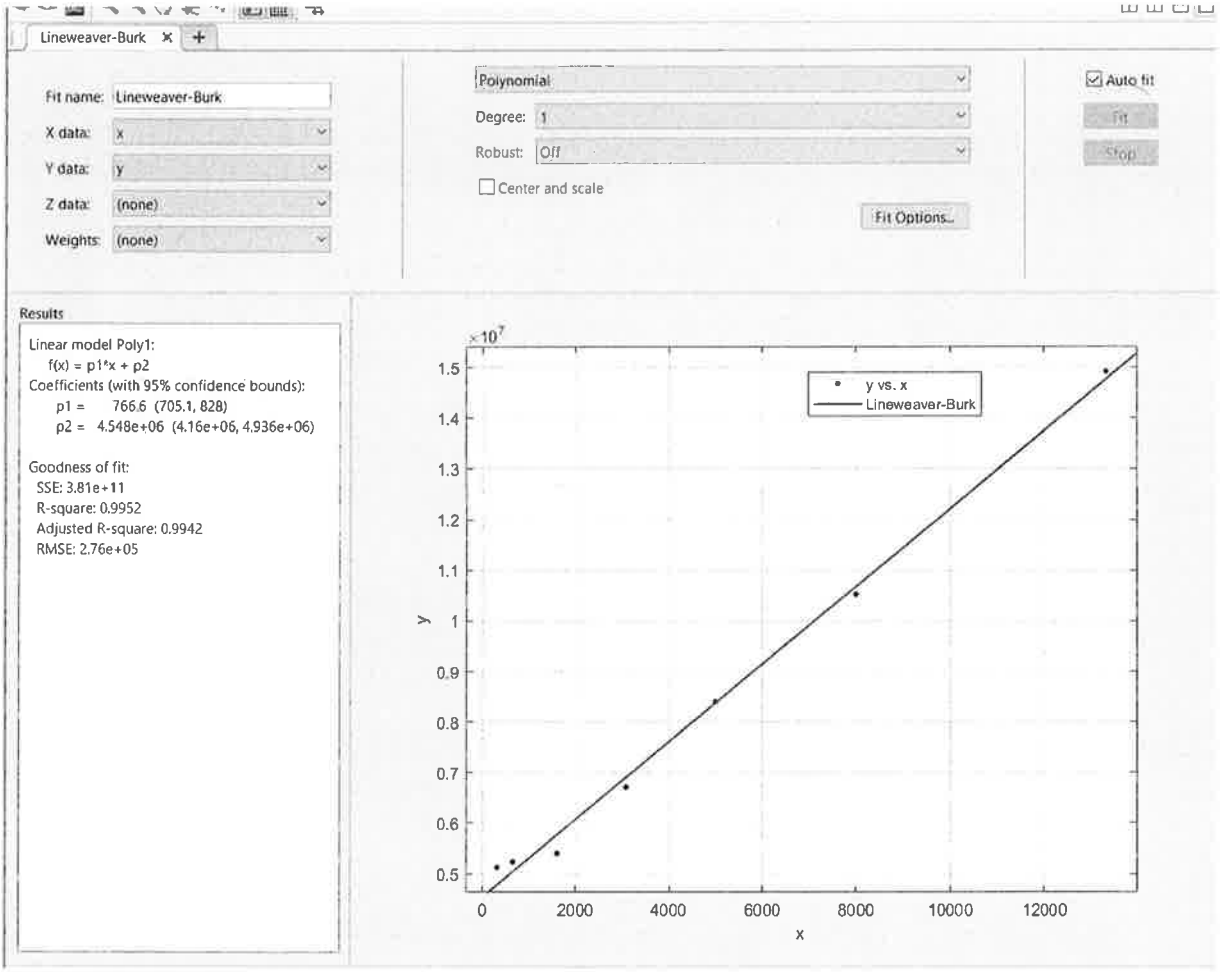
CHEM-C3220 - Kemiallinen dynamiikka

5. laskuharjoitus 2.12.2020

1. >> S=[7.5 12.5 20.0 32.5 62.5 155.0 329.0]*1e-5;
>> R=[0.067 0.095 0.119 0.149 0.185 0.191 0.195]*1e-6;
>> x=1./S;y=1./R;
>> cftool



Leikkauspiste = $1/R_{max}$ ja kulmakerroin = K_m/R_{max}. Leikkauspiste = p2 = $(4.55 \pm 0.40)\cdot 10^6$ → $\underline{R_{max} = (2.20 \pm 0.20)\cdot 10^{-7}\ \text{M/s}}$

Kulmakerroin = p1 = 767 ± 61 → $K_m = (767 \pm 61)(2.20 \pm 0.20)\cdot 10^{-7}$ M = $\underline{(0.17 \pm 0.03)\ \text{mM}.}$

2. Lasku Excel-taulukossa MyCourses:ssa.

3.

$$S + H \xrightarrow{k_1} E + 2H$$

$$E + H \xrightarrow{k_2} E + X$$

$$\frac{dS}{dt} = -k_1 SH$$

$$\frac{dH}{dt} = k_1 SH - k_2 EH$$

$$\frac{dE}{dt} = k_1 SH$$

Aja Matlab-ohjelma "runkiiva"

4.

$$E + S \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} ES \xrightarrow{k_2} E + P \underset{k_{-I}}{\overset{k_I}{\rightleftharpoons}} EP$$

$$[E]_0 = [E] + [ES] + [EP] \qquad [EP] = K_I [E][P]$$

$$[E]_0 = [E]\left(1 + K_I [P]\right) + [ES]$$

$$\frac{d[ES]}{dt} = k_1 [E][S] - (k_{-1} + k_2)[ES] = 0$$

$$[ES] = \frac{k_1 [E][S]}{k_{-1} + k_2} = \frac{[E][S]}{K_m}$$

$$[E]_0 = [E]\left(1 + K_I [P] + \frac{[S]}{K_m}\right)$$

$$[E] = \frac{[E]_0}{1 + K_I [P] + [S]/K_m}$$

$$[ES] = \frac{[E]_0 [S]}{K_m + K_m K_I [P] + [S]}$$

$$v = \frac{k_2 [E]_0 [S]}{[S] + K_m\left(1 + K_I [P]\right)} = \frac{d[P]}{dt}$$

$$\frac{1}{v} = \frac{1}{v_{max}} + \frac{K_m\left(1 + K_I [P]\right)}{v_{max}[S]}$$

$$\frac{d[P]}{dt} = \frac{P_{max}\left([S]_0 - [P]\right)}{\left([S]_0 - [P]\right) + K_m\left(1 + K_I [P]\right)}$$

Aja Matlab-ohjelm. "runP1"

5.

$$F(v) = \frac{\sqrt{\pi m^3}}{\sqrt{2kT}} \underbrace{\frac{4}{\sqrt{\pi}} x^2 e^{-x^2}}_{\int_0^\infty = 1} \qquad x = \frac{mv^2}{2kT} = \frac{Mv^2}{2RT}$$

$v = 300$ m/s $T = 298$ K $\Rightarrow x = 0.7265$

$v = 600$ m/s $T = 298$ K $\Rightarrow x = 2.9061$

$v = 300$ m/s $T = 1000$ K $\Rightarrow x = 0.2165$

$v = 600$ m/s $T = 1000$ K $\Rightarrow x = 0.8660$

Lasketaan integraali $\int_{300}^{600} x^2 e^{-x^2} dx$ Mathematican avulla

298 K: 78.7 %

1000 K: 31.0 %

```
In[1]:= Integrate[4 / Sqrt[Pi] * x^2 * Exp[-x^2],
          {x, 0.7265, 2.9061}]

Out[1]= 0.787056

In[2]:= Integrate[4 / Sqrt[Pi] * x^2 * Exp[-x^2],
          {x, 0.2165, 0.8660}]

Out[2]= 0.310287
```