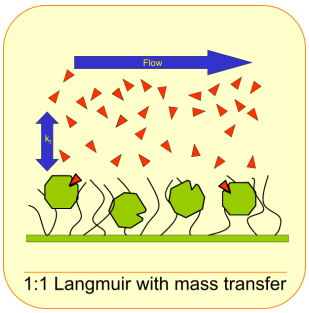
1.1. 1:1 interaction with mass transfer - kt



1:1 Langmuir with mass transfer

Binding of analyte (A) to the ligand (L) on the sensor chip is in principle a two-step event. First, the analyte is transferred from the bulk solution (A_{bulk}) towards the sensor chip surface ($A_{surface}$). Second, the binding of the analyte to the ligand takes place. The first step is also known as mass transfer and is driven by convection and diffusion (3). Both events have their specific rate constants. The coefficient for mass transfer (k_t) is the same in both directions (1).

The coefficient for mass transfer is calculated without taking into account the mass of the analyte. The mass transfer rate (k_t) is in RU M^{-1} s^{-1}.

It is assumed that the flow in the cell is sufficiently high so that there is no depletion or accumulation of analyte in solution and that the analyte concentration remains constant.

Reaction equation

$$A_{bulk} \underset{k_t}{\overset{k_t}{\rightleftharpoons}} A_{surface} + L \underset{k_d}{\overset{k_a}{\rightleftharpoons}} LA \qquad (0.1)$$

Differential equations

$$\frac{d[A_{surface}]}{dt} = k_t \cdot ([A_{bulk}] - [A_{surface}]) - (k_a \cdot [L] \cdot [A_{surface}] - k_d \cdot [LA])$$

$$\frac{d[L]}{dt} = -(k_a \cdot [L] \cdot [A_{surface}] - k_d \cdot [LA]) \qquad (0.2)$$

$$\frac{d[LA]}{dt} = (k_a \cdot [L] \cdot [A_{surface}] - k_d \cdot [LA])$$

$[A_{surface}]_0 = 0$
$[A_{bulk}] = C_{analyte}$
$[L]_0 = R_{max}$
$[LA]_0 = 0$

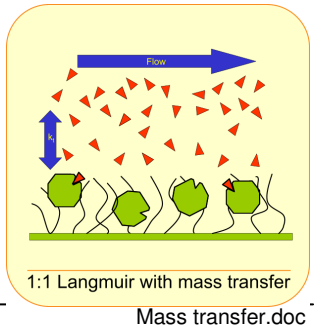
Parameters

$[A_{bulk}]$ = analyte concentration in buffer in M
$[A_{surface}]$ = analyte concentration at surface of sensor chip in M
[L] = concentration of free ligand in RU
[LA] = concentration of ligand-analyte complex in RU
k_a = rate constant for association in M^{-1} s^{-1}
k_d = rate constant for dissociation in s^{-1}
k_t = coefficient for mass transfer in RU M^{-1} s^{-1}

Result of the fitting

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

1:1 interaction with mass transfer – km



1:1 Langmuir with mass transfer

Binding of analyte (A) to the ligand (L) on the sensor chip is in principle a two step-event. First, the analyte is transferred from the bulk solution (A_{bulk}) towards the sensor chip surface ($A_{surface}$). Second, the binding of the analyte to the ligand takes place. The first step is also known as mass transfer and is driven by convection and diffusion (3). Both events have their particular rate constants. The coefficient for mass transfer (k_m) is the same in both directions.

This model is different in the way the mass transfer is calculated. The k_m is calculated with a term for the mass of the analyte. The mass transfer rate (k_m) is given as the diffusion rate in m s^{-1} (2).

It is assumed that the flow in the cell is sufficiently high so that there is no depletion or accumulation of analyte in solution and that the analyte concentration remains constant.

Reaction equation

$$A_{bulk} \underset{k_m}{\overset{k_m}{\rightleftharpoons}} A_{surface} + L \underset{k_d}{\overset{k_a}{\rightleftharpoons}} LA \qquad (0.3)$$

Differential equation

$$\frac{d[L]}{dt} = -\left(\left(\frac{k_a}{1+k_a\cdot[L]}{10^9\cdot Mr\cdot k_m}\right)\cdot[L]\cdot[A] - \left(\frac{k_d}{\frac{1+k_a\cdot[L]}{10^9\cdot Mr\cdot k_m}}\right)\cdot[LA]\right)$$

$$\frac{d[LA]}{dt} = \left(\frac{k_a}{\frac{1+k_a\cdot[L]}{10^9\cdot Mr\cdot k_m}}\right)\cdot[L]\cdot[A] - \left(\frac{k_d}{\frac{1+k_a\cdot[L]}{10^9\cdot Mr\cdot k_m}}\right)\cdot[LA] \qquad (0.4)$$

[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}
k_m = mass transfer constant in m s^{-1}
Mr = molecular mass of analyte in Dalton
10^9 = conversion factor between molar concentration and RU

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;

A=$2-$3|0;

L=-$3|Rmax;

LA=$3|0;
```

(0.5)

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

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.

Download zip-file

Explanation document	Mass transfer.pdf
Integrated models	Mass transfer.pdf and *.mdl
Numeric model	Mass transfer numeric.pdf and *.mdl
Example data	Mass transfer.txt
Example data	Mass transfer.ble

Example data:

Concentrations: 5, 10, 20, 40, 80, 160 nM

References

1. **BIACORE AB**; BiaEvaluation 3.0; Biacore AB; 1997.
2. **BIACORE AB**; BiaEvaluation 3.0. 1999.
3. **Glaser, R. W.**; Antigen-antibody binding and mass transport by convection and diffusion to a surface: a two-dimensional computer model of binding and dissociation kinetics. *Anal.Biochem.* **(213)**: 152-161; 1993.