Unit 5—Kinetics

Ch 14

Reaction rates, *ch 14.1, 14.2*

Define:

Chemical kinetics

Reaction rate

What factors change the rate at which an Alka-Seltzer tablet reacts with water?

Draw particles for the reaction A(*g*) → B(*g*)

Before rxn starts	Some time later	After half of A has reacted	Rxn completion

$$Average\ Rate = -\frac{\Delta[A]}{\Delta T}$$

$$Average\ Rate = \frac{\Delta[B]}{\Delta T}$$

What is happening to A? What is happening to B?

Why is the average rate for A negative?

By convention, rates are always expressed as ____________ quantities.

Average rate of reaction example

$A(g) \rightarrow B(g)$

Time (s)	0.00	10.0	20.0	30.0	40.0
Moles of A	0.124	0.110	0.088	0.073	0.054

The average rate of disappearance of A between 10 s and 20 s is _________.

The average rate of disappearance of A between 20 s and 30 s is _________.

What is the difference between average rate and instantaneous rate?

How is the rate of disappearance of A related to the appearance of B in the example above?

How are the rates of disappearance/appearance related for $2\ HI(g) \rightarrow H_2(g) + I_2(g)$?

What rule can you write for generic rates?

Introduction to rate laws, *ch 14.3*

Write the equation for a generic rate law:

What is k? Is it always the same or does it change?

Rate law example

Determine the rate law and rate constant using initial reaction rate for the following reaction:

$$2\ NO + 2\ H_2 \rightarrow N_2 + 2\ H_2O$$

Experiment Number	[NO] (*M*)	$[H_2]$ (*M*)	Initial Rate (*M*/s)
1	0.10	0.10	1.23×10^{-3}
2	0.10	0.20	2.46×10^{-3}
3	0.20	0.10	4.92×10^{-3}

Practice 1

1. Determine the rate law and rate constant using initial reaction rate for the following reaction:

$$OCl^- + I^- \rightarrow OI^- + Cl^-$$

$[OCl^-]$ (*M*)	$[I^-]$ (*M*)	Rate (*M*/s)
1.5×10^{-3}	1.5×10^{-3}	1.36×10^{-4}
3.0×10^{-3}	1.5×10^{-3}	2.72×10^{-4}
1.5×10^{-3}	3.0×10^{-3}	2.72×10^{-4}

2. Determine the rate law and rate constant using initial reaction rate for the following reaction. Then calculate the rate when [NO] = 0.050 M and $[H_2]$ = 0.150 M.

$$2\ NO + 2\ H_2 \rightarrow N_2 + 2\ H_2O$$

Experiment Number	[NO] (*M*)	$[H_2]$ (*M*)	Initial Rate (*M*/s)
1	0.10	0.10	1.23×10^{-3}
2	0.10	0.20	2.46×10^{-3}
3	0.20	0.10	4.92×10^{-3}

Another example

Determine the rate law and rate constant for the reaction $2\,A + B \rightarrow C + D$

Experiment	Initial [A] (mol L^{-1})	Initial [B] (mol L^{-1})	Initial rate of formation of C (mol L^{-1} min^{-1})
1	0.125	0.375	2.2×10^{-4}
2	0.375	0.375	6.5×10^{-4}
3	0.750	0.750	2.7×10^{-3}

Practice 2

1. Determine the rate law and the rate constant. Calculate the initial rate of change of [A] in experiment 3 as well as the initial value of [B] in experiment 4. $2\,A + B \rightarrow C + D$

Experiment	Initial [A] (mol L^{-1})	Initial [B] (mol L^{-1})	Initial rate of formation of C (mol L^{-1} min^{-1})
1	0.25	0.75	4.3×10^{-4}
2	0.75	0.75	1.3×10^{-3}
3	1.50	1.50	5.3×10^{-3}
4	1.75	?	8.0×10^{-3}

For the reaction $2\,NO + Br_2 \rightarrow 2\,NOBr$ with the rate law rate = $k[NO]^2[Br_2]$:

What is the order with respect to NO?

What is the order with respect to Br_2?

What is the overall reaction order?

Practice 3

Reaction	Rate law	Order with respect to		Overall reaction order
$2\ NO_2 + F_2 \rightarrow 2\ NO_2F$	Rate = $k[NO_2][F_2]$	NO_2	F_2	
$2\ NO + O_2 \rightarrow 2\ NO_2$	Rate = $k[O_2][NO]^2$	NO	O_2	
$NO + N_2O_5 \rightarrow 3\ NO_2$	Rate = $k[N_2O_5]$	NO	N_2O_5	

Concentration changes and rate laws, *ch 14.3, 14.4*

What do rate laws tell us? How are they useful?

Briefly explain first order reactions.

Briefly explain second order reactions.

Briefly explain zero order reactions.

More details for first order reactions:

First order reactions example

$CH_3 - N \equiv C \rightarrow CH_3 - C \equiv N$ The reaction is a first order reaction. At 230.3˚C, $k = 6.29 \times 10^{-4}\ s^{-1}$.

If $[CH_3 - N \equiv C]$ is 1.00×10^{-3} M initially, what is $[CH_3 - C \equiv N]$ after 1.000×10^3 s?

More details for second order reactions:

Second order reactions example 2

The following reaction is second order in [A] and the rate constant is 0.039 $M^{-1}s^{-1}$. A → B The concentration of A was 0.30 M at 23 s. The initial concentration of A was __________ M.

More details for zero order reactions:

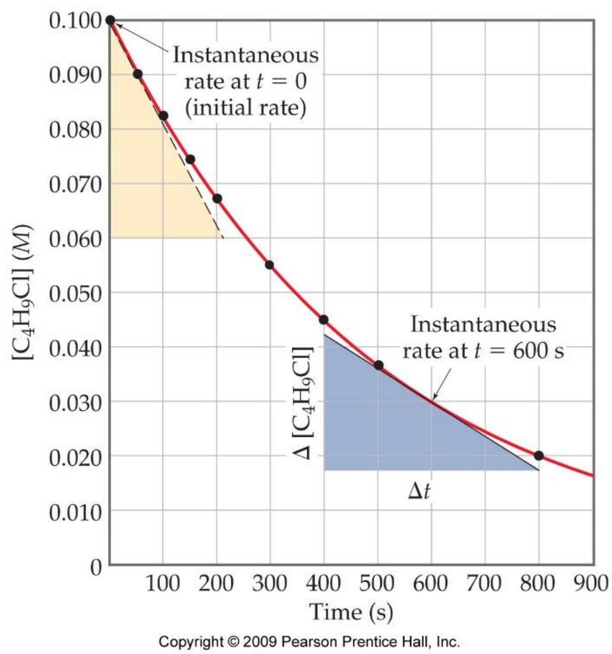
Practice 4

NO_2 → NO + ½ O_2. Determine if the reaction is zero, first, or second order in NO2, then write the rate law and determine k.

Time (s)	**[NO_2] (M)**
0.0	0.01000
5.0	0.00787
10.0	0.00649
20.0	0.00481
30.0	0.00380

Practice 5

The graph shows a first order reaction. Determine the half-life ($t_{½}$)and reaction constant (k).



Important equations

Elementary reactions, *ch 14.6*

What is an elementary reaction?

What does molecularity mean?

Define and give examples for:

Unimolecular

Bimolecular

Termolecular

Why are termolecular reactions rare?

Practice 6

2. $H_2 + Br_2 \rightarrow 2\ HBr$
    a. If the reaction occurs in a single elementary reaction, predict its rate law.

    b. If experimental studies show a different rate law, what can you conclude?

3. $2\ NO + Br_2 \rightarrow 2\ NOBr$
    a. Write the rate law for this reaction, assuming it involves a single elementary reaction.

    b. Is a single elementary reaction likely for this reaction? Why/why not?

Collision model, *ch 14.5*

To react, molecules must _____________.

What importance does molecule orientation play during collisions?

What importance does energy play during collisions?

Why do higher temperatures generally result in faster reactions?

Why does increasing the concentration of a reactant or reactants generally increase the rate of a reaction?

Why does changing the surface area affect the rate of a reaction?