

Catalysts and Activation Energy

- A catalyst is a substance speeds up a reaction but is chemically unchanged

1. A catalyst participates in a chemical reaction, but **does not undergo permanent change-overall**, the catalyst is **neither generated nor consumed**.



Automobiles are now equipped with catalytic converters containing mixture of catalysts to reduce the emission through reaction.



- To increase the rate of a reaction you need to increase the **proportion of successful collisions**.
- **Catalysts increase the rate of reaction** by providing an alternative way for the reaction to happen which has a **lower activation energy**.

Catalyst

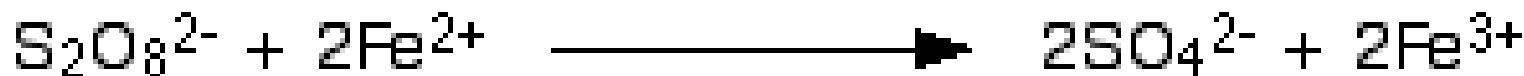
A catalyst participates in a chemical reaction, but **does not undergo a permanent change-overall**, the catalyst is **neither generated nor consumed**.

Two type of Catalysts

1. Homogenous and 2. heterogeneous catalysts

Homogeneous catalyst -A catalyst is in the same phase (gases and solutions) as the reactants is a **homogeneous catalyst**. It is effective, but recovery is difficult.

Ex- The reaction between persulphate ions and iodide ions (catalyst to be iron(II))



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Source	Pollutants	Catalysts	Note
Gasoline engines	Nitrogen oxides (NO _x), hydrocarbons (HC _s) and carbon monoxide (CO)	Pt/Pd/Rh/Ce _x Zr _{1-x} O ₂ /(La, Ba) – Al ₂ O ₃ on ceramic and metallic monoliths	Stoichiometric air to fuel ratio
Diesel engines (light vehicles)	NO _x , HC _s , CO	Pt/Pd/Rh/BaO/Al ₂ O ₃ on ceramic and metallic monoliths	Switch from oxidizing to reducing conditions
Diesel engines (heavy)	NO _x , HC _s , CO	V ₂ O _x / TiO ₂ on ceramic monolith	Use of ammonia or urea as reductant

vehicles, trucks and busses)		(NO _x reduction), Pt, Pd / Al ₂ O ₃ on ceramic and metallic monoliths (CO and HC oxidation)	
Diesel engines	Particulate	(i) Cerium and iron oxides (ii) Pt/ Al ₂ O ₃ (iii) Cu, V and K based catalysts	(i) Ce or Fe fuel additives to generate in situ the catalysts during the combustion; (ii) the catalyst oxidises NO to NO ₂ , which then oxidizes the particulate
Power plants, gas turbines, waste incinerators	NO _x	V ₂ O ₅ -WO ₃ /TiO ₂ on ceramic monolith	In the case of waste incinerators, simultaneous destruction of NO _x and dioxins
Gas turbines	CO, HC _s	Pt, Pd / Al ₂ O ₃ on ceramic and metallic monoliths	
Nitric acid production plants	NO _x	CuO-NiO/ Al ₂ O ₃ or Cu-La/ Y	Possible partial conversion of N ₂ O
Nitric acid, adipic acid or caprolactame production plants	N ₂ O	Rh/Ce-ZrO ₂ , Rh/ hydrotalcites	Possible partial conversion of N ₂ O
Chemical plants, refineries, paintings, etc...	Volatile organic compounds (VOC _s)	Pt, Pd / Al ₂ O ₃ on ceramic and metallic monoliths	
Refineries	H ₂ S, CS ₂ , COS	Al ₂ O ₃ or TiO ₂ (Fe ₂ O ₃ / Al ₂ O ₃)	Claus and Super Claus Processes
Waste water treatment from chemical, petrochemical, paper and electronic industry etc...	Organic compounds	Ru / TiO ₂ ----- TiO ₂ (anatase)	Catalytic oxidation with air ----- Photocatalytic process for diluted situations
Hospitals and public places	Organic compounds and bacteria	TiO ₂ (anatase)	Photocatalytic process



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2. Heterogeneous Catalyst

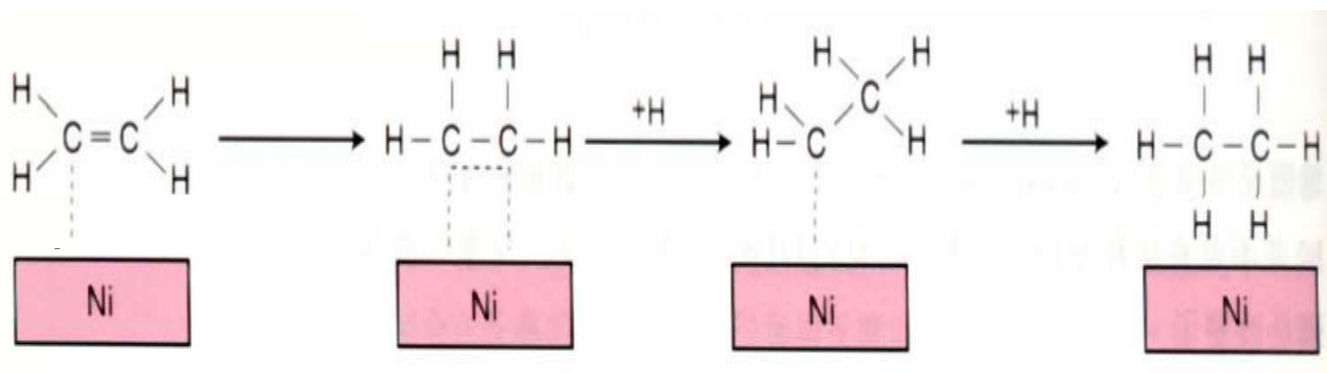
When the catalyst is in a different phase (**usually solid state**) than reactants (and products), the process involve **heterogeneous catalysis**. **Chemisorption**, **absorption**, and **adsorption** cause reactions to take place via different pathways.

❖ e.g. decomposition of H_2O_2 with MnO_2 as catalyst

❖ e.g. hydrogenation of ethene (Ni as Catalyst)



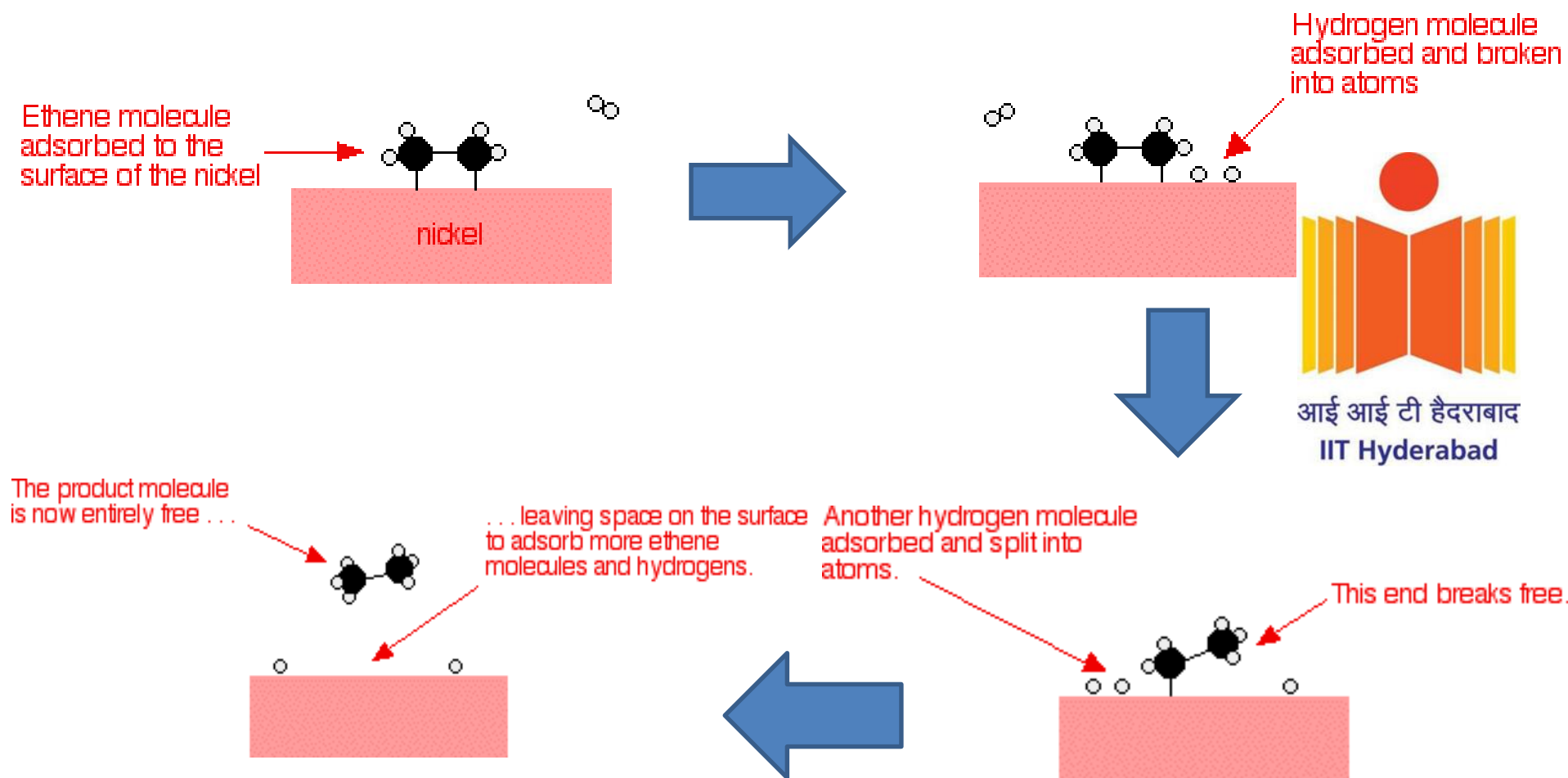
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Physisorption

Chemisorption

Heterogeneous catalysis



Heterogeneous catalysis

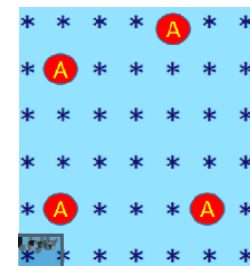
Many gaseous or solution phase reactions can be catalyzed on an appropriate solid surface-many transition metals and their compounds are used as effective catalysts.

Not all the surface atoms are effective for catalysis; those that are effective are called active sites.

Theory of heterogeneous catalyst was given by Langmuir.

A reaction taking place on the surface is supposed to consist of 4 consecutive steps

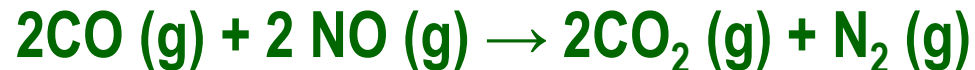
1. Adsorption of reactants on the surface.
2. Diffusion of reactants along the surface to reach the active site
3. Reaction at active site to form adsorbed product
4. Desorption and diffusion of product from the surface to the bulk.



Example of Heterogeneous Catalysis

Carbon monoxide, CO, and nitric oxide, NO, found in automobile emissions are partially responsible for the formation of photochemical smog.

Automobiles are now equipped with catalytic converters containing mixture of catalysts to reduce the emission through reaction.



The method by which this process is believed to occur on a Rh surface is illustrated in the next slide

Mechanism of Heterogeneous Catalysis



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a) *adsorption* of CO and NO

b) *diffusion* and dissociation of NO

c) combination of CO and O to form CO_2 , N atoms to form N_2 , along with *desorption* of products

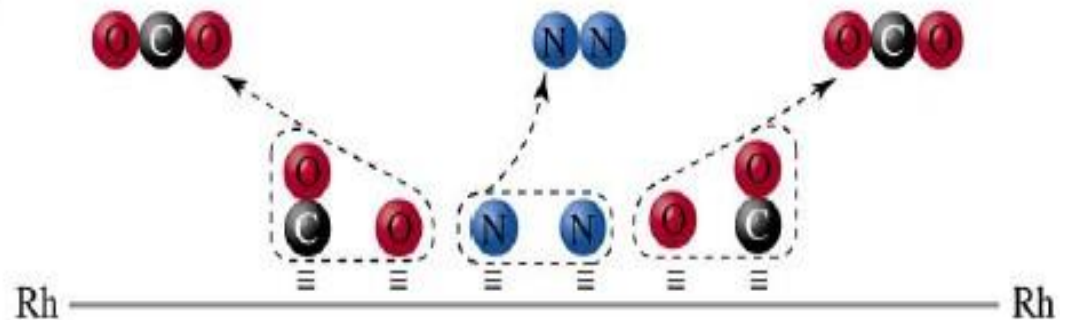
(dissociation & combination processes are equivalent to *reaction* step)



(a)

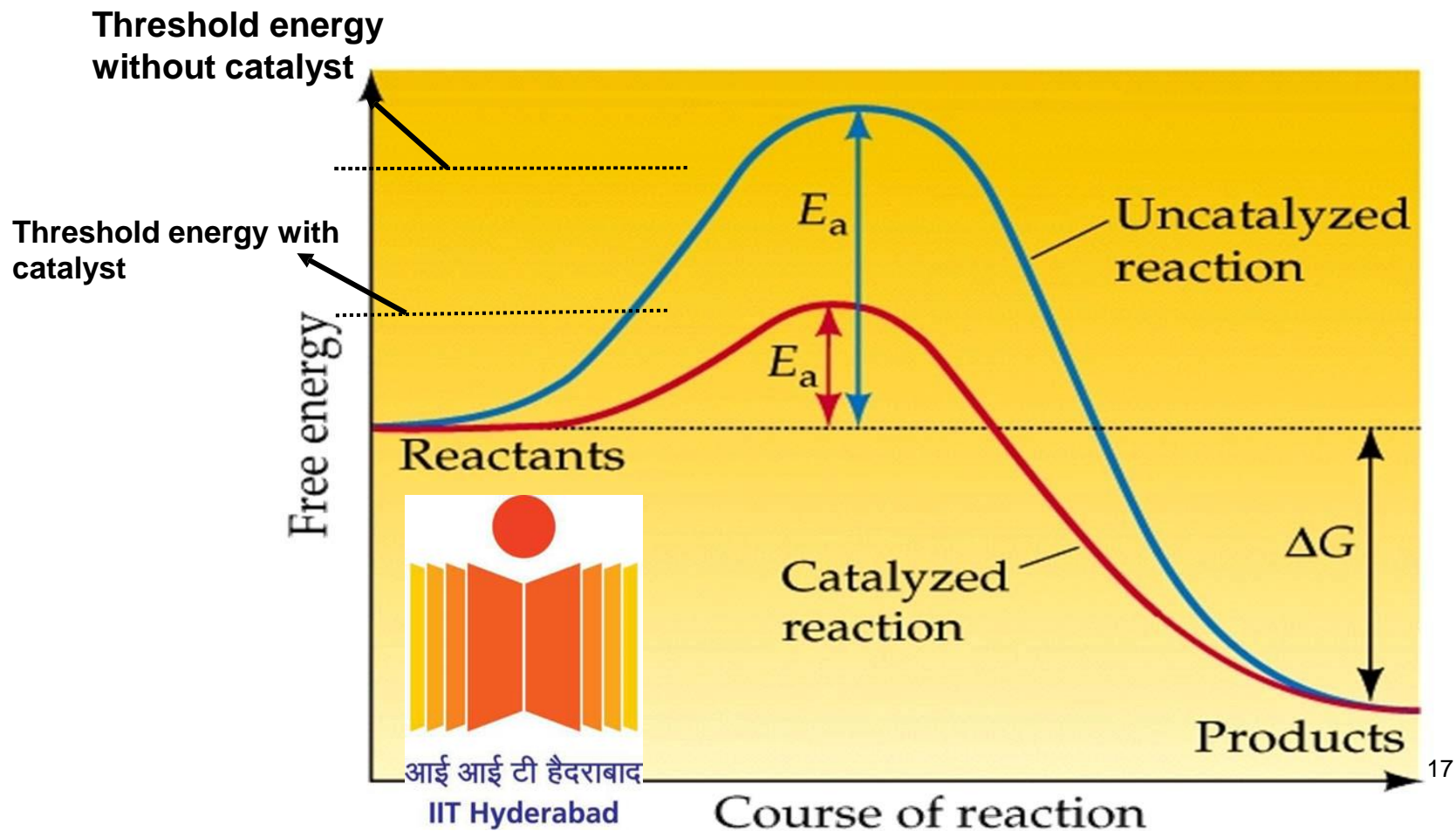


(b)

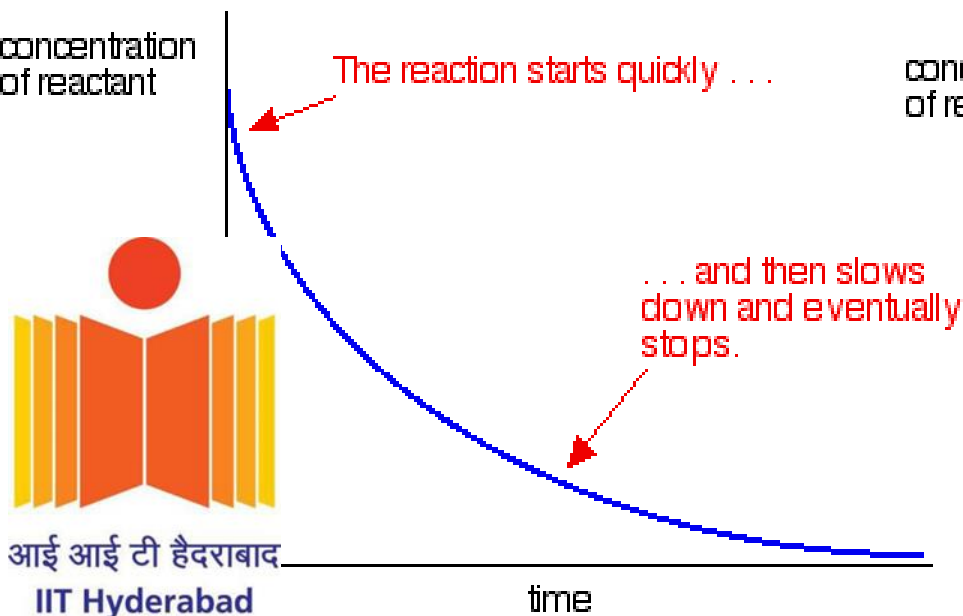


(c)

Catalysts Influences the Energy Profile

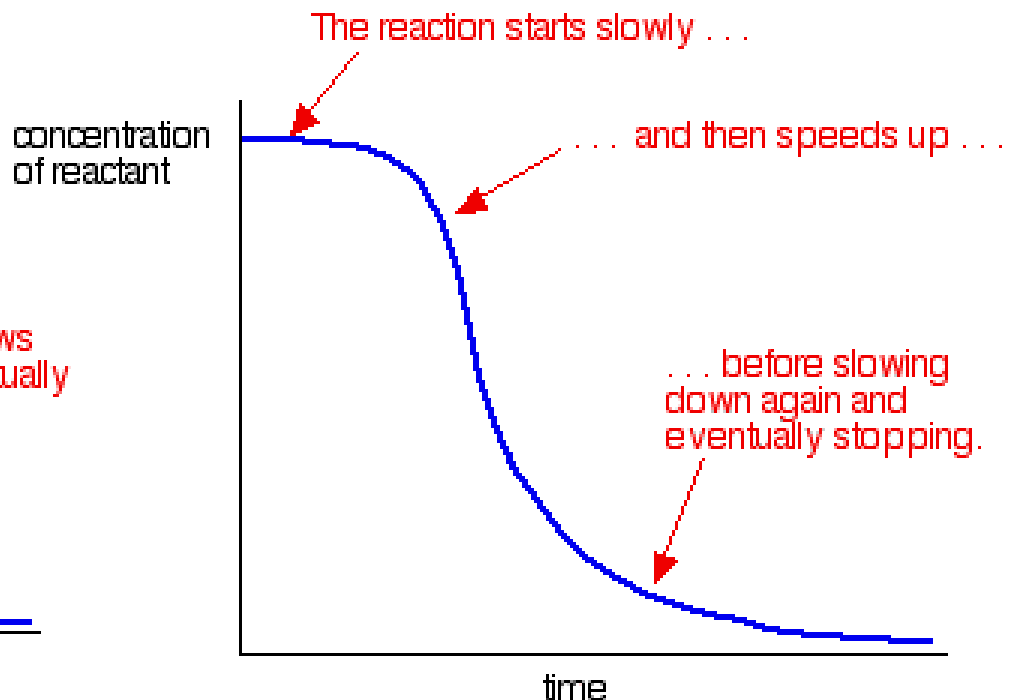


Most reactions give a rate curve which looks like this:



Concentrations are high at the beginning and so the reaction is fast - shown by a rapid fall in the reactant concentration. As things get used up, the reaction slows down and eventually stops as one or more of the reactants are completely used up.

An example of autocatalysis gives a curve like this:



As catalyst begins to be formed in the mixture, the reaction speeds up - getting faster and faster as more and more catalyst is formed. Eventually, of course, the rate falls again as things get used up.

In overall catalysts



- ❖ A catalyst **changes** the **rate of reaction**
- ❖ **Does not take part** in the reaction
- ❖ Provides a **convenient surface** for the reaction to occur
- ❖ Particles **gather on the catalyst surface** – Collide more frequently
 - Resulting in more collisions giving a reaction because of the new route of reaction

e.g. **H_2O_2** is bit stable at Room Temperature

In presence of **catalyst MnO_2** cause it to decompose fast