Modelling of deposition velocities and indoor concentrations of pollutant gases.

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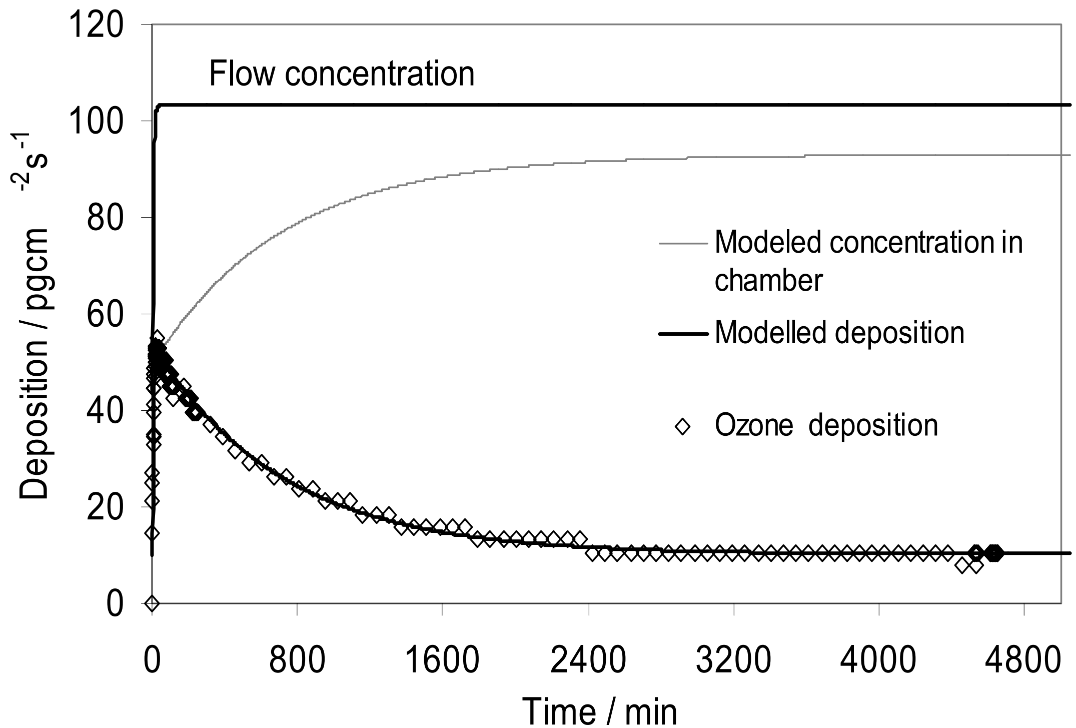
Ozone deposition to materials

Modelling of the,
- humidity,
- temperature,
- air flow

dependent deposition velocity, from experimental measurements.

Equilibrium deposition velocities and 1st order rate constants. Concrete floor tile (RH =70%, T = 22°C):



$$v_d(eq) = k_r \frac{k_a}{k_r + k_d}(RH)$$

$k_{ads} = 3.5*10^{-4}$ cms^{-1}

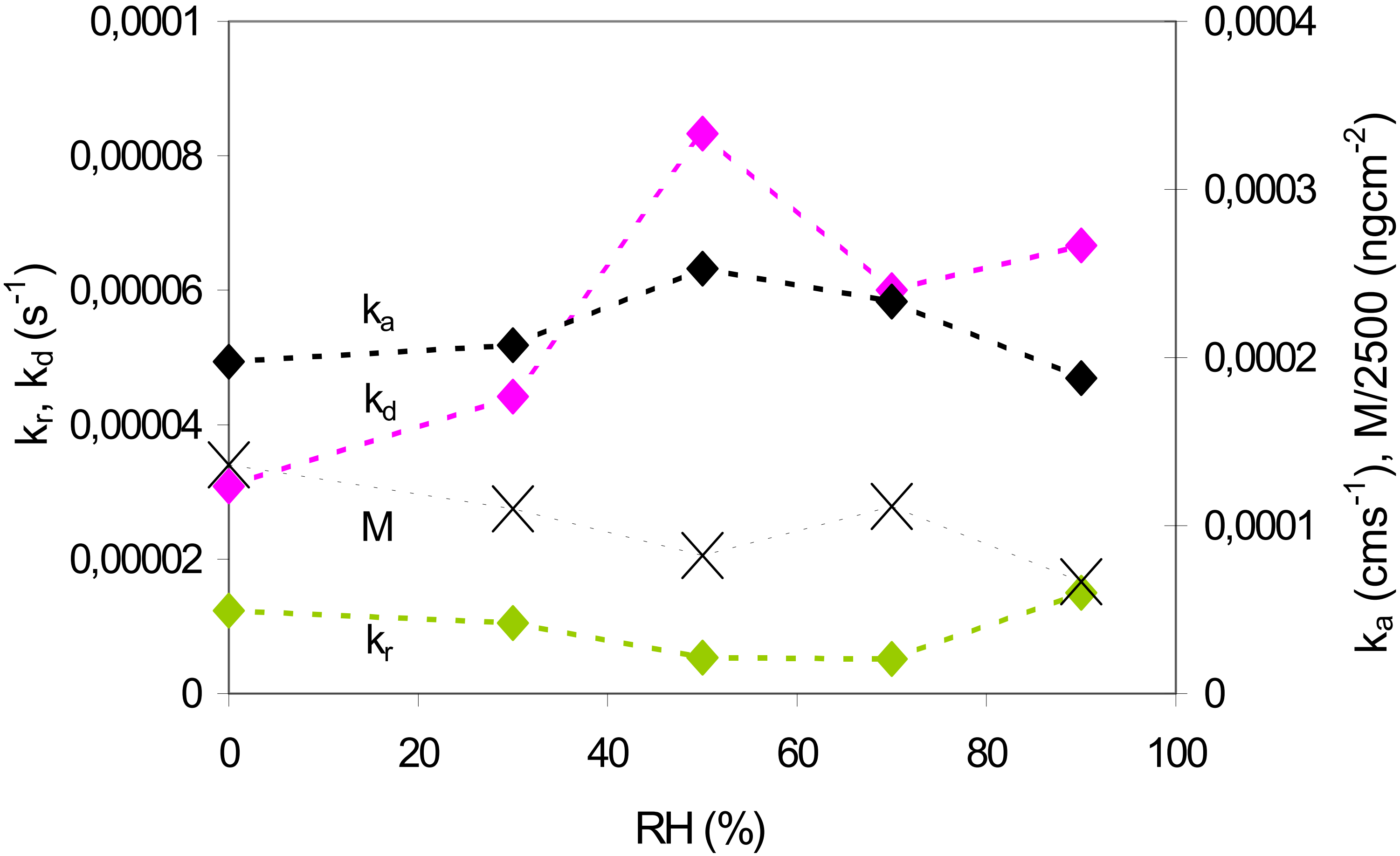
$k_{des} = 2.8*10^{-5}$ s^{-1}

$k_r = 4.5*10^{-6}$ s^{-1}

Humidity modelling

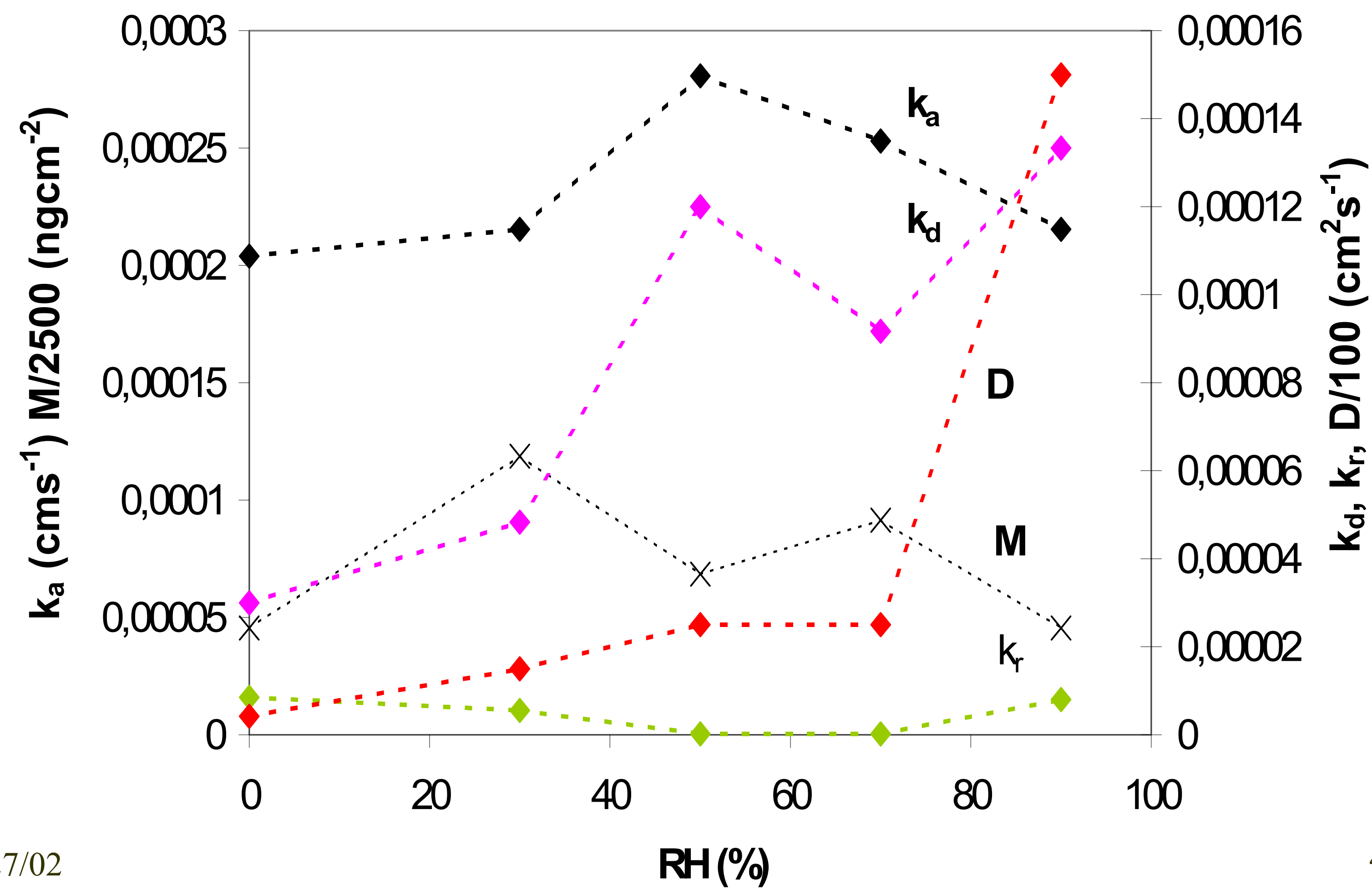
1st order rate constants

Concrete floor tile:



Modelled with diffusion from the surface

Concrete floor tile:

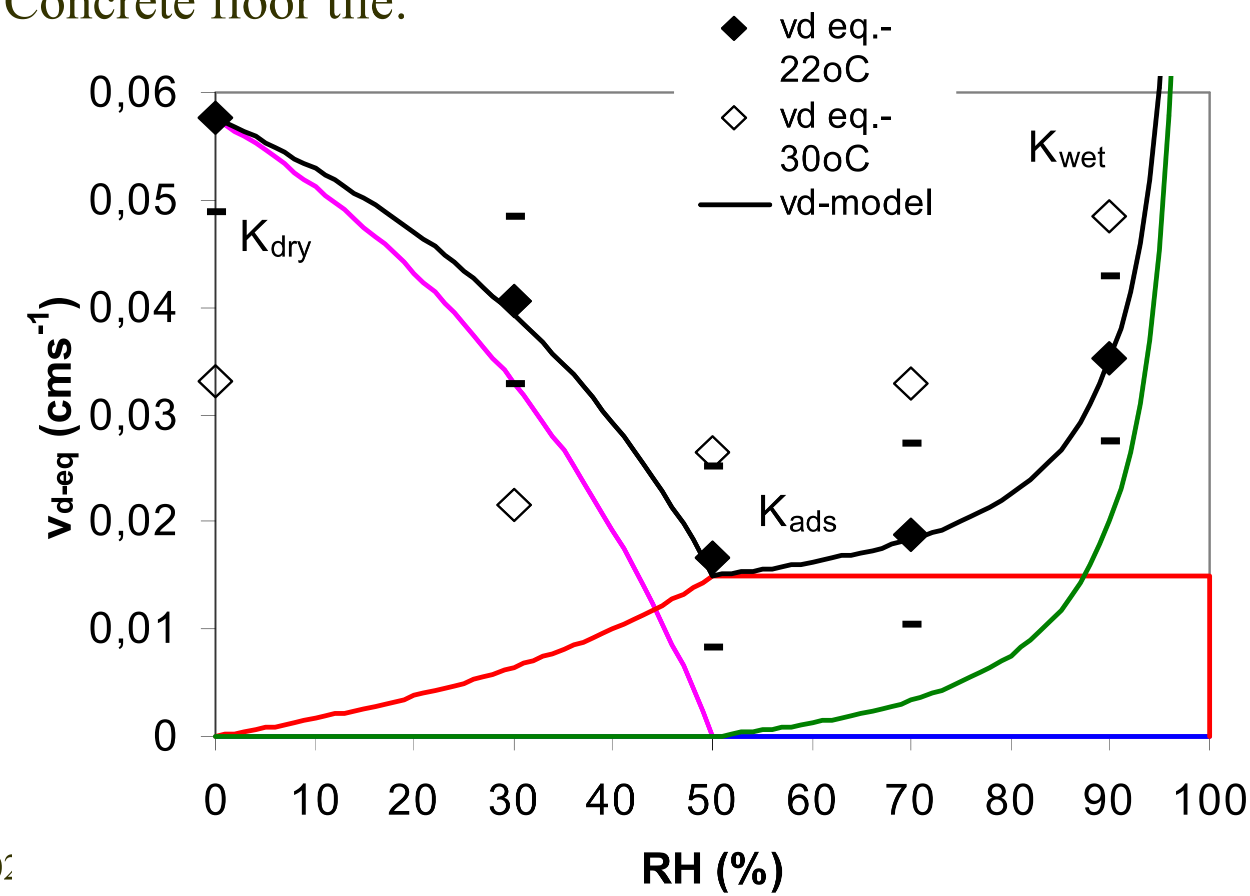


2^{nd} order rate constants

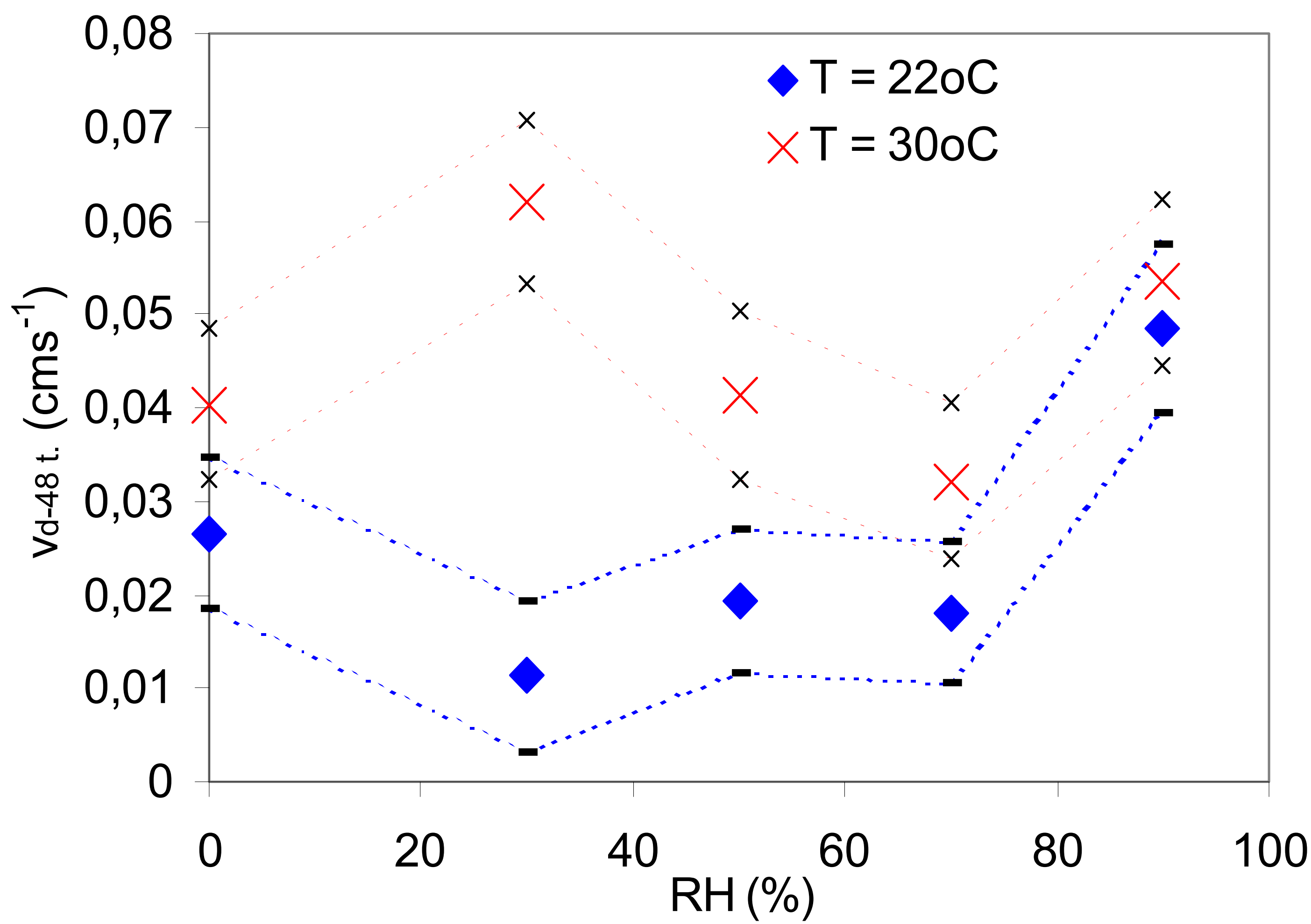
$m \leq 1$, $\mathbf{v_d = K_{dry}(1\text{-}m) + K_{ads}m}$, m = number of mono-layers of water, from BET isotherm.

$m > 1$, $\mathbf{v_d = K_{ads} + K_{wet}(m\text{-}1)}$

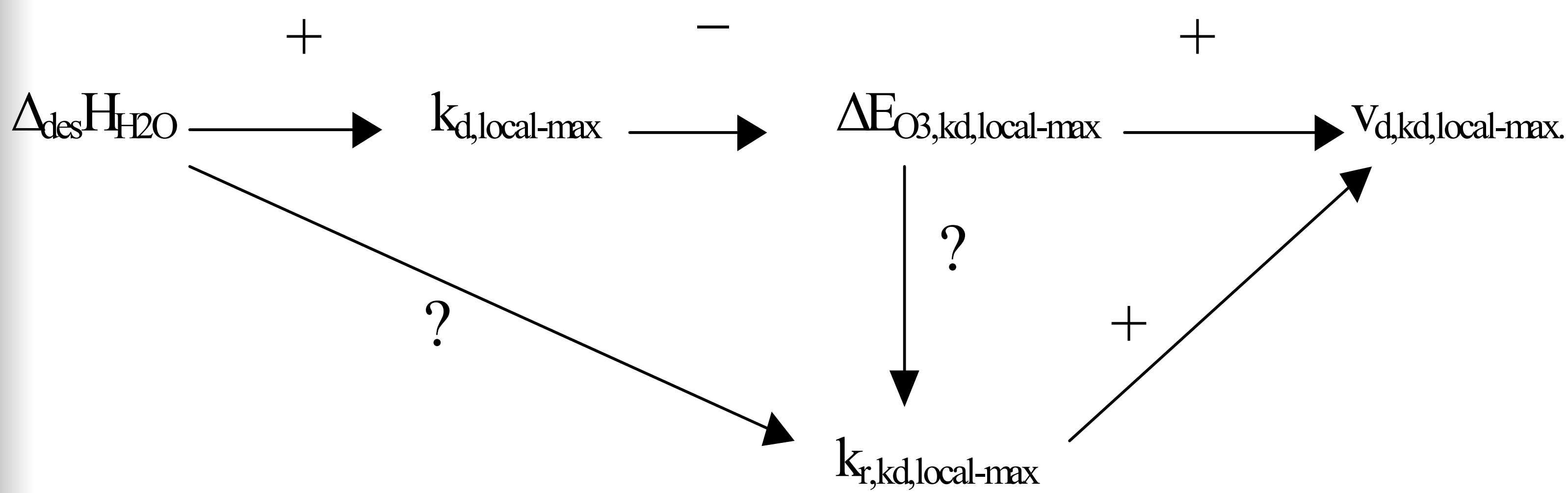
Concrete floor tile:



Linoleum floor covering:



Hypothesised dependencies of, v_d, on bonding strength of water, $\Delta_{des}H_{H2O}$, and on 1st order rate constants.

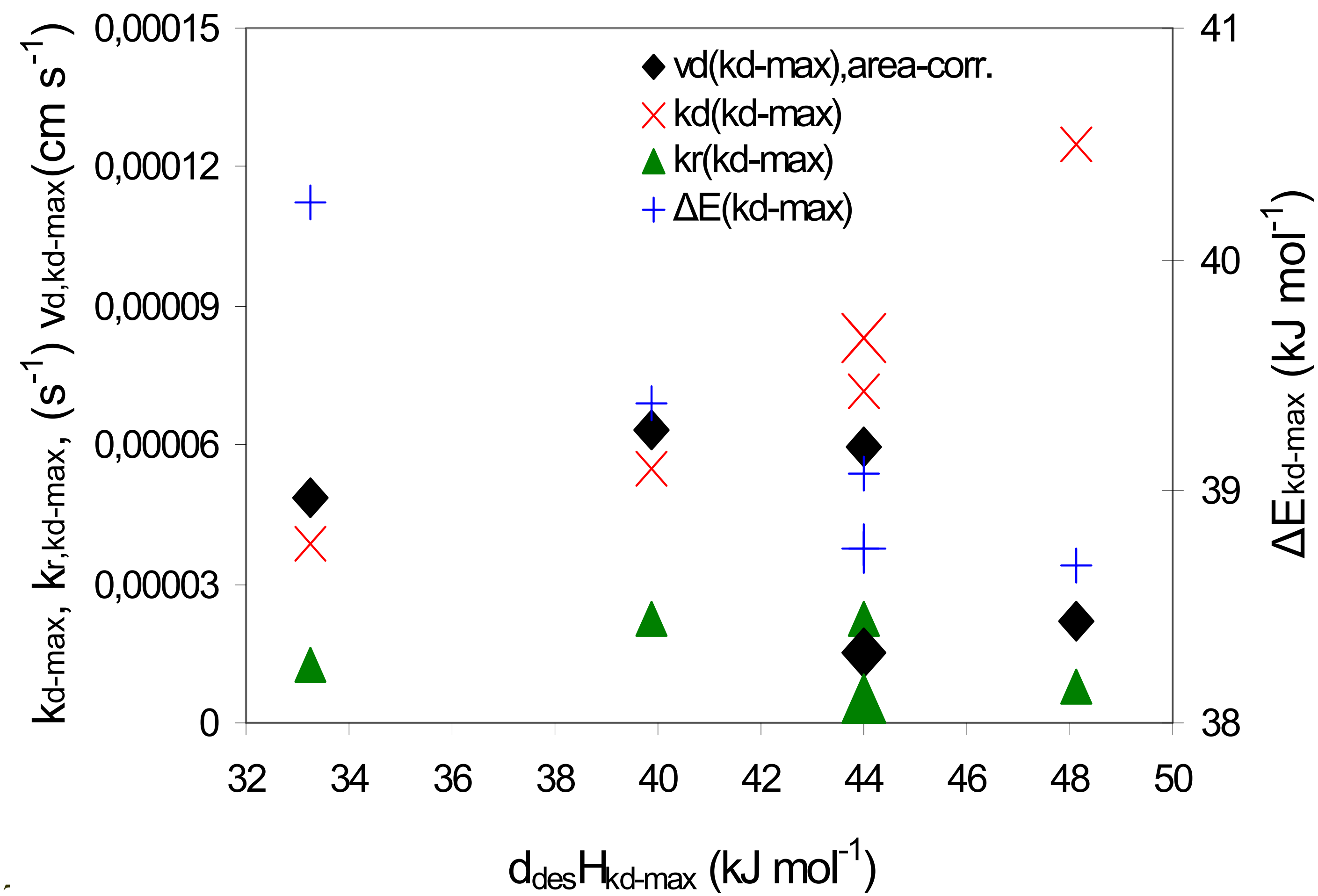


$$\Delta E = E_{a.d} - E_{a.a} = RT \ln \frac{A_d}{A_a} + RT \ln \frac{k_a}{k_d}$$

(van’t Hoff eq. for adsorption)

Correlation of v_d with bonding strength of water, $\Delta_{des}H_{H2O}$, and 1st order rate constants, at m = 1.

5 sample materials:



Equations (T = 22°C):

$$k_a = A_1 \Delta H^2 - B_1 \Delta H + C_1$$

$$k_d = A_2 \Delta H^2 - B_2 \Delta H + C_2$$

$$\Delta E = E_{a.d} - E_{a.a} = RT \ln \frac{A_d}{A_a} + RT \ln \frac{k_a}{k_d}$$

k_r = normal distribution of k_r around $\Delta E_{mean} = 39.8\ kJ\ mol^{-1}$.

<u>Temperature dependencies</u> were given from the Arrhenius equation:

$$k = A e^{-\frac{E_a}{RT}}$$

<u>And:</u>

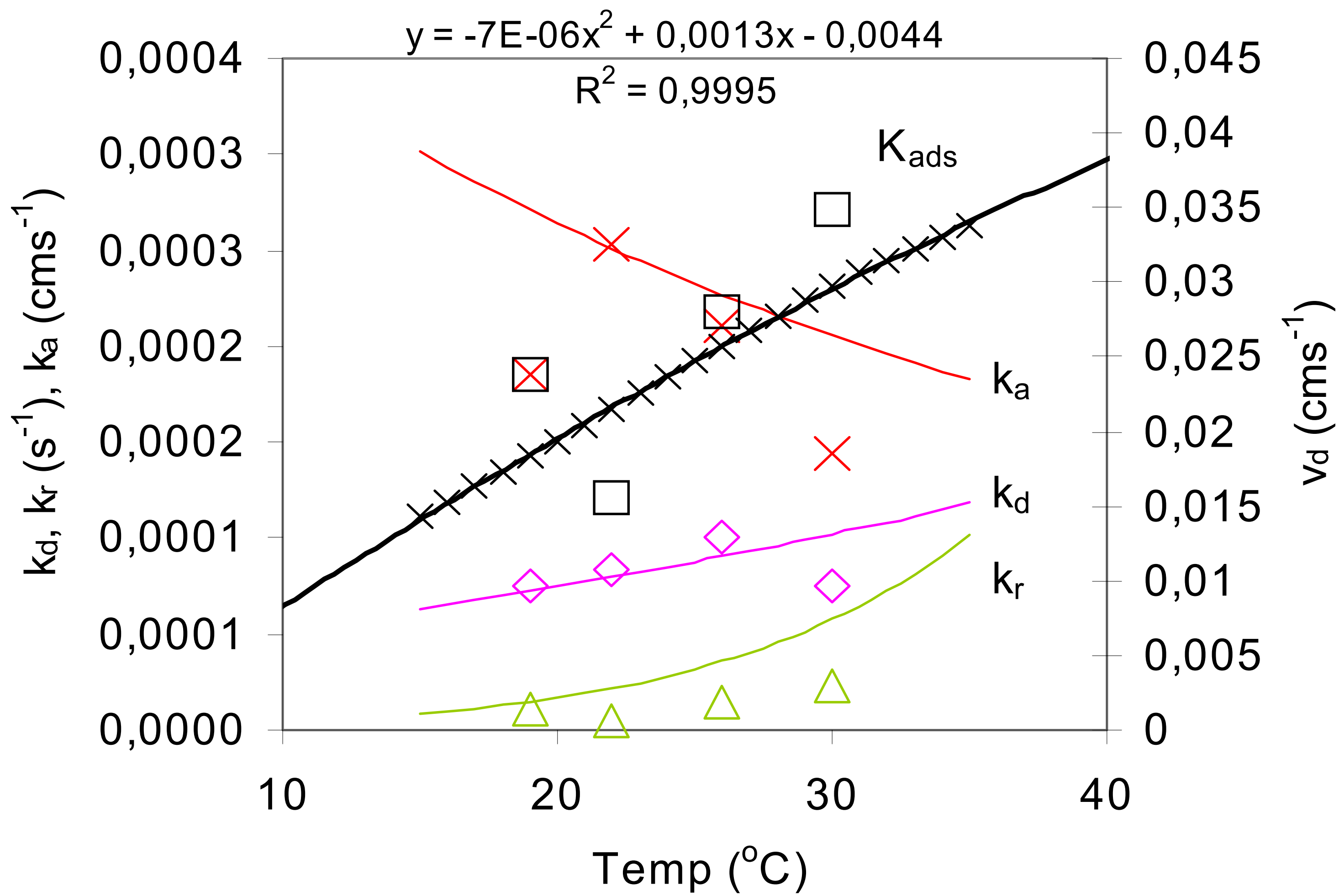
$$K_{ads} = k_r \cdot \frac{k_a}{k_r + k_d} (\Delta H_{H2O}, T)$$

$K_{dry}(\Delta H_{H2O},T)$ and $K_{wet}(\Delta H_{H2O},T)$ were found from humidity and temperature(RH = 50%) modelling.

All constants were adjusted for real areas.

Temperature modelling (RH = 50%):

Concrete floor tile:



Turbulence modelling:

Assumptions:

- Turbulence depends on linear air flow velocity and is only a result of air exchange.
- Experimental flow dependent v_d-values are valid for real indoor settings.

At small turbulence intensity in exp. chamber:

$$v_t = \frac{1}{\tan^{-1}\left(\delta\sqrt{\frac{K_e}{D}}\right)}\left(D^{1-\frac{1}{m}} K_e^{\frac{1}{m}}\right) \quad , \quad K_e = k_0^2 \frac{du}{dy}$$

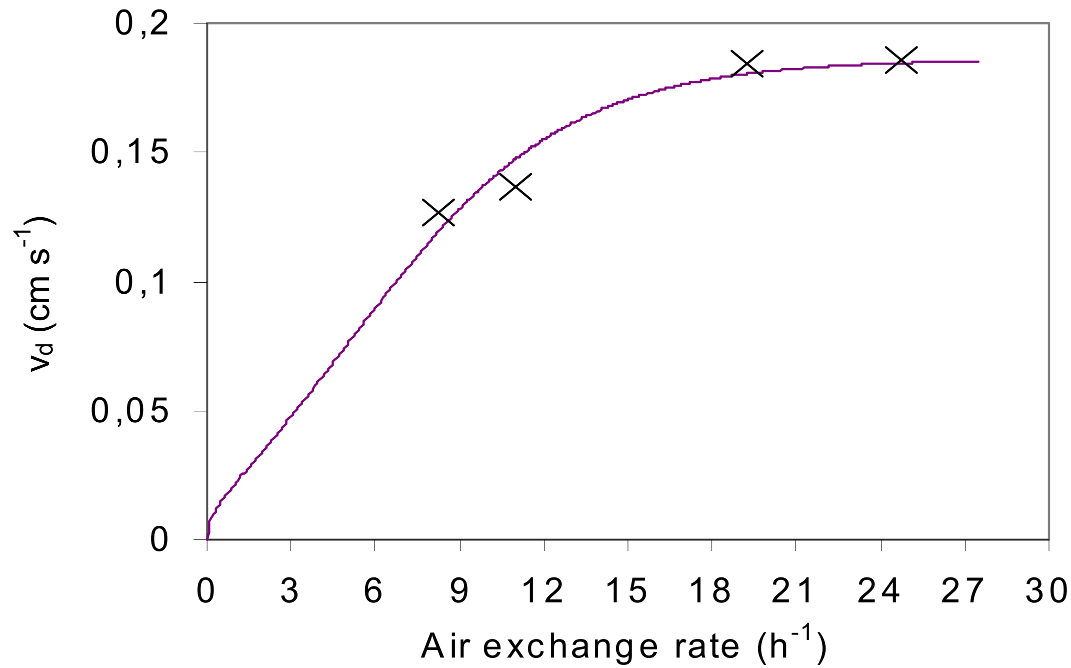
$k_0 = 0.4$,

$m = 2$,

$\delta(K_e)$ and $dy = \exp(-\mathbf{A}u)$

(Corner and Pendelbury 1951)

"A" was found from fit of: $v_d = \left(\frac{1}{v_t} - \frac{1}{v_s} \right)^{-1}$ to experimental data.



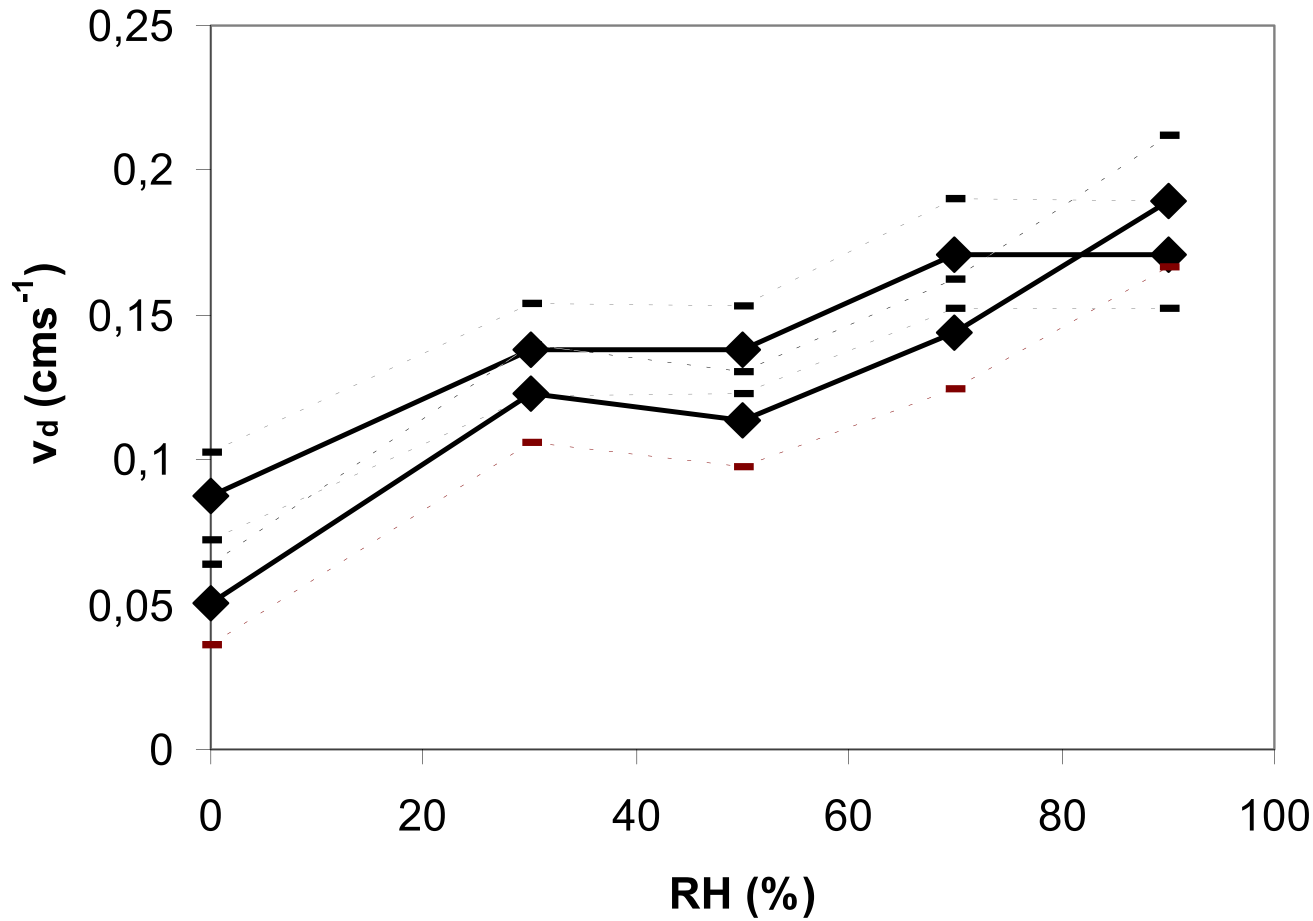
Model data were then adjusted using:

$$v_d = \left(\frac{1}{v_t} - \frac{1}{v_s} \right)^{-1} \quad \text{with:} \quad v_t = \left(DK_e \right)^{\frac{1}{2}}$$

Modelling of SO_2 deposition on indoor materials.
- Humidity and temperature dependence.

Measured deposition velocities at 48 h. (T = 22°C).

Smooth concrete floor tile:



Modelled deposition velocities at 48 h. (T = 22ºC).