IT Skill for Chemist

What is the Trapezoidal Rule?

The trapezoidal rule is a numerical integration method used to approximate the area under a curve. It is especially helpful when the exact integration is difficult or when only discrete experimental data points are available.

Formula:

For a function f(x) over the interval [a,b] divided into n equal subintervals of width $h=\frac{b-a}{n}$ the trapezoidal rule is:

$$\int_a^b f(x)dx \approx \frac{h}{2}[f(x_0) + 2f(x_1) + 2f(x_2) + \ldots + 2f(x_{n-1}) + f(x_n)]$$

Where: $x_0 = a$, $x_n = b$ and $f(x_i)$ are the values of the function at those points

Application in Chemistry

The trapezoidal rule is widely used in analytical and physical chemistry, especially when integrating experimental data. Here are some key applications:

1. Spectrophotometry (UV/Vis, IR, NMR)

- Purpose: To calculate area under absorption peaks, which is proportional to concentration.
- Use: When the absorption vs. wavelength graph is given as data points, the area is calculated using the trapezoidal rule to determine:
  - Concentration (via Beer-Lambert Law)
  - Molar absorptivity

2. Thermodynamics

- Purpose: To evaluate changes in properties such as enthalpy or entropy when data is given as discrete points.
- Use: For example:
  - Calculating entropy change from $\frac{Cp}{T}$ vs T
  - Calculating heat from Cp vs. T

$\Delta S=\int_{T1}^{T2} \frac{Cp}{T} dT$ (approximated by trapezoidal rule)

3. Chromatography

- **Purpose**: To calculate **peak areas** from chromatograms to determine quantity of analytes.
- **Use**: When peaks are irregular and data points are recorded by instruments.

4. Kinetics

- **Purpose**: To determine the **rate of reaction** when concentration vs. time data is not continuous.
- **Use**: Estimating the area under the curve or average rate over intervals.

Example: Spectrophotometric Peak Area

Suppose absorbance data is given as:

Wavelength (nm)	Absorbance
400	0.00
410	0.10
420	0.40
430	0.60
440	0.40
450	0.10
460	0.00

Using the trapezoidal rule with h=10

$$A \approx \frac{10}{2}[0 + 2(0.10 + 0.40 + 0.60 + 0.40 + 0.10) + 0]$$

=5[2.00]=10.00

Problem involving entropy change using the trapezoidal rule

You are given heat capacity (C_p) data for a substance at different temperatures. Calculate the **entropy change** ΔS from **300 K to 400 K** using the formula:

$$\Delta S = \int_{T1}^{T2} \frac{Cp}{T} dT$$

Given data:

Temperature T(K)	Heat capacity C_p (J/mol.K)
300	28.0
320	29.2
340	30.1
360	31.0
380	31.8
400	32.5

Answer:

Step-1

Temperature T(K)	Heat capacity C_p (J/mol.K)	C_p/T(J/mol.K^2)
300	28.0	0.0933
320	29.2	0.0913
340	30.1	0.0885
360	31.0	0.0861
380	31.8	0.083
400	32.5	0.0813

Step-2: Apply the Trapezoidal Rule

$\Delta S \approx \frac{h}{2}$ $[f(x_0) + 2 f(x_1) + 2 f(x_2) + \ldots\ldots + 2 f(x_{n-1}) + f(x_n)]$

h= 20K (constant interval)

$f(T) = C_p/T$

$\Delta S \approx \frac{20}{2}$ $[0.0933 + 2 (0.0913 + 0.0885 + 0.0861 + 0.0837) + 0.0813]$

$\Delta S \approx$ 10[0.0933+2(0.3496)+0.0813]

=10[0.8738] J/mol.K

=8.738 J/mol.K