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

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

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.

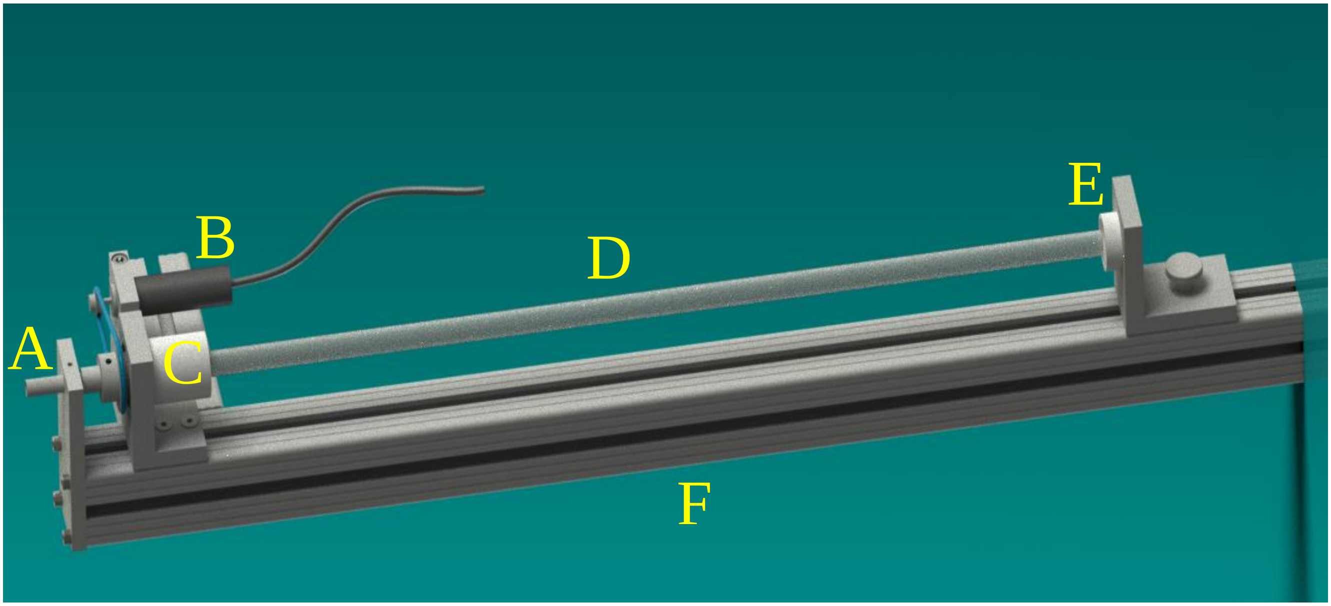

Figure S.1. Air-dried continuous rotating coating tool (ACRO). (A) flushing gas inlet; (B) motor with a driving belt; (C) fastened tubing holder; (D) coated flow tube; (E) loosened tubing holder; (F) foothold.

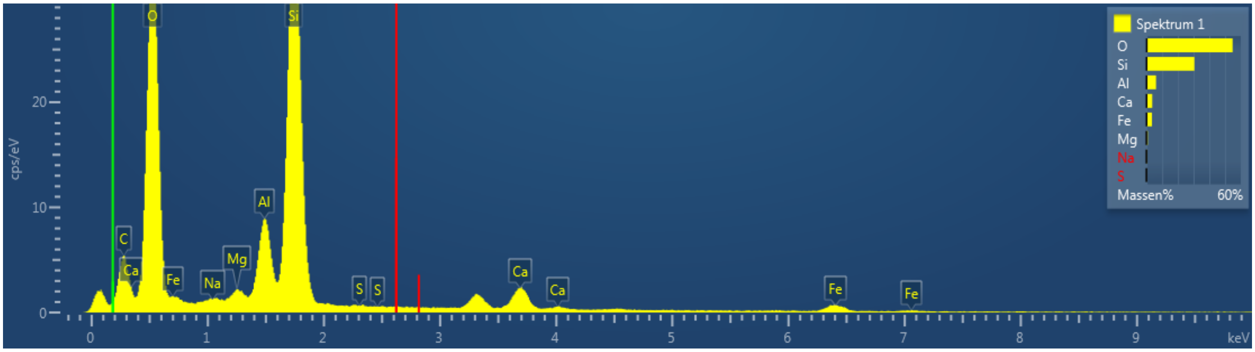

Figure S.2. Energy Dispersive X-ray (EDX) analysis of the soil sample.

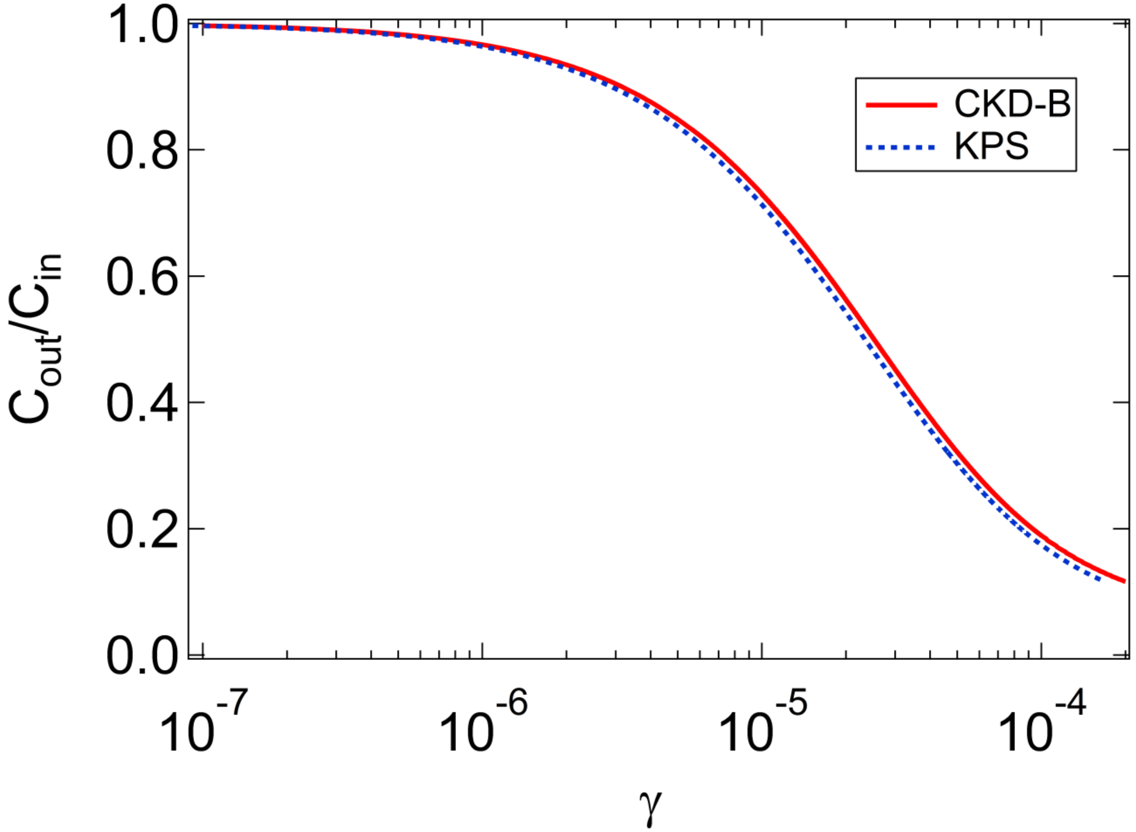

Figure S.3. Transmittance C_{out}/C_{in} versus uptake coefficients derived from both CKD-B and KPS methods, for specified dimensionless length $z^* = 0.385$ under our experimental conditions.

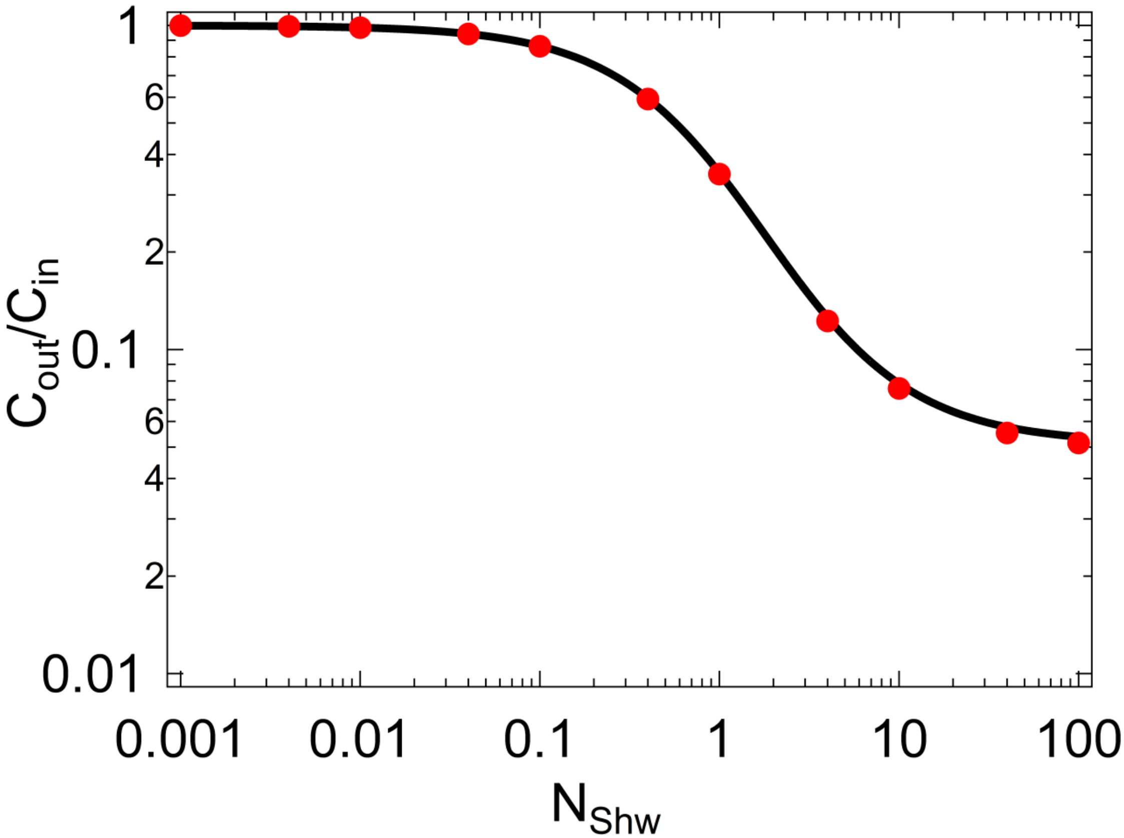

Figure S.4. Transmittance C_{out}/C_{in} versus Sherwood number N_{Shw}, for specified dimensionless length z^{*} = 0.385 under our experimental conditions. The red dots represent the values from Table I in the reference of Murphy et al., (1987); the black line denotes values from our calculations.

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*_min: the minimum value of the uptake coefficient; *g*_max: the maximum value of the uptake coefficient; *g*_*n*: the number of values of *g* from *g*_min to *g*_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.

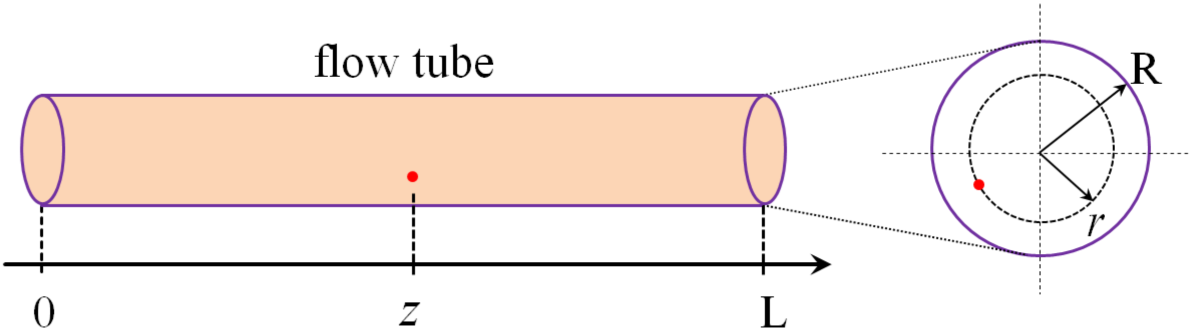

Figure S.5. Schematic of the axial and radial position (*z*, *r*) in a flow tube with length of *L* and radius of *R*.

(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*_min, *g*_max and *g*_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

```
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

```
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;
```

pdex1bc.m

```
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
```