

Introduction

Modern Methods in Heterogeneous Catalysis

F.C. Jentoft, October 21, 2005

Literature

G.A. Somorjai: Introduction to surface chemistry and catalysis, Wiley New York [u.a.] 1994

Jens Hagen: Technische Katalyse: eine Einführung, VCh Weinheim 1996

B.C. Gates: Catalytic Chemistry, John Wiley & Sons, New York 1997

G. Ertl, H. Knözinger, J. Weitkamp, [Eds.]: Handbook of heterogeneous catalysis: VCh Weinheim 1997

J.M. Thomas, W.J. Thomas: Principles and practice of heterogeneous catalysis, Weinheim [u.a.] VCh 1997

B. Cornils, W.A. Herrmann, R. Schlögl, C.-H. Wong (Eds.): Catalysis from A to Z, Wiley-VCh Weinheim 2000

R.I. Masel: Chemical kinetics and catalysis, Wiley-Interscience New York [u.a.] 2001

J.W. Niemantsverdriet: Spectroscopy in Catalysis, Wiley-VCh Weinheim 2002

James F. Haw (Ed.): In-Situ Spectroscopy in Heterogeneous Catalysis, Wiley-VCh Weinheim 2002

I. Chorkendorff, J.W. Niemantsverdriet: Concepts of Modern Catalysis and Kinetics, Wiley-VCh Weinheim 2003

Catalysis Definition – First Description



Jöns Jakob Berzelius
(1779–1848)

Berzelius' Ideas of "Catalytic Power" (1835)

- ❖ the ability of substances "to awaken affinities, which are asleep at a particular temperature, by their mere presence and not by their own affinity"
- ❖ used to explain conversion of starch to sugar by acid, hydrogen peroxide decomposition by metals, conversion of ethanol to acetic acid by Pt
- ❖ chose "catalysis" in analogy to "analysis"
- ❖ stated that catalysis was more common than believed, part of inorganic and organic nature, in living plants and animals thousands of catalytic processes may proceed

M.W. Roberts, Catalysis Lett. 67,1 (2000)

G. Ertl and T. Gloya, Z. Phys. Chem. 217 (2003) 1207-1219

Reactions on Berzelius' "Catalytic Power"

Liebig to Wöhler, June 2, 1837:

Weisst Du denn nicht, dass die Esel, welche in Deutschland Bücher schreiben, seine [Berzelius] katalytische Kraft ohne zu prüfen, annehmen und unsern Kindern in den Kopf setzen werden, weil sie bequem und die Faulheit begünstigend ist?

Don't you know that the idiots who write books in Germany will adopt his [Berzelius'] catalytic power without scrutinization, and will teach it to our children because it [the catalytic power] is convenient and favors the laziness?

Berzelius und Liebig, Ihre Briefe von 1831-1845, Hrsg. T. Reschke, WiSoMed 1978, Göttingen

Catalysis Definition

Ostwald's Definition of Catalysis (1894)

- ❖ "catalysis is the acceleration of a slowly proceeding chemical reaction through the presence of a foreign substance"
- ❖ "the acceleration occurs without a change of the energetic situation"
- ❖ "at the end of the reaction the foreign substance can be considered as removed"

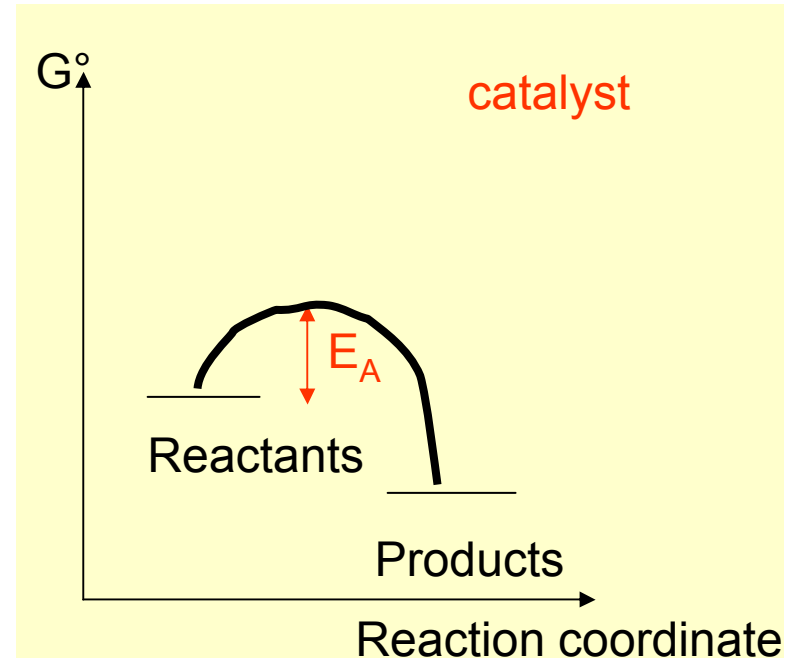
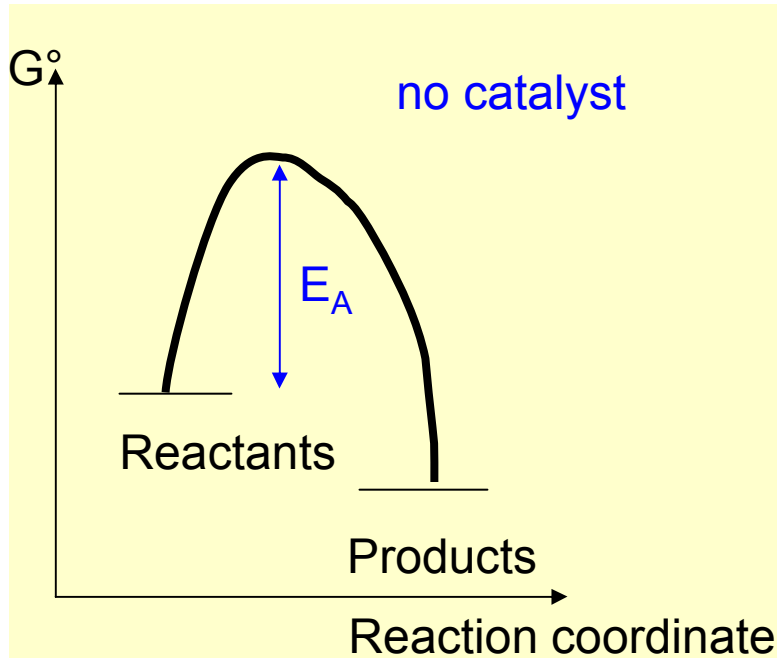
Stohmann, Z. Biol. 31 (1894) 364-391

W. Ostwald, Z. Phys. Chem. 15 (1894) 705-706

G. Ertl and T. Gloyna, Z. Phys. Chem. 217 (2003) 1207-1219

N.I Rodnyj, Ju.I. Solowjew, Wilhelm Ostwald, Teubner, Leipzig 1977.

Modern Catalysis Picture



- ❖ Thermodynamics of reaction remain unchanged
- ❖ Catalyst influences reaction rate by changing the reaction coordinate and the nature of transition states or intermediates

Types of Catalysis

- ❖ Biocatalysis

catalyzed reactions where the catalyst is an enzyme

- ❖ Homogeneous catalysis

catalysis with the catalyst in the same phase as the reactant

- ❖ Heterogeneous catalysis

1) catalysis with the catalyst in a different phase than the reactants, and 2) with the catalyst on solid, porous material or impregnated in such material

Biocatalysis (Nov.4, 2005)

❖ Enzymes as catalysts

highly efficient, i.e. very fast and very selective!

mild conditions (T, p)... but also very sensitive (T,pH)

catalase



Rate: 10^7 molecules/s

Catalyst	$E_a / \text{kJ} \cdot \text{mol}^{-1}$
None	73
iodide ion	54
Pt surface	46
iron(III)	40
Catalase	4

Homogeneous Catalysis (Feb. 17, 2006)

Phases/catalyst reactants	Type of cat.	Examples of cat. reaction
<i>Homophasic</i>		
Liquid	*Acids, protons	*Esterification
	*Lewis acids	*Isomerization
	*Bases	*Alkylation
	*Organometals	*Aldolization
Gaseous		*Condensation
		*C-C bond formation
	NO/NO ₂ [NOHSO ₄]	*Lead chamber proc.
	NO ₂ /HCl [NOCl]	*Kellogg Kelchlor proc.
	Oxygen	*LDPE synthesis
	Halogens	*Chlorinations
	Halides	*Eastman MMA
		*Goodyear/SD isoprene
	Radicals (*initiators)	*Radical reactions
	H-Hal	*Demethanation
<i>Heterophasic</i>		
Liquid/liquid	*Organometals	two-phase operation, *Hydroformylation *Shell SHOP

Homogeneous catalysis helps with understanding! Ideas can be transferred from solution chemistry to surface chemistry (e.g. in acid catalysis, 18.2.05)

Heterogeneous Catalysis

Advantages

- ❖ easy separation of product and catalysts
- ❖ high catalyst lifetimes
- ❖ particularly acid catalysis: fewer corrosion and disposal problems
- ❖ ca. 80 % of industrial catalytic processes are heterogeneous

Applications

- ❖ production of chemicals
- ❖ cleaning of waste and exhaust gas streams (environmental catalysis)
- ❖ energy conversion (fuel cells)

Largest Processes in Heterogeneous Catalysis

Reaction	Catalyst
Catalytic cracking of crude oil	Zeolites
Hydrotreating of crude oil	Co-Mo, Ni-Mo, Ni-W (sulfidic form)
Reforming of naphtha (to gasoline)	Pt, Pt-Re, Pt-Ir
Alkylation	H ₂ SO ₄ , HF, solid acids
Polymerization of ethylene, propylene, a.o.	Cr, TiCl _x /MgCl ₂
Ethylene epoxidation to ethylene oxide	Ag
Vinyl chloride (ethylene + Cl ₂)	Cu (as chloride)
Steam reforming of methane to CO + H ₂	Ni
Water-gas shift reaction	Fe (oxide), Cu-ZnO
Methanation	Ni
Ammonia synthesis	Fe
Ammonia oxidation to NO and HNO ₃	Pt-Rh
Acrylonitrile from propylene and ammonia	Bi-Mo, Fe-Sb (oxides)
Hydrogenation of vegetable oils	Ni
Sulfuric acid	V (oxide)
Oxidation of CO & hydrocarbons (car exhaust)	Pt, Pd
Reduction of NO _x (in exhaust)	Rh, vanadium oxide

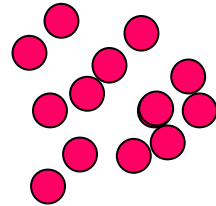
Catalysis: A Multidisciplinary Problem

1. Physical Chemistry

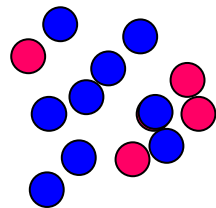
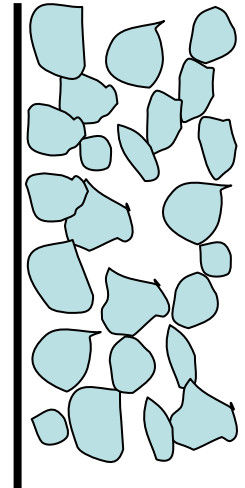
- ❖ Thermodynamics of target reaction
- ❖ Kinetics
- ❖ Analytical techniques (e.g. spectroscopy)

3. Reaction Engineering

- ❖ Reactors, catalyst formulation



A



A, B

2. Organic and Inorganic Chemistry

- ❖ Reactants
- ❖ Catalysts

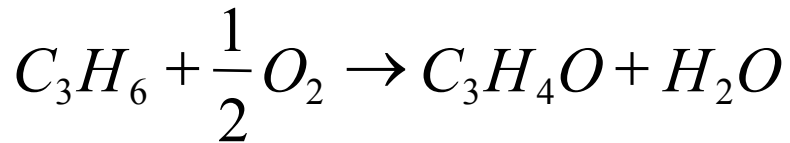
4. Theoretical Chemistry

5. Physics

6. Biosciences (enzymes)

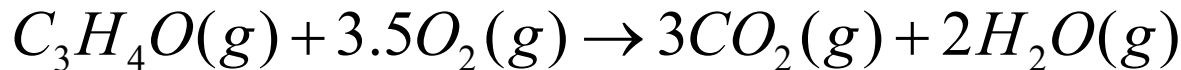
Partial vs. Total Oxidation

- ❖ Oxidation of propene to acrolein

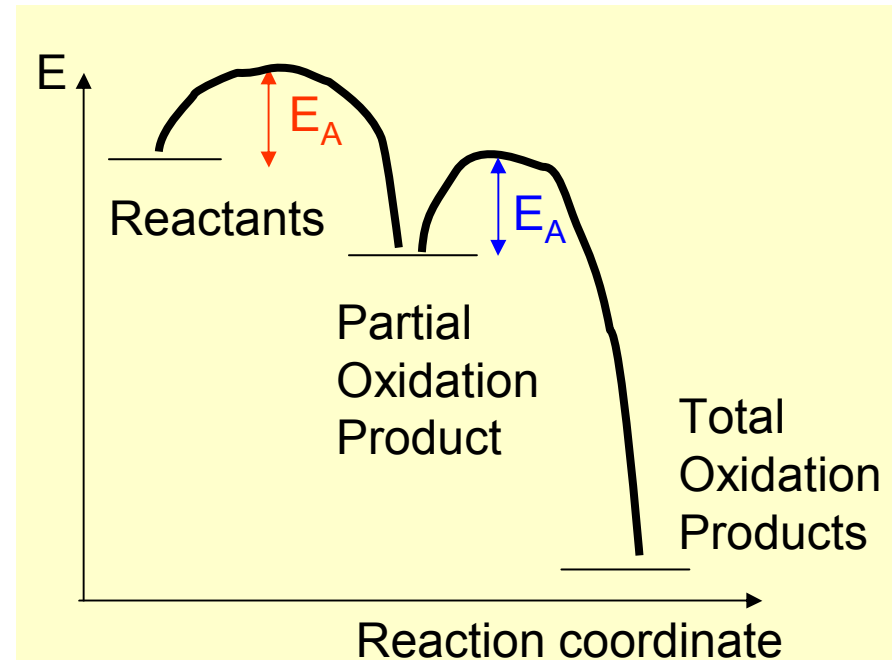


$$\Delta_r H^\circ = -427 \text{ kJ mol}^{-1}$$

- ❖ Oxidation of acrolein to CO_2



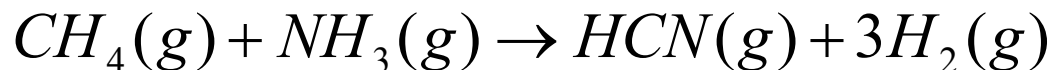
$$\Delta_c H^\circ = -1633 \text{ kJ mol}^{-1}$$



need to control reaction temperature

HCN Synthesis

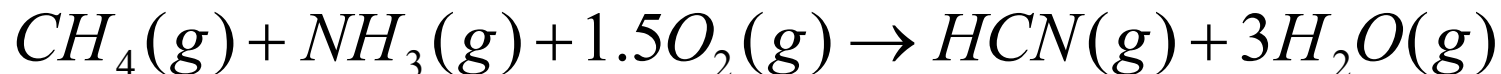
- ❖ BMA or Degussa process:



$$\Delta_r H^\circ = + 256 \text{ kJ mol}^{-1}$$

runs at 1300°C, process needs large amount of energy

- ❖ Andrussov process



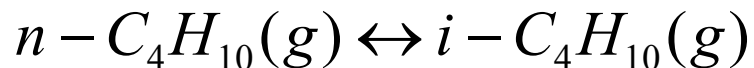
$$\Delta_r H^\circ = - 474 \text{ kJ mol}^{-1}$$



Both possibilities (oxidative/non-ox.) may be feasible

Isomerization

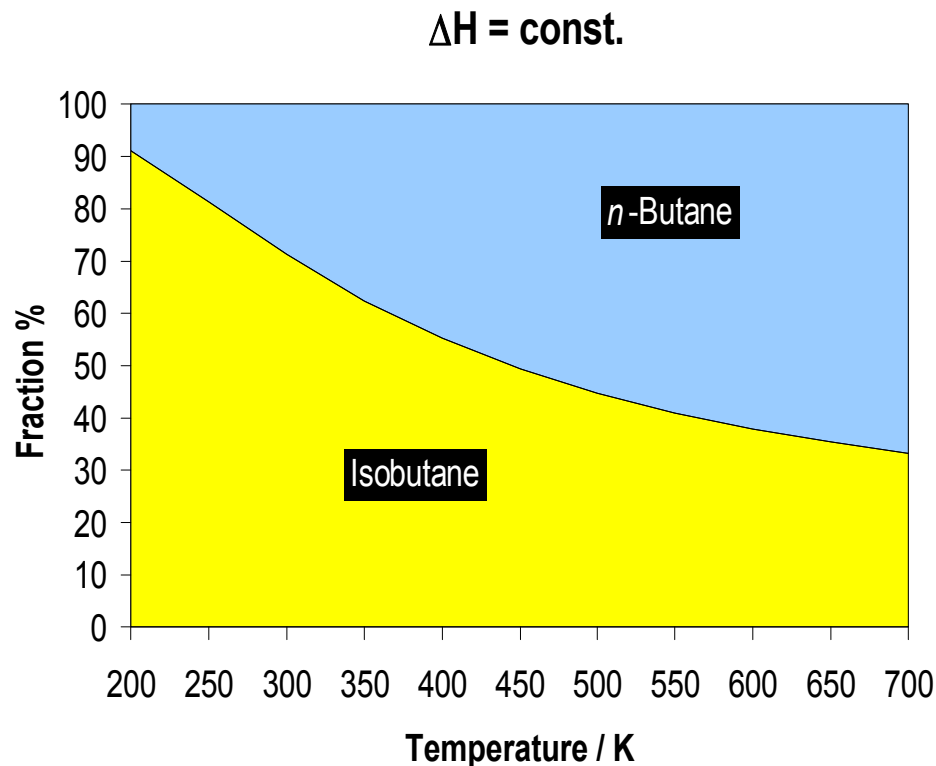
❖ Isomerization of butane



$$\Delta_r H^\circ = -7 \text{ kJ mol}^{-1}$$

$$\Delta_r S^\circ = -15 \text{ J mol}^{-1}$$

$$\Delta_r G^\circ = -2.3 \text{ kJ mol}^{-1}$$



Start your research by calculating the thermodynamics of your reaction!

Kinetics: Rate Equations

- ❖ Typical rate equation:

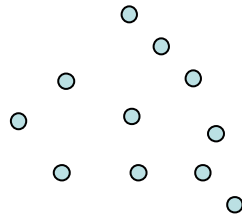
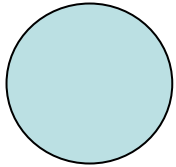
$$r = k[A]^a[B]^b[C]^c \dots$$

- ❖ With r the reaction rate in units of mol/l per time
- ❖ With a, b, c , the individual reaction order with respect to a particular reactant and the total reaction order n the sum of the exponents
- ❖ With $[A]$, $[B]$, $[C]$ the reactant concentrations
- ❖ With k the rate constant in units of min^{-1} for a first order reaction, for higher orders in inverse units of concentration in different powers

$$\left[\text{min}^{-1} \left(\frac{l}{mol} \right)^{n-1} \right]$$

Rates in Heterogeneous Catalysis

❖ Rate with respect to mass or surface area of the catalyst



$$\left[\frac{\text{mol}}{\text{min } g_{\text{catalyst}}} \right]$$

$$\left[\frac{\text{mol}}{\text{min } m^2_{\text{catalyst surface}}} \right]$$

How to Derive a Rate Equation I

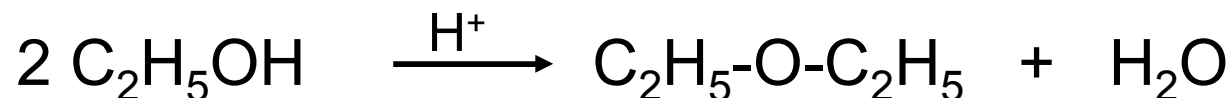


Table 4-2

KINETICS OF DEHYDRATION OF ETHANOL CATALYZED BY SULFONATED
POLY(STYRENE-DIVINYLBENZENE) AT $120 \pm 1^\circ\text{C}^a$

$10^4 \times r$, mol/(min·g of Catalyst)	$P_{\text{C}_2\text{H}_5\text{OH}}$, atm	$P_{\text{H}_2\text{O}}$, atm	$P_{\text{C}_2\text{H}_5\text{-O-C}_2\text{H}_5}$, atm	P_{argon} , atm
1.19	1.00	0.00	0.00	0.00
0.81	0.65	0.00	0.35	0.00
0.47	0.42	0.00	0.58	0.00
0.30	0.59	0.41	0.00	0.00
0.12	0.40	0.60	0.00	0.00
0.65	0.58	0.00	0.00	0.42
0.60	0.47	0.00	0.00	0.53
0.41	0.33	0.00	0.00	0.67
0.25	0.20	0.00	0.00	0.80
0.57	0.75	0.25	0.00	0.00
0.24	0.55	0.45	0.00	0.00
0.08	0.38	0.62	0.00	0.00

^a The catalyst was 8% cross-linked gel-form resin having 5.2 meq of $-\text{SO}_3\text{H}$ groups per gram.

How to Derive a Rate Equation II

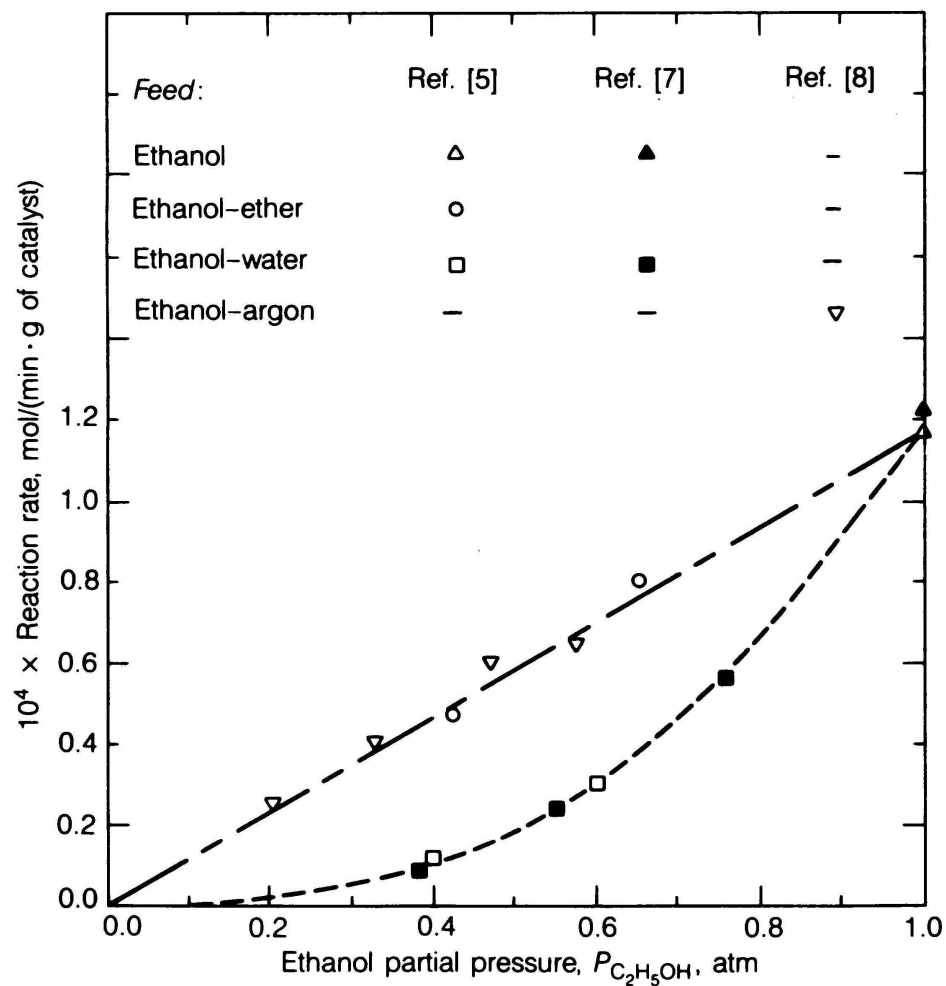


Figure 4-9

Kinetics of ethanol dehydration catalyzed by sulfonic acid resin at 120°C. The curves are from Eq. 4-24 with the parameter values of Table 4-3.

How to Derive a Rate Equation III

Table 4-3
COMPARISON OF SUGGESTED FORMS OF RATE EQUATIONS WITH THE DATA OF TABLE 4-2

Equation ^a		k' ^b	K_A, atm^{-1}	K_W, atm^{-1}	Sum of Squares of Deviations of Predicted and Observed Values of Rate, $[\text{mol}/(\text{min} \cdot \text{g of catalyst})]^2$
A	$r = \frac{k' P_A}{1 + K_A P_A + K_W P_W}$	$(1.20 \pm 0.09) \times 10^{-4}$	$(3.8 \pm 100) \times 10^{-3}$	3.28 ± 0.52	1.9×10^{-10}
B	$r = \frac{k' P_A^2}{1 + K_A P_A + K_W P_W}$	-0.0178 ± 0.056	-150 ± 470	-290 ± 910	7.4×10^{-11}
C	$r = \frac{k' P_A^2}{(1 + K_A P_A + K_W P_W)^2}$	$(8.21 \pm 1.1) \times 10^{-4}$	1.65 ± 0.20	2.70 ± 0.33	1.4×10^{-10}
D	$r = \frac{k' P_A}{(1 + K_A P_A + K_W P_W)^2}$	$(1.20 \pm 0.08) \times 10^{-4}$	$(7.9 \pm 44) \times 10^{-4}$	1.32 ± 0.14	1.4×10^{-10}

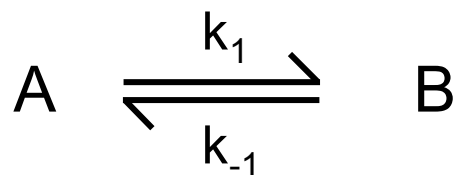
^a Parameter values estimated by a nonlinear least squares fitting technique; r has dimensions of $\text{mol}/(\text{min} \cdot \text{g of catalyst})$; A = ethanol; W = water.

^b k' has units of $\text{mol}/(\text{min} \cdot \text{g of catalyst} \cdot \text{atm})$ in Eqs. A and D and units of $\text{mol}/(\text{min} \cdot \text{g of catalyst} \cdot \text{atm}^2)$ in Eqs. B and C.

Temperature Dependence of Rate Constant

- ❖ Once a rate equation has been established, a rate constant can be calculated
- ❖ The rate constant is temperature dependent
- ❖ There are three different ways to derive this relation:
 - Arrhenius Theory
 - Collision Theory
 - Transition State Theory (Eyring)

Arrhenius Theory



$$K = \frac{k_1}{k_{-1}}$$

$$\left(\frac{\partial \ln K}{\partial T} \right)_p = \frac{\Delta H}{RT^2}$$

van't Hoff's Equation

$$\left(\frac{\partial \ln k_1}{\partial T} \right) - \left(\frac{\partial \ln k_{-1}}{\partial T} \right) = \frac{\Delta H}{RT^2}$$

$$\left(\frac{\partial \ln k_1}{\partial T} \right) = \frac{E_1}{RT^2} \quad \left(\frac{\partial \ln k_{-1}}{\partial T} \right) = \frac{E_{-1}}{RT^2} \quad E_1 - E_{-1} = \Delta H$$

Arrhenius Theory

$$\ln k = \ln A - \frac{E_A}{RT}$$

- ❖ With E the apparent activation energy in kJ mol^{-1}
 A the frequency factor
- ❖ Plot of $\ln k$ vs. $1/T$ gives a slope of $-E_A/R$
which allows the calculation of the activation energy
- ❖ A rule of thumb: the rate doubles for 10 K rise in temperature

Example for Arrhenius Plot

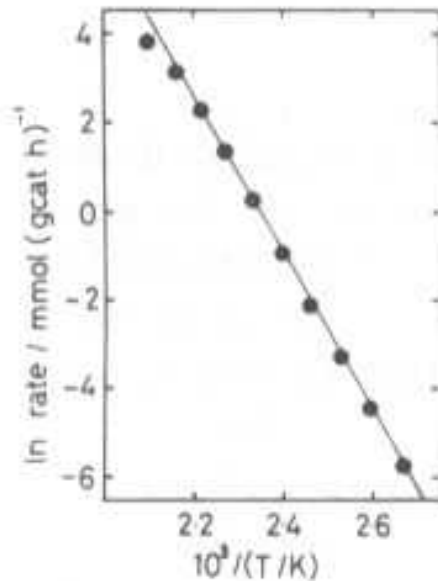


Fig. 2. Arrhenius plot for hydrogenolysis of n-butane over 1% Ru/Al₂O₃ (H₂:n-butane = 10:1) [1].

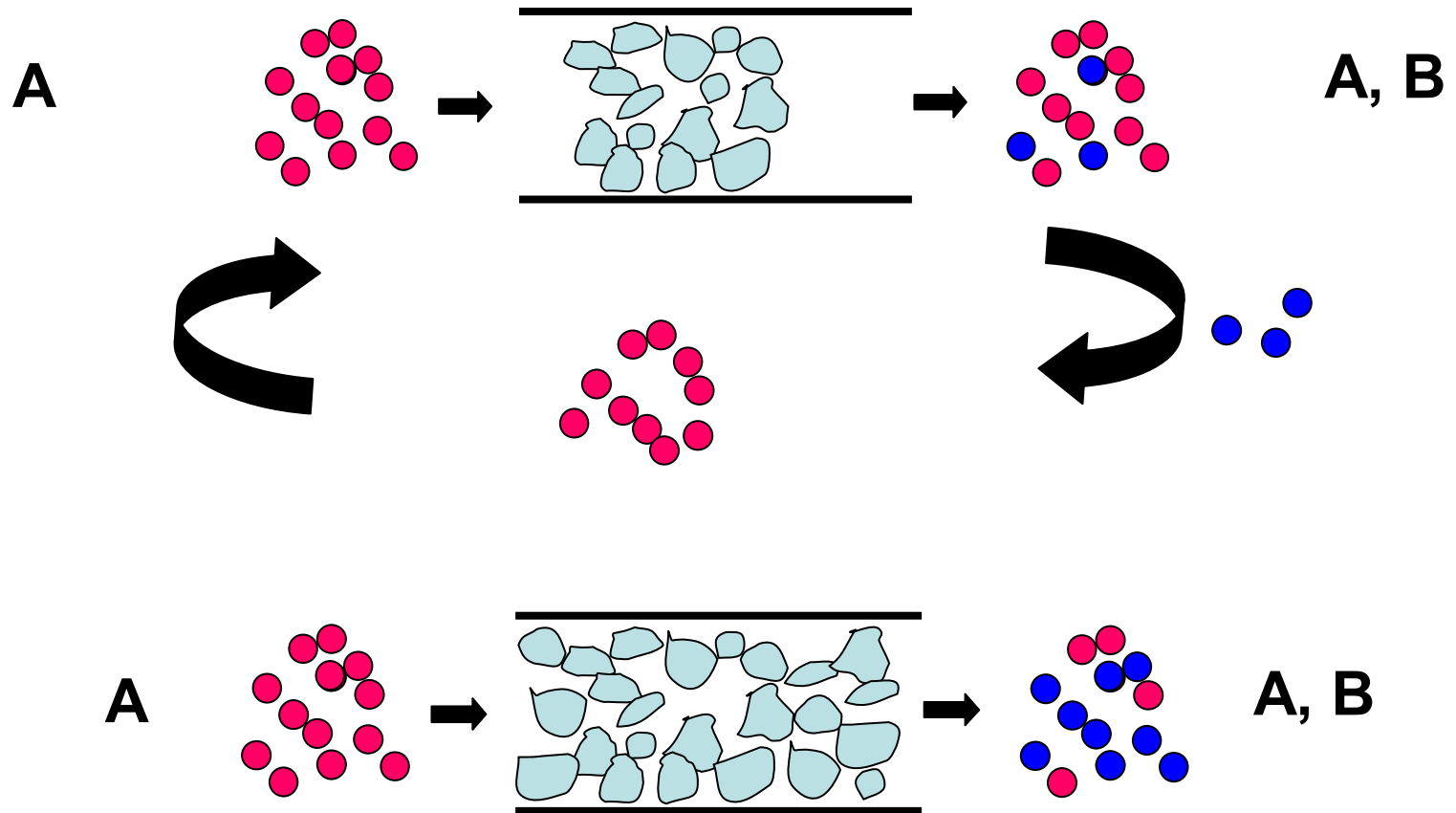
2 different slopes may indicate change in mechanism or change from reaction to diffusion control

What Kinetics Will (Not) Deliver...

- ❖ Reaction rates
- ❖ Rate equation / reaction order
- ❖ Rate constant
- ❖ Apparent activation energies

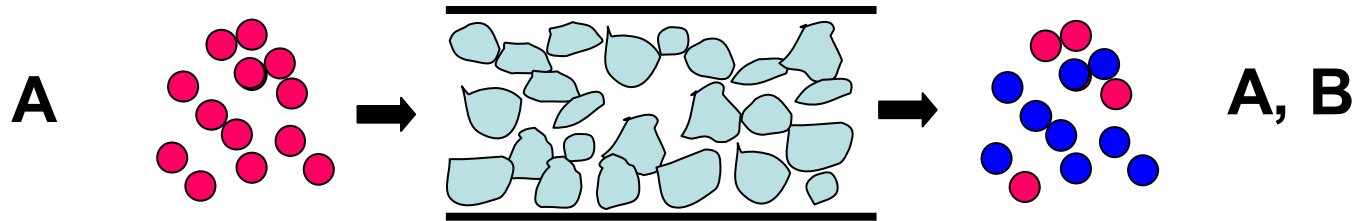
- ❖ Will not deliver a mechanism.....
- ❖ But any mechanism we think of should be consistent with the kinetic data....

Catalyst Characteristics: Activity



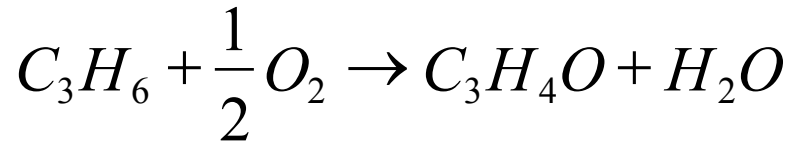
❖ activity is vague term, better: rate constants

Conversion



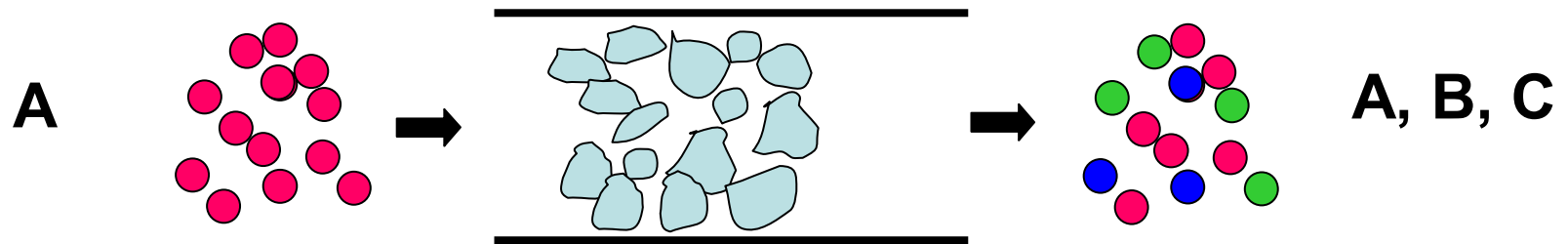
Conversion X (in %)

❖ the fraction of the reactant(s) that has been converted



❖ there can be conversion with respect to different reactants, e.g. oxidation reactions

Selectivity



- ❖ ratio of rates
- ❖ extremely important: unconverted reactant can be recycled – a valuable reactant converted to unwanted side products is lost!

Selectivity S (in %)

- ❖ e.g. moles of desired product/moles of all products

Yield

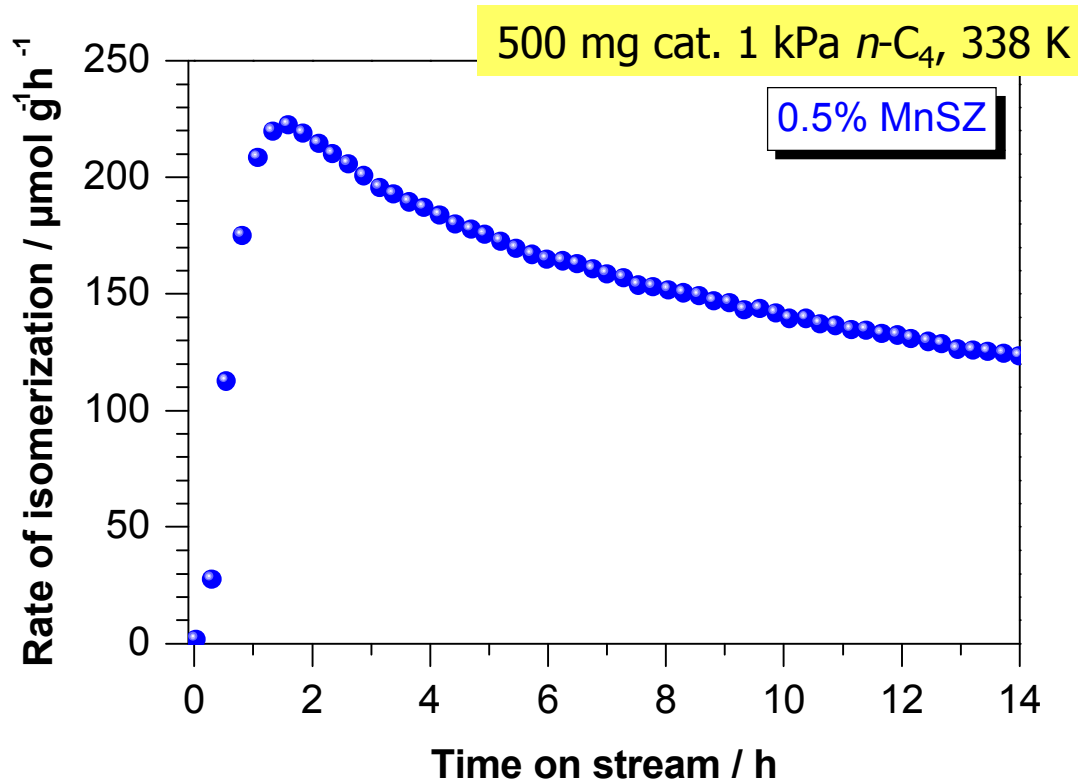
Yield Y (in%)

- ❖ the product of X and S

Space Time Yield (STY)

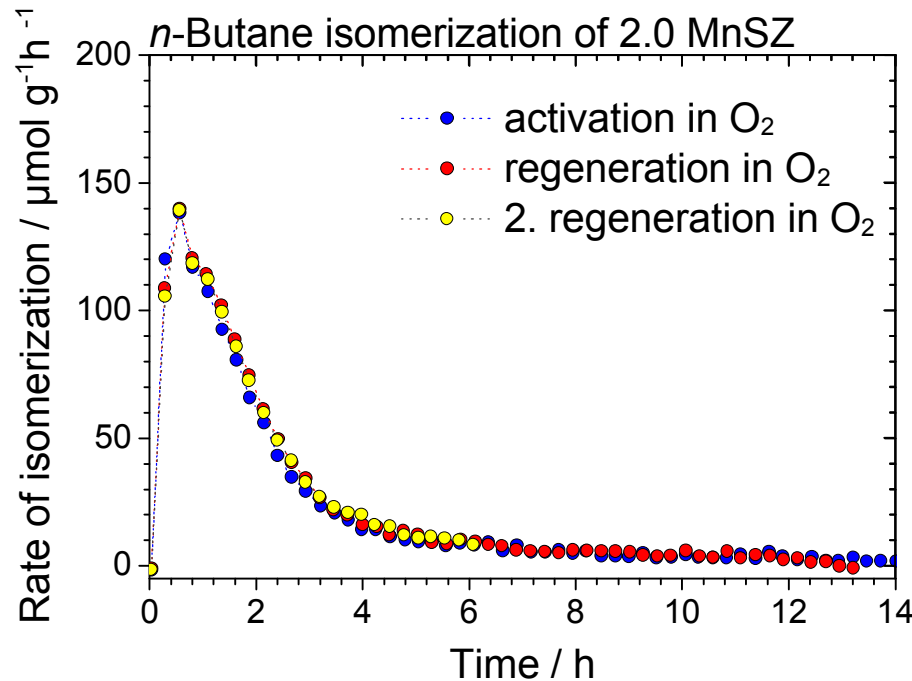
- ❖ differently defined for continuous and discontinuous operation
- ❖ continuous process:
$$(\text{feed} \times \text{conversion} \times \text{selectivity}) / (\text{reactor volume} \times \text{time})$$
- ❖ discontinuous process:
$$(\text{input} \times \text{conversion} \times \text{selectivity}) / (\text{reactor volume} \times \text{time of reaction})$$

Catalyst Characteristics: Stability



❖ rate of deactivation

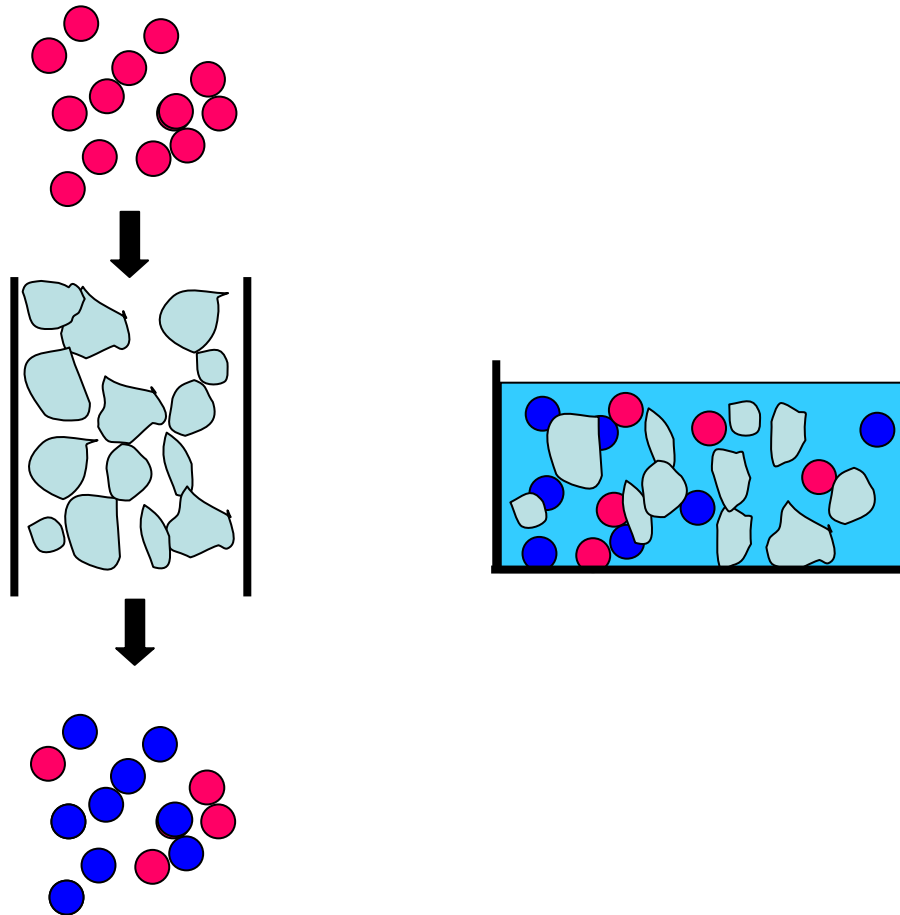
Catalyst Characteristics: Regenerability



- ❖ e.g. cracking catalysts in refineries are constantly regenerated in separate recycle reactor

Reaction Engineering

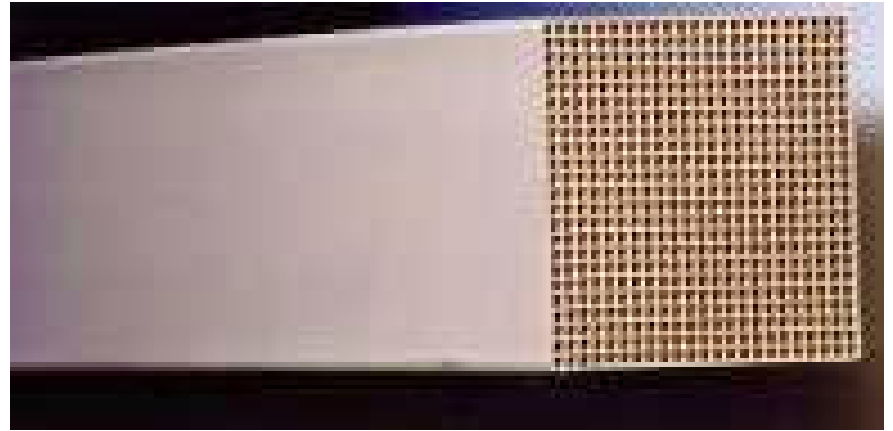
- ❖ Reactor type (Feb. 17, 2006) and catalyst formulation, reaction conditions



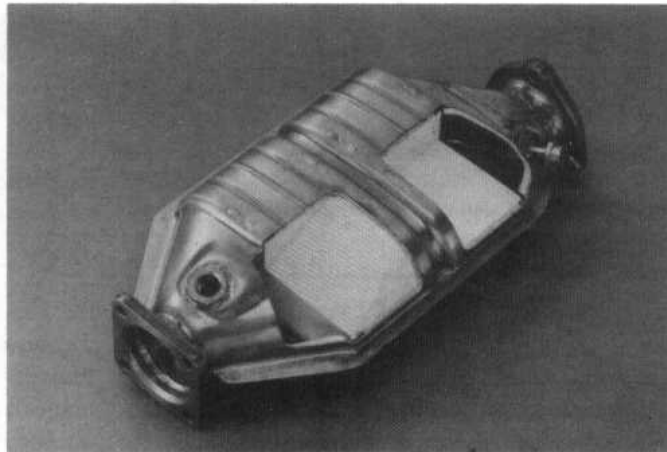
Catalyst Formulations



extrudates



NOx catalyst, stationary power plants



three-way converter

Example Three-Way Converter

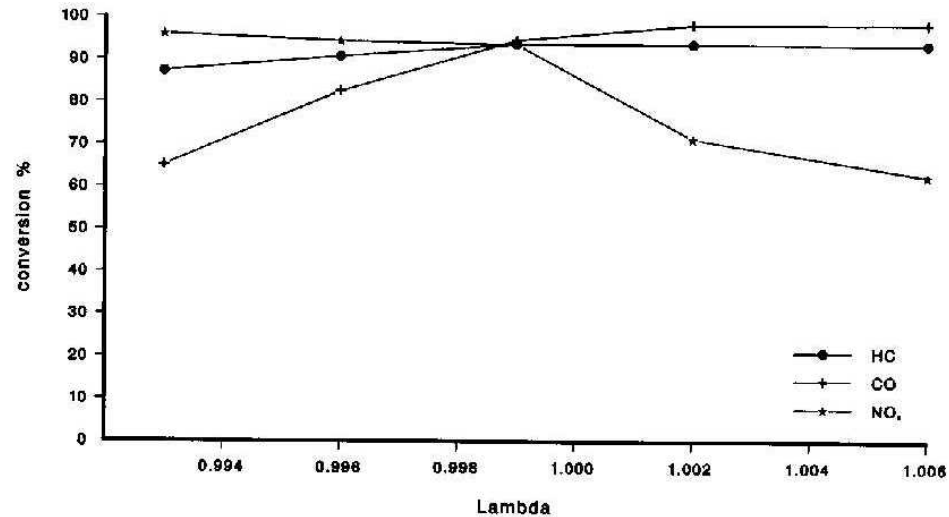
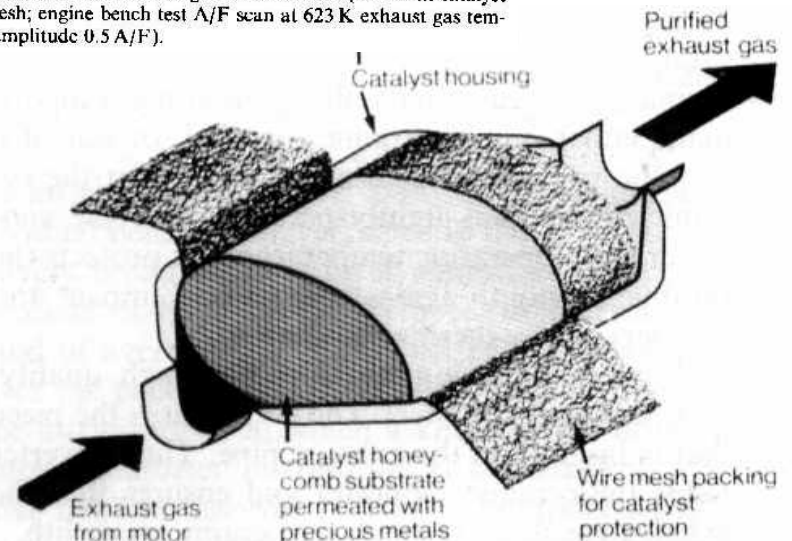
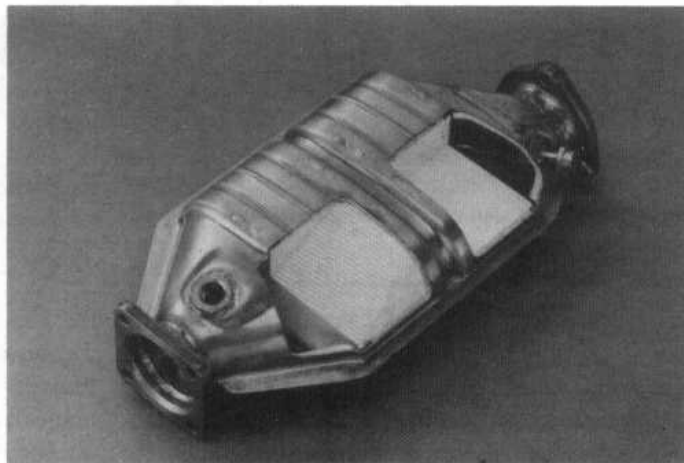
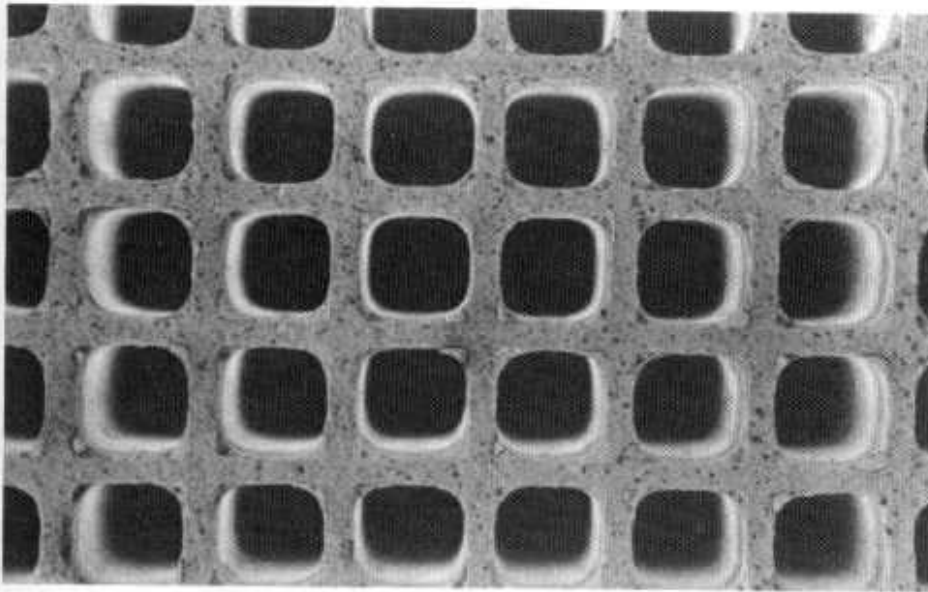


Figure 51. Conversion of CO, HC and NO_x over a three way catalyst as a function of the exhaust gas lambda value (monolith catalyst with 62 cells cm⁻², three-way formulation with Pt: 1.42 g l⁻¹, Rh: 0.28 g l⁻¹), fresh; engine bench test A/F scan at 623 K exhaust gas temperature; space velocity 60 000 Nl l⁻¹ h⁻¹; dynamic conditions frequency 1 Hz; amplitude 0.5 A/F).

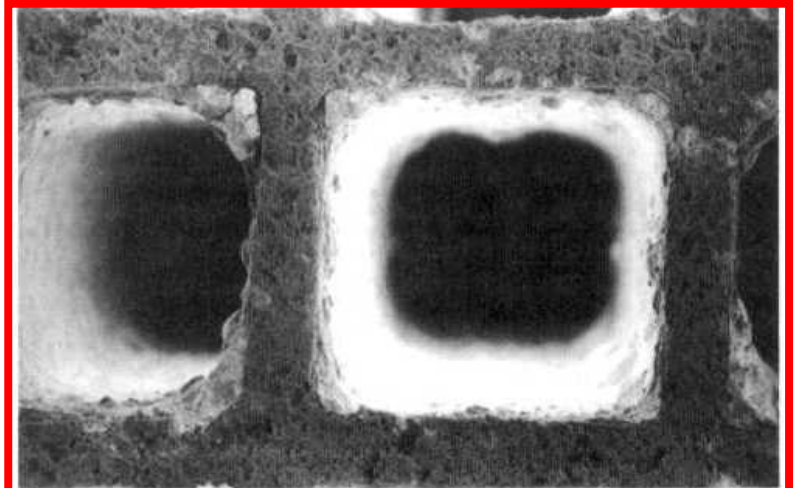


Monolith + Washcoat



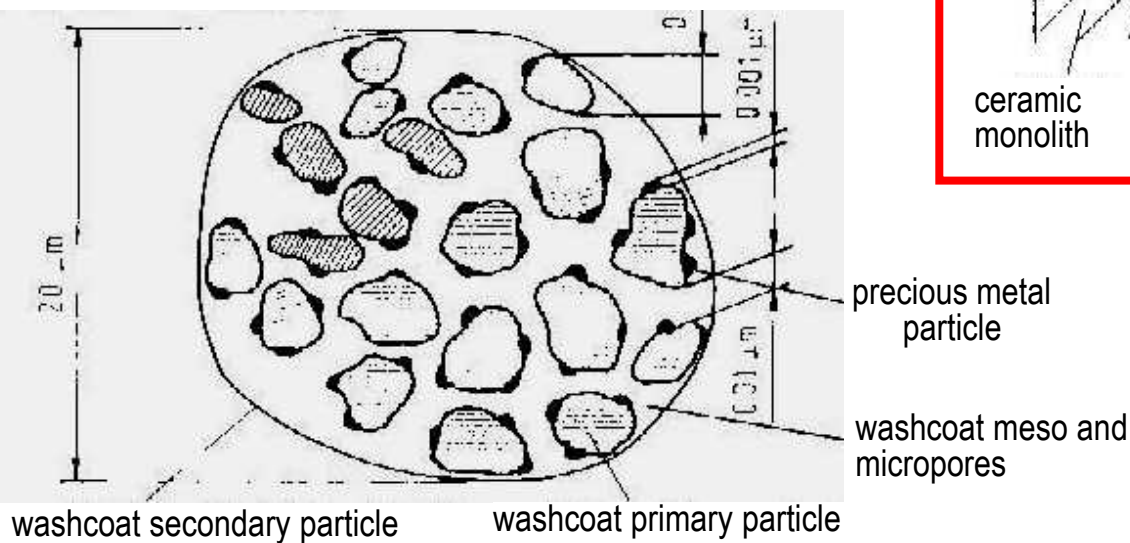
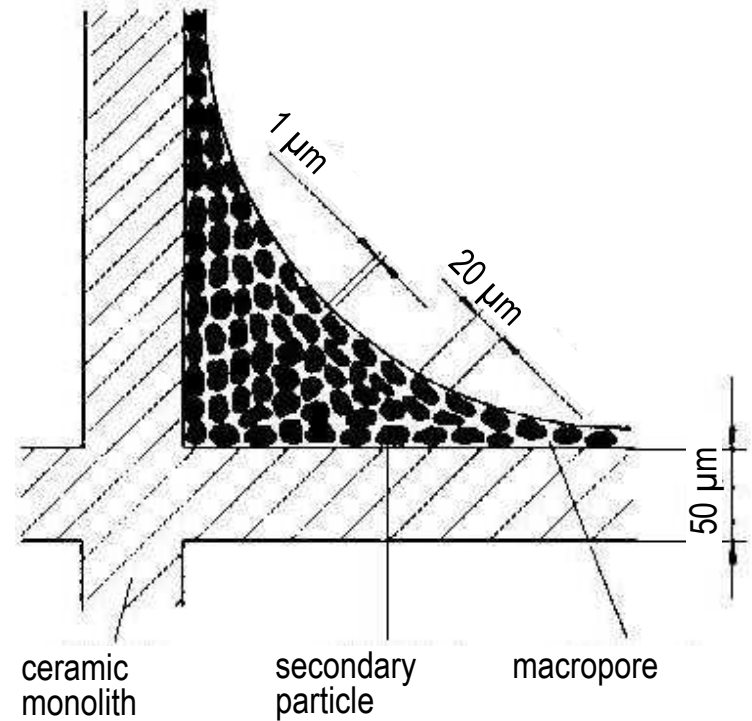
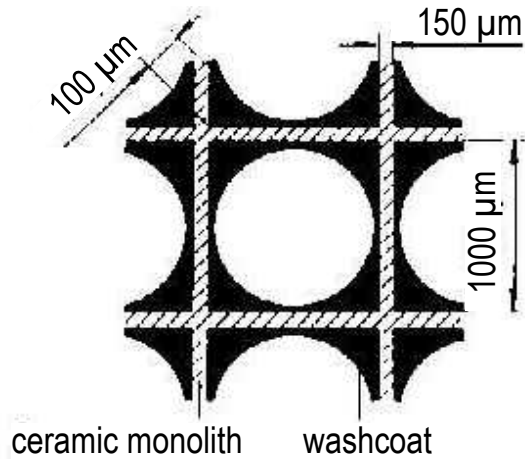
Close-up view of ceramic monolithic support with 62 cells/cm²

❖ Pt/Rh on washcoated monolith

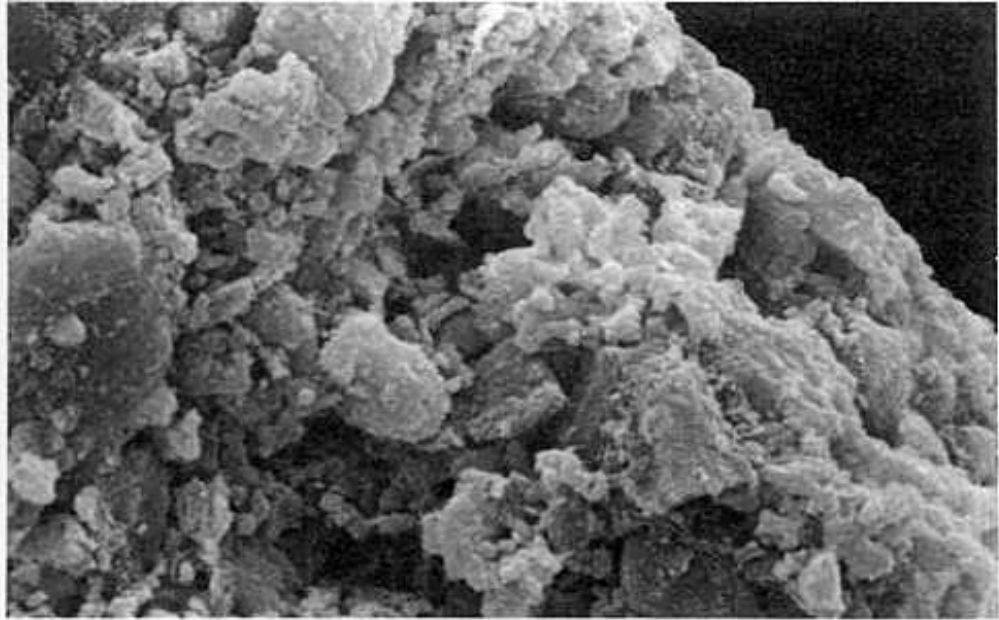


Close-up view of a channel of a washcoated ceramic ceramic monolith

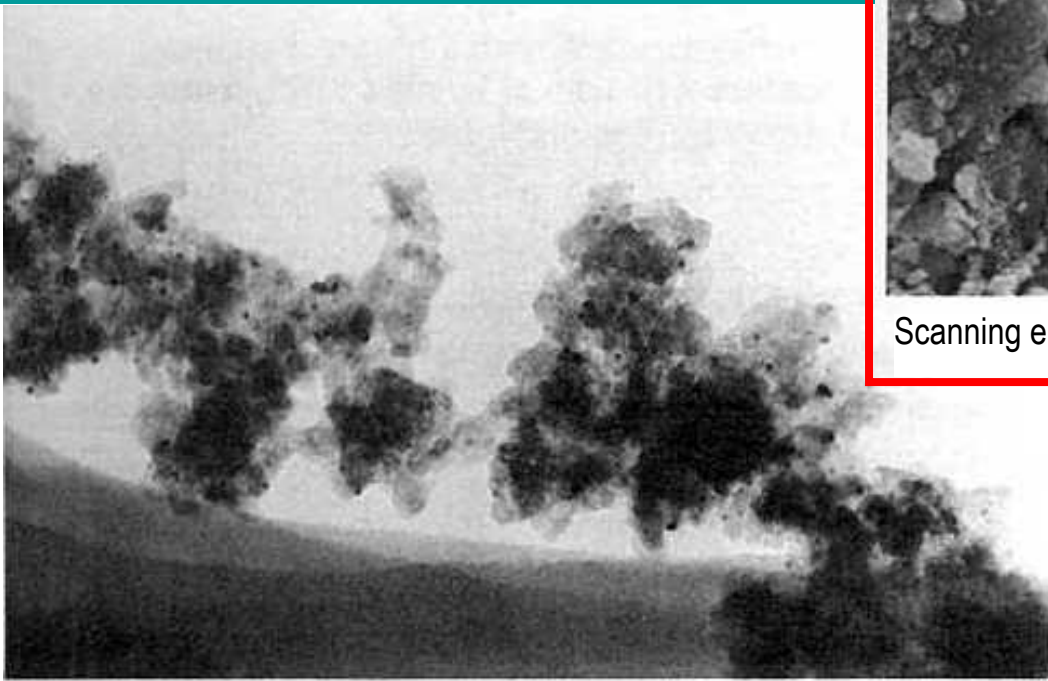
Washcoat Dimensional Details



Images of Washcoat



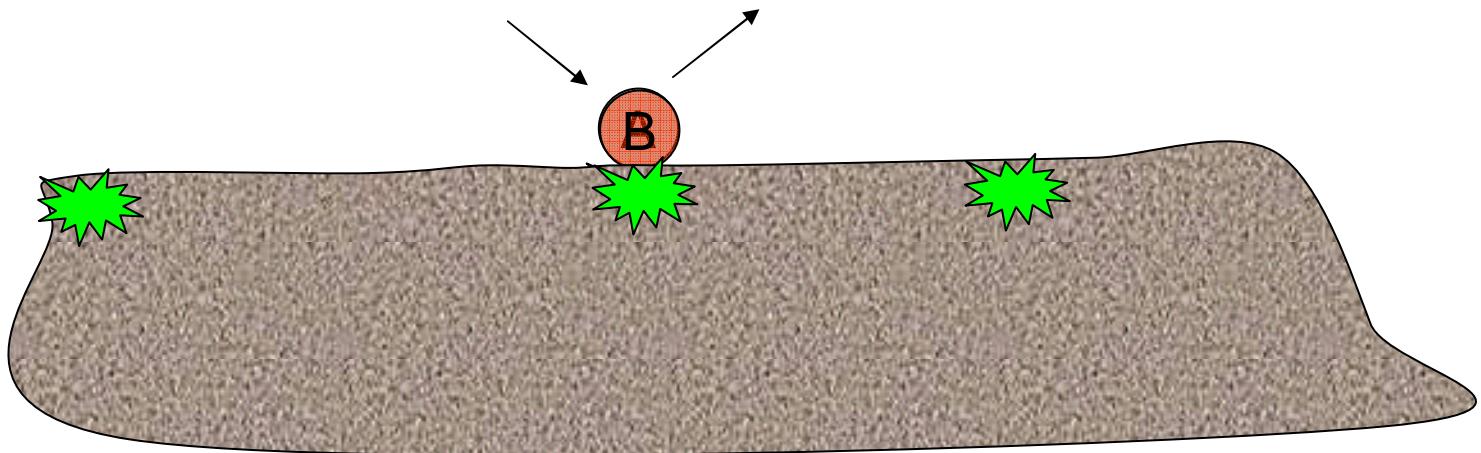
Scanning electron microscopic image of a washcoat layer



Transmission electron microscopic image of precious metals on a washcoat particle

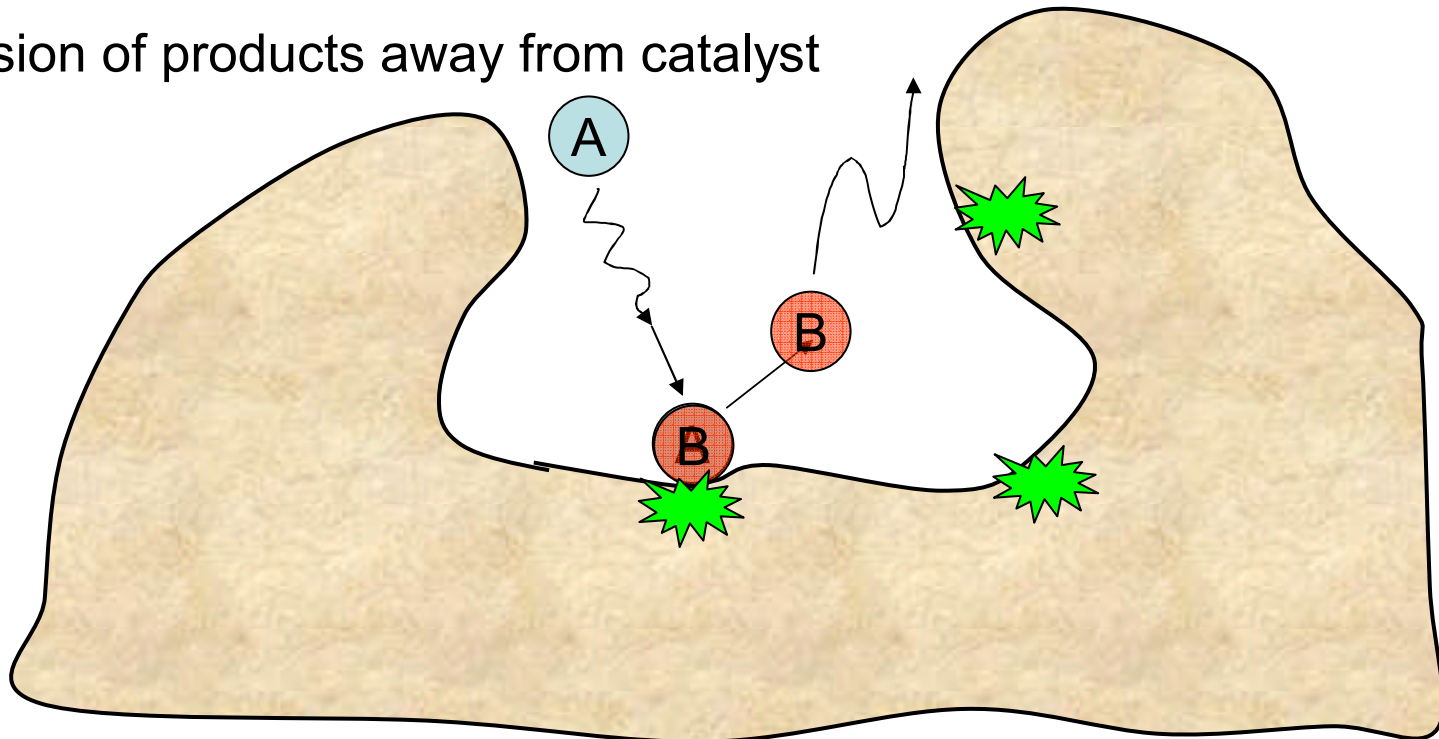
Minimal Number of Reaction Steps in Heterogeneous Catalysis

1. Adsorption of reactant on catalyst surface
2. Reaction
3. Desorption of products from catalyst surface



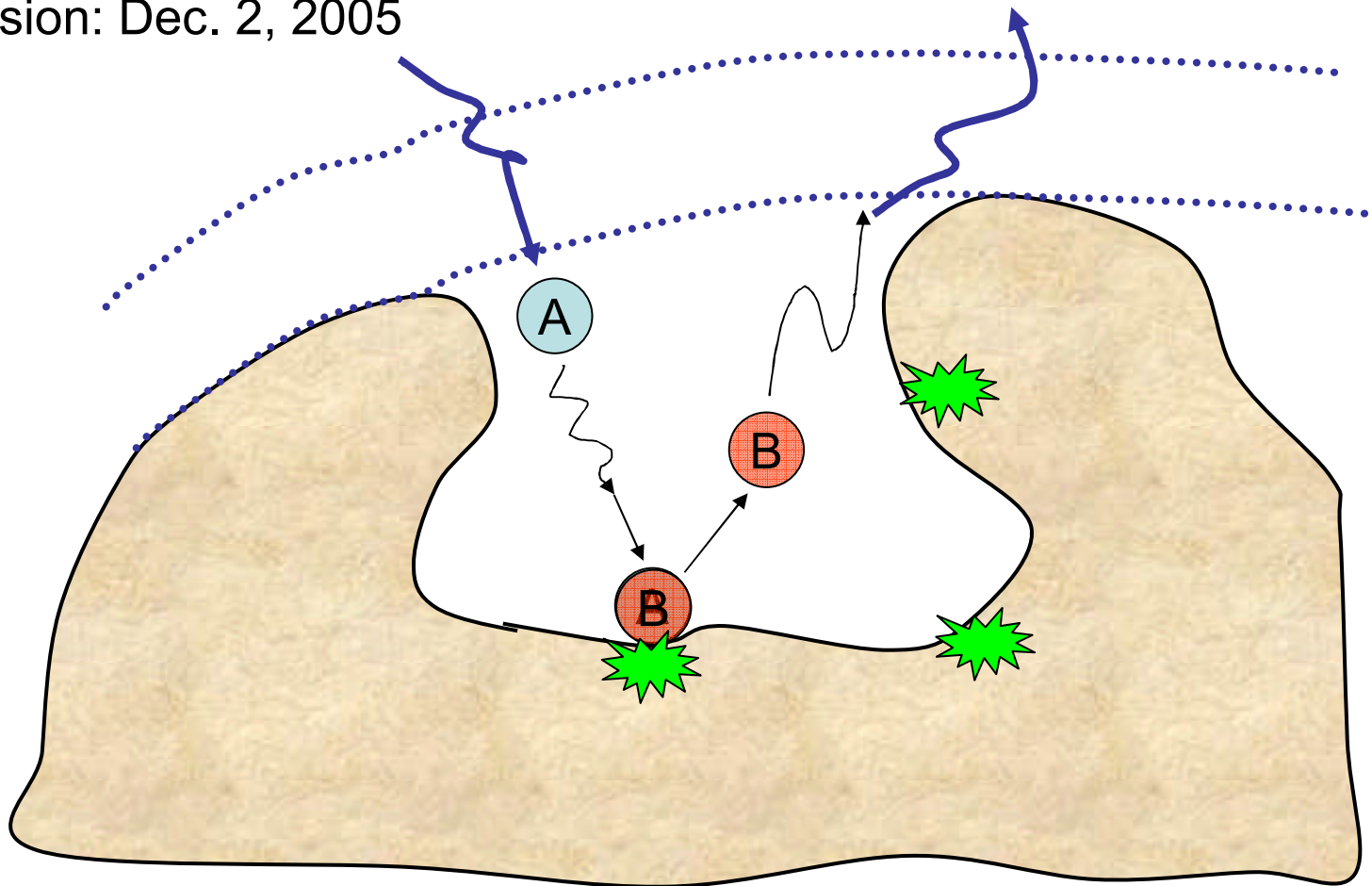
Reaction Steps in Heterogeneous Catalysis

1. Diffusion of reactant to catalyst
2. Adsorption of reactant on catalyst surface
3. Reaction
4. Desorption of products from catalyst surface
5. Diffusion of products away from catalyst



Reaction Steps in Heterogeneous Catalysis

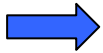
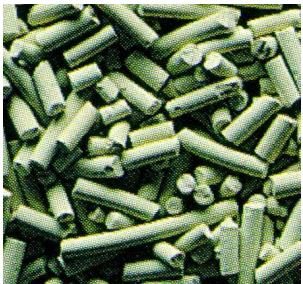
- ❖ film diffusion (total of 7 steps)
- ❖ diffusion can become rate-limiting!
- ❖ diffusion: Dec. 2, 2005



Understanding a Catalyst: Breaking Down the Problem

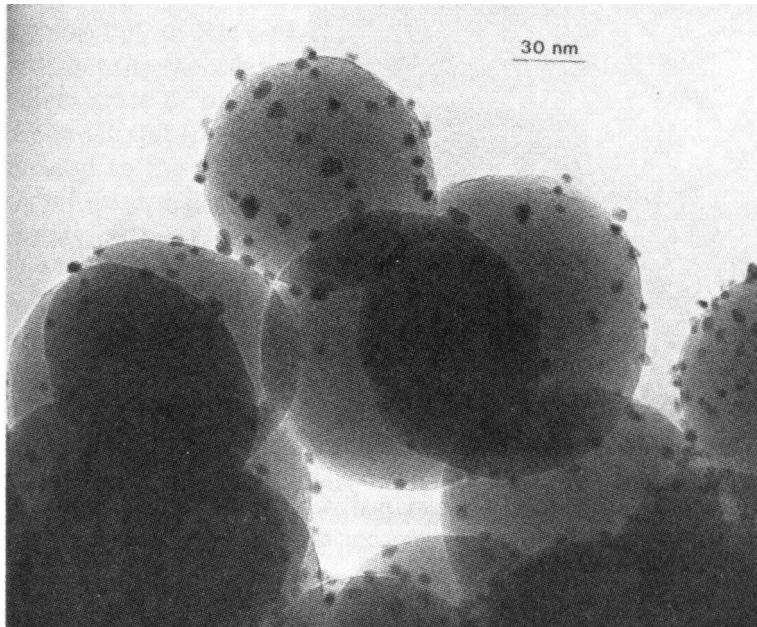
Catalyst
formulation

“Active material”



structural complexity
chemical complexity

Examples: Structural & Chemical Complexity



transmission electron microscopy: Rh/SiO₂

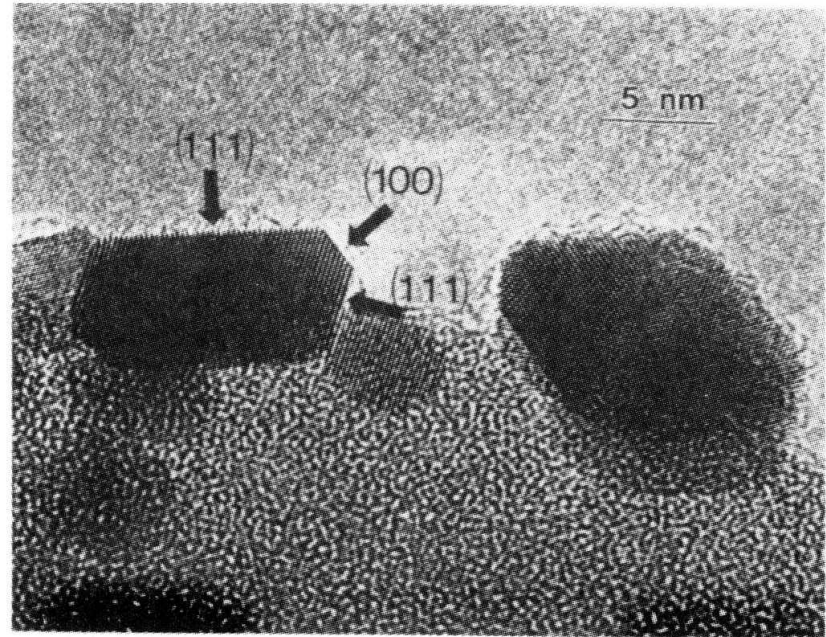


Figure 6-39

Electron micrograph of a supported metal catalyst, Rh/TiO₂ [84]. The resolution is so high that different crystal faces of the metal particle can be discerned. [Courtesy of Professor A. Datye.]

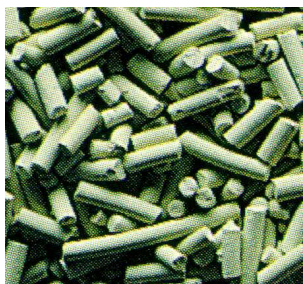
- ❖ precious metals are supported to increase active metal surface area
- ❖ which facets are exposed
- ❖ TEM: Oct. 28, 2005
- ❖ surface and bulk structure (Nov. 4 & 11, 2005)

Breaking Down the Problem

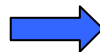
Catalyst
formulation

“Active material”

Model systems (examples)
(Nov. 18, 2005 & Jan. 6, 2006)



structural complexity
chemical complexity



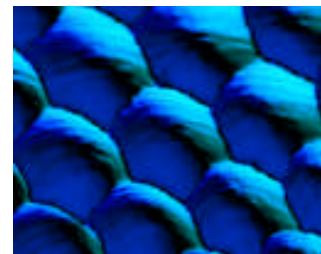
2-dimensional models / flat
surfaces
single crystals of metals,
oxide layers

metal foil

cluster models
supported on single/polycrystalline material

·
·
·

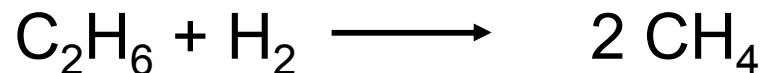
reduce structural and/or chemical
complexity
demonstrate validity of model



STM: Pt (111)
image: IBM

Role in Catalysis? Structure Sensitivity!

- ❖ rate per exposed metal surface area is a function of the metal particle size / the exposed facet plane
- ❖ active site an ensemble of atoms
- ❖ example: the hydrogenolysis of ethane



- ❖ also: ammonia synthesis (reactions involving C-C, N-N bond breaking)

Structure Sensitivity

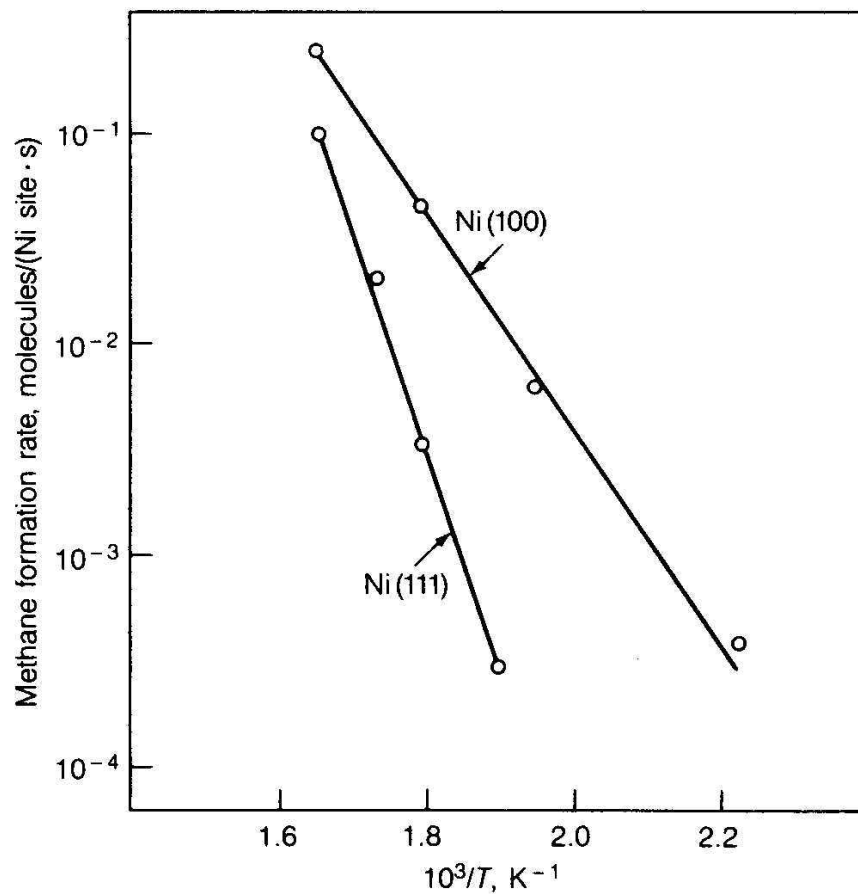
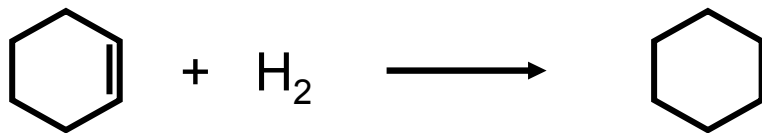


Figure 6-45

Rates of ethane hydrogenolysis catalyzed by two Ni single-crystal surfaces [98]. Data demonstrate that the reaction is structure sensitive.

Structure Insensitivity (1969)

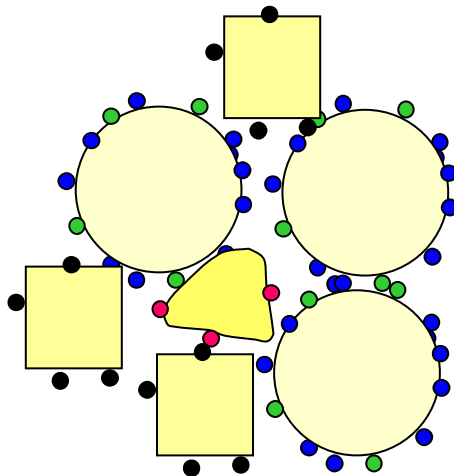
- ❖ rate per exposed metal surface area is NOT a function of the metal particle size
- ❖ active site 1-2 atoms
- ❖ example: the hydrogenation of cyclohexene



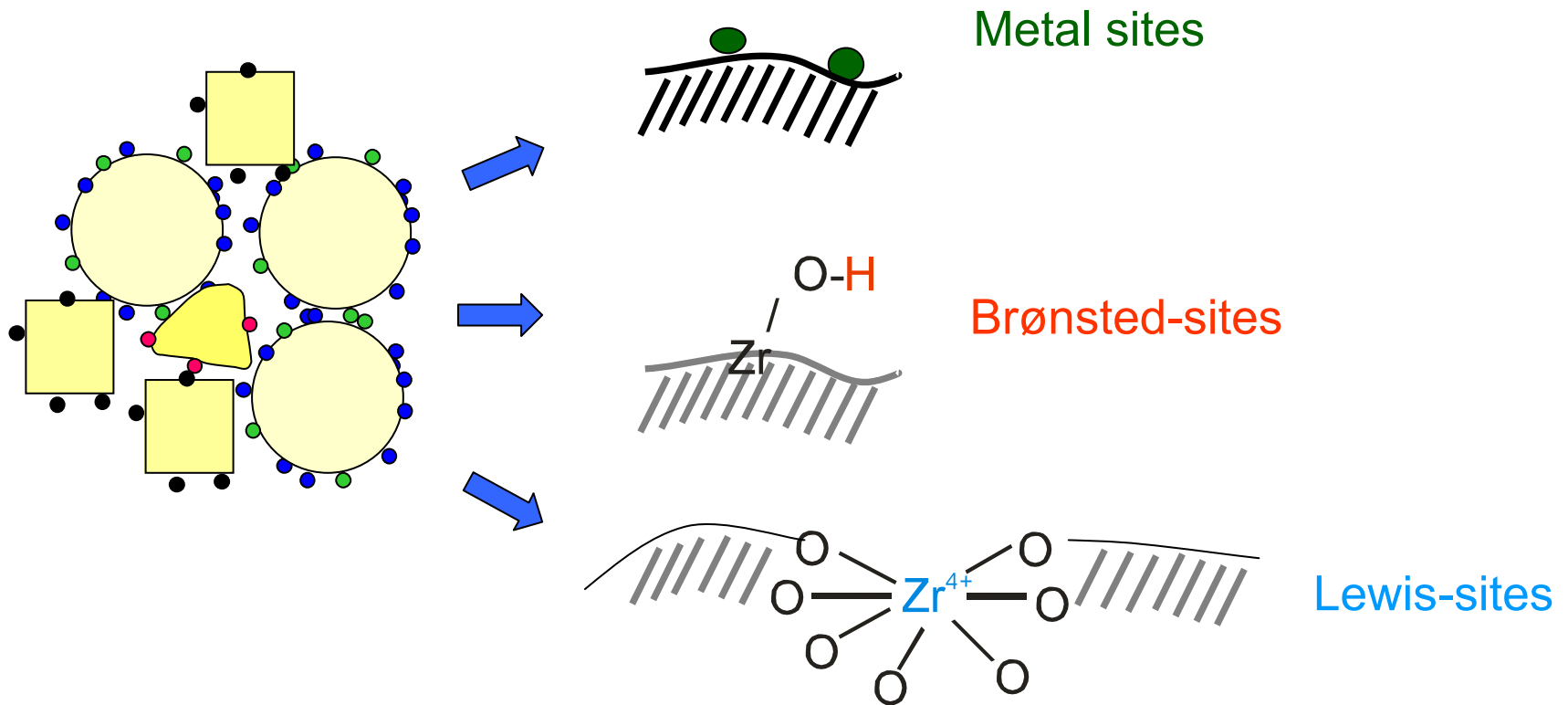
Concept of Active Sites

Hugh Stott Taylor 1925

- ❖ “only a small fraction of the surface is active”
- ❖ “the amount of surface which is catalytically active is determined by the reaction catalyzed”



Examples for Surface Sites



Questions:

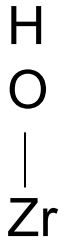
Type?

Number / density?

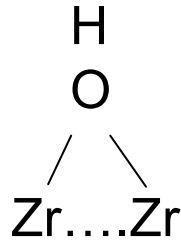
„Strength“ (interaction with a certain molecule)?

Oxide Surfaces

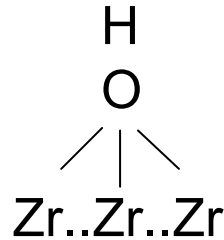
- ❖ can be terminated by O or M^{x+} or mixture (may depend on environment)
- ❖ can be terminated by foreign ions
- ❖ most frequently surfaces feature OH groups:



type I

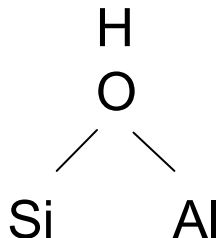


type II



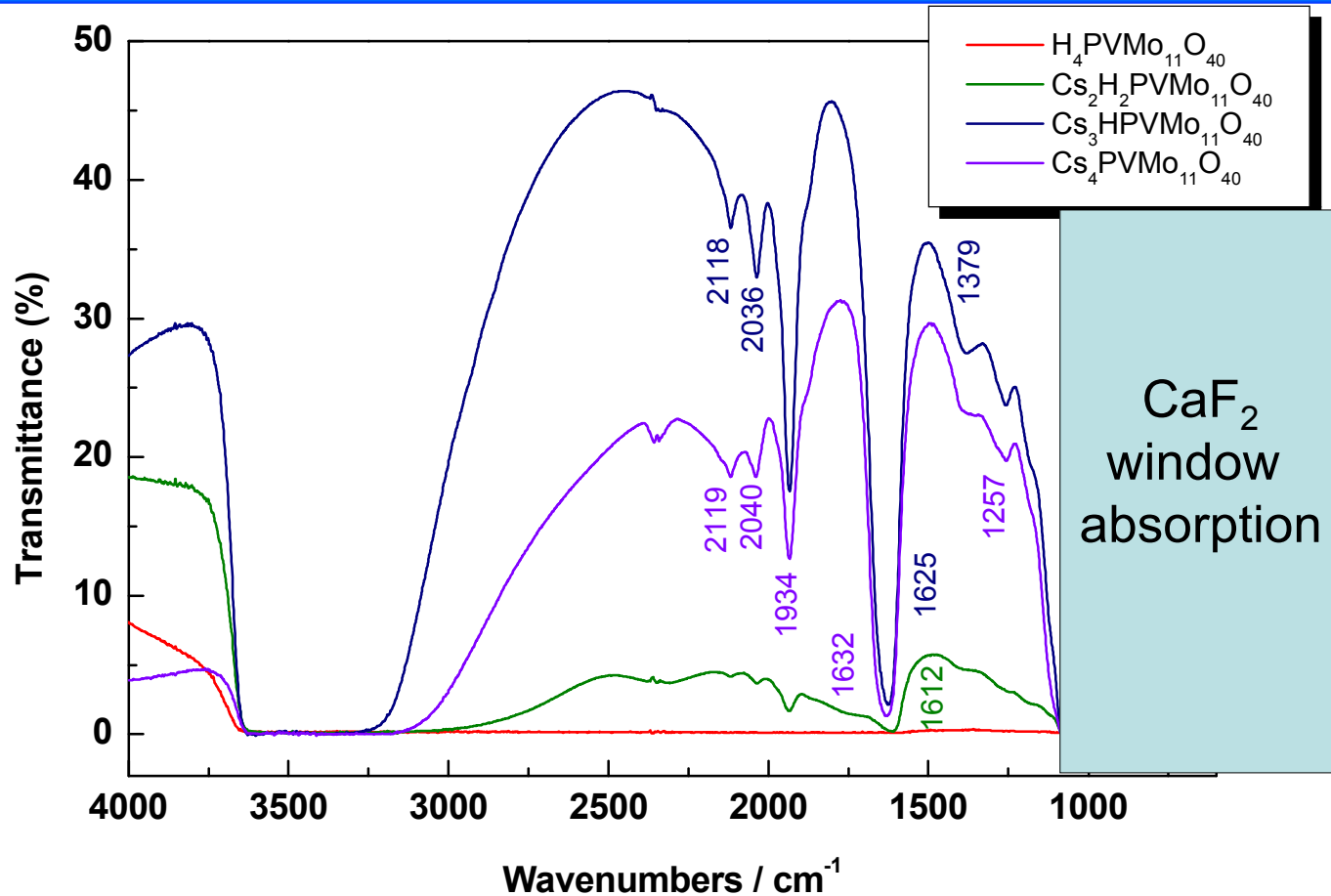
type III

- ❖ zeolite OH groups inside the pores



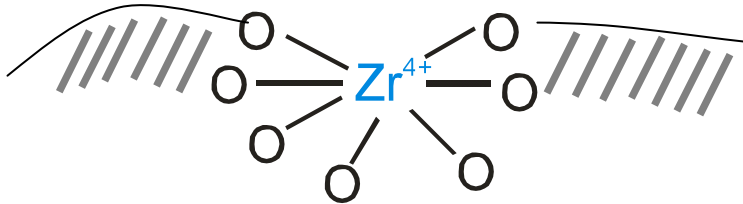
OH groups can be
Brønsted acids = proton donors
Brønsted bases = proton acceptors

Detection of OH-Groups



- ❖ IR spectroscopy, NMR spectroscopy
- ❖ band position or chemical shift delivers information

Lewis Sites



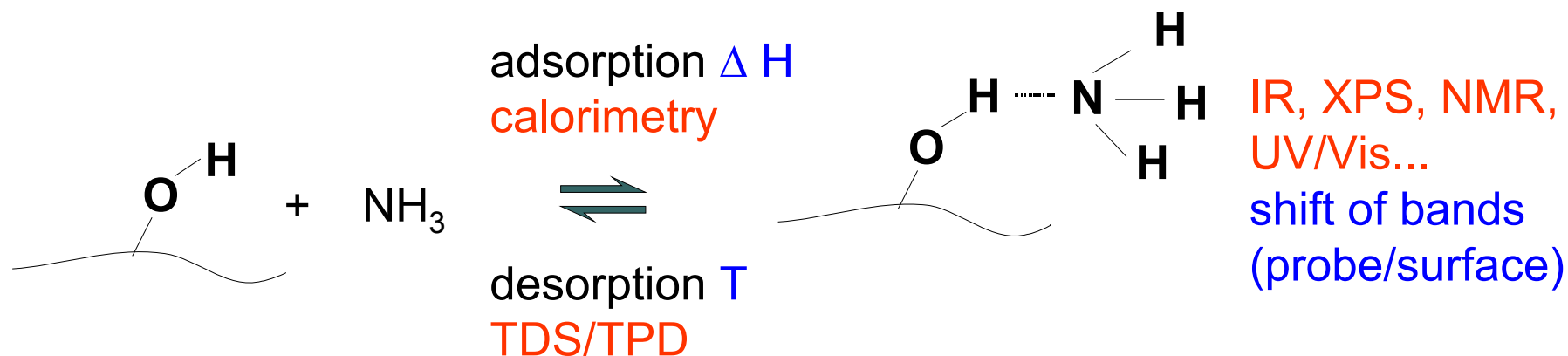
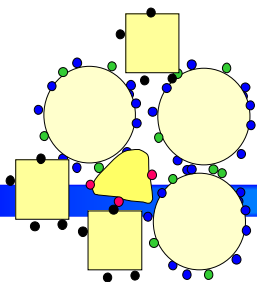
Lewis-sites

coordinatively unsaturated (cus) metal cations (acidic, electron pair acceptors)

oxygen anions (basic, electron pair donors)

- ❖ note: on a surface, acidic and basic sites (Brønsted and/or Lewis) can coexist (would neutralize each other in solution)
- ❖ only detectable in an adsorption experiment

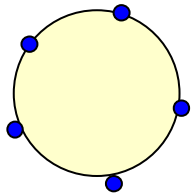
Probing Sites by Chemisorption



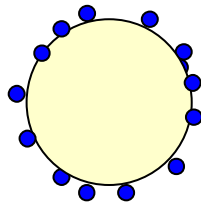
Different methods to follow adsorption (Nov. 18, 2005) deliver different information

- ❖ Isotherms: number of sites
- ❖ Spectroscopies: type, strength (but not number unless extinction coefficient known)
- ❖ Calorimetry (Dec. 2, 2005) , TDS (Nov. 25, 2005): number and strength (but not type)

Turn Over Frequency (1966)



low site density



high site density

❖ Rate with respect to number of active sites

❖ Turnover frequency (TOF) is the number of molecules formed per active site per second (in a stage of saturation with reactant, i.e. a zero order reaction with respect to the reactant)

$$\left[\frac{\text{molecules}}{\text{site } s} \right] = [s^{-1}]$$

TOF, TON, Catalysis

❖ TON

Total number of product formed molecules per active site

$$\text{TON} = \text{TOF} \times \text{catalyst life time}$$

❖ $\text{TON} = 1$ stoichiometric reaction

$\text{TON} \geq 10^2$ catalytic reaction

$\text{TON} = 10^6\text{-}10^7$ industrial application

❖ TON origins from enzyme kinetics, definitions vary

Examples for TOFs

Table 3

Turnover frequencies (TOF) of various reactions^a

Reaction	Feed	TOF molecule/site·sec	Relative TOF
Cracking	Hexane	0.0469	1
	Nonane	0.150	3.2
	Dodecane	1.07	23
Isomerization	<i>m</i> -Xylene	10.6	226
Polymerization	Propylene	40.7	868
Cracking	1-Hexene	36.7	782
	1-Heptene	56.7	1209
Skeletal isom.	1-Hexene	$>5 \times 10^3$	$> 1 \times 10^5$
Double-bond shift	1-Hexene	4.7×10^4	1×10^6

^aWith ZSM-5 catalyst, 1 atm pressure, 450°C.

Because the reactions have different activation energies, the relative TOFs will be different at other temperatures.

Catalyst Synthesis

Catalyst	Transformation	Examples
Metals	hydrogenation, dehydrogenation	Fe, Ni, Pt, Ag, Ru
Semiconducting oxides	oxidation	NiO, ZnO mixed oxides
Insulating oxides	dehydration	Al ₂ O ₃ , SiO ₂ , MgO
Acids	polymerization, isomerization cracking, alkylation	HF, H ₃ PO ₄ , H ₂ SO ₄ , SiO ₂ / Al ₂ O ₃ , zeolites



catalysts are developed empirically (trial and error)
with input from experience

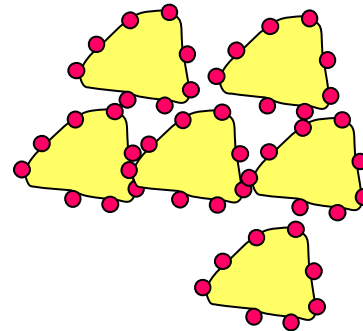
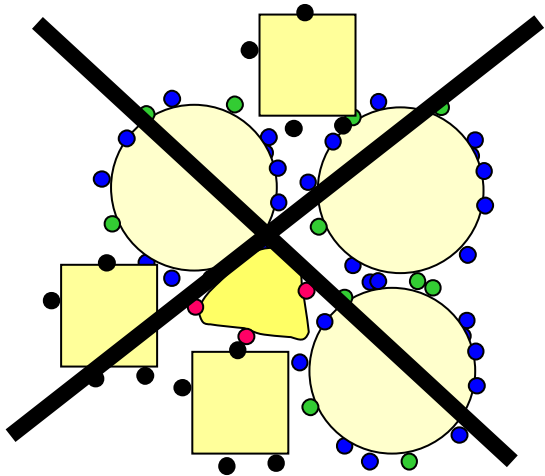
Catalysis Research: Motivation

Fundamental understanding

- ❖ active site
- ❖ reaction mechanism

Targeted synthesis

- ❖ Goal: once active structure is known synthesis can be targeted



knowledge-derived catalyst synthesis