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# Catalysts and catalytic processes and their driving forces

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**Middlesbrough - Victorian town**

Middlesbrough – Town mus



# Middlesbrough - Transporter bridge



Middlesbrough Institute of Modern Art (mima)





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## Teesside University - Main entrance





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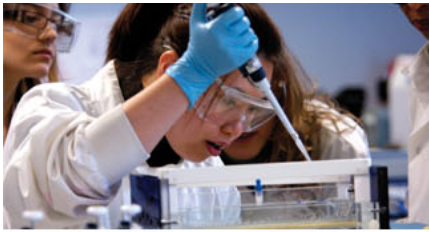
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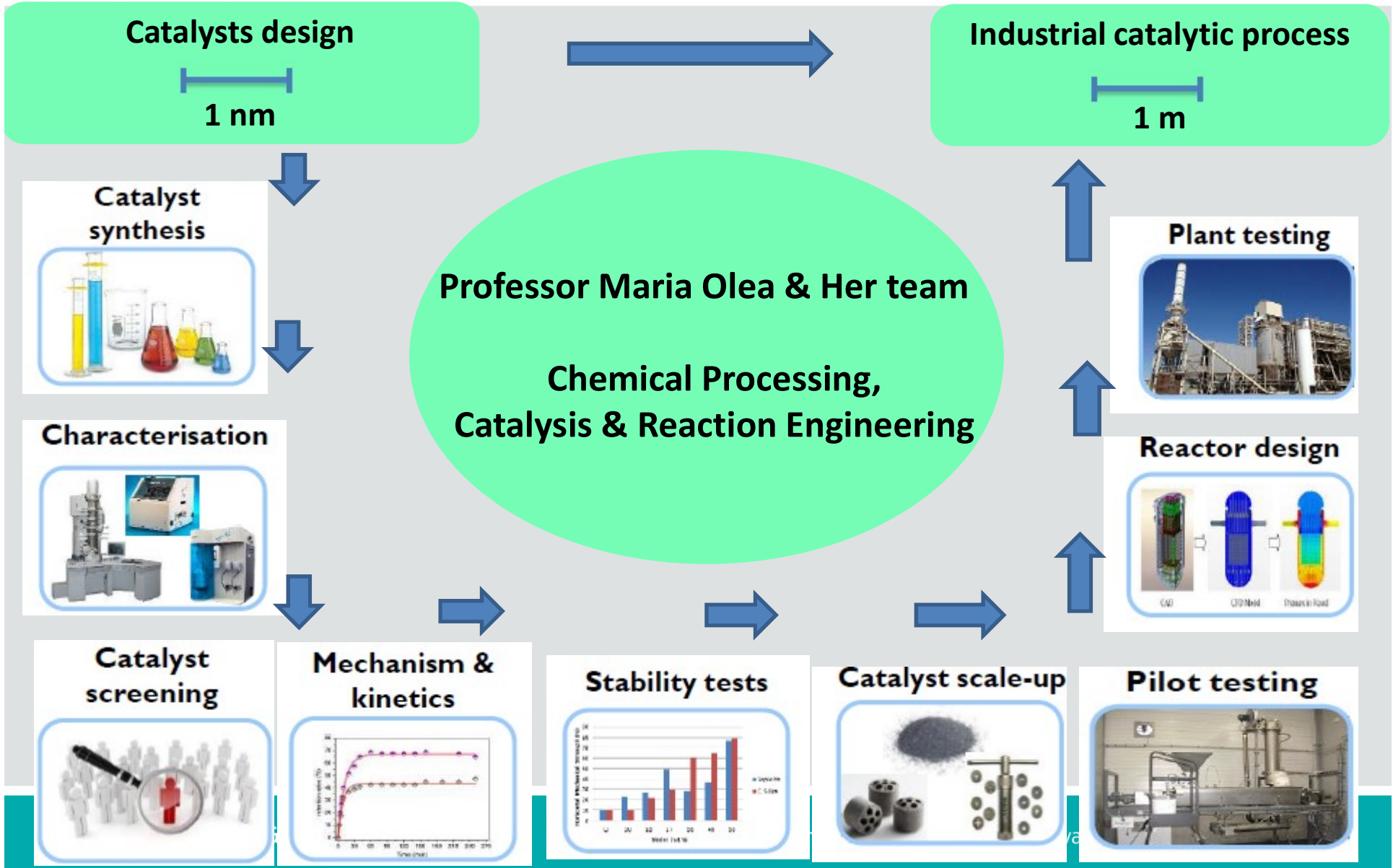
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## What is Catalysis?

- **Catalysis is the process of modifying a chemical reaction with the use of a catalyst;**
- **Catalysis modifies only the chemical reactions which are possible (spontaneous) from thermodynamic point of view!**
- **$\Delta G < 0$ ;  $\Delta G = \Delta H - T * \Delta S$ ; *spontaneous reaction*;**
- **$\Delta G = 0$ ; *equilibrium*;**
- **$\Delta G > 0$ ; *non – spontaneous reaction*.**



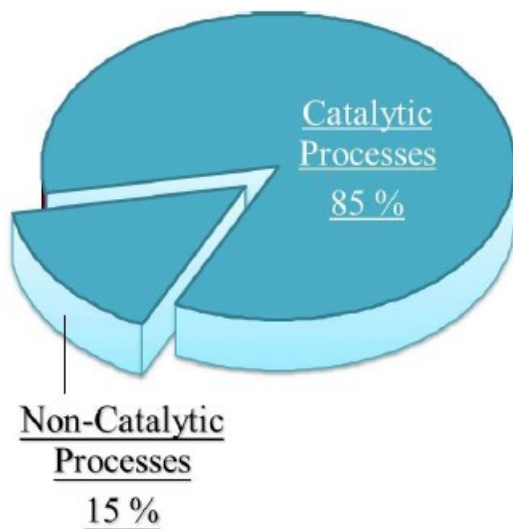
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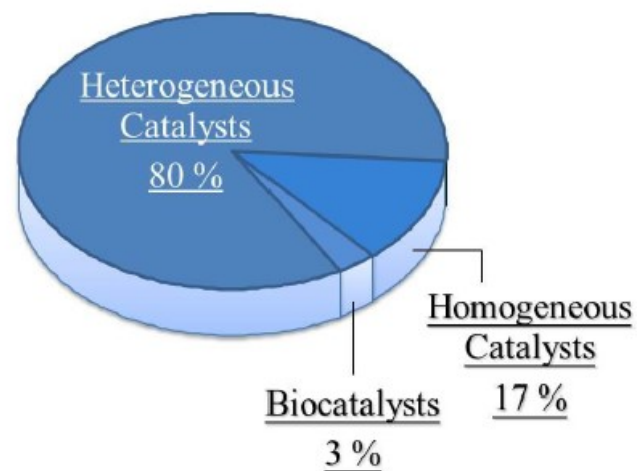


## Role of Catalysis in Chemical Manufacture

### All Chemical Processes



### Catalytic Processes



G. Rothenberg, *Catalysis: Concepts and Green Applications*, Wiley-VCH, 2008



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## Milestones of Catalysis Application in the 20th Century



Ammonia Synthesis-Food

.....



Automotive Emission Control-Air

.....



Oil Refining-Energy

.....

<https://mycourses.aalto.fi/pluginfile.php/663748/course/section/109647/Lecture%201%20Introduction.pdf>



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## Catalysts? What are they?

- ✓ Chemicals that increase the rate of reaction without being used in the reaction itself;
- ✓ Lower the **activation energy** of a chemical reaction by increasing the frequency of collisions between reactants, altering the orientation of reactants so that more collisions are effective, reducing intramolecular bonding within reactant molecules, or donating electron density to the reactants.
- ✓ Presence of a catalyst helps a reaction to proceed more quickly to equilibrium; both the forward and reverse reaction rates are affected by the catalyst, i.e. the  $E_a$  for both directions is decreased; the equilibrium constant is not changed by the presence of a catalyst; the relative concentrations of the reactants and products do not change.





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## Catalysts properties

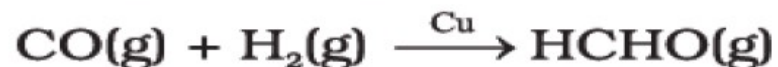
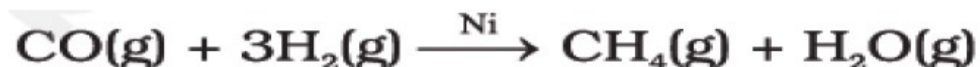
### Activity

The activity of a catalyst depends upon the strength of chemisorption to a large extent. The reactants must get adsorbed reasonably strongly on to the catalyst to become active.

### Selectivity

The selectivity of a catalyst is its ability to direct a reaction to yield a particular product.

For example -:



### Stability

The number of reactions performed by each active site before it decays or becomes inactive.



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## Catalysts? What are they?

- Catalysts can be classified as either heterogeneous or homogeneous.
- Heterogeneous catalysts work by the adsorption of reactant molecules.
- The surface activity of a catalyst can be reduced by poisoning.
- Impurities in the reactants result in the industrial catalysts having to be regenerated or renewed.
- Catalytic converters are fitted to cars to catalyse the conversion of poisonous carbon monoxide and oxides of nitrogen to carbon dioxide and nitrogen.



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# Catalyst poisoning

- In heterogeneous catalysis Catalyst poisoned by a chemical binding to surface
- Poison bonds irreversibly with catalyst
- Sulphur and lead are two examples of catalyst poisons



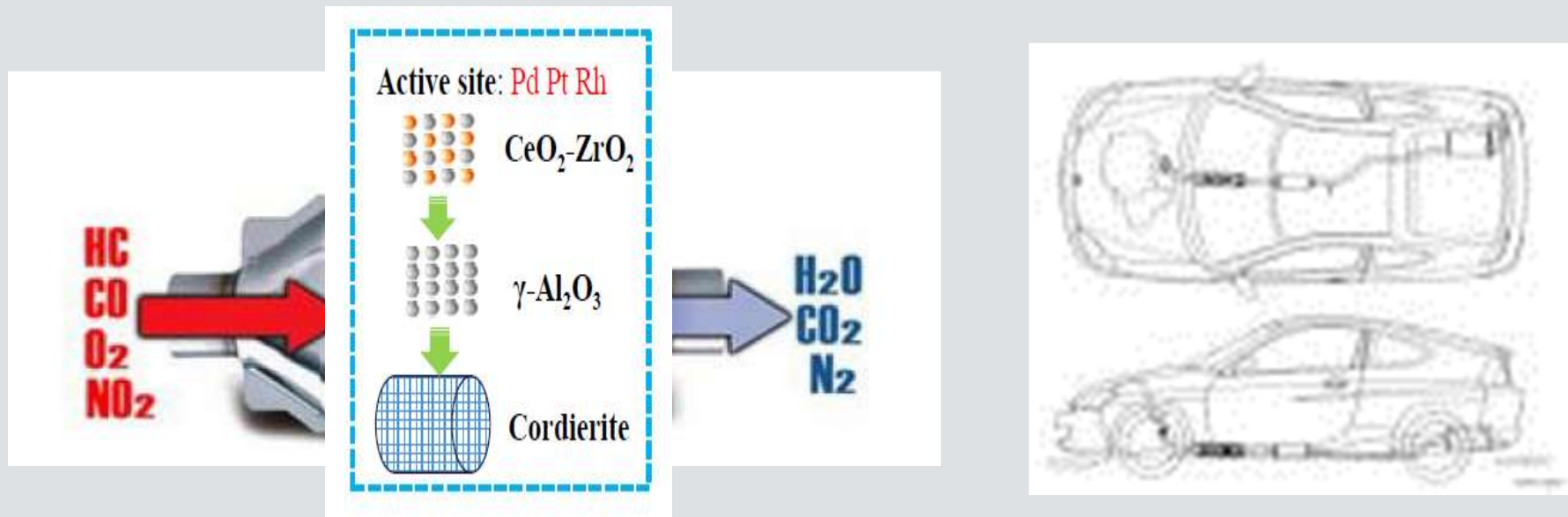
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## Catalytic Converters – Three-way catalyst

- Found in car exhaust systems
- Reduce levels of pollutant gases
- Pollutants react in exhaust to form less harmful gases.





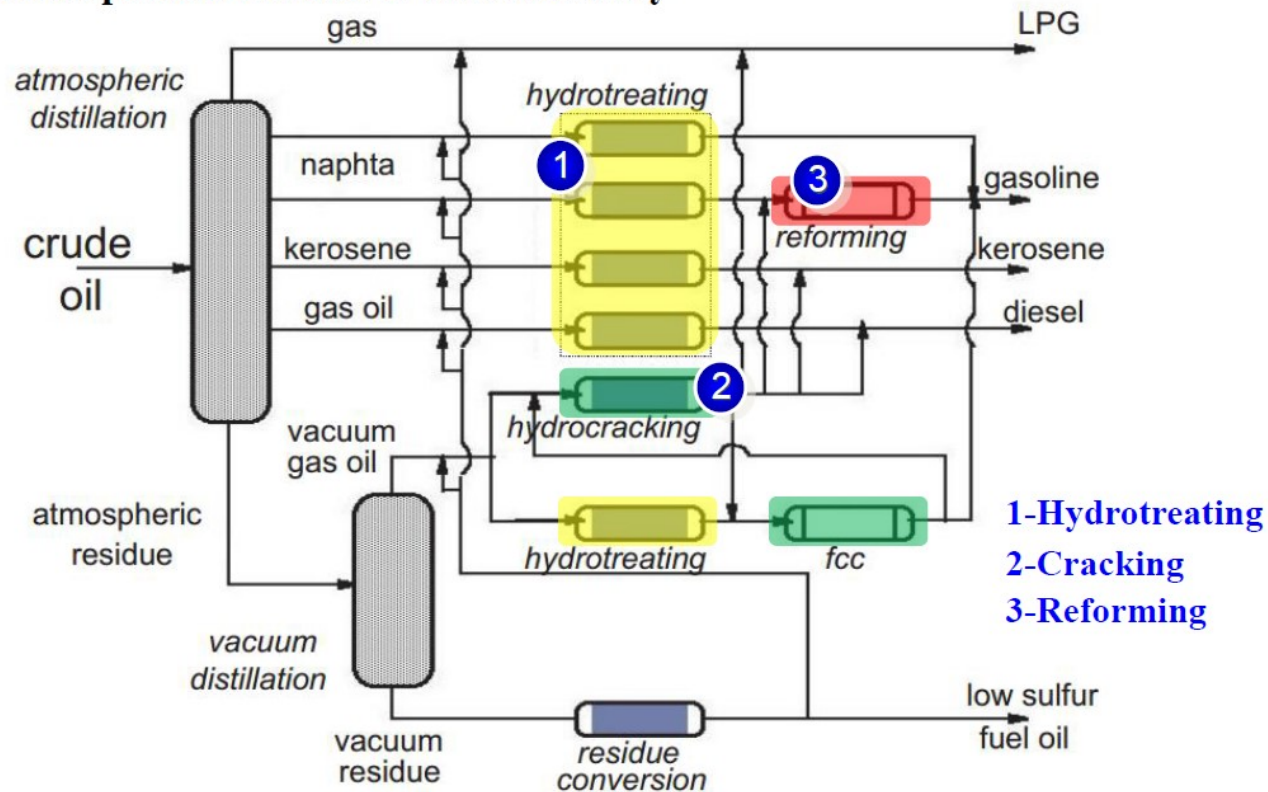
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## Oil Refining

Simplified process scheme of an oil refinery



I. Chorkendorff and J.W. Niemantsverdriet, Concepts of Modern Catalysis and Kinetics, Wiley-VCH, 2003 & 2007

<https://mycourses.aalto.fi/pluginfile.php/663748/course/section/109647/Lecture%201%20Introduction.pdf>



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## Oil Refining – cont'd

### Hydrotreating

HDS, HDO, HDN, HDA

Co-MoS<sub>2</sub>/Al<sub>2</sub>O<sub>3</sub>, Ni-WS<sub>2</sub>/Al<sub>2</sub>O<sub>3</sub>, Ni-MoS<sub>2</sub>/Al<sub>2</sub>O<sub>3</sub>

### Cracking

$C_{16}H_{34} \rightarrow C_8H_{18} + C_8H_{16}$

Amorphous silica-aluminas and zeolites

### Reforming

$n-C_5H_{12} \rightarrow i-C_5H_{12}$ ,  $C_6H_{14} \rightarrow C_6H_6$

Bifunctional catalysts, Pt-Re/Al<sub>2</sub>O<sub>3</sub>, Pt-Ir/Al<sub>2</sub>O<sub>3</sub>

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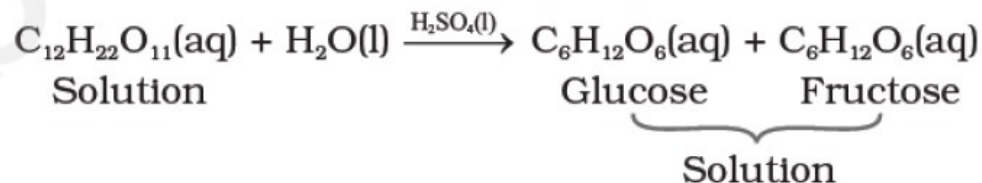


## Homogeneous catalysts

When the reactants and the catalyst are in the same phase (i.e., liquid or gas), the process is said to be homogeneous catalysis.

For e.g -:

Hydrolysis of sugar is catalysed by H<sup>+</sup> ions furnished by sulphuric acid.



### Advantages

- Good contact with reactants .

[www.ncert.nic.in/NCERTS/l/l/ech105.pdf](http://www.ncert.nic.in/NCERTS/l/l/ech105.pdf)

### Disadvantages\_\_\_\_\_

- Catalysis needs to be separated after reaction
- Catalyst recovery may be difficult because the temperature for the distillation can destroy the catalyst



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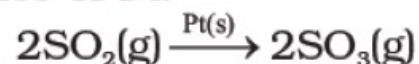
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## Heterogeneous catalysts

The catalytic process in which the reactants and the catalyst are in different phases is known as heterogeneous catalysis.

For e.g -: Oxidation of sulphur dioxide into sulphur trioxide in the presence of Pt.



The reactant is in gaseous state while the catalyst is in the solid state.

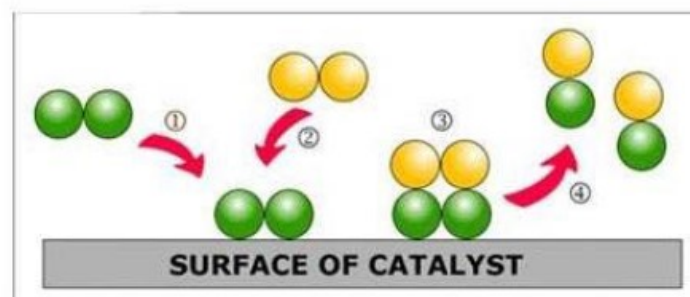
### Advantages

- There is little difficulty in separating and recycling the catalyst.

### Disadvantages

- There is a lower effective concentration of catalyst since the reaction occurs

only on the exposed active surface. ([www.knockhardy.org.uk](http://www.knockhardy.org.uk))







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## Heterogeneous catalysts

- Catalyst is usually solid
- Reactants are **adsorbed** onto surface
- Adsorb – *formation of weak bonds*



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## Absorption vs Adsorption



**Absorption**



**Adsorption**



**Bulk (Volume)  
Phenomenon**



**Surface  
Phenomenon**



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## Heterogeneous catalysts

**Powders:**



**Microspheres:**



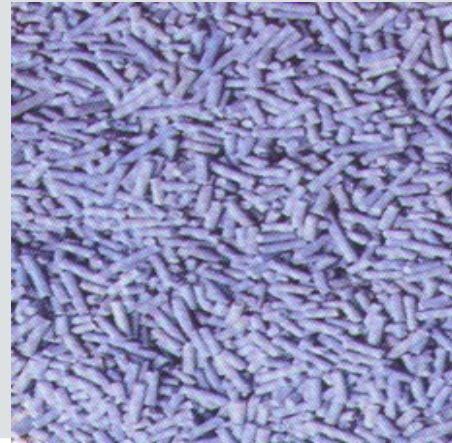
**Spheres:**



**Granules:**



**Extrudates:**



**Miniliths:**





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## Heterogeneous catalysts

### Catalyst particles

Extrudate	D=1-5 mm L = 3-30 mm	Fixed bed reactor
Pellet	D=3-10 mm H=3-10 mm	Fixed bed reactor
Granule	D=1-20 mm	Fixed bed reactor
Bead	D=1-5 mm	Fixed bed reactor
Sphere	D=1-5 mm	Fixed bed reactor
Sphere	D=20-100 $\mu\text{m}$	Fluidized bed & Slurry bed reactors

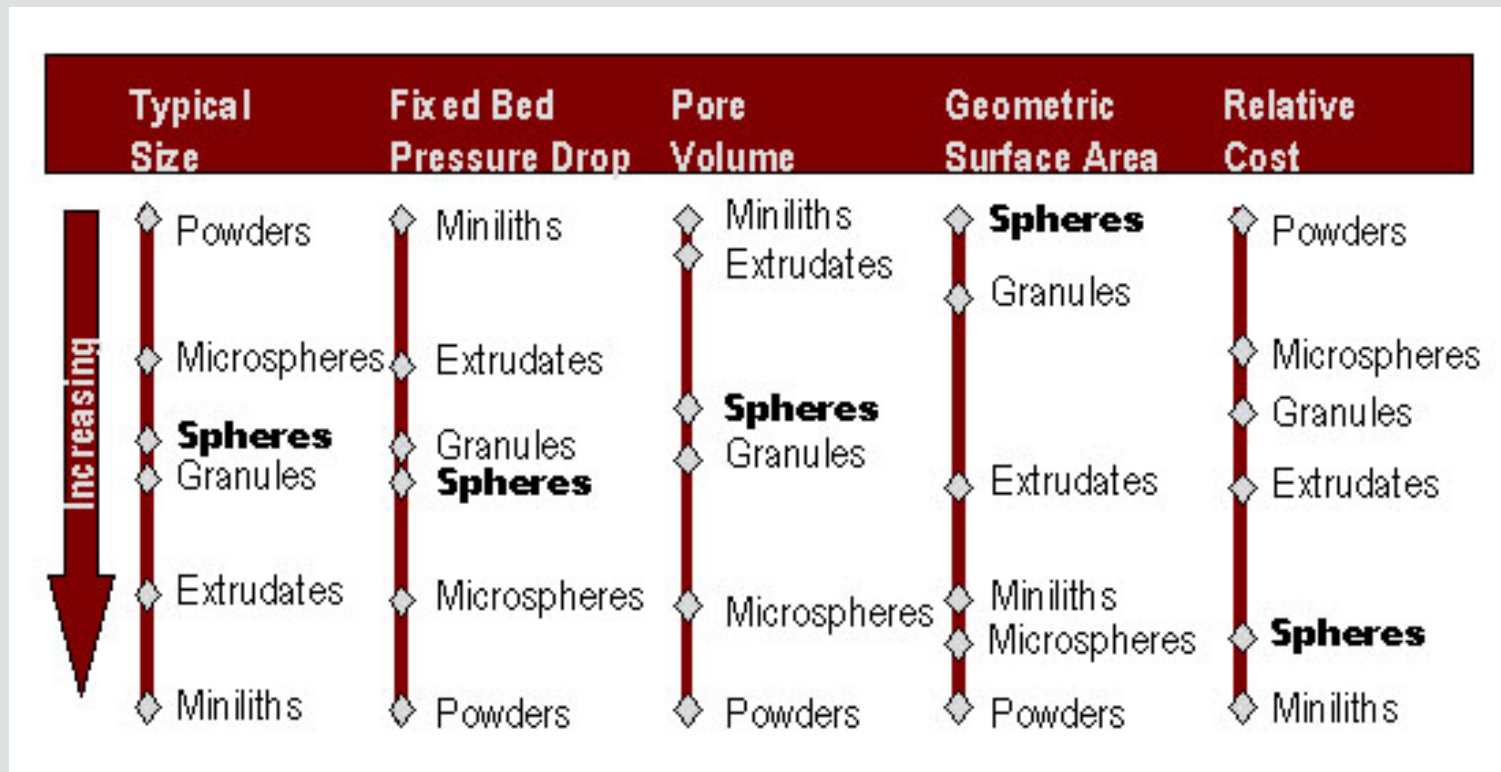


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## Heterogeneous catalysts



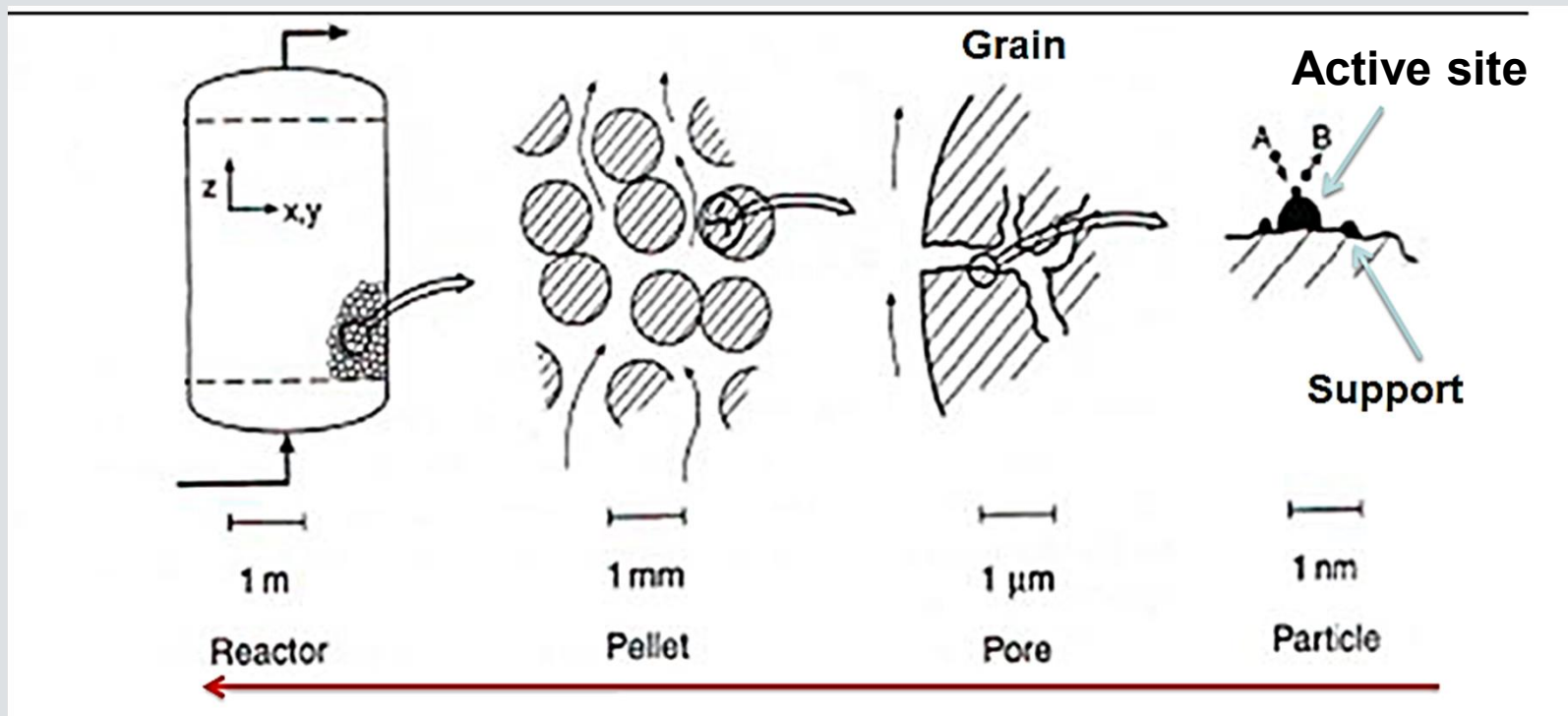


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## Catalysts? What are they?



(L. D. Schmidt – The engineering of chemical reactions, 2<sup>nd</sup> Edition, Oxford University Press, 2005, p.278, modified)



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## Activation energy

- ✓ In chemistry, activation energy, also called threshold energy, is a term introduced in 1889 by Svante Arrhenius that is defined as the energy that must be overcome in order for a chemical reaction to occur.

≈ the minimum energy necessary for a specific chemical reaction to occur. The activation energy of a reaction is usually denoted by  $E_a$ .

- ✓ Basically, the activation energy is the height of the potential barrier (sometimes called the energy barrier) separating two minima of potential energy (of the reactants and of the products of reaction). For chemical reaction to have noticeable rate, there should be noticeable number of molecules with the energy equal or greater than the activation energy.



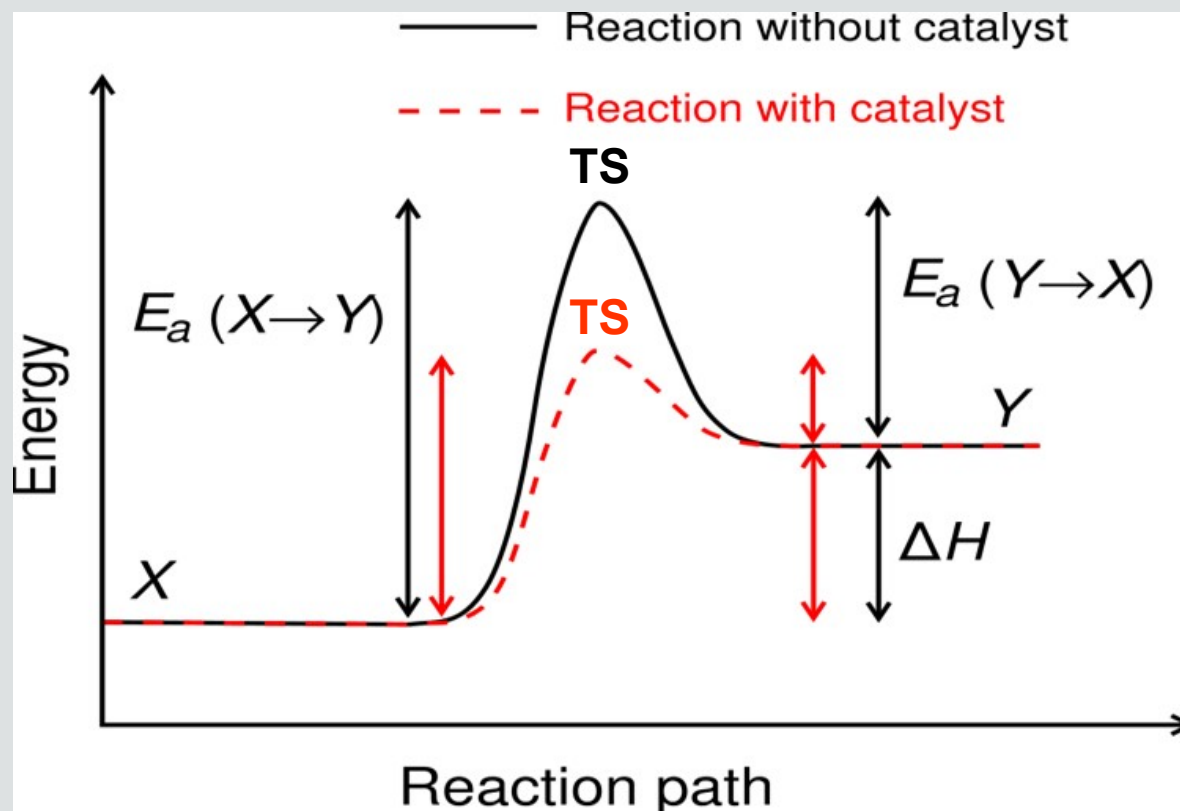
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## Reaction path

TS = Transition state (it is not an intermediate!)



### Discussion:

- Is the forward reaction endothermic or exothermic? Why?
- Some questions for the reverse reaction.





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## Major points

- 1) **Why reactions have barriers?**
- 2) **How catalysts avoid/reduce these barriers?**
- 3) **Why thermochemistry of the catalyst-substrate complex is so important?**



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## Major points

### 1) Why reactions have barriers?

Usually, reactions have barriers because:

- a) closed shell orbitals repel
- b) steric strains to reach TS
- c) most reactions except ion-molecule and radical recombination have some barrier since molecule has to rearrange to reach TS.



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## Major points

### 2) How catalysts avoid/reduce these barriers?

Many catalysts have a vacant orbital that can accept an electron or electron pair, dramatically lowering barriers, completely changing reaction path: Transition Metals, Lewis acids, Free Radicals. Many catalysts are charged: acids, bases, metal ions, oxides.

Some catalysts provide a path that avoids steric strain, e.g.  $\text{H}_2\text{O}$  can pass protons around.

A few catalysts are less dramatic: they don't change the reaction path much, but instead have some weak interactions which stabilize the TS more than the reactants. Each H-bond is worth 5 kcal/mol; enough van der Waals contacts can add up.



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## Major points

### 3) Why thermochemistry of the catalyst-substrate complex is so important?

- ✓ Moving from catalyst + reactants to catalyst + products - with a fixed free energy difference; avoiding any steps with free energy differences much larger than this – they will introduce effective activation energies (even if there is no kinetic barrier beyond the intermediate's thermochemistry). Best if the intermediates are all intermediate in energy between reactants + catalyst and products + catalyst.
- ✓ Another critical aspect of thermochemistry is the strength of the catalyst-substrate binding. If the binding is too weak, rates will be low because not enough catalyst-substrate complex – not effectively using the catalyst, and most of the substrate is reacting some other way rather than through the desired catalytic route. If binding is too strong, kinetics will be controlled by difficulty getting substrate off the binding site.
- ✓ Barriers usually highly correlated with thermo: exothermic reactions have low barriers. So you can usually accelerate a process by making the rate-limiting step more exothermic.



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## Transition - State Theory

- Also called **activated-complex theory**, or **theory of absolute reaction rates**, a conception of chemical reactions or other processes that involve rearrangement of matter as proceeding through a continuous change in the relative positions and potential energies of the constituent atoms and molecules. Between the initial and final arrangements of atoms or molecules there exists an intermediate configuration for which the **energy** arising from interatomic and intermolecular forces (potential energy) reaches a maximum. The activated complex is a hypothetical transient molecule considered to be in a state of equilibrium with the atoms or molecules in the initial state and therefore amenable (to some extent) to specification of thermodynamic properties.

-The **activation energy** is the difference in energy content between atoms or molecules in an activated or transition-state configuration and the corresponding atoms and molecules in their initial configuration.



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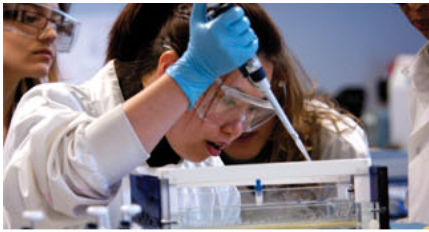
## Discussion

1. Draw the Energy – Reaction path diagram for the exothermic process:



2. Elementary vs non-elementary reactions!

3. How does the presence of a catalyst change the thermodynamic equilibrium constant of a reaction?



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## Driving force - Conceptual understanding

- Each process has a driving force!
- The process will occur as long as the driving force is acting upon it;
- The process rate depends on the driving force:  
*rate = constant X driving force!*
- Multiphase (heterogeneous) processes - there is an interface between different phases through which mass transfer occurs.

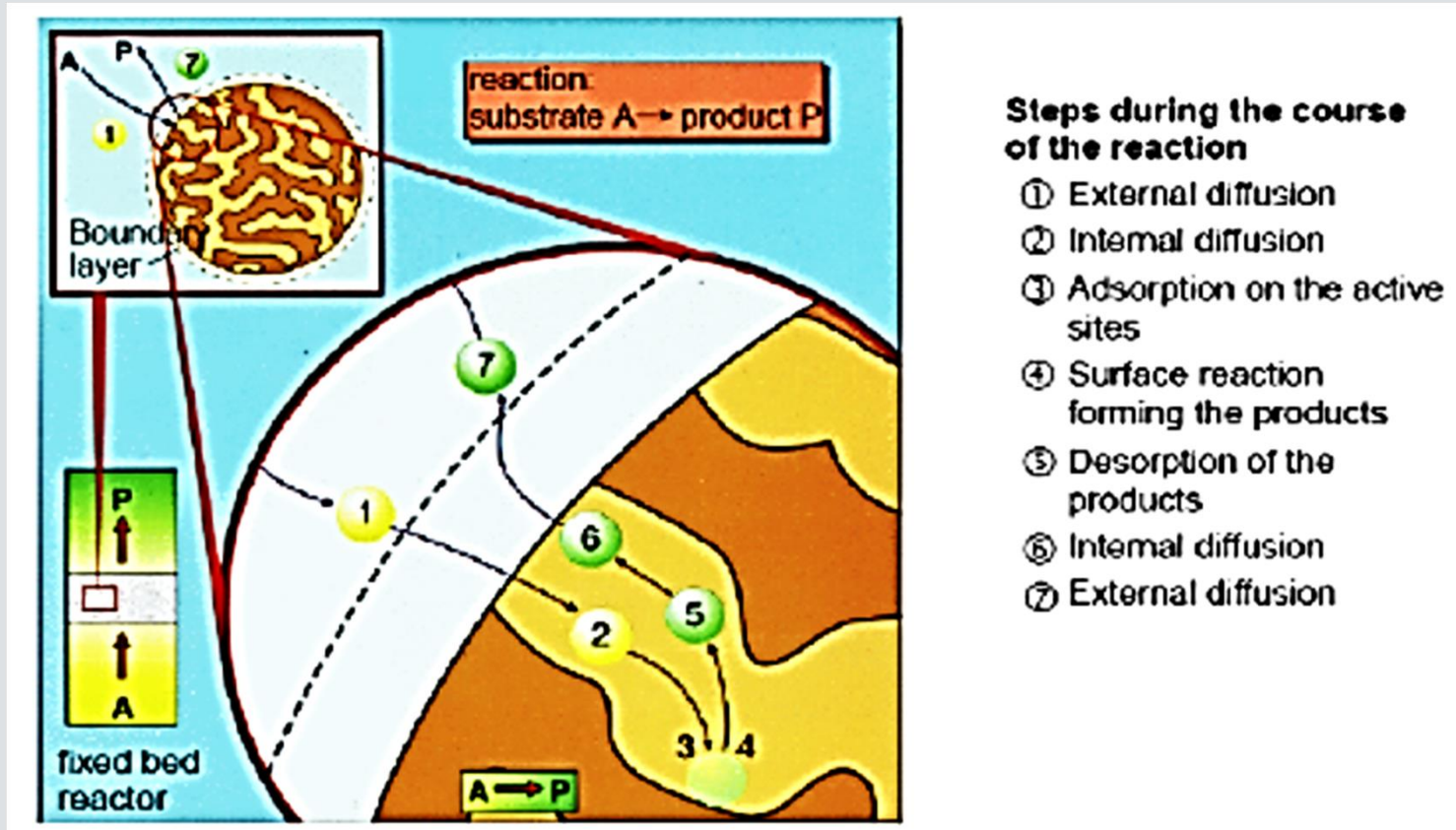


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## Heterogeneous catalysis



Steps 3, 4, 5: reactive steps, surface processes

Steps 1, 2, 6, 7: involve only mass transfer & transport and not chemical transformation





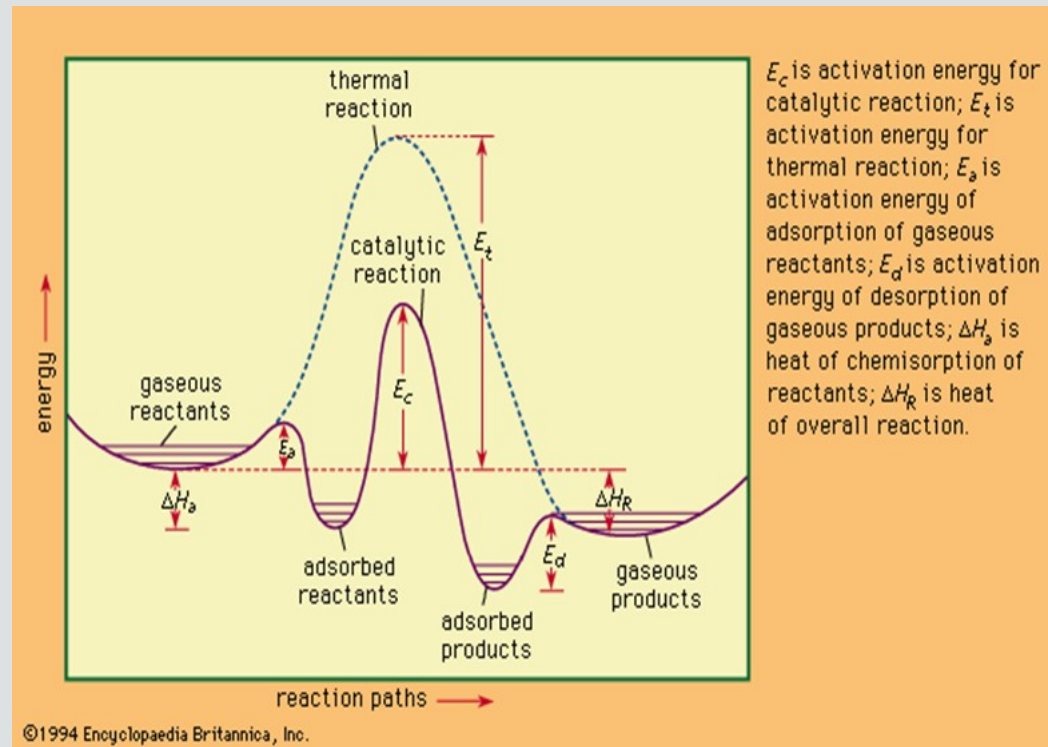
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## Heterogeneous catalysis - Driving force and rate determining step (RDS)

Steps 3, 4, 5: adsorption – reaction - desorption



**RDS – the slowest step; in steady-state – Overall rate of reaction = rate of RDS; any of Heterogeneous catalysis steps could be RDS.**

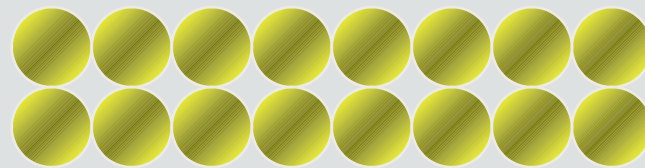


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**Driving force and rate determining step**  
**Steps 3, 4, 5: reactive steps, surface processes**



***Catalyst***



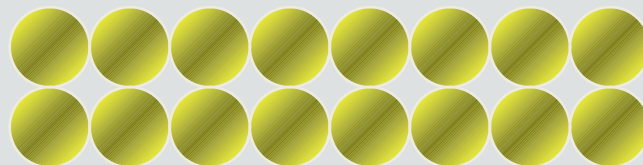
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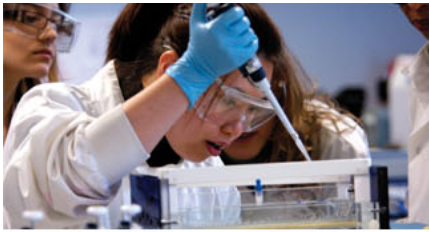


Steps 3, 4, 5: reactive steps, surface processes – cont'd

**Reactant A**



**Catalyst**



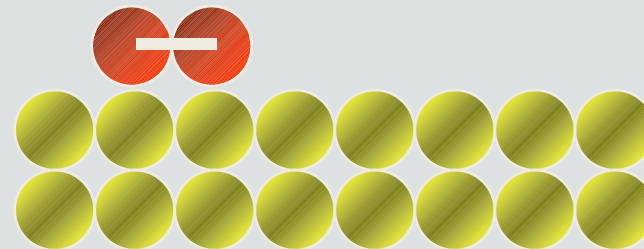
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Steps 3, 4, 5: reactive steps, surface processes – cont'd

- Adsorption occurs at **active site**



**Catalyst**

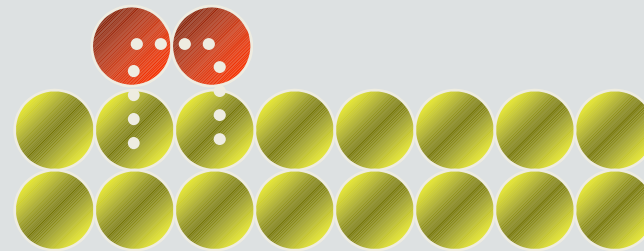


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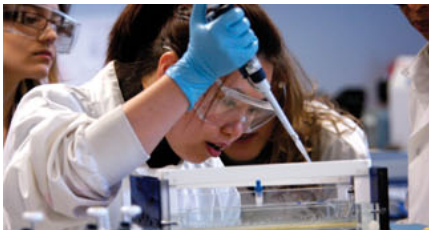
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Steps 3, 4, 5: reactive steps, surface processes – cont'd



**Catalyst**



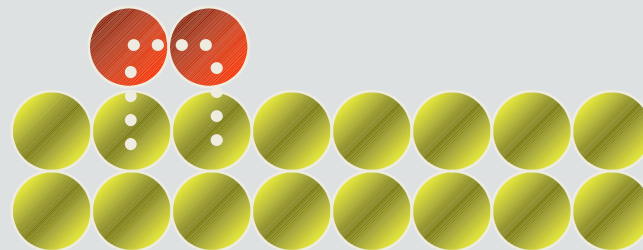
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## Steps 3, 4, 5: reactive steps, surface processes – cont'd

**Reactant B**



**Catalyst**

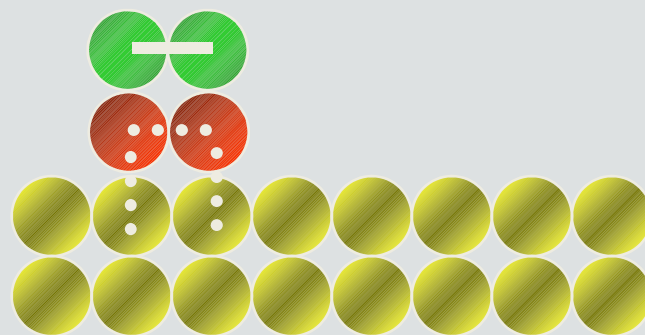


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Steps 3, 4, 5: reactive steps, surface processes – cont'd



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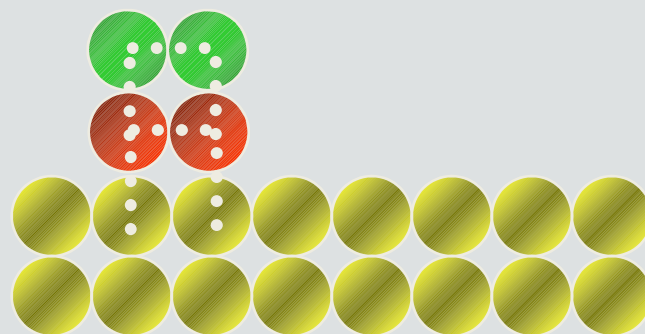


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Steps 3, 4, 5: reactive steps, surface processes – cont'd



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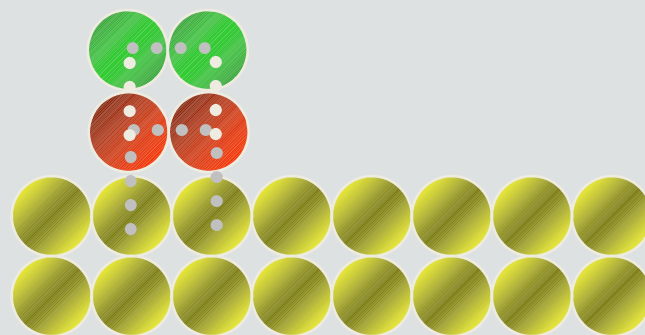


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Steps 3, 4, 5: reactive steps, surface processes – cont'd



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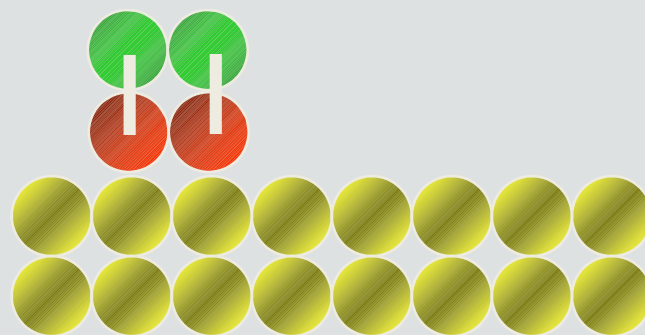


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Steps 3, 4, 5: reactive steps, surface processes – cont'd



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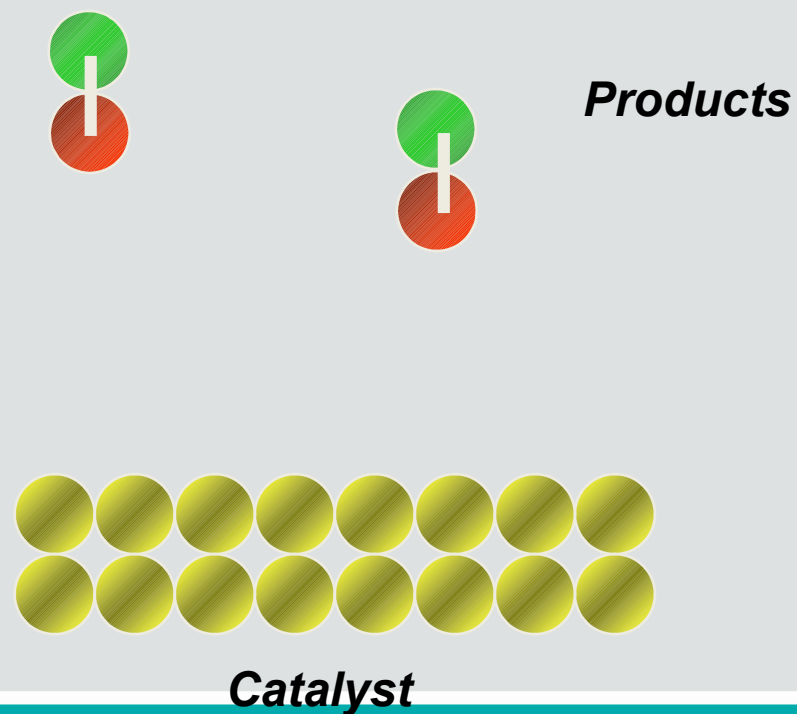


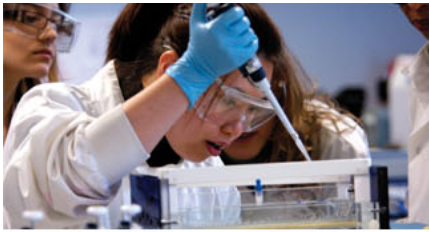
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## Steps 3, 4, 5: reactive steps, surface processes – cont'd



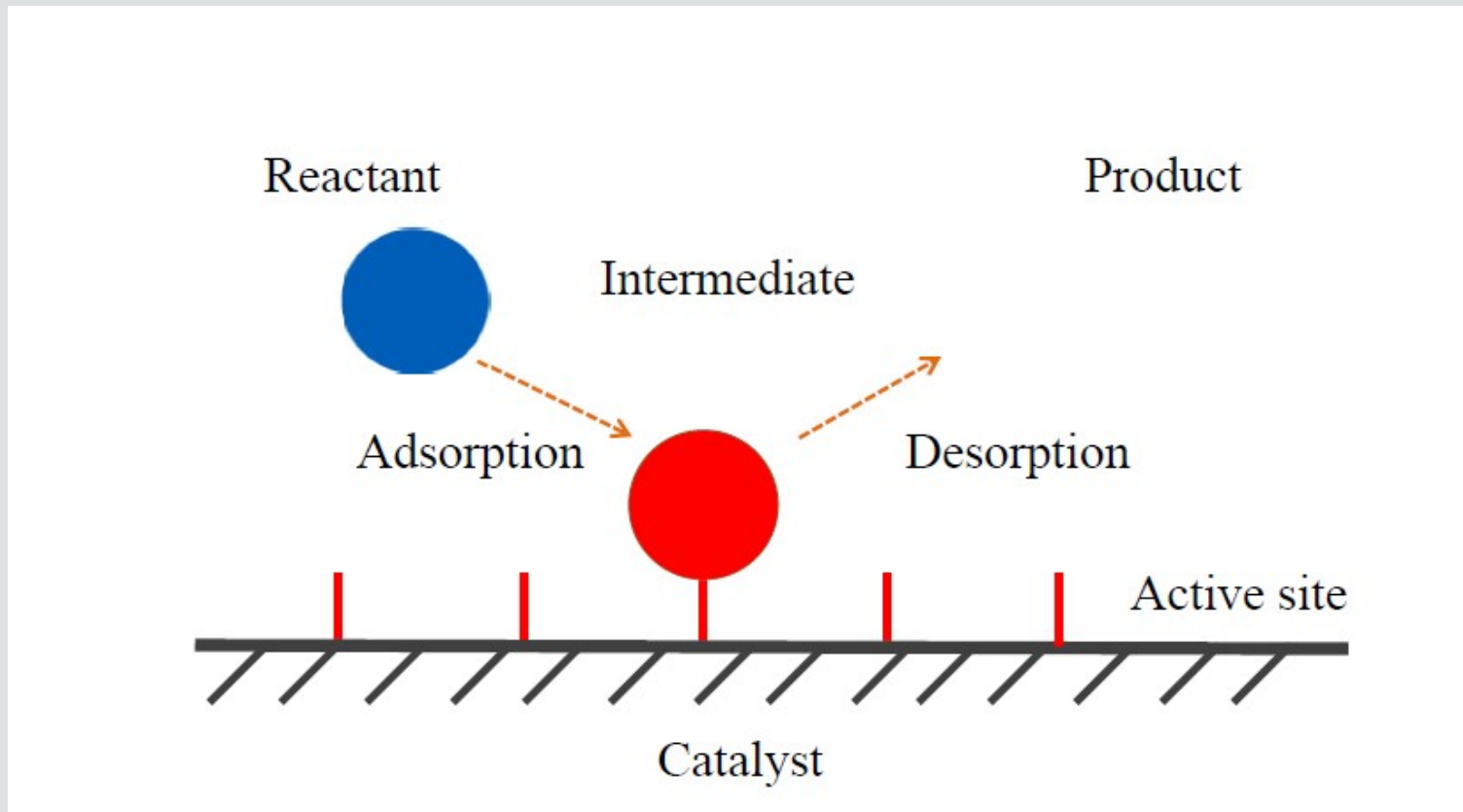


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## Driving force and rate determining step (RDS) – Adsorption - Desorption



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## Driving force and rate determining step (RDS) – Adsorption

### ● Comparison:

	Physisorption	Chemisorption
Enthalpy of adsorption, kJ/mol	5-20	40-80
Activation energy	Zero	Typically low
Number of adsorption layers	Multiple	Single
Strength	Weak	Strong
Selectivity	No	Yes
Common	Exothermic	

- Spontaneous process,  $\Delta G < 0$
- The movement of adsorbates is limited from three dimensional space to two-dimensional plane,  $\Delta S < 0$
- $\Delta G = \Delta H - T\Delta S < 0 \Rightarrow \Delta H < 0$

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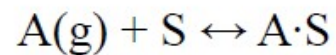
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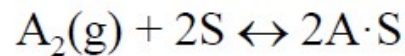
## Driving force and rate determining step (RDS) – Adsorption

### ● Adsorption

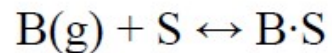
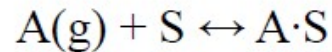
a) Molecular adsorption



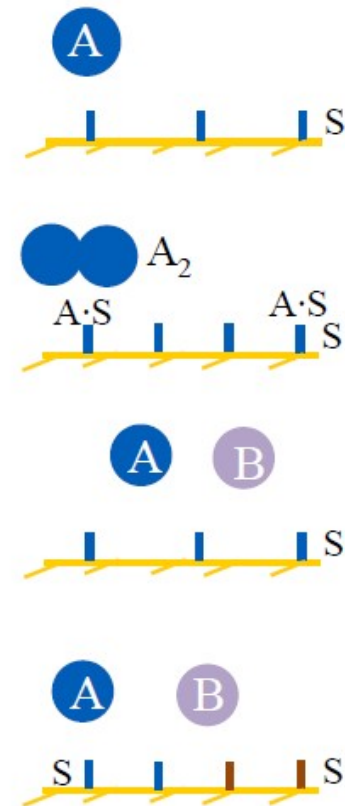
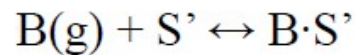
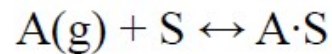
b) Dissociative adsorption



c) Competitive adsorption



d) Adsorption on different types of sites



<https://mycourses.aalto.fi/pluginfile.php/663748/course/section/109647/Lecture%201%20Introduction.pdf>



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## Driving force and rate determining step (RDS) – Adsorption

### a) Molecular adsorption, nondissociatively:

$$r_{AD} = k_a \left( P_{CO} C_v - \frac{C_{CO \cdot s}}{K_A} \right) \text{ rate} = \text{constant} \times \text{driving force!}$$

- $k_A$ ,  $k_{-A}$ ,  $K_A$  are temperature dependent
  - $k_A$  and  $k_{-A}$  increase with increasing temperature
  - $K_A$  decreases with increasing temperature (adsorption is exothermic reaction)

**Driving force = Distance from the (adsorption) equilibrium!**

**How can the rate of adsorption be increased?**

<https://mycourses.aalto.fi/pluginfile.php/663748/course/section/109647/Lecture%201%20Introduction.pdf>



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## Driving force and rate determining step (RDS) – Desorption

### ● Desorption

- The rate of desorption of C:

***rate = constant X driving force!***

$$r_{DC} = k_D(C_{C.S} - P_C C_V / K_{DC})$$

Where  $K_{DC}$  is the desorption equilibrium constant  $K_D = k_D / k_{-D}$

**Driving force = Distance from the (desorption) equilibrium!**





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## Driving force and rate determining step (RDS) – Surface reaction

### Case: chemical reaction determines the reaction rate



concentration of C on the catalyst surface

$$-r_A = k f(C_{A,S}, C_{B,S}, C_{C,S})$$

**rate = constant X driving force!**

- Diffusion at the outer surface and inside the catalyst particles significantly faster than chemical reaction
- Concentrations near active sites in pores  $\approx$  concentrations in bulk phase

How can the rate of surface reaction be increased?

$$k = A \exp\left(-\frac{E_a}{RT}\right)$$

**Driving force = Reaction will occur as long as there are reactants on or near the active site!**

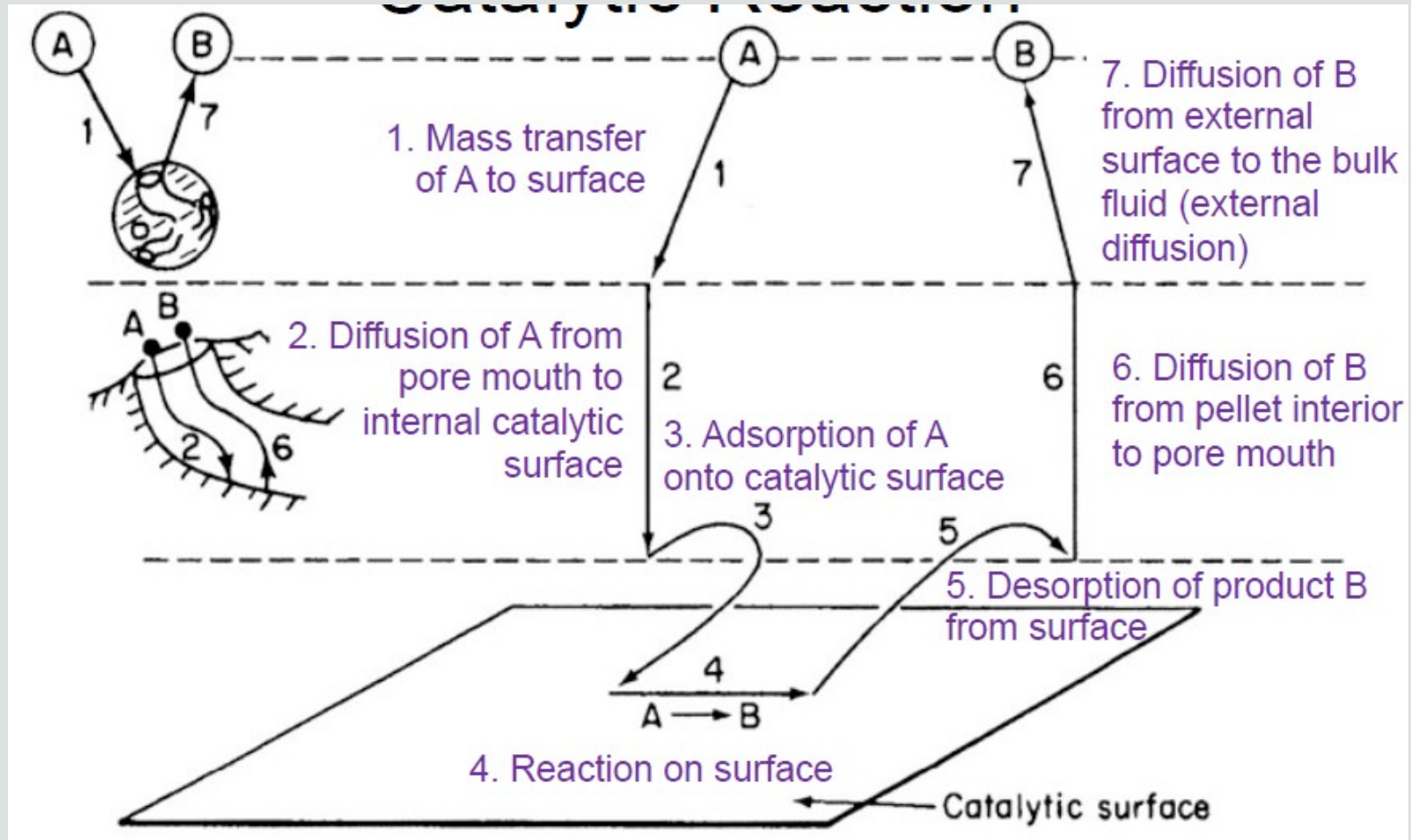


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## Driving force and rate determining step (RDS) – External diffusion



[http://umich.edu/~elements/5e/powerpoints/2013lectures/Lec27\\_PDF.pdf](http://umich.edu/~elements/5e/powerpoints/2013lectures/Lec27_PDF.pdf)

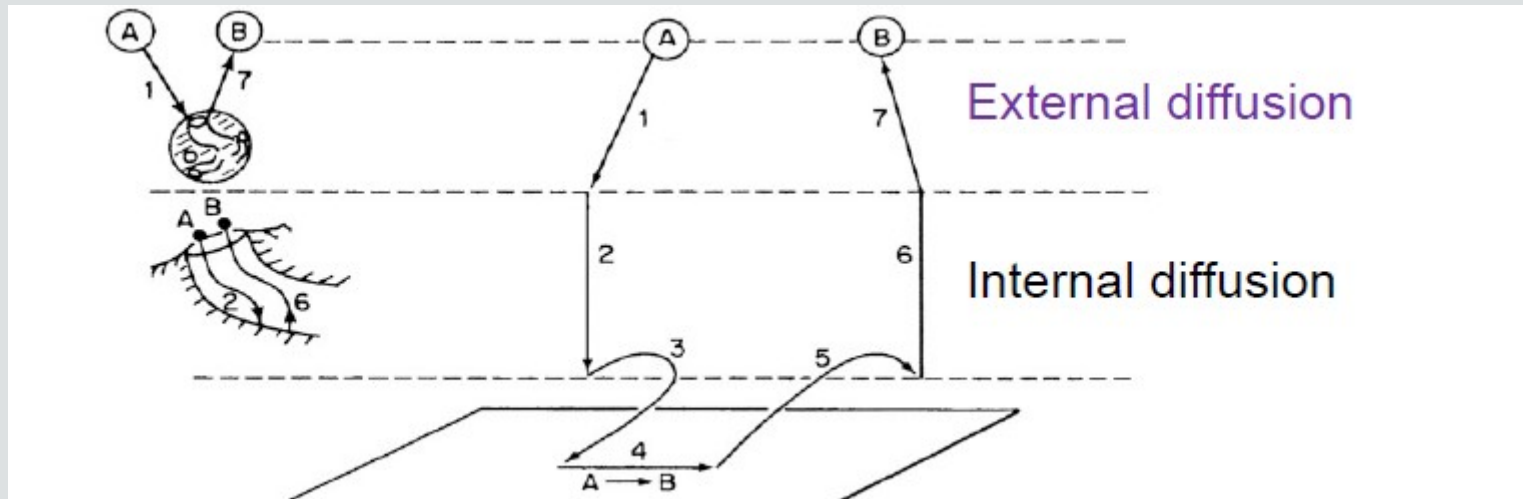


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## Driving force and rate determining step (RDS) – External diffusion



[http://umich.edu/~elements/5e/powerpoints/2013lectures/Lec27\\_PDF.pdf](http://umich.edu/~elements/5e/powerpoints/2013lectures/Lec27_PDF.pdf)



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## Driving force and rate determining step (RDS) – External diffusion

# Definition of diffusion and mass transfer

- **Diffusion:** Spontaneous mixing of atoms or molecules due to thermal motion

Driving force of diffusion is the concentration gradient  
(movement from higher concentration to lower one)

↳ The gradient causes a molar flux  $W_A$  in the direction of concentration gradient

- **Mass transfer:** Transfer of a mass species through the bulk of a fluid or a solid matrix  
Diffusion is a kind of mass transfer



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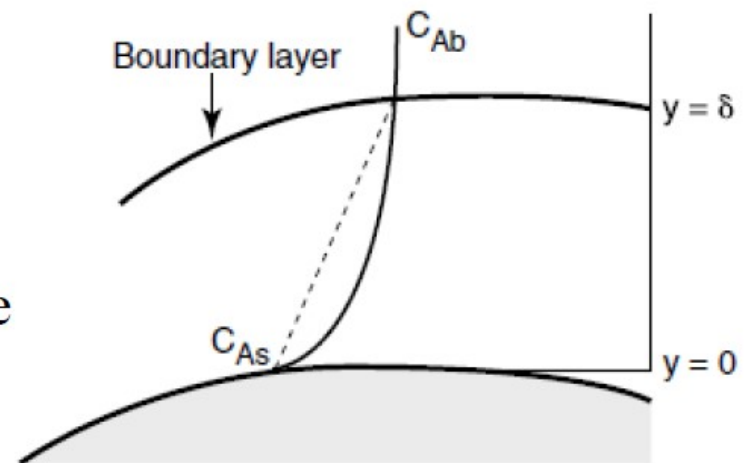
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## Driving force and rate determining step (RDS) – External diffusion

### Diffusion of reactants to the catalyst particle outer surface is slow

- Diffusion resistance can cause a concentration gradient  $\Rightarrow$  bulk concentration  $\neq$  concentration on the outer surface



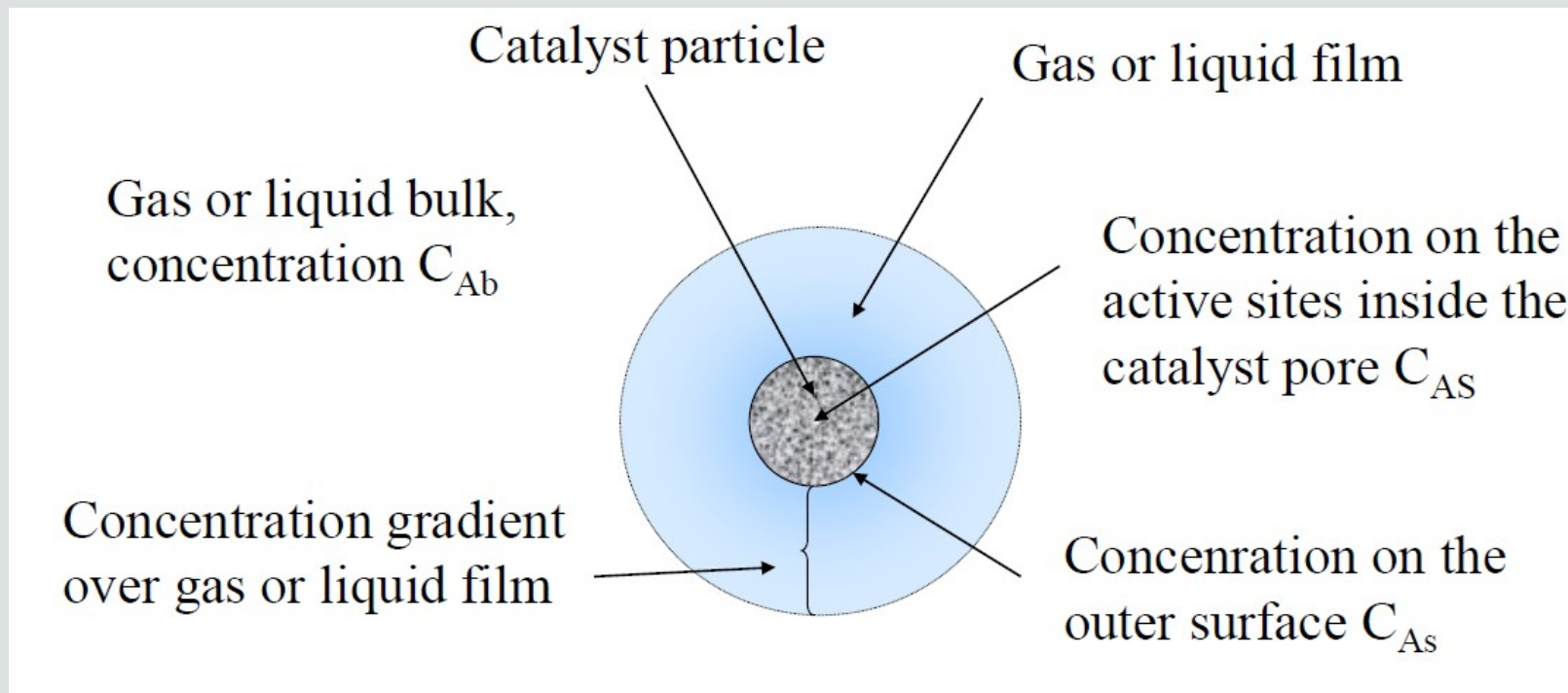


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## Driving force and rate determining step (RDS) – External diffusion



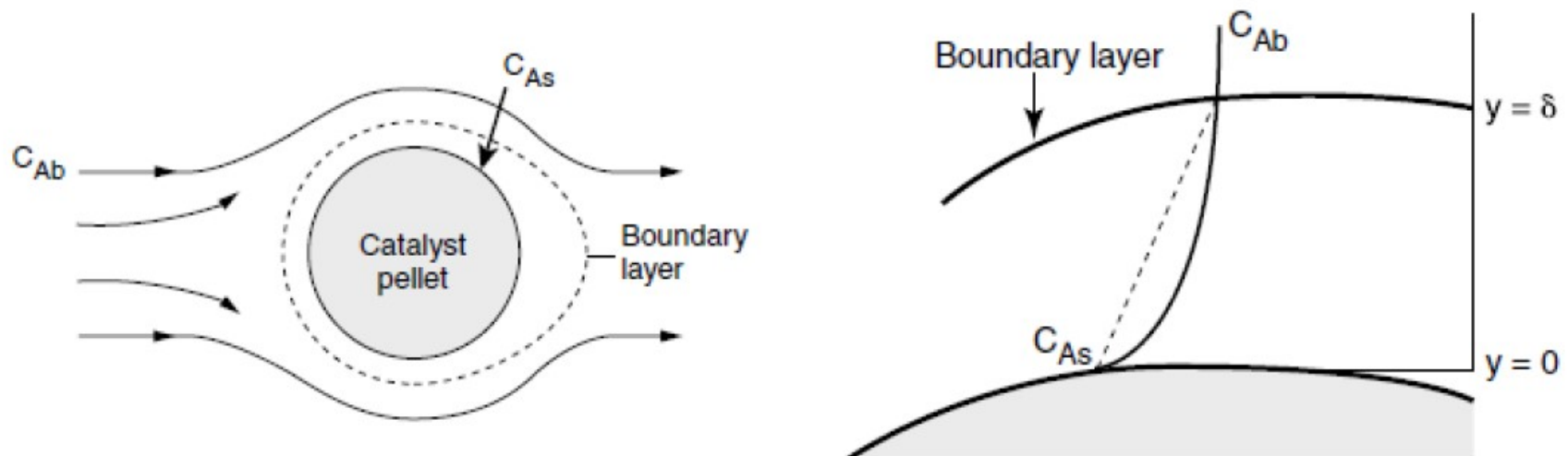


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## Driving force and rate determining step (RDS) – External diffusion



$$\Rightarrow W_A = \frac{D_{AB}}{\delta} (C_{Ab} - C_{As}) \quad (13)$$

$k_c$  (mass transfer coefficient)

**rate = constant X driving force!**

**How can the rate of external diffusion be increased?**

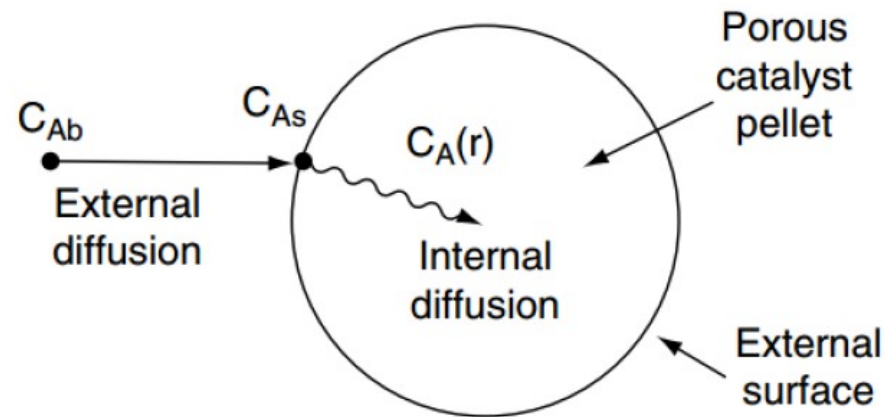


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## Driving force and rate determining step (RDS) – Internal diffusion



*Fig 7.6 Mass transfer and reaction steps for a catalyst pellet.*

- May affect the overall reaction rate
- Reactant concentrations at the exit of pores higher than inside the pores (opposite for the products)
- Concentration gradients in the particles can be calculated





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## Driving force and rate determining step (RDS) – Internal diffusion

For a first order reaction

$$-r_A = \eta \cdot (k_1 C_{As})$$

$$-r_A = \frac{3}{R} \sqrt{\frac{D_e}{k_1}} \cdot (k_1 C_{As}) = \frac{3}{R} \sqrt{D_e k_1} C_{As}$$

***rate = constant X driving force!***

**How can the rate of internal diffusion be increased?**

**Driving force = Reaction will occur as long as there are reactants on or near the active site, brought there by internal diffusion!**



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Summary

**Let's write it together!**



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*Thank you for your attention!*