GRAPHICAL PRESENTATION OF EXPERIMENTAL DATA

In «y = ax + b» equation, there are two sets of values:

Constant: fixed values in the equation;

slope (a) and intercept (b)

Variable: “x” and “y”;

x: time, **y:** concentration

.

- **Variables** may be classified as **independent** and **dependent** variables:

Independent variable:

- **Fixed** variable in an experiment, .
- Represented by "**x**,"
- Example: **time**

Dependent variable:

- **Measurable** variable in an experiment
- Represented by "**y**"
- Stands alone on one side of an equation.
- Example: **Concentration** (vitamin conc., pigment conc., the number of m.o.'s etc).

- **<u>Example 2.1:</u>** The loss of ascorbic acid in orange juice during storage (at 10^{o}C) will be studied. For this experiment, define the dependent and independent variables.
  - Independent variable (x): ……
  - Dependent variable (y): ……

Graph

- Graph shows the relation between **dependent** and **independent** variables.
- **Independent variable** is plotted on horizontal axis (abscissa, x).
- **Dependent variable** is plotted on vertical axis (ordinate, y).

Experimental data can be fitted to an equation using the following techniques

- *Graphical method (practical, but not concise)*
- *Linear regression (statistical meth, very concise)*

In both methods, **slope** and **intercept** are determined.

Equation of straight line

The equation of straight line which passes at least two points is expressed by the following equation:

$$y = a(x) + b$$

a : Slope,

b : Intercept.

Slope: Ratio of the change in “y” variable to the change in “x” variable.

In terms of the deterioration kinetic of foods;

slope is the change in the quality factor (concentration) in question (interest) over time.

Slope is calculated by placing the (x_1,y_1) and (x_2,y_2) coordinates in the following equation:

$$\textbf{Slope (a)} = \frac{y_2 - y_1}{x_2 - x_1} = \frac{\Delta y}{\Delta x}$$

- **Intercept (y-intercept)**; The point on the ordinate, when x=0.

  To find y-intercept, straight line is **extrapolated** to the point to cross the ordinate, when x=0.

Graphical method

- Original experimental data are plotted to form a straight line.
- Best-fitting line is passed through the data points by using «**the freehand method of curve fitting**.»
- Two points are marked on the straight line, and the coordinates are determined; (x1, y1) and (x2, y2), and then, the **slope** is calculated from these coordinates
- The **intercept** is calculated from the straight line.

Plotting the experimental data

- ***First step:*** Determine the independent (x) and dependent variable (y)

- ***Second step:*** The titles of axes are written on the center of each scale.

- ***Third step:*** Determine increments for both “x” and “y” scales. For that, take into consideration of the smallest and largest values and then determine increments.

For example; in an experiment, orange juice samples were taken in 0, 5, 9, 16, 22, 28 days from storage and analyzed for ascorbic acid content (55, 51, 44, 40, 37 and 30 mg/100 mL, respectively). Find out the increments in «x» and «y» axes.

- ***Fourth step:*** Experimental data are plotted on a arithmetic or semi-log graph paper depending on the relationship between «x» and «y» values. (our purpose is to obtain the **best** straight line)

  Experimental data are marked in cartesian system by using circle, square, rectangular, triangle or asterix symbols, **not using point**,

- ***Fifth step:*** Draw straight line which takes into consideration of all points (not necessarily passing the most points)

- ***Sixth step:*** Mark two points on straight line and determine coordinates of these points ((x_1 y_1) and (x_2 y_2)).

✓ Calculate **slope** using these coordinate values.

✓ Extrapolate straight line to “y” axis to determine **y-intercept.**

- ***Seventh step:*** Determine the equation of straight line by using **slope** and **intercept** values.

$$y = a\,(x) + b$$

Example 2.2: Plotting the experimental data

- The change in ascorbic acid (aa) content of pasteurized orange juice during storage at 30°C was studied. AA contents of periodically drawn samples from storage were determined by HPLC method and results are given in Table 2.1.

- Plot the experimental data in an arithmetic graph paper.

- Determine **slope**, **intercept** and the **equation** describing aa degradation during storage of orange juice at 30°C.

- Give the **units** of slope and intercept.

- Calculate **«% aa degraded»** and **«% aa retained»** after 3 and 7 days of storage at 30°C.

Table 1 AA contents of orange juice stored at 30°C

Time (days)	AA concentration (mg L^{-1})
2	457
4	305
5	251
6	148

Solution

- ***First step:*** Determine the independent (x) and dependent variable (y)

  x →

  y →

- ***Second step:*** The titles of axes are written on the each scale by centering the scale.

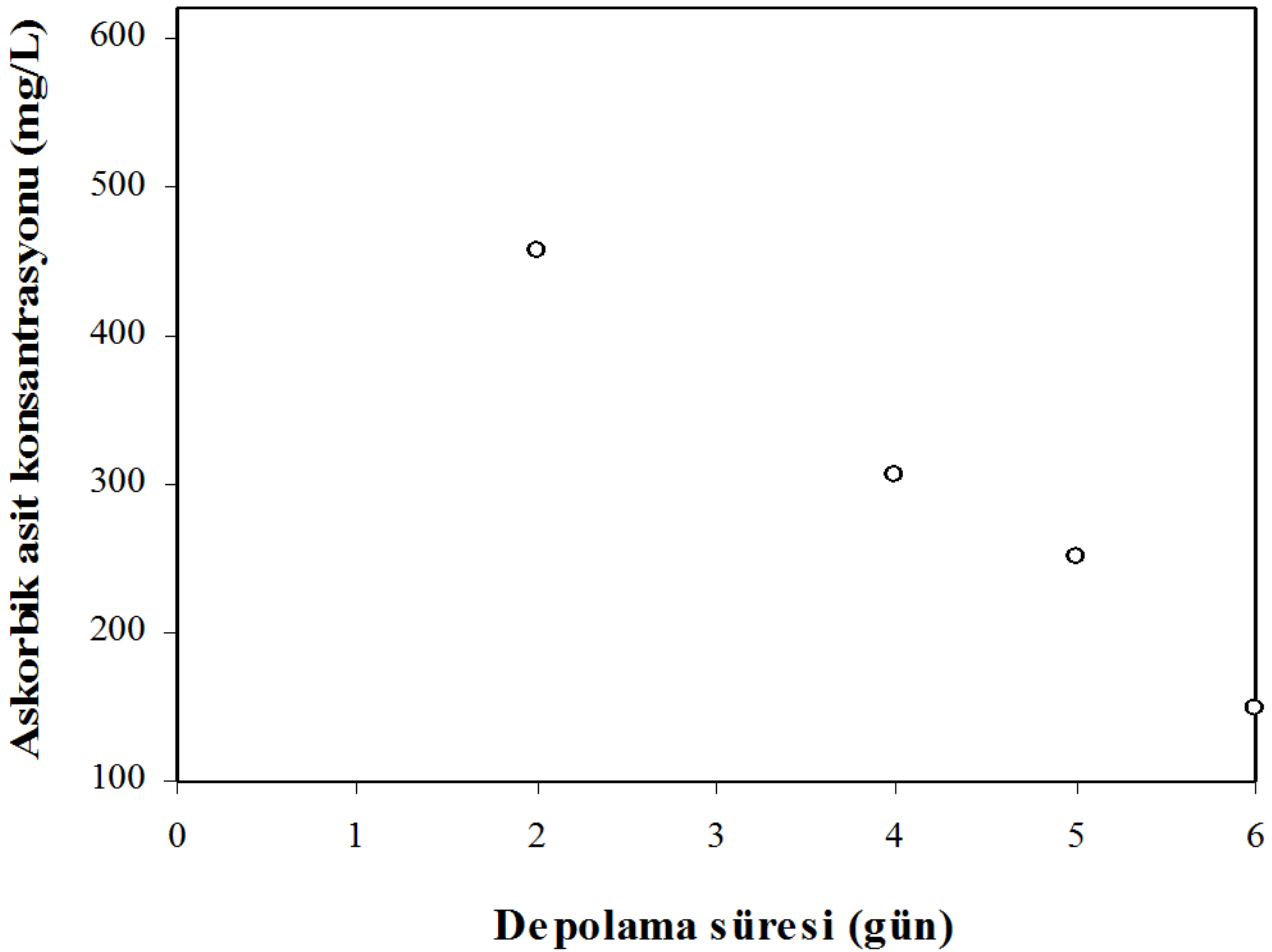
- ***Third step:*** Determine the increments for both “x” and “y” scales.

For that, take into consideration of the smallest and the largest values and then determine the increments.

- For esthetical reason, «y» axis should not be started from «0.»

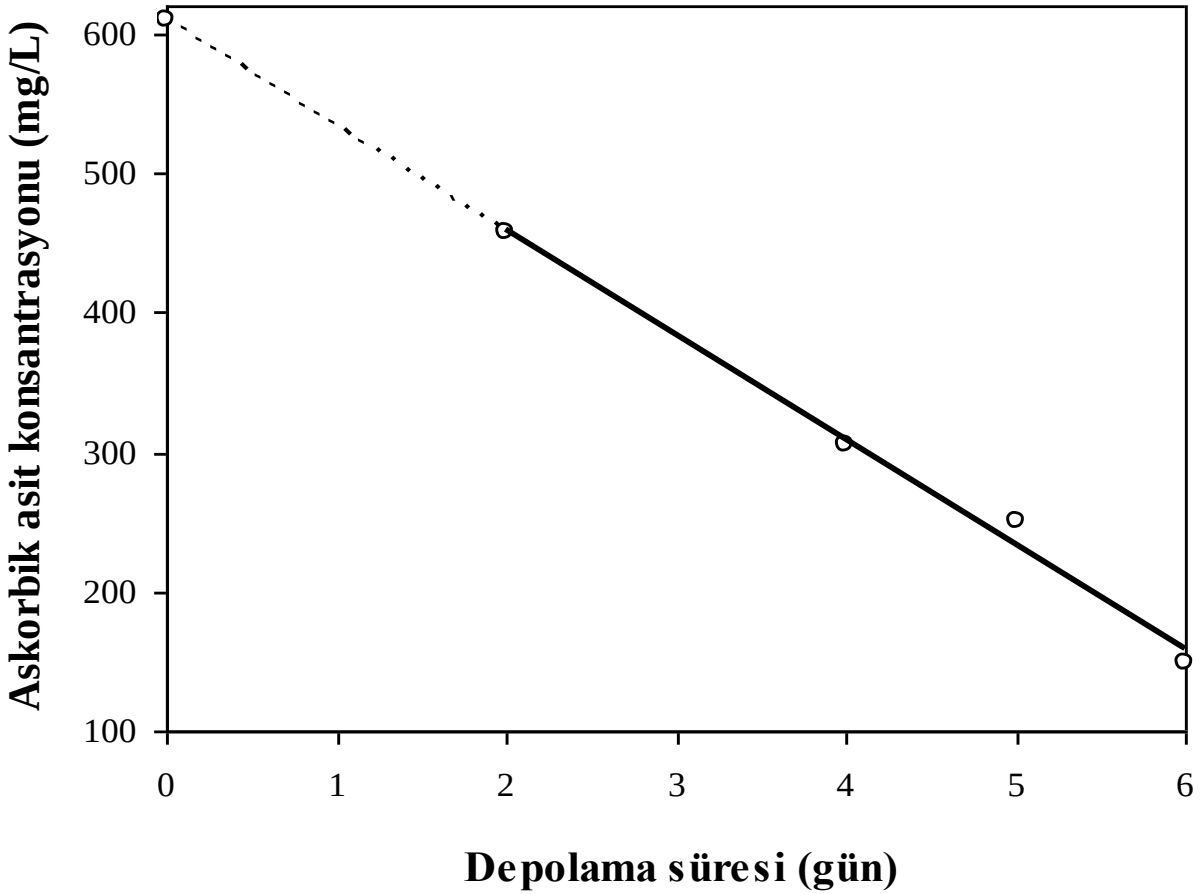
- Although there was no need for starting «x» from «0», «x» axis **should be** started from «0» in order to calculate intercept.

- **Fourth step:** Experimental data are plotted on an arithmetic graph paper.



- ***Fifth step:*** Draw straight line which «almost includes all the points» by using the freehand method of curve fitting (Figure 2).

Figure 2.3 Drawing straight line by the freehand method of curve fitting



- ***Sixth step:*** Mark two points on straight line and determine coordinates of these points; (300, 4.10) ve (400 2.75) By using these coordinate values, calculate **slope** from the equation.

$$\text{Slope (a)} = \frac{y2 - y1}{x2 - x1} = \frac{400 - 300}{2.75 - 4.10} = -74.07 \text{ mg/L day}$$

Interpretation: **??????????**

$$\text{Slope (a)} = \frac{y2 - y1}{x2 - x1} = \frac{400 - 300}{2.75 - 4.10} = -74.07 \text{ mg/L day}$$

Interpretation: For each «single» day, 74.07 mg of aa was degraded from 1 L of orange juice.

For the determination of **intercept**, straight line is extrapolated to “y” axis by marking dotted lines.

intercept (b) = ?????

intercept (b) = 610 mg/L

- ***Seventh step:*** Determine the equation of line by using slope and intercept values.

$$y = -74.07x + 610$$

Eight step: To calculate the aa content of orange juice after 7 days of storage.

***Put* «7» in place of (x) in the** equation.

$$x = 7 \rightarrow y = -74.07\,x + 610$$

$$y = -74.07\,(7) + 610$$

$$y = 91.51 \text{ mg } L^{-1}$$

- ***Nineth step:*** «%» of aa degraded in orange juice after 7 days of storage was calculated from the following equation.

$$\%\text{degraded} = \frac{\text{amount of aa degraded}}{\text{amount of aa at the beginning}} (100)$$

$$\%\text{retained} = \frac{\text{amount of undegraded aa}}{\text{amount of aa at the beginning}} (100)$$

$$\%\text{degraded} = \frac{610 - 91.51}{610}(100) = 85\%$$

$$\%\text{reatined} = \frac{91.51}{610}(100) = 15\%$$

After 7 days of storage at 30°C:

- **85%** of aa was degraded.
- **15%** of aa was retained.

After 3 days of storage at 30°C:

- **36.4%** of aa was degraded.
- **63.6%** of aa was retained.

Example 2.3:

When the «Y» kg of water is added to 1 kg of food material containing (X) kg of water, water content of the material is raised to 35%. Determine the equation defining this situation.

Solution: Water ratio of food material is defined with the following equation.

$$\frac{\text{.....}}{\text{.....}} (100) = 35$$

Solution: Water ratio of food material is defined with the following equation.

$$\frac{x + y}{1 + y}(100) = 35$$

This equation is rearranged to show the "slope-intercept" form:

$$y = -1.538\,x + 0.538$$

This is the equation which describes the relationship between the water needed to be added to 1 kg food and the mositure content (%) of this food, which will contain 35% moisture after water addition.

«x» and «y» variables

x: Moisture content of food (%)

y: Amount of water needed to be added to 1 kg food (kg)

This equation is plotted to the arithmetic graph paper

$$y = -1.538\,x + 0.538$$

- **First point:** **Clue;** y-intercept value.

  x= ?, then y = ? (**?, ?**).

- **Second point:** **Clue;** x-intercept value.

  y= ?, then x = ? (**?, ?**).

$$y = -1.538\,x + 0.538$$

- **First point:** **Clue;** y-intercept value.

  x= 0, then y = ???.

- **Second point:** **Clue;** x-intercept value.

  y= 0, then x = ???.

$$y = -1.538\,x + 0.538$$

- **First point:** **Clue;** y-intercept value.

  x= 0, then y = 0.538.

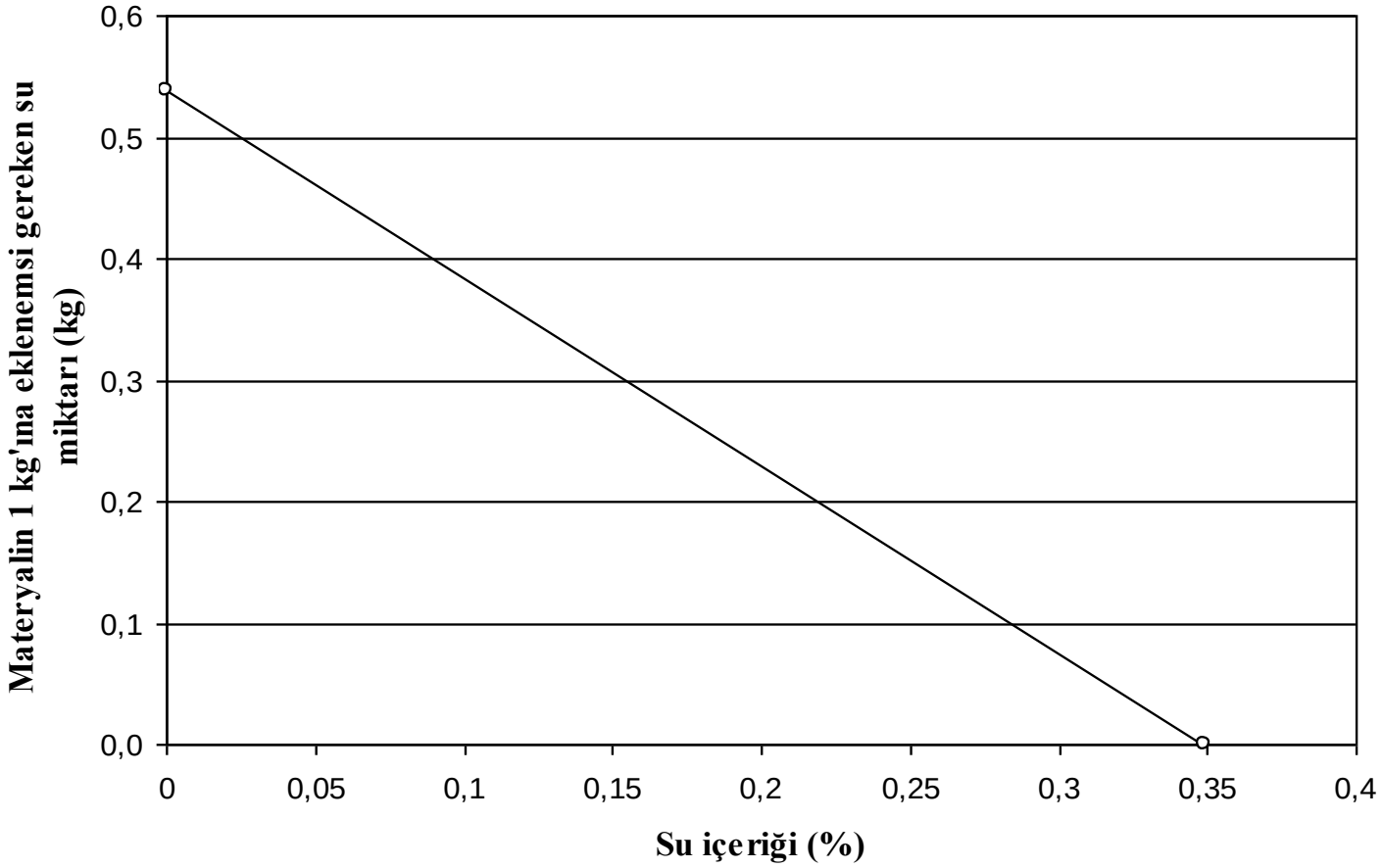
- **Second point:** **Clue;** x-intercept value.

  y= 0, then x = 0.35.

- **Negative sign of slope** shows that straight line will go straight down.

- Of course, straight line **must** pass from these two data points (**Figure 2.4**).

Figure 2.4 Graph for the equation of «Y = -1.538 X + 0.538»



Interpretation of the graph

- **At any point on the straight line, the food will contain 35% water**
- …….. kg water should be added to 1 kg food material containing **0% water**, then the water content of food material will be 35%.
- ……. kg water should be added to 1 kg food material containing **10% water**, then the water content of food material will be 35%.

- **0.538** kg water should be added to 1 kg food material containing **0% water** **(x=0)**, then the water content of food material will be 35%.

- **0.384** kg water should be added to 1 kg food material containing **10% water** **(x=0.1)**, then the water content of food material will be 35%.