## Factor analysis of the influence of environmental conditions on

## VOCs emissions from medium density fibreboard and the

## correlation of the factors with fitting parameters

Huiqi Shao,<sup>a</sup> Yifan Ren,<sup>a</sup> Yan Zhang,<sup>b</sup> Chuandong Wu,<sup>a</sup> Wenhui Li<sup>a</sup> and Jiemin Liu,<sup>\*a</sup>

<sup>a</sup> School of Chemistry and Biological Engineering, University of Science and Technology Beijing, Beijing 100083, China.

<sup>b</sup> School of Science, Beijing University of Civil Engineering and Architecture, Beijing

100044, China

\* Corresponding author, Jiemin Liu, email: liujm@ustb.edu.cn

| Table S1 Determinatior | n conditions | of TD-GCMS |
|------------------------|--------------|------------|
|------------------------|--------------|------------|

| Instruments | Parameters                | Values                                             |
|-------------|---------------------------|----------------------------------------------------|
| TD          | Tube desorption           | 280 °C                                             |
|             | temperature               |                                                    |
|             | Tube desorption time      | 10 min                                             |
|             | Cold trap temperature     | Low: 20 °C; high: 280 °C                           |
|             | Cold trap desorption time | 3 min                                              |
|             | Cold trap sorbent         | Tenax TA                                           |
|             | Transfer line temperature | 200 °C                                             |
|             | Split ratio               | 30:1                                               |
| GC          | Injector temperature      | 280 °C                                             |
|             | Column                    | DB-5MS, 60 m × 0.25 mm × 0.25 μm                   |
|             | Carrier gas               | He, constant flow, 1.2 mL·min <sup>-1</sup>        |
|             | Temperature program       | The initial temperature was held at 50 °C          |
|             |                           | for 2 min, then heated at the rate of 5            |
|             |                           | °C·min <sup>-1</sup> to 225 °C and held for 2 min. |
| MS          | lon source                | EI, 70 eV                                          |
|             | Ion source temperature    | 230 °C                                             |
|             | Quadrupole temperature    | 150 °C                                             |
|             | Mass range                | Scan mode, 40-350 m/z                              |
|             | Transfer line temperature | 280 °C                                             |

| Compounds        | Exponential fitting  |        | Linear fitting |        | Logarithmic fitting |        | Polynomial fitting        |        | Power fitting       |        |
|------------------|----------------------|--------|----------------|--------|---------------------|--------|---------------------------|--------|---------------------|--------|
|                  | Formula              | R²     | Formula        | R²     | Formula             | R²     | Formula                   | R²     | Formula             | R²     |
| n-Butyl acetate  | y=2.1361             | 0.9905 | y=2.2268x      | 0.9978 | y=0.8879ln(x)       | 0.9856 | y=-0.7564x <sup>2</sup> + | 1      | y=3.9228            | 0.9951 |
|                  | e <sup>0.7473x</sup> |        | +2.0189        |        | +3.8229             |        | 2.9101x+1.893             |        | x <sup>0.3005</sup> |        |
| Ethylbenzene     | y=0.1163             | 0.9796 | y=0.218x       | 0.9959 | y=0.0872ln(x)       | 0.9895 | y=-0.1006x <sup>2</sup> + | 0.9997 | y=0.2935            | 0.9994 |
|                  | e <sup>1.1341x</sup> |        | +0.1002        |        | +0.2771             |        | 0.3089x+0.0835            |        | x <sup>0.4596</sup> |        |
| PGMEA            | y=0.6876             | 0.9314 | y=1.0998x      | 0.9401 | y=0.4435ln(x)       | 0.9499 | y=-1.3048x <sup>2</sup> + | 0.9643 | y=1.5862            | 0.9529 |
|                  | e <sup>1.0233x</sup> |        | +0.6169        |        | +1.5126             |        | 2.2786x+0.3997            |        | x <sup>0.4152</sup> |        |
| p/m-Xylene       | y=0.4873             | 0.8700 | y=1.7428x      | 0.9447 | y=0.7168ln(x)       | 0.9927 | y=-2.7938x <sup>2</sup> + | 0.9891 | y=2.0569            | 0.9554 |
|                  | e <sup>1.7329x</sup> |        | +0.3389        |        | +1.7718             |        | 4.2667x-0.1261            |        | x <sup>0.7285</sup> |        |
| o-Xylene         | y=1.1052             | 0.9732 | y=1.154x       | 0.9879 | y=0.4643ln(x)       | 0.9935 | y=-0.7562x <sup>2</sup> + | 0.9957 | y=2.0421            | 0.9975 |
|                  | e <sup>0.7513x</sup> |        | +1.0467        |        | +1.9856             |        | 1.8372x+0.9208            |        | x <sup>0.3052</sup> |        |
| Isopropyl        | y=0.0755             | 0.9712 | y=0.2369x      | 0.9861 | y=0.0936ln(x)       | 0.9574 | y=0.0527x <sup>2</sup> +  | 0.9870 | y=0.2677            | 0.9845 |
| benzene          | e <sup>1.5537x</sup> |        | +0.0522        |        | +0.2433             |        | 0.1893x+0.0609            |        | x <sup>0.6276</sup> |        |
| 1, 2, 4-         | y=0.0858             | 0.9658 | y=0.1878x      | 0.9909 | y=0.0755ln(x)       | 0.9945 | y=-0.1234x <sup>2</sup> + | 0.9988 | y=0.2407            | 0.9991 |
| Trimethylbenzene | e <sup>1.2591x</sup> |        | +0.0712        |        | +0.2238             |        | 0.2992x+0.0506            |        | x <sup>0.5138</sup> |        |

Table S2 The fitting results of  $a_1$  with relative humidity

Table S3 The fitting results of  $a_1$  with the air change rate

| Compounds        | Exponential fitting  |        | Linear fitting |        | Logarithmic fitting |        | Polynomial fitting       |        | Power fitting              |        |
|------------------|----------------------|--------|----------------|--------|---------------------|--------|--------------------------|--------|----------------------------|--------|
|                  | Formula              | R²     | Formula        | R²     | Formula             | R²     | Formula                  | R²     | Formula                    | R²     |
| n-Butyl acetate  | y=0.5833             | 0.7069 | y=-0.1823x     | 0.5661 | y=-0.297ln(x)       | 0.7580 | y=0.1728x <sup>2</sup> - | 0.7987 | y=0.2824                   | 0.8508 |
|                  | e <sup>-0.604x</sup> |        | +0.5827        |        | +0.3679             |        | 0.7902x+0.9547           |        | x <sup>-0.931</sup>        |        |
| PGMEA            | y=0.6651             | 0.6461 | y=-0.1662x     | 0.5682 | y=-0.269ln(x)       | 0.7519 | y=0.1471x <sup>2</sup> - | 0.7718 | y=0.4241                   | 0.7991 |
|                  | e <sup>-0.376x</sup> |        | +0.6739        |        | +0.4777             |        | 0.6834x+0.9904           |        | <b>x</b> <sup>-0.589</sup> |        |
| p/m-Xylene       | y=0.2923             | 0.7223 | y=-0.0855x     | 0.5848 | y=-0.137ln(x)       | 0.7640 | y=0.0721x <sup>2</sup> - | 0.7749 | y=0.1456                   | 0.8367 |
|                  | e <sup>-0.576x</sup> |        | +0.2837        |        | +0.1824             |        | 0.3392x+0.4389           |        | x <sup>-0.872</sup>        |        |
| o-Xylene         | y=0.5942             | 0.7568 | y=-0.1671x     | 0.6119 | y=-0.267ln(x)       | 0.7888 | y=0.1358x <sup>2</sup> - | 0.7967 | y=0.3037                   | 0.8680 |
|                  | e <sup>-0.554x</sup> |        | +0.5678        |        | +0.3695             |        | 0.6447x+0.8601           |        | <b>x</b> <sup>-0.834</sup> |        |
| 1, 2, 4-         | y=0.0501             | 0.6651 | y=-0.0142x     | 0.5646 | y=-0.023ln(x)       | 0.7378 | y=0.0115x <sup>2</sup> - | 0.7357 | y=0.0272                   | 0.7796 |
| Trimethylbenzene | e <sup>-0.506x</sup> |        | +0.0498        |        | +0.033              |        | 0.0548x+0.0746           |        | <b>x</b> <sup>-0.77</sup>  |        |

| Compounds        | Exponential fitting  |        | Linear fitting |        | Logarithmic fitting |        | Polynomial fitting        |        | Power fitting       |        |
|------------------|----------------------|--------|----------------|--------|---------------------|--------|---------------------------|--------|---------------------|--------|
|                  | Formula              | R²     | Formula        | R²     | Formula             | R²     | Formula                   | R²     | Formula             | R²     |
| n-Butyl acetate  | y=0.0118             | 0.8857 | y=0.0113x      | 0.8820 | y=0.0044ln(x)       | 0.8312 | y=0.0138x <sup>2</sup> -  | 0.9062 | y=0.0205            | 0.8544 |
|                  | e <sup>0.6913x</sup> |        | +0.0112        |        | +0.0202             |        | 0.0012x+0.0135            |        | x <sup>0.2724</sup> |        |
| Ethylbenzene     | y=0.0147             | 0.8856 | y=0.0274x      | 0.9091 | y=0.0109ln(x)       | 0.8952 | y=0.0062x <sup>2</sup> +  | 0.9100 | y=0.0369            | 0.9072 |
|                  | e <sup>1.1269x</sup> |        | +0.0127        |        | +0.0348             |        | 0.0217x+0.0137            |        | x <sup>0.4576</sup> |        |
| PGMEA            | y=0.0038             | 0.9340 | y=0.0089x      | 0.9647 | y=0.0036ln(x)       | 0.9588 | y=-0.0016x <sup>2</sup> + | 0.9653 | y=0.0111            | 0.9661 |
|                  | e <sup>1.3007x</sup> |        | +0.0031        |        | +0.0103             |        | 0.0104x+0.0029            |        | x <sup>0.5307</sup> |        |
| p/m-Xylene       | y=0.0085             | 0.7590 | y=0.0135x      | 0.7772 | y=0.0048ln(x)       | 0.6271 | y=0.0498x <sup>2</sup> -  | 0.9716 | y=0.018             | 0.6112 |
|                  | e <sup>0.9625x</sup> |        | +0.0074        |        | +0.0178             |        | 0.0315x+0.0157            |        | x <sup>0.3465</sup> |        |
| o-Xylene         | y=0.0086             | 0.6108 | y=0.0102x      | 0.6267 | y=0.004ln(x)        | 0.6142 | y=0.0107x <sup>2</sup> +  | 0.6394 | y=0.0167            | 0.6205 |
|                  | e <sup>0.8186x</sup> |        | +0.0081        |        | +0.0163             |        | 0.0005x+0.0099            |        | x <sup>0.331</sup>  |        |
| Isopropyl        | y=0.0129             | 0.4683 | y=0.0199x      | 0.4782 | y=0.008ln(x)        | 0.4760 | y=0.0228x <sup>2</sup> -  | 0.4896 | y=0.0293            | 0.4877 |
| benzene          | e <sup>1.0012x</sup> |        | +0.012         |        | +0.0282             |        | 0.0006x+0.0158            |        | x <sup>0.4099</sup> |        |
| 1, 2, 4-         | y=0.0087             | 0.7973 | y=0.0234x      | 0.8225 | y=0.0092ln(x)       | 0.7955 | y=0.0199x <sup>2</sup> +  | 0.8335 | y=0.0276            | 0.8147 |
| Trimethylbenzene | e <sup>1.4167x</sup> |        | +0.0066        |        | +0.0255             |        | 0.0054x+0.0099            |        | x <sup>0.5745</sup> |        |

Table S4 The fitting results of  $\mathsf{b}_1$  with relative humidity

Table S5 The fitting results of  $b_1$  with the air change rate

| Compounds        | Exponential fitting  |        | Linear fitting |        | Logarithmic fitting |        | Polynomial fitting          |        | Power fitting       |        |
|------------------|----------------------|--------|----------------|--------|---------------------|--------|-----------------------------|--------|---------------------|--------|
|                  | Formula              | R²     | Formula        | R²     | Formula             | R²     | Formula                     | R²     | Formula             | R²     |
| n-Butyl acetate  | y=0.0059             | 0.4113 | y=0.0013x      | 0.4862 | y=0.0014ln(x)       | 0.2919 | y=0.0012x <sup>2</sup> -    | 0.6780 | y=0.0073            | 0.2356 |
|                  | e <sup>0.16x</sup>   |        | +0.0058        |        | +0.0075             |        | 0.0028x+0.0083              |        | x <sup>0.1702</sup> |        |
| PGMEA            | y=0.0033             | 0.5342 | y=0.0009x      | 0.6211 | y=0.001ln(x)        | 0.4216 | y=0.0006x <sup>2</sup> -    | 0.7570 | y=0.0043            | 0.3489 |
|                  | e <sup>0.1873x</sup> |        | +0.0032        |        | +0.0044             |        | 0.0013x+0.0046              |        | x <sup>0.2128</sup> |        |
| p/m-Xylene       | y=0.0044             | 0.4023 | y=0.0006x      | 0.4429 | y=0.0007ln(x)       | 0.3354 | y=0.0001x <sup>2</sup> +    | 0.4479 | y=0.0051            | 0.2906 |
|                  | e <sup>0.1161x</sup> |        | +0.0044        |        | +0.0052             |        | 0.0003x+0.0046              |        | x <sup>0.1387</sup> |        |
| o-Xylene         | y=0.0042             | 0.4015 | y=0.0007x      | 0.4590 | y=0.0009ln(x)       | 0.3315 | y=0.0002x <sup>2</sup> -8E- | 0.4799 | y=0.005             | 0.2749 |
|                  | e <sup>0.1413x</sup> |        | +0.0042        |        | +0.0051             |        | 05x+0.0047                  |        | x <sup>0.1644</sup> |        |
| 1, 2, 4-         | y=0.0045             | 0.4484 | y=0.0011x      | 0.5385 | y=0.0013ln(x)       | 0.3743 | y=0.0006x <sup>2</sup> -    | 0.6049 | y=0.0057            | 0.2952 |
| Trimethylbenzene | e <sup>0.1877x</sup> |        | +0.0044        |        | +0.0059             |        | 0.0009x+0.0057              |        | x <sup>0.214</sup>  |        |



Fig. S1 Fitting of TVOC emission rates with single exponential model at ACR 1.0 h<sup>-1</sup> and

different relative humidity: (a) 20%; (b) 30%; (c) 50%; (d) 70%.



**Fig. S2** Fitting of acetic acid butyl ester emission rates with single exponential model at ACR 1.0 h<sup>-1</sup> and different relative humidity: (a) 20%; (b) 30%; (c) 50%; (d) 70%.



Fig. S3 Fitting of a PGMEA emission rates with single exponential model at ACR 1.0  $h^{\text{-1}}$  and

different relative humidity: (a) 20%; (b) 30%; (c) 50%; (d) 70%.



Fig. S4 Fitting of m/p-Xylene emission rates with single exponential model at ACR 1.0 h<sup>-1</sup> and





**Fig. S5** Fitting of o-Xylene emission rates with single exponential model at ACR 1.0  $h^{-1}$  and different relative humidity: (a) 20%; (b) 30%; (c) 50%; (d) 70%.



Fig. S6 Fitting of Ethylbenzene emission rates with single exponential model at ACR 1.0 h<sup>-1</sup> and

different relative humidity: (a) 20%; (b) 30%; (c) 50%; (d) 70%.



Fig. S7 Fitting of Isopropyl benzene emission rates with single exponential model at ACR 1.0



 $h^{\mbox{-}1}$  and different relative humidity: (a) 20%; (b) 30%; (c) 50%; (d) 70%.

**Fig. S8** Fitting of 1,2,4-Trimethylbenzene emission rates with single exponential model at ACR 1.0 h<sup>-1</sup> and different relative humidity: (a) 20%; (b) 30%; (c) 50%; (d) 70%.



Fig. S9 Fitting of TVOC concentrations with single exponential model at RH 50% and different

ACR: (a) 0.5 h<sup>-1</sup>; (b) 1.0 h<sup>-1</sup>; (c) 2.0 h<sup>-1</sup>; (d) 3.0 h<sup>-1</sup>.



Fig. S10 Fitting of Acetic acid butyl ester concentrations with single exponential model at RH



50% and different ACR: (a) 0.5  $h^{-1}$ ; (b) 1.0  $h^{-1}$ ; (c) 2.0  $h^{-1}$ ; (d) 3.0  $h^{-1}$ .

**Fig. S11** Fitting of PGMEA concentrations with single exponential model at RH 50% and different ACR: (a)  $0.5 h^{-1}$ ; (b)  $1.0 h^{-1}$ ; (c)  $2.0 h^{-1}$ ; (d)  $3.0 h^{-1}$ .



Fig. S12 Fitting of p/m-Xylene concentrations with single exponential model at RH 50% and

different ACR: (a) 0.5  $h^{-1}$ ; (b) 1.0  $h^{-1}$ ; (c) 2.0  $h^{-1}$ ; (d) 3.0  $h^{-1}$ .



Fig. S13 Fitting of o-Xylene concentrations with single exponential model at RH 50% and

different ACR: (a) 0.5  $h^{-1}$ ; (b) 1.0  $h^{-1}$ ; (c) 2.0  $h^{-1}$ ; (d) 3.0  $h^{-1}$ .