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Integrated Rate Laws

Finally a use for calculus!

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What is a rate?

It's a "delta/delta"!

Rate of reaction = $\frac{\Delta \text{concentration}}{\Delta \text{time}}$

In other words, it is a differential.

As you MAY recall from calculus, if you take a small enough delta (difference) you end up with a derivative!

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A rate as a derivative

Rate of reaction = $\frac{\Delta \text{concentration}}{\Delta \text{time}}$

If Δtime is small enough, we have:

$\text{Rate of reaction} = \frac{-d[\text{reactant}]}{dt}$

Why "-"? Because you are losing reactants and the rate should always be positive.

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Solving the equation

$$\int_{[A]_{initial}}^{[A]_{final}} \frac{d[A]}{[A]} = - \int_{time=0}^{final\ time} k dt$$
$$\ln[A]_{final} - \ln[A]_{initial} = -kt$$

This is the only equation we really need. This is called the "integrated rate law" ...well, because we integrated the rate law. ☺

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What it means...

$$\ln[A]_{final} - \ln[A]_{initial} = -kt$$

What it means is that the concentration at any time decays logarithmically from the initial concentration. If I rearrange the equation a little:

$$\ln[A]_{final} = -kt + \ln[A]_{initial}$$

What does this look like to you?

Yes, it is the equation of a straight line (y=mx+b)!

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Using the integrated rate law

$$\ln[A]_{final} = -kt + \ln[A]_{initial}$$

If you know k and the initial concentration, you could calculate the concentration at any time.

For example, if I know k=0.015 s⁻¹ and I start with 0.250 M A, how much A is left after 1 minute?

Beware the units. 1 minutes = 60 seconds. Since k is in s⁻¹, I need my time to be in seconds.

Plug and chug, baby!

$$\ln[A]_{final} = -0.015s^{-1} \times 60s + \ln(0.250\ M)$$
$$\ln[A]_{final} = -2.256$$
$$[A]_{final} = e^{-2.256} = 0.102\ M$$

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Using the integrated rate law

$$\ln[A]_{final} = -kt + \ln[A]_{initial}$$

$$\ln[A]_{final} = -0.015s^{-1} \cdot 60s + \ln(0.250M)$$

$$\ln[A]_{final} = -2.286$$

$$[A]_{final} = e^{-2.286} = 0.102M$$

You can see the power of the integrated rate law. I can determine the remaining concentration of reactants at any second in time! (And, using stoichiometry, I could determine the concentration of products at any second in time!)

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Compare the integrated rate law to the rate law

$$\ln[A]_{final} = -kt + \ln[A]_{initial}$$

$$\text{Rate} = k[A]$$

For the same problem, the rate law only allows me to calculate the initial rate of the reaction:

$$\text{Rate} = (0.015s^{-1})(0.250M) = 0.00375M/s$$

I could also calculate the RATE for any specific concentration. But I can't know how long it takes me to get to that new concentration.

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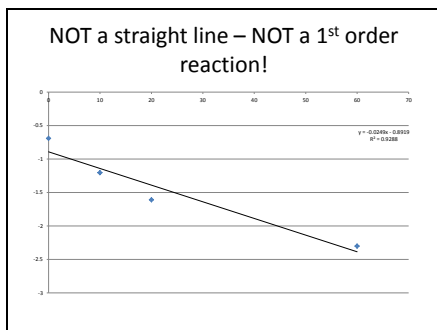
Other uses of the integrated rate law

$$\ln[A]_{final} = -kt + \ln[A]_{initial}$$

It's a straight line. Scientists LOVE LOVE LOVE straight lines!

If you have a reaction that you KNOW is 1st order, you could measure the [A] at a number of different times and plot the data and you'll get a straight line where the slope=-k. So you could use the equation to find the rate constant.

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This works for other orders of reaction also.

For a second order reaction:

$$\text{Rate} = k[A]^2$$

You get an integrated rate law

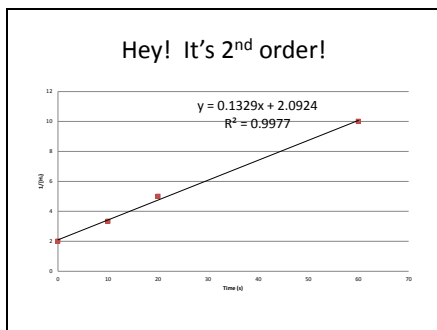
$$\frac{1}{[A]_{\text{final}}} = kt + \frac{1}{[A]_{\text{initial}}}$$

Same idea, it's a straight line ($y = mx+b$) where:

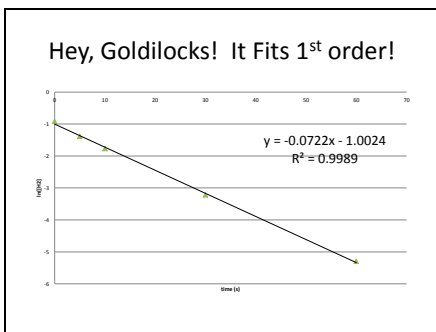
Slope = k

Intercept = $\frac{1}{[A]_{\text{initial}}}$

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What if I don't want to or can't make a graph?

- A. Find someone who can make a graph.
- B. Copy the answer from the person next to me.
- C. Calculate the rate of the reaction and see if the rate is constant or if the $\ln(\text{rate})$ is constant or $1/\text{rate}$ is constant.
- D. Calculate the slope between data points and see if they are constant.

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What if I don't want to make a graph?

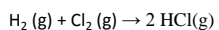
$\text{N}_2(\text{g}) + 3 \text{Cl}_2(\text{g}) \rightarrow 3 \text{NCl}_3(\text{g})$

Given the following data, determine the rate law.

Time	$[\text{N}_2(\text{g})]$ (M)
0 min	0.40
5 min	0.25
10 min	0.17
30 min	0.04
60 min	0.005

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The following reaction is 1st order in Cl₂ and 1st order overall.



2 M H₂ and 2 M Cl₂ was placed in a 5 L flask at 298 K. The initial rate was 3.82x10⁻³ M/s. What was the rate after 10 minutes? How much HCl had been made after 10 minutes?

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$$\text{Rate} = k[\text{Cl}_2]$$

$$\text{Rate} = 1.92 \times 10^{-3} \text{ s}^{-1} (0.632 \text{ M}) = 1.2135 \times 10^{-3} \text{ M/s}$$

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How much HCl?

Just stoichiometry folks...

I started with 10 moles Cl₂ :

$$\frac{2 \text{ mol}}{\text{L}} \times 5 \text{ L} = 10 \text{ moles initial}$$

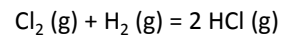
I end up with:

$$\frac{0.632 \text{ mol}}{\text{L}} \times 5 \text{ L} = 3.16 \text{ mol left}$$

So...

$$10 \text{ moles initial} - 3.16 \text{ mol left} = 6.84 \text{ mol reacted!}$$

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$$6.84 \text{ mol Cl}_2 \text{ reacted} \frac{2 \text{ mol HCl}}{1 \text{ mol Cl}_2}$$
$$= 13.68 \text{ mol HCl}$$
