REACTION TYPES AND ORDERS

- Chemical reactions occur in foods during both **processing** (pasteurization and sterilization) and **storage**.

- **Degradation reactions**: Result in the loss of quality. (Must be minimized.)

- **Formation reactions**: Produce desirable or undesirable flavor or color. (Must be maximized or minimized)

Reaction kinetics deals with:

- The mechanisms of the chemical reactions

- **Reaction rates**

- As a food engineer, we only deal with the **substrates** and the **products**.

- **Intermediate products** are usually not very important because they are formed and used immediately. (Difficult to measure)

- Exceptions in foods, **HMF,**hydroxymethylfurfural
  - HMF formed during browning as an intermediate products.
  - HMF gives estimate about ongoing browning reactions.
  - HMF can easily be measured.

Reaction kinetics in food science

- <u>**Degradation of food constituents**</u>
- Formation of products
- Inactivation and growth of m.o.'s
- Inactivation and activation of enzymes

Difference between chemical and food engineering in terms of reaction kinetics

- **Chemical engineers** determines the conditions for high output.

  Therefore, their intention is to increase the reaction rate.

- **Food engineers** look for the conditions to reduce the reaction rate to preserve the substrates (**preserving the quality).**

Reaction types

- monomolecular reactions
- “bimolecular reactions

Monomolecular recations

- Involves with a single reactant.
- Examples:

$$A \xrightarrow{k_1} B \text{ (product)}$$

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C \text{ (product)}$$

$$A \xrightarrow{k_1} B + A \xrightarrow{k_2} C \text{ (product)}$$

Bimolecular reactions

- Involves with two reactans. The reactants may the same or different.

$$\mathbf{A + B \xrightarrow{k_1} C\ (product)}$$

$$\mathbf{A + B \xrightarrow{k_1} C\ (product) + D\ (product)}$$

Reaction rate

To calculate the reaction rate, we simply take into consideration of the change in the concentrations of either one of the reactants or the products per unit of time (which coefficent in the equation???).

$$\text{Reaction rate} = \frac{\text{Amount of substrate consumed (A)}}{\text{Time period}} \quad (\text{rate, “–”})$$

$$\text{Reaction rate} = \frac{\text{conc. of «A» at } t_2 \text{ time} - \text{conc. of «A» at } t_1 \text{ time}}{t_2 - t_1}$$

$$\text{Reaction rate} = \frac{\text{Amount of product formed (C)}}{\text{Time period}} \quad \text{(rate, “+”)}$$

$$\text{Reaction rate} = \frac{\text{C at } t_2 \text{ time} - \text{C at } t_1 \text{ time}}{t_2 - t_1}$$

Unit for reaction rate

$$\frac{mol/L}{s} = \frac{mol}{L\ s} = mol/(L\ s)$$

or,

$$\frac{mg/L}{s} = \frac{mg}{L\ s} = mg/(L\ s)$$

To determine the reaction rate in foods

- In food applications, take the food samples from processing or storage for certain time-intervals (such as every hour) and then analyze the content of food for the selected **reactant** or the **product**.

Anthocyanins + O_2 → ??????????

Sugar + amino acid → **Brown pigments**

Right or wrong?

- What is the reaction rate for sour cherry juice?

Right or wrong?

- What is the reaction rate for **anthocyanins** in sour cherry juice?

Right or wrong?

- What is the reaction rate for **anthocyanins** in **sour cherry juice** stored at **10^{o}C**?

- **What type of data would you need in order to calculate the reaction rate for anthocyanins in sour cherry juice stored at 10^{o}C?**

Concentration units for food constituents

- mg/100 mL,
- mg/L, mg/kg (ppm)
- μg/L, μg/kg (ppb)

Example 1 : Mg reacts with HCl and 448 cm^3 of H_2 gas is formed at 0°C and 1 atm pressure in 20 s. Find out the reaction rate for the H_2 gas formed in «mol s^{-1}».

$$Mg \quad + \quad 2HCl \quad \rightarrow \quad MgCl_2 \quad + \quad H_2$$

Interpretation: In every 1 s, 0.001 mole H_2 gas is formed during the reaction between Mg and HCl.

Example 2: What is the average rate of reaction (mole L^{-1} s^{-1}) of the following reaction when $[Sn^{++}]$ changes from 0.56 mole L^{-1} to 0.51 mole L^{-1} in 15 s. Also find the reaction rate for Fe^{++}.

$$2Fe^{+++}(aq) + Sn^{++}(aq) \rightarrow 2Fe^{++}(aq) + Sn^{+++}(aq)$$

Choosing the time period

- Time period is selected depending on the rate of the reaction.
- **Fast occurring reactions**: Select the small time periods, such as «second» or «min.»
  - For enzymatic reactions, choose «second,»
  - For microbial inactivations, choose «minute,»
  - For anthocyanin degradation, choose «minute» or «hour» depending on temperature.

- **Slow occurring reactions:** Select large time periods, such as «days,» «week,» or «month.»

  For carotenoid degradation, choose «days» or «week» depending on temperature.

Reaction rates and coefficients

When the reaction rate is known for a reactant or a product, the coefficients of the reaction's balanced equation is used to find the rates with respect to the other species.

Example (combustion of propane)

$$C_3H_8 + 5O_2 \rightarrow 3\,CO_2 + 4\,H_2O$$

- 5 moles of oxygen must be consumed per unit of time for each mole of propane used in the same time. Therefore, in this reaction, oxygen must react 5 times faster than propane.

- Similarly, CO_2 forms 3 times faster than propane reacts and water 4 times faster.

Example 3: Butane burns with oxygen to give carbon dioxide and water.

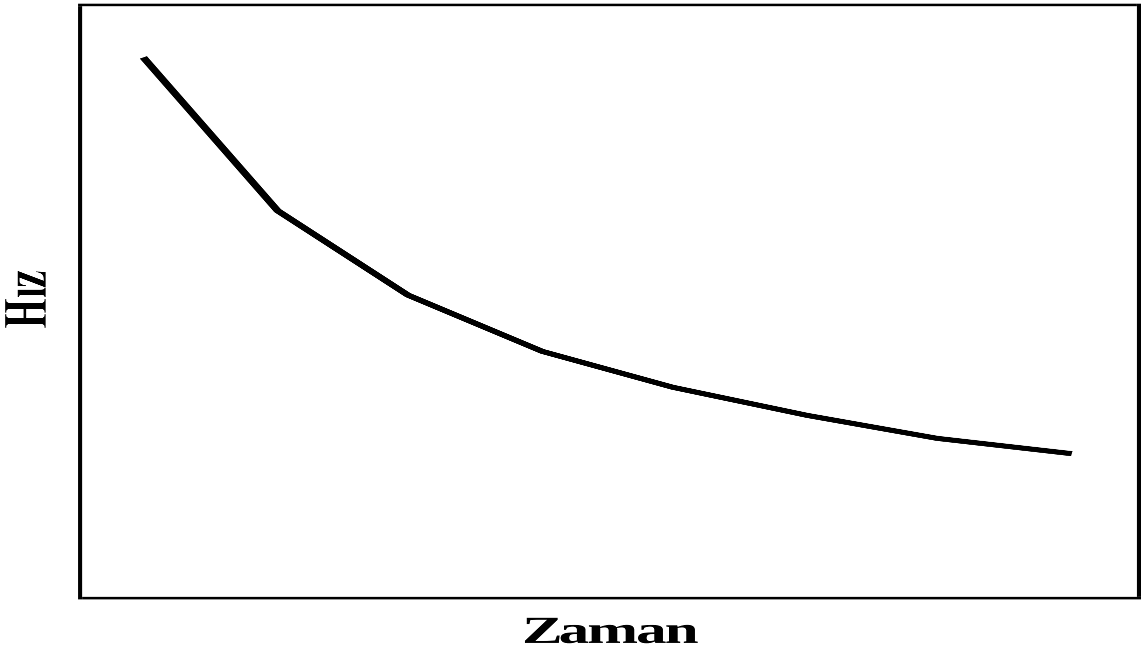
$$2\ C_4H_{10} \quad + \quad 13\ O_2 \quad \rightarrow \quad 8\ CO_2 \quad + \quad 10\ H_2O$$

If at a certain time, the butane conc. is decreasing at a rate 0.20 mol L^{-1} s^{-1}, what is the rate at which the oxygen conc. is decreasing, an what is the rate at which the CO_2 conc. is increasing?

Change of reaction rate with time

- Reaction rate is generally is **not constant** throughout the reaction and changes as the reactants are used up.

Effect of time on reaction rate



Reaction rates are generally higher at the beginning of the reaction when the high amount of reactants are present.

Example 4: The data for the decomposition of hydrogen iodide (HI) at 508°C is given in Table 1. Plot the data on an arithmetic scaled graph paper and determine the reaction rate for HI at 100 s.

$$2\,HI \rightarrow H_2 + I_2$$

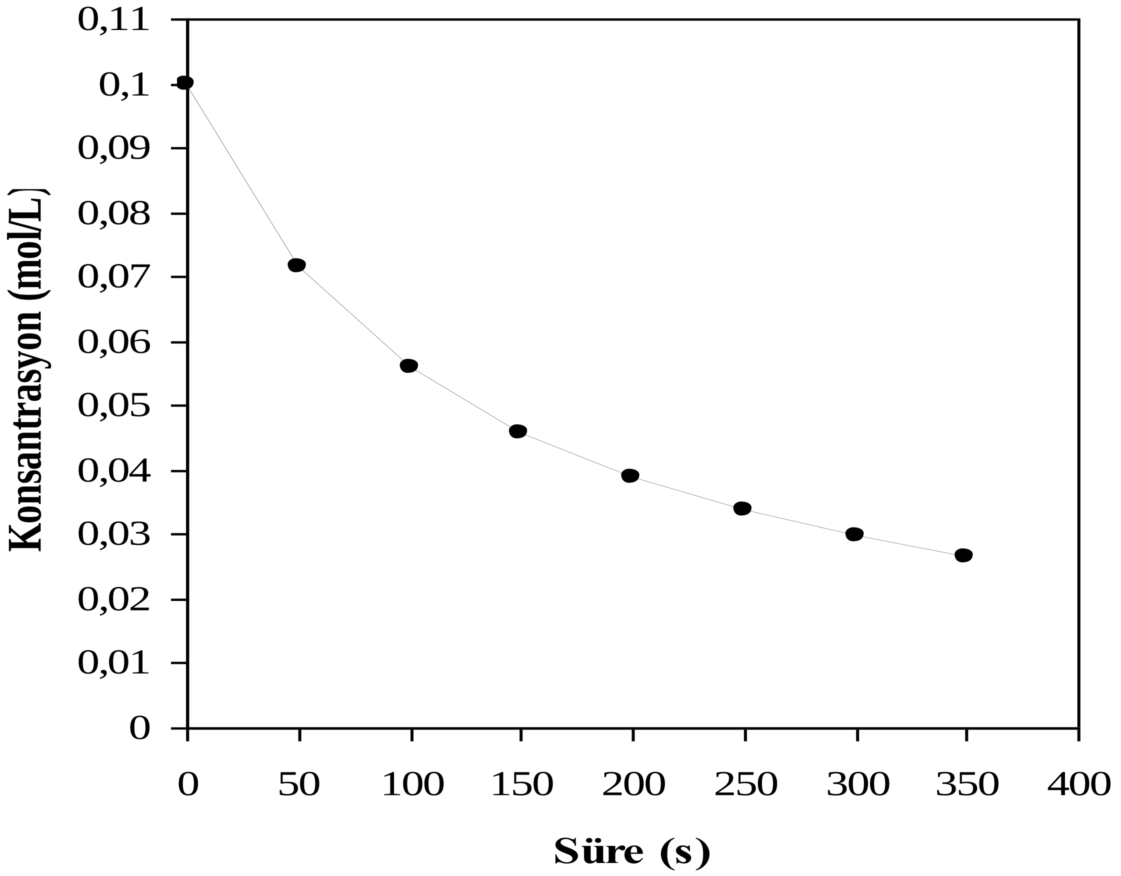
Table 1 Data at 508°C for the decomposition of HI

Time (s)	Concentration (mol L^{-1})
0	0.1000
50	0.0716
100	0.0558
150	0.0457
200	0.0387
250	0.0336
300	0.0296
350	0.0265

Solution

- Data is plotted on an arithmetic scaled graph paper.

Change in concentration of HI with time at 508°C



- Concentration of HI drops rapidly during the first 50 s. This indicates that the reaction occurs fast during the first 50 s.

- Between 300 and 350 s, concentration changes by only a small amount, so the rate has slowed down considerably.

- Conclusion: The steeper (dik) the curve, the higher is the rate.

- The rate at which HI is consumed at any particular time can be determined from the slope of the tangent drawn at 100 s.

- The slope of tangent is determined by taking coordinates of the two points and calculating the ratio of the change in concentration to the change in time.

Answer: rate (HI) =-2.5 x 10^{-4} mol/(L s)

Concentration and rate

The rate of a chemical reaction is proportional to the product of the molar concentrations of the reactants or products.

$$A + B \rightarrow C + D$$

$$\text{Rate } \alpha \ [A]^{n} [B]^{m}$$

$$\text{Rate } \alpha \ [C]^{x} [D]^{y}$$

The values of the exponents ***n*** and ***m*** need to be found experimentally.