 | 81.0                  | 9.0                 | 0.85| 0.90|
|           | D+2 | 112.4                 | 10.6                | 0.79| 0.86|
| Random Forest | D+0 | 62.4                  | 7.9                 | 0.90| 0.93|
|           | D+1 | 106.1                 | 10.3                | 0.83| 0.85|
|           | D+2 | 156.3                 | 12.5                | 0.73| 0.76|
Table S6. Precision and recall of DNN-ALL and CMAQ models by four categories: "good" (PM2.5 ≤ 15 μgm-3), "moderate" (16 μgm-3 ≤ PM2.5 ≤ 35 μgm-3), "bad" (36 μgm-3 ≤ PM2.5 ≤ 75 μgm-3), and "very bad" (76 μgm-3 ≤ PM2.5).

| Model   | Day | Precision |          |          |          |          |          |          |          |          |
|---------|-----|-----------|----------|----------|----------|----------|----------|----------|----------|----------|
|         |     | Good      | Moderate | Bad      | Very bad | Total    | Good      | Moderate  | Bad      | Very bad | Total    |
| DNN-ALL | D+0 | 0.83      | 0.71     | 0.88     | 1.0      | 0.86     | 0.70      | 0.85      | 0.71     | 1.0      | 0.82     |
|         | D+1 | 0.83      | 0.61     | 0.64     | 0.0      | 0.52     | 0.38      | 0.79      | 0.70     | 0.0      | 0.47     |
|         | D+2 | 0.79      | 0.59     | 0.56     | 0.0      | 0.49     | 0.42      | 0.67      | 0.75     | 0.0      | 0.46     |
| CMAQ    | D+0 | 0.74      | 0.67     | 0.64     | 0.0      | 0.51     | 0.64      | 0.68      | 0.67     | 0.0      | 0.50     |
|         | D+1 | 0.85      | 0.69     | 0.54     | 0.0      | 0.52     | 0.65      | 0.67      | 0.70     | 0.0      | 0.51     |
|         | D+2 | 0.82      | 0.69     | 0.42     | 0.0      | 0.48     | 0.69      | 0.63      | 0.55     | 0.0      | 0.47    |
Table S7. AQI performance of the DNN-ALL and Random Forest model.

| Model     | Day | ACC (%) | POD (%) | FAR (%) | F1-score (%) |
|-----------|-----|---------|---------|---------|--------------|
| DNN-ALL   | D+0 | 77.8    | 70/90   | 72.7    | 11.1 2/18    | 80            |
|           | D+1 | 64.4    | 58/90   | 71.4    | 31.8 7/22    | 70            |
|           | D+2 | 61.1    | 55/90   | 76.2    | 40.7 11/27   | 67            |
| Random    | D+0 | 75.6    | 68/90   | 77.3    | 19.0 4/21    | 79            |
| Forest    | D+1 | 61.1    | 55/90   | 76.2    | 33.3 8/24    | 71            |
|           | D+2 | 48.9    | 44/90   | 71.4    | 50.0 15/30   | 58            |