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Supplement of

Uptake of gaseous formaldehyde by soil surfaces: a combination of adsorption/desorption equilibrium and chemical reactions

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<table>
<thead>
<tr>
<th>Initial HCHO con. $C_m$ (ppb)</th>
<th>RH (%)</th>
<th>$\gamma^a \times 10^5$</th>
<th>$\gamma^b \times 10^5$</th>
<th>$\gamma^c \times 10^5$</th>
<th>$\gamma^d \times 10^5$</th>
<th>$\gamma^e \times 10^5$</th>
<th>$\gamma^f \times 10^5$</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>0</td>
<td>17.9 ± 0.7</td>
<td>17.2 ± 1.7</td>
<td>17.0 ± 1.6</td>
<td>17.4 ± 0.8</td>
<td>17.1 ± 0.8</td>
<td>16.7 ± 1.3</td>
</tr>
<tr>
<td>10</td>
<td>40</td>
<td>7.4 ± 1.2</td>
<td>6.3 ± 0.9</td>
<td>4.9 ± 0.6</td>
<td>4.3 ± 0.8</td>
<td>3.8 ± 0.9</td>
<td>3.5 ± 0.8</td>
</tr>
<tr>
<td>20</td>
<td>0</td>
<td>16.7 ± 0.3</td>
<td>16.3 ± 0.6</td>
<td>15.8 ± 0.7</td>
<td>15.5 ± 0.8</td>
<td>15.3 ± 0.8</td>
<td>15.4 ± 0.4</td>
</tr>
<tr>
<td>20</td>
<td>40</td>
<td>7.2 ± 1.0</td>
<td>6.6 ± 0.4</td>
<td>5.1 ± 0.3</td>
<td>4.1 ± 0.1</td>
<td>3.5 ± 0.1</td>
<td>3.2 ± 0.1</td>
</tr>
<tr>
<td>30</td>
<td>0</td>
<td>16.0 ± 0.8</td>
<td>15.5 ± 1.2</td>
<td>14.8 ± 1.2</td>
<td>14.8 ± 0.9</td>
<td>14.6 ± 1.2</td>
<td>14.2 ± 0.9</td>
</tr>
<tr>
<td>30</td>
<td>10</td>
<td>11.6 ± 0.3</td>
<td>9.4 ± 0.3</td>
<td>7.5 ± 0.2</td>
<td>6.3 ± 0.2</td>
<td>5.5 ± 0.1</td>
<td>4.8 ± 0.1</td>
</tr>
<tr>
<td>30</td>
<td>20</td>
<td>10.4 ± 0.5</td>
<td>7.8 ± 0.5</td>
<td>5.8 ± 0.3</td>
<td>4.7 ± 0.2</td>
<td>3.9 ± 0.2</td>
<td>3.3 ± 0.1</td>
</tr>
<tr>
<td>30</td>
<td>30</td>
<td>9.4 ± 0.3</td>
<td>6.5 ± 0.3</td>
<td>4.7 ± 0.3</td>
<td>3.8 ± 0.3</td>
<td>3.1 ± 0.3</td>
<td>2.7 ± 0.2</td>
</tr>
<tr>
<td>30</td>
<td>40</td>
<td>7.1 ± 0.6</td>
<td>6.3 ± 0.5</td>
<td>4.5 ± 0.4</td>
<td>3.4 ± 0.4</td>
<td>2.9 ± 0.2</td>
<td>2.5 ± 0.2</td>
</tr>
<tr>
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<td>50</td>
<td>7.6 ± 0.3</td>
<td>6.0 ± 0.2</td>
<td>4.2 ± 0.2</td>
<td>3.3 ± 0.1</td>
<td>2.7 ± 0.1</td>
<td>2.3 ± 0.1</td>
</tr>
<tr>
<td>30</td>
<td>60</td>
<td>7.8 ± 0.1</td>
<td>6.1 ± 0.2</td>
<td>4.4 ± 0.2</td>
<td>3.6 ± 0.2</td>
<td>3.0 ± 0.2</td>
<td>2.6 ± 0.2</td>
</tr>
<tr>
<td>30</td>
<td>70</td>
<td>7.7 ± 0.4</td>
<td>6.0 ± 0.3</td>
<td>4.3 ± 0.2</td>
<td>3.4 ± 0.2</td>
<td>2.9 ± 0.2</td>
<td>2.5 ± 0.2</td>
</tr>
<tr>
<td>40</td>
<td>0</td>
<td>13.5 ± 0.7</td>
<td>13.3 ± 0.5</td>
<td>13.1 ± 0.5</td>
<td>12.8 ± 0.5</td>
<td>12.7 ± 0.4</td>
<td>12.7 ± 0.3</td>
</tr>
<tr>
<td>40</td>
<td>40</td>
<td>6.9 ± 0.1</td>
<td>6.1 ± 0.2</td>
<td>4.5 ± 0.2</td>
<td>3.5 ± 0.2</td>
<td>2.9 ± 0.1</td>
<td>2.5 ± 0.1</td>
</tr>
</tbody>
</table>

$^a$Uptake coefficients at uptake time period of 5 min. $^b$10 min. $^c$20 min. $^d$30 min. $^e$40 min. $^f$50 min.

The error bars represent one standard deviation of three replicates.

**Table S.1.** Calculated HCHO uptake coefficients as a function of initial HCHO concentration, relative humidity and uptake time period.
Figure S.1. Air-dried continuous rotating coating tool (ACRO). (A) flushing gas inlet; (B) motor with a driving belt; (C) fastened tubing holder; (D) coated flow tube; (E) loosened tubing holder; (F) foothold.
Figure S.2. Energy Dispersive X-ray (EDX) analysis of the soil sample.
Figure S.3. Transmittance $C_{\text{out}}/C_{\text{in}}$ versus uptake coefficients derived from both CKD-B and KPS methods, for specified dimensionless length $z^* = 0.385$ under our experimental conditions.
Figure S.4. Transmittance $C_{\text{out}}/C_{\text{in}}$ versus Sherwood number $N_{\text{Shw}}$, for specified dimensionless length $z^* = 0.385$ under our experimental conditions. The red dots represent the values from Table I in the reference of Murphy et al., (1987); the black line denotes values from our calculations.
Matlab code mannul

(1) Parameters definition

The parameters adopted in the provided code are defined as follows:

$L$: flow tube length; $R$: flow tube radius; $z$: axial position; $r$: radial position; $F$: volume flow rate of carrier gas in flow tube; $D$: diffusion coefficient of analyte in the carrier gas under experimental conditions; $T_0$: standard temperature, 273K; $P_0$: standard pressure, 101kPa; $T$: temperature at experimental conditions; $P$: pressure at experimental conditions; $g$: the uptake coefficient; $g_{\text{min}}$: the minimum value of the uptake coefficient; $g_{\text{max}}$: the maximum value of the uptake coefficient; $g_{\text{n}}$: the number of values of $g$ from $g_{\text{min}}$ to $g_{\text{max}}$; $x$: the dimensionless form of radius position $r$, $x = r/R$, ranging from 0 to 1; $t$: the dimensionless form of axial position $z$, $t = z \times \pi \times D / (2 \times F) \times (T_0/T) \times (P/P_0)$, ranging from 0 to $t_0$; $t_0$: $t_0 = L \times \pi \times D / (2 \times F) \times (T_0/T) \times (P/P_0)$; $u$: analyte concentration at the axial and radial position (dimensionless) of $(t, x)$; $v$: analyte mean molecular speed; $N$: Sherwood number.

For the axial and radial position $(z, r)$ in a flow tube, see Fig. S.5.

![flow tube](image)

**Figure S.5.** Schematic of the axial and radial position $(z, r)$ in a flow tube with length of $L$ and radius of $R$.

(2) Parameters input

Open all the *.m files and input the following parameters: $L$, $R$, $F$, $D$, $T$, $P$ and $v$ according to the specific experimental conditions applied. Note that $g_{\text{min}}$, $g_{\text{max}}$ and $g_{\text{n}}$ should be specified in advance and also for the numbers ($n$) of $t$ and $x$ within their effective ranges. In principle, the larger the $n$ input, the more precise the results are.

(3) Results output

After input/change of the parameters, please SAVE the parameters setting. Then RUN the Main.m file. A red process bar will show as the code is running. Please wait until the calculation ends. The output results include two tables and two plots:

```
table_g = [g', end_mean_u'] = table [γ, C_{out}/C_{in}]
```
table_N = [N', end_mean_u'] = table [N_{Shw}, C_{out}/C_{in}]

plot(g, end_mean_u) = plot (γ, C_{out}/C_{in})

plot(N, end_mean_u) = plot (N_{Shw}, C_{out}/C_{in})

The tables and plots will be saved automatically into the folder in which the *.m files are located.

Matlab code

**Main.m**

```matlab
function Main()
L = 0.25;
% the length of the flow tube, 0.25 m
F = 1*10^{-3}/60;
% the sample volume flow rate, 1.6667e-005 m^3/s
D = 0.0000177;
% HCHO diffusion coefficient in N2 at 296k and 101kPa, 0.0000177 m^2/s
T0 = 273;
% temperature at standard conditions, 273 K
P0 = 101;
% pressure at standard conditions, 101 kPa
T = 296;
% temperature at experimental conditions, 296 K
P = 101;
% pressure at experimental conditions, 101 kPa
t0=L*pi*D/(2*F)*(T0/T)*(P/P0);
g_min= 1e-7;
g_max = 1e-4;
g_n = 100;
% g is uptake coefficient, g_n is the number of g between g_min and g_max
pdex1(t0,g_min,g_max,g_n)
```

**pdex1.m**

```matlab
function pdex1(t0,g_min,g_max,g_n)
m = 1;
x = linspace(0,1,100);
% x = r* = r/R, x ranging from 0 to 1, r is radial position, R is the
% radius of the flow tube
t = linspace(0,t0,100);
% t = z* = z*pi*D/(2*F)*(T0/T)*(P/P0), z is axial position, z ranging from
% 0 to L, t ranging from 0 to t0, t0 corresponding to the whole length of
```
% the flow tube (dimensionless)
g = linspace(g_min,g_max,g_n);
% g is uptake coefficient, g_n is number of g between g_min and g_max
global g_i
h = waitbar(0,'Please wait...');
steps = length(g);
for i=1:length(g)
    g_i = g(i);
    sol = pdepe(m,@pdex1pde,@pdex1ic,@pdex1bc,x,t);
    u = sol(:,:,1);
    N_f(g(i))
    end_mean_u(i) = mean(u(end,:));
    waitbar(i / steps)
end
close(h)
table_g = [g',end_mean_u'];
xlswrite(['results,g',num2str(t0),'-',num2str(g_min),'.xls'], table_g)
figure
plot(g,end_mean_u)
xlabel('Uptake coefficient')
ylabel('Cout/Cin')
title ('Cout/Cin vs Uptake coefficient')
saveas(gcf, ['results,g',num2str(t0),'-',num2str(g_min),'.fig'],'fig')
close gcf
N = N_f(g);
table_N = [N',end_mean_u'];
xlswrite(['results,N',num2str(t0),'-',num2str(g_min),'.xls'], table_N)
figure
plot(N,end_mean_u)
xlabel('Sherwood Number')
ylabel('Cout/Cin')
title('Cout/Cin vs Sherwood Number')
saveas(gcf, ['results,N',num2str(t0),'-',num2str(g_min),'.fig'],'fig')
close gcf

pdex1pde.m

function [c,f,s] = pdex1pde(x,t,u,DuDx)
c = 1-x^2;
f = DuDx;
s = 0;

pdex1ic.m

function u0 = pdex1ic(x)
u0 = 1;
function [pl,ql,pr,qr] = pdex1bc(xl,ul,xr,u,t)
global g_i;
pl = 0;
ql = 0;
pr = N_f(g_i)*u;
qr = 1;

N_f.m

function N = N_f(g)
v = 457.16;
% mean molecular velocity of HCHO, 457.16 m/s
R = 0.0035;
% flow tube radius, 0.0035 m
D = 0.0000177;
% HCHO diffusion coefficient in N2 at 296k and 101kPa, 0.0000177 m^2/s
N = 0.5*(v*R/D).*g./(2-g);
% Sherwood number