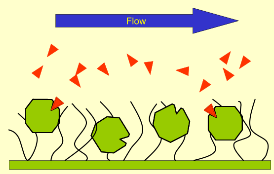
1.1. Langmuir one to one interaction

The reaction between immobilized ligand (L) and analyte (A) can be assumed to follow pseudo first-order kinetics (3, 1, 4, 2). During the association phase the number of formed complex (LA) increases as a function of time. After binding, when the analyte concentration drops to zero, a time-dependent dissociation follows. The interaction is equivalent and independent for all binding sites (5).



1:1 Langmuir interaction

It is assumed that the flow in the cell is sufficiently high so that there is no depletion or accumulation of analyte in solution, that the analyte concentration remains constant during the association phase, that the analyte concentration is zero and there is no analyte rebinding during the dissociation phase.

Reaction equation

$$L + A \underset{k_d}{\overset{k_a}{\rightleftarrows}} LA \tag{1.1}$$

Differential equations

$$\frac{d[L]}{dt} = -\left(k_a \cdot [L] \cdot [A] - k_d \cdot [LA]\right)$$
$$\frac{d[LA]}{dt} = k_a \cdot [L] \cdot [A] - k_d \cdot [LA] \tag{1.2}$$

[A] $= C_{analyte}$
$[L]_0 = R_{max}$
$[LA]_0 = 0$

Parameters

[L] = concentration of free ligand in RU
[A] = concentration of free analyte in M
[LA] = concentration of ligand-analyte complex in RU
k_a = association rate constant in $M^{-1}\ s^{-1}$
k_d = dissociation rate constant in s^{-1}

Integrated rate equations

$$R = R_{eq}\left(1 - e^{-(k_a \cdot C + k_d)(t - t_0)}\right)$$
$$R = R_0 \cdot e^{-k_d (t - t_0)} \tag{1.3}$$

$$R_{eq} = \frac{k_a \cdot C}{k_a \cdot C + k_d} \cdot R_{max}$$

Result of the fitting

[Analyte]	Conc
ka (1/Ms)	ka
kd (1/s)	kd
KD (M)	kd/ka
Rmax (RU)	Rmax
RI (RU)	RI
Req (RU)	ka*Conc*Rmax/(ka*Conc+kd)

Numeric model

```
LA+$1*RI1;

$1=(sign(t-ton1)-sign(t-(ton1+c_time)))/2;

$2=kt*($1*conc-A);

$3=ka*L*A*-kd*LA;                                   (1.4)

A=$2-$3|0;
```

conc = concentration of analyte in M
ton1 = start time of analyte injection
c_time= duration of the injection in seconds

```
L=-$3|Rmax;
LA=$3|0;
```

The numeric model can be added to the general tab of the models in the BiaEvaluation 4.1 software of Biacore. The model takes a mass transfer parameter in the form of k_t.

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Explanation document	Langmuir one to one.pdf
Integrated model	Langmuir one to one integrated.pdf and *.mdl
Numeric model	Langmuir one to one numeric.pdf and *.mdl
Example data	Langmuir one to one.txt
Example data	Langmuir one to one.ble

Example data:

Concentrations: 10, 20, 40, 80, 160 nM

References

1. **BIACORE AB**; BiaEvaluation 3.0; Biacore AB; 1997.
2. **Bjorquist, P. and Bostrom, S.**; Determination of the kinetic constants of tissue factor/factor VII/factor VIIA and antithrombin/heparin using surface plasmon resonance. *Thromb.Res.* **(85)**: 225-236; 1997.
3. **Chaiken, I. M.**; *Anal.Biochem.* **(212)**: 457-468; 1993.
4. **Jonsson, U. et al**; Real-time biospecific interaction analysis using surface plasmon resonance and a sensor chip technology. *Biotechniques* **(11)**: 620-627; 1991.
5. **O'Shannessy, D. J. and Winzor, D. J.**; Interpretation of deviations from pseudo-first-order kinetic behavior in the characterization of ligand binding by biosensor technology. *Anal.Biochem.* **(236)**: 275-283; 1996.