Syntax of equation - basic rule

1. In general follow the Excel equation formulation rules.
2. Start with **"y="**
3. No space
4. Case sensitive
5. Independent variable (x data) is **x1**.
6. Parameters are **p1, p2, p3**,… (Numbers have to be sequential.)
7. Parameter values are always positive.
8. Maxium parameter count is 8.
9. No differentials

Examples)

Polynomial equation: y=p1*x1^2+p2*x1+p3

Exponential equation (single exponential decay): y=p1*exp(-p2*x1) [p1 is an initial value, p2 is rate constant, and x1 is usually a time.]

Michaelis-Menten equation: y=p1*x1/(p2+x1) [p1 is Vmax, p2 is Kd, and x1 is a reactant concentration.]

Syntax of equation - special cases

1. **Using Newton-Raphson method (Please see references for the details about Newton-Raphson method described elsewhere.)**

…Before evaluating sum of square value root value is numerically calculated by real-valued function and is assigned to fitting equation.

Syntax)

A root variable: **n1**

Real-valued function (Newton Raphson equation) to find rood value: start with **"f="** (*x: f(x)* = 0)

Example) **Competitive Inhibition**

Equilibrium binding of reactants (A and B) in the presence of competitive inhibitor (I)

$A + B \leftrightarrow AB$

$A + I \leftrightarrow AI$

If added A concentration is 20 and added B concentration is 40…

Real-valued function to find rood value: f=20-n1*40/(p1+n1)-n1*x1/p2

Fitting equation for evaluating sum of square values: y= n1*40/(p1+n1)

n1: free A concentration (unknown)

x1: Added I concentration (independent variable: x values)

p1: Dissociation constant (Kd) of (A + B reaction)

p2: Dissociation constant (Ki) of (A + I reaction)

y: Concentration of AB complex (y data values, usually experimentally found by activity and in this case activity of AI complex is assumed to be zero.)

2. Equation contains integration.

…rare case when equation contains integral equation parts.

Syntax)

Integral equation part starts with **"I1=", "I2=", "I3=",…(**multiple number of integral equation accepted) followed by "lower range number : upper range number : increment:", then write integrating equation. (Range number part can contain p1, p2,…,x1, x2,…,c1, c2…)

Integration variable: t1, t2, t3….

Calculation speed heavily depends on range values and increments.

Example)

This is not a real case but …

$$y = a * x + \int_0^{100} \exp(-bt)\, dt$$

is written as…

```
I1=0:100:1:exp(-p1*t1)  …(*Increment in this case is 1.)
y=p2*x1+I1
```