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# Characterization of organic release kinetics in particleboard by the dual model fitting methodology

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**Table S1 Determination conditions of TD-GC-MS**

| | |
|---|---|
| **TD** | |
| Adsorption tube type | Tenax-TA |
| Tube desorption temperature | 280 ℃ |
| Tube desorption time | 15 min |
| Cold trap temperature | Low: -20 ℃; High: 300 ℃ |
| Cold trap desorption time | 3 min |
| Transfer line temperature | 150 ℃ |
| **GC** | |
| Injector temperature | 270 ℃ |
| Column | HP-5MS, 30 m × 250 μm × 0.25 μm |
| Carrier gas | He |
| Constant flow | 1.4 mL·min$^{-1}$ |
| Temperature program | The initial temperature was held at 30℃ for 2 min, then heated at the rate of 30℃·min$^{-1}$ to 250℃ and held for 1min.， then heated at the rate of 6℃·min$^{-1}$ to 300℃ and held for 1 min |
| **MS** | |
| Ion source EI | 70 eV |
| Ion source temperature | 200 ℃ |
| Quadrupole temperature | 150 ℃ |
| Mass range Scan mode | 10-1000 amu |
| Transfer line temperature | 280 ℃ |

**Table S2. Important detectable of particle board**

| Compound Name | Boiling Point (°C) | Vapor Pressure (mmHg) | Qualitative ion (*m/z*) | Quantitative ion (*m/z*) |
|---|---|---|---|---|
| Methyl mercaptan | 6 | 1536 ( 20 °C) | 48 | 47 |
| Isoprene | 34 | 550 ( 25 °C) | 68 | 67 |
| Formic acid | 100-101 | 52 ( 37 °C) | 46 | 45 |
| Dimethyl acetal | 64 | 187.1 (25 °C) | 75 | 59 |
| Butenone | 80 | 310 ( 55 °C) | 70 | 55 |
| Butyraldehyde | 75 | 90 ( 20 °C) | 72 | 57 |
| Acetic acid | 117-118 | 11.4 ( 20 °C) | 60 | 45 |
| Trichloromethane | 61 | 160 ( 20 °C) | 118,85 | 83 |
| Tetrahydrofuran | 66 | <0.01 ( 25 °C) | 72 | 71 |
| Dichloroethane | 82-84 | 83.9 (25 °C) | 98 | 62 |
| 1,4-Dioxane | 101 | 27 ( 20 °C) | 88 | 58 |
| Toluene | 110-111 | 22 ( 20 °C) | 92 | 91 |
| Cyclohexanone | 155 | 3.4 ( 20 °C) | 98 | 55 |
| Phenol | 182 | 0.35 ( 25 °C) | 94 | 66 |
| 2-Methylphenol | 191 | 0.3 ( 20 °C) | 108 | 107 |
| Octanoic acid | 237 | 1 ( 78 °C) | 115 | 101 |
| Naphthalene | 218 | 0.03 ( 25 °C) | 128 | 127 |
| Nonanoic acid | 268-269 | <0.1 ( 20 °C) | 158 | 129 |
| p-tert-Butylphenol | 236-238 | 1 ( 70 °C) | 150 | 135 |
| 1-Methylnaphthalene | 240-243 | 0.1 (25 °C) | 142 | 141 |
| Phthalic anhydride | 284 | <0.01 ( 20 °C) | 148 | 104 |
| Decanoic acid | 268-270 | 15 ( 160 °C) | 172 | 129 |
| Dibutyl phthalate | 340 | 1 ( 147 °C) | 223,205 | 149 |

**Table S3 Biexponential model fitting parameters for toluene release**

| Fitting parameter name | Fitting parameter value |
|---|---|
| Release rate for Phase 1 | 0.11 |
| Decay constant for Phase 1 | 1.9 |
| Release rate for Phase 2 | 0.012 |
| Decay constant for Phase 2 | 0.003 |
| Emission factor | $E(t)=0.11*e^{-1.9t}+0.012*e^{-0.003t}$ |

**Table S4 Mass transfer model fitting parameters for toluene release**

| **Parameters set in the experiment** | | | | | | |
|---|---|---|---|---|---|---|
| $A(m^2)$ | δ(m) | $V(m^3)$ | | $Q(m^3/s)$ | β | |
| 0.5 | 0.009 | 1 | | 1/3600 | 0.0045 | |
| **Theoretical parameters derived from software** | | | | | | |
| $D_s(m^2/s)^{\#}$ | K | $h_m(m/s)$ | a | $Bi_m/K$ | q | $G_1$ |
| 3.39E-10 | 7.06E+02 | 0.000424 | 66.37 | 15.94 | 1.414 | 102.504 |
| **Parameters obtained by fitting the experimental data** | | **The equation corresponding to the linear fit of the data** | | | | |
| $C_0(\mu g/m^3)$ | $D_m(m^2/s)$ | $b=\ln(3.06E-06*C_0)$ | | | | |
| 1.7E+06 | 1.6E-11 | $k=-24683.9*D_m$ | | | | |

# Software estimation value of $D_m$, the same below.

**Table S5 Biexponential model fitting parameters for dimethyl acetal**

| Fitting parameter name | Fitting parameter value |
|---|---|
| Release rate for Phase 1 | 0.0677 |
| Decay constant for Phase 1 | 1.16 |
| Release rate for Phase 2 | 0.0114 |
| Decay constant for Phase 2 | 0.01 |
| Emission factor | $E(t)=0.0677*e^{-1.16t}+0.0114*e^{-0.01t}$ |

**Table S6 Mass transfer model fitting parameters for dimethyl acetal**

| **Parameters set in the experiment** | | | | | | |
|---|---|---|---|---|---|---|
| $A(m^2)$ | $\delta(m)$ | $V(m^3)$ | $Q(m^3/s)$ | $\beta$ | | |
| 0.5 | 0.009 | 1 | 1/3600 | 0.0045 | | |
| **Theoretical parameters derived from software** | | | | | | |
| $D_s(m^2/s)$ | K | $h_m(m/s)$ | a | $Bi_m/K$ | q | $G_1$ |
| 2.56E-08 | 73.98 | 0.000506 | 0.88 | 2.4 | 0.746 | 1.17426 |
| **Parameters obtained by fitting the experimental data** | | | **The equation corresponding to the linear fit of the data** | | | |
| $C_0(\mu g/m^3)$ | $D_m(m^2/s)$ | | $b=\ln(7.4E-05*C_0)$ | | | |
| 4.3E+03 | 3.9E-10 | | $k=-6870.6*D_m$ | | | |

**Table S7 Biexponential model fitting parameters for decanoic acid**

| Fitting parameter name | Fitting parameter value |
|---|---|
| Release rate for Phase 1 | 0.022 |
| Decay constant for Phase 1 | 0.26 |
| Release rate for Phase 2 | 0.001 |
| Decay constant for Phase 2 | 0.005 |
| Emission factor | $E(t)=0.022*e^{-0.26t}+0.001*e^{-0.005t}$ |

**Table S8 Mass transfer model fitting parameters for decanoic acid**

| **Parameters set in the experiment** | | | | | | |
|---|---|---|---|---|---|---|
| $A(m^2)$ | $\delta(m)$ | $V(m^3)$ | $Q(m^3/s)$ | $\beta$ | | |
| 0.5 | 0.009 | 1 | 1/3600 | 0.0045 | | |
| **Theoretical parameters derived from software** | | | | | | |
| $D_s(m^2/s)$ | K | $h_m(m/s)$ | a | $Bi_m/K$ | q | $G_1$ |
| 4.28E-12 | 5.047E06 | 0.000352 | 5257 | 0.15 | 0.297 | 10351.8 |
| **Parameters obtained by fitting the experimental data** | | **The equation corresponding to the linear fit of the data** | | | | |
| $C_0(\mu g/m^3)$ | $D_m(m^2/s)$ | $b=\ln(1.3E-09*C_0)$ | | | | |
| 5.0E+08 | 2.3E-09 | $k=-1089*D_m$ | | | | |

**Table S9 Biexponential model fitting parameters for phenol**

| Fitting parameter name | Fitting parameter value |
|---|---|
| Release rate for Phase 1 | 0.0045 |
| Decay constant for Phase 1 | 0.0048 |
| Release rate for Phase 2 | 0.003 |
| Decay constant for Phase 2 | 0.13 |
| Emission factor | $E(t)=0.0045*e^{-0.0048t}+0.003*e^{-0.13t}$ |

**Table S10 Mass transfer model fitting parameters for phenol**

| **Parameters set in the experiment** | | | | | | |
|---|---|---|---|---|---|---|
| $A(m^2)$ | $\delta(m)$ | $V(m^3)$ | $Q(m^3/s)$ | $\beta$ | | |
| 0.5 | 0.009 | 1 | 1/3600 | 0.0045 | | |
| **Theoretical parameters derived from software** | | | | | | |
| $D_s(m^2/s)$ | K | $h_m(m/s)$ | a | $Bi_m/K$ | q | $G_1$ |
| 2.83E-10 | 2.47E+04 | 0.000439 | 79.5 | 0.565 | 0.534 | 151.763 |
| **Parameters obtained by fitting the experimental data** | | | **The equation corresponding to the linear fit of the data** | | | |
| $C_0(\mu g/m^3)$ | $D_m(m^2/s)$ | | $b=\ln(2.95E-07*C_0)$ | | | |
| 7.3E+06 | 3.98E-10 | | $k=-3520.4*D_m$ | | | |