Supplement S1. Formulas for statistical evaluation indexes

1. Mean Bias

$$\mathrm{MB} = \frac{1}{\mathrm{N}} \sum_{1}^{N} (\mathrm{Sim} - \mathrm{Obs})$$

2. Mean Average Gross Error

$$\mathrm{MAGE} = \frac{1}{N} \sum_{1}^{\mathrm{N}} |Sim - Obs|$$

3. Root Mean Square Error

$$\mathrm{RMSE} = \sqrt{\frac{1}{N} \sum_{1}^{N} (Sim - Obs)^2}$$

4. Index of agreement, IOA

$$\mathrm{IOA} = 1 - \frac{\sum_{i=1}^{N} (Sim - Obs)^2}{\sum_{i=1}^{N} (|Sim - \overline{Obs}| + |Obs - \overline{Obs}|)^2}$$

5. Wind Normalized Mean Bias

$$\mathrm{WNMB} = \frac{\sum_{i=1}^{N} (Sim - Obs)}{N \times 360^{\circ}} \times 100\%$$

3. Wind Normalized Mean Error

$$\mathrm{WNME} = \frac{\sum_{i=1}^{N} |Sim - Obs|}{N \times 360^{\circ}} \times 100\%$$

6. Mean Fractional Bias

$$\mathrm{MFB} = \frac{2}{N} \sum_{1}^{\mathrm{N}} \left(\frac{Sim - Obs}{Sim + Obs} \right)$$

7. Mean Fractional Error

$$\mathrm{MFE} = \frac{2}{N} \sum_{1}^{\mathrm{N}} \left| \frac{Sim - Obs}{Sim + Obs} \right|$$

8.Correlation coefficient (R)

$$\mathrm{R} = \frac{1}{N} \sum_{i=1}^{N} \left[\frac{(Sim - \overline{Sim})(Obs - \overline{Obs})}{S_p S_o} \right]$$

$$S_P = \left[\frac{1}{N} \sum_{i=1}^{N} (Sim - \overline{Sim})^2 \right]^{\frac{1}{2}}$$

$$S_o = \left[\frac{1}{N} \sum_{i=1}^{N} (Obs - \overline{Obs})^2 \right]^{\frac{1}{2}}$$

Supplement S2 Supplementary figures

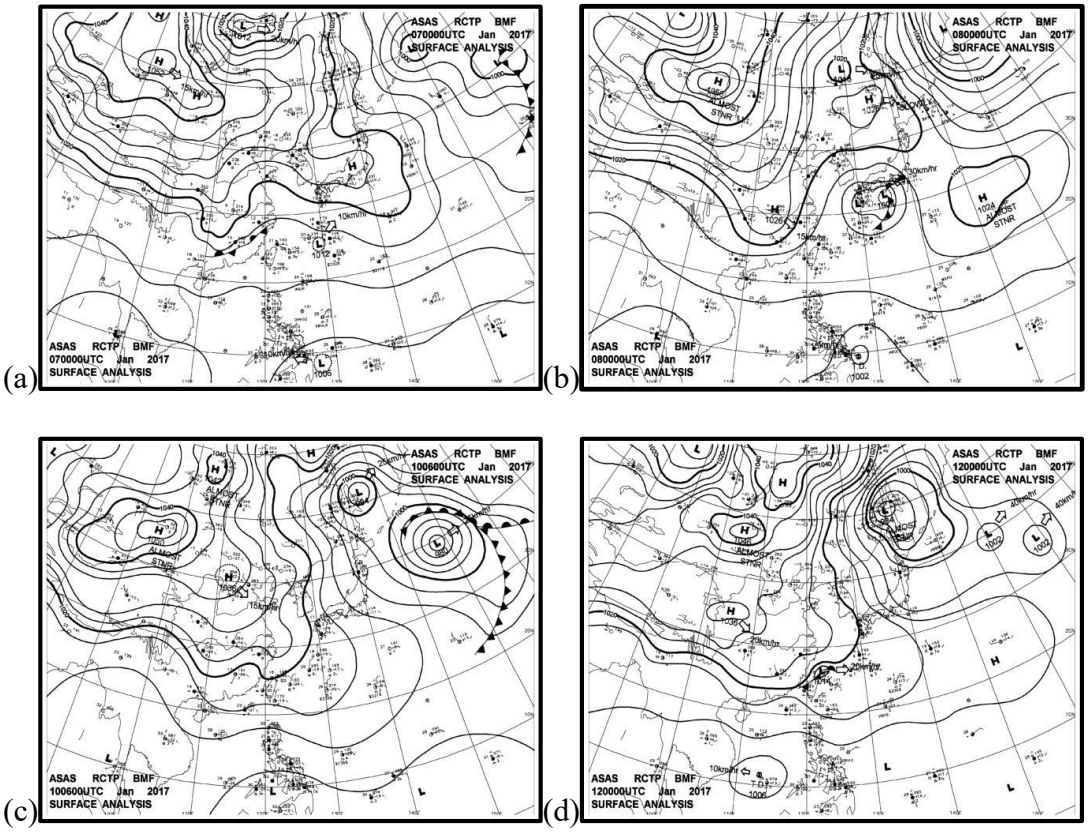

Fig. S2.1 The surface weather map on 08:00 LST Jan 7th (a), 08:00 LST Jan 8th (b),14:00 LST Jan 10th (c), and 08:00 LST Jan 12th (d) 2017

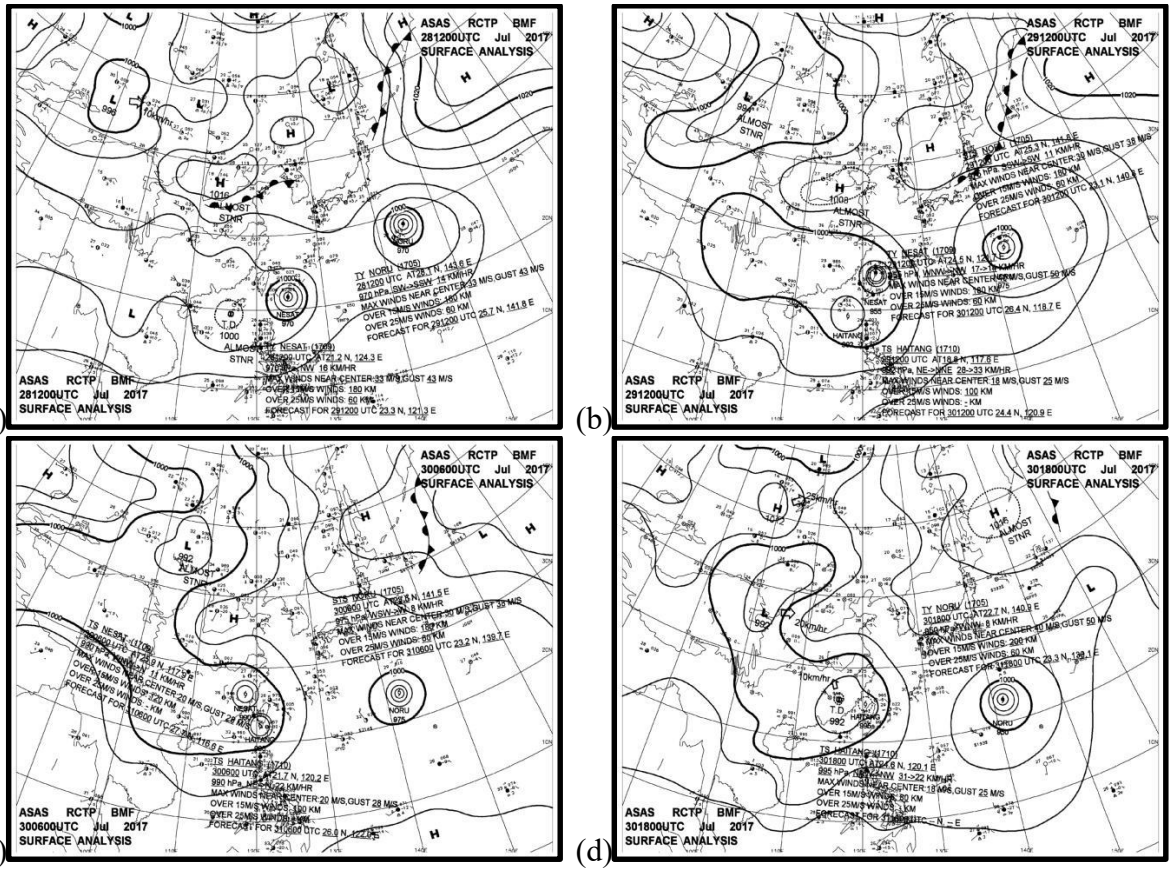

Fig. S2.2 The surface weather map on 20:00 LST July 28th (a), 20:00 LST July 29th (b), 14:00 LST July 30th (c), and 02:00 LST July 31st (d) 2017

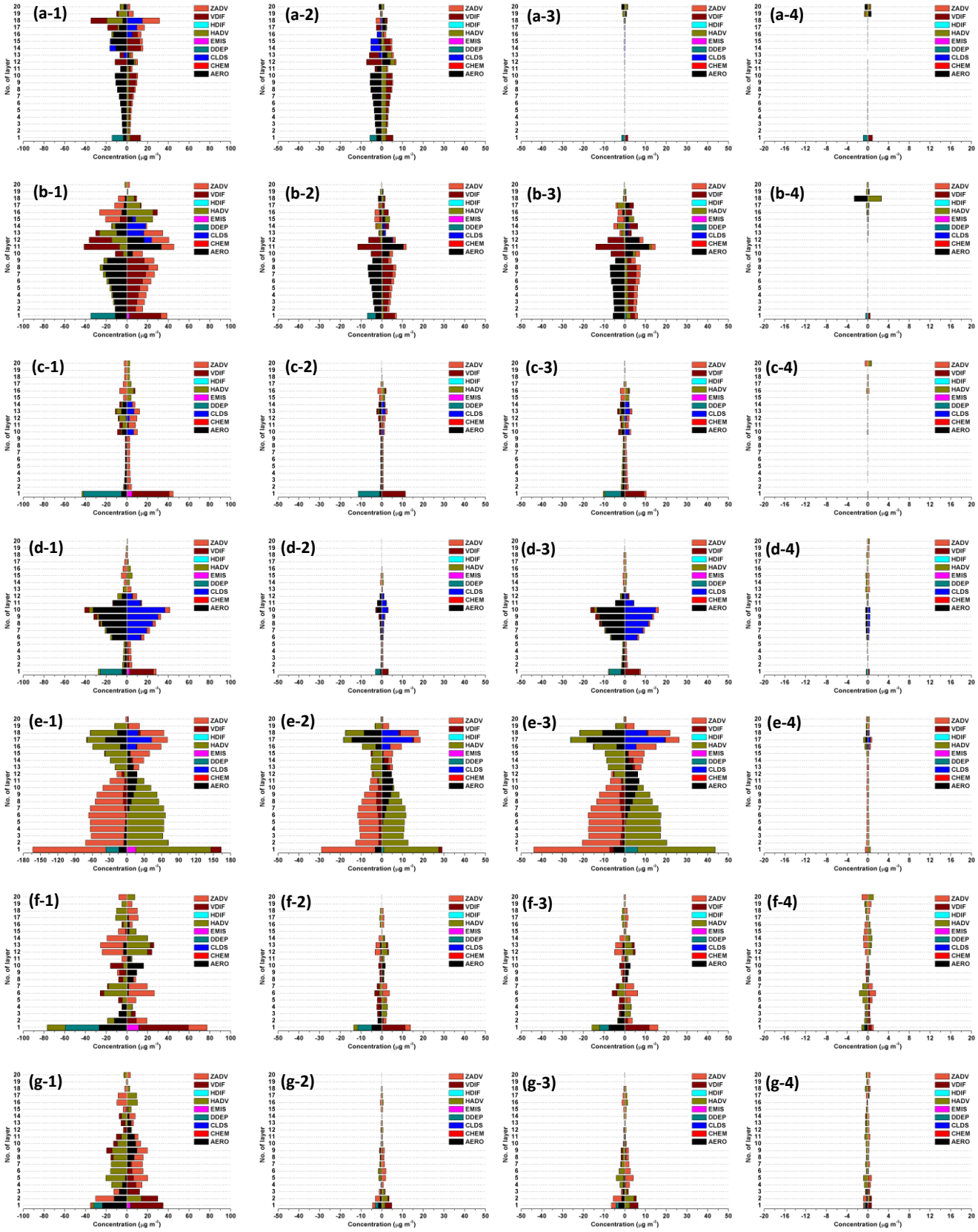

Fig. S2.3 The hourly average contribution of physical process at each layer on Jan 9th 2017, a,b,c,d,e,f, and g represent #17, #18, #19, #20, BQ, ZM, and CY, respectively；1, 2, 3, and 4 represent influence of total emissions, BRIB, YRDIB, and PRDIB, respectively.

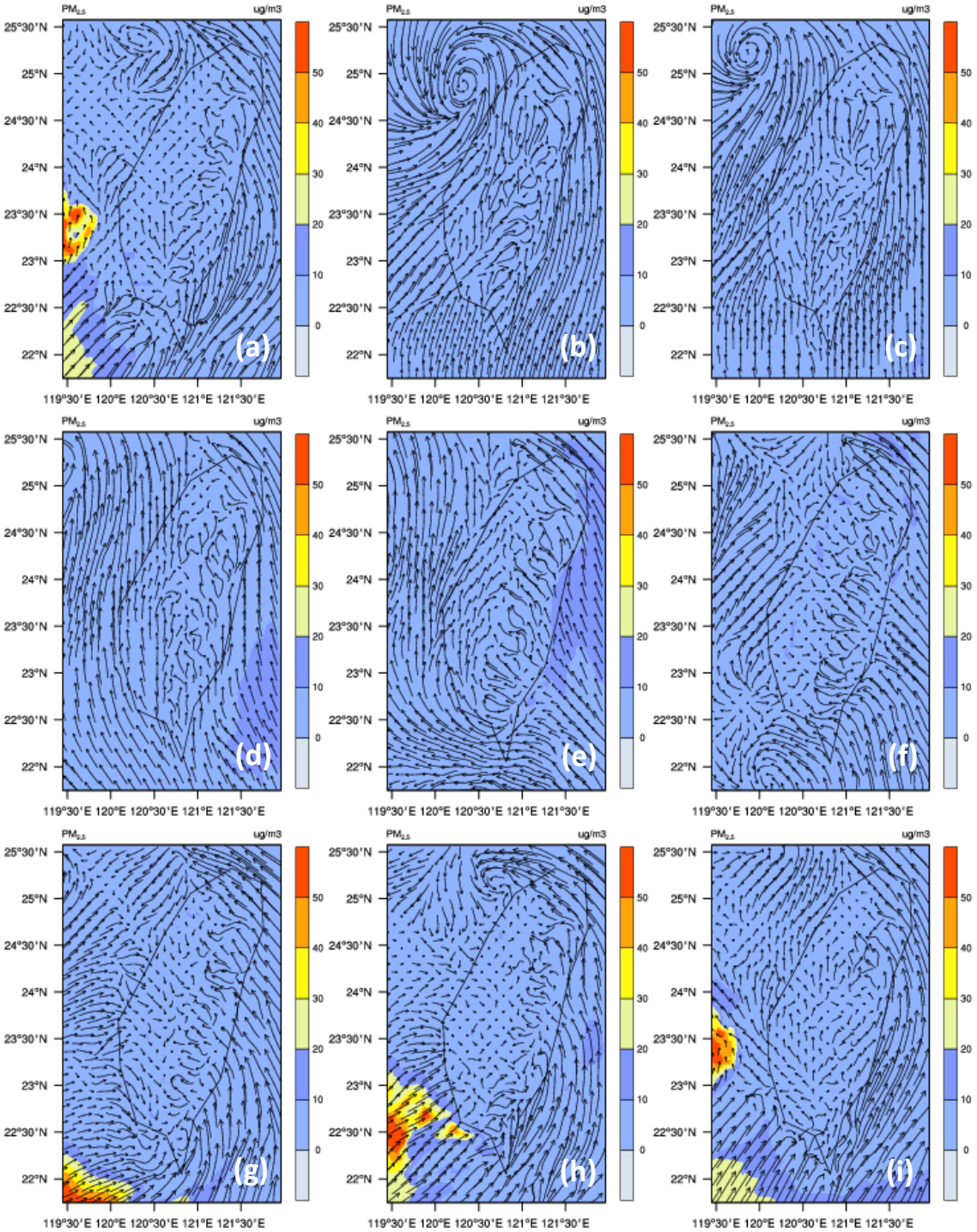

Fig. S2.4 The every 3 hour simulated wind vector and $PM_{2.5}$ distribution on the event at 00:00 LST (a) 03:00 LST (b) 06:00 LST (c) 09:00 LST (d) 12:00 LST (e) 15:00 LST (f) 18:00 LST (g) 21:00 (h) July 30 2017.

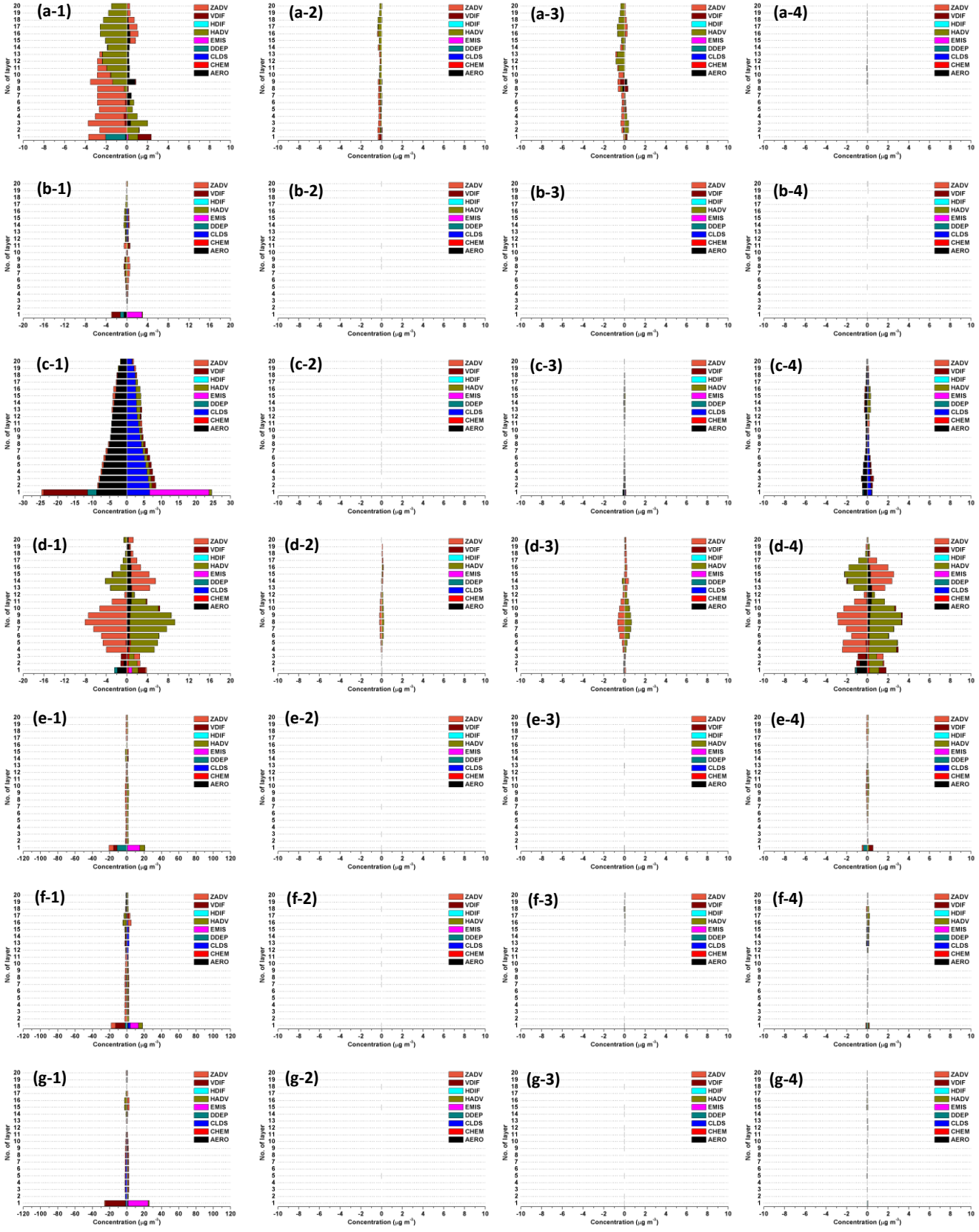

Fig. S2.5 The hourly average contribution of physical process at each layer on July 30th 2017, a,b,c,d,e,f, and g represent #17, #18, #19, #20, BQ, ZM, and CY, respectively；1, 2, 3, and 4 represent influence of total emissions, BRIB, YRDIB, and PRDIB, respectively.