

**Q1: The significance of pore structure and surface area in heterogeneous catalysis?**

**A1:** If a catalyst is used in a reaction the rate of product formation is a function of the available surface area and so it follows that the greater the amount of surface area accessible to the reactants, the larger is the throughput. Surface area is by no means the only physical property which determines the extent of adsorption and catalytic reaction. Equally important is the pore structure of the catalyst material or support, which, although contributing to the total surface area. This is because the distribution of pore sizes in a given catalyst preparation may be such that some of the internal surface area is completely inaccessible to large reactant molecules and, furthermore, may restrict the rate of conversion to products by impeding the diffusion of reactants and products throughout the porous medium.

**Q2: What are adsorption isotherms and adsorption isobar?**

**A2:** The equilibrium distribution of adsorbate molecules between the surface of the adsorbent and the gas phase is dependent upon pressure, temperature, the nature and area of the adsorbent, and the nature of the adsorbate. An adsorption isotherm shows how the amount adsorbed depends upon the equilibrium pressure of the gas at constant temperature: an adsorption isobar, how the amount adsorbed varies with temperature at constant pressure

**Q3: What is Knudsen diffusion?**

**A3:** Knudsen diffusion is a means of [diffusion](#) that occurs when the scale length of a system is comparable to or smaller than the mean free path of the particles involved. For example in a long pore with a narrow diameter (2–50 nm) because molecules frequently collide with the pore wall. In practice, Knudsen diffusion applies only to gases because the [mean free path](#) for molecules in the liquid state is very small, typically near the diameter of the molecule itself.

Knudsen diffusion coefficient is given by  $D_K = \frac{2}{3} r \sqrt{\frac{8RT}{\pi M}}$

**Q4: What is effective diffusivity?**

**A4:** A porous mass of solid usually contains pores of non-uniform cross-section which pursue a very tortuous path through the particle and which may intersect with many other pores. Thus the flux predicted by an equation for normal bulk diffusion (or for Knudsen diffusion) should be multiplied by a geometric factor which takes into account the tortuosity and the fact that the flow will be impeded by that fraction of the total pellet volume which is solid. It is therefore expedient to define an effective diffusivity  $D_e$ , in such a way that the flux of material may be thought of as flowing through an equivalent homogeneous medium. We may then write:  $D_e = D \frac{\psi}{\tau}$  where  $D$  is the normal diffusion coefficient (either Bulk or Knudsen as appropriate),  $\psi$  is the porosity of the particles and  $\tau$  is a tortuosity factor.

**Q5: What are zeolites?**

**A5:** Zeolites are three-dimensional, microporous, crystalline solids with well-defined structures that contain aluminum, silicon, and oxygen in their regular framework; cations and water are located in the pores. The silicon and aluminum atoms are tetrahedrally coordinated with each other through shared oxygen atoms. Zeolites have void space (cavities or channels) that can host cations, water, or other molecules. Because of their regular and reproducible structure, they behave in a predictable fashion.

**Q6: How do zeolites function as ion exchangers?**

**A6:** The framework aluminum and silicon are bound to each other through shared oxygen atoms. The  $\text{SiO}_4$  units are neutral:  $\text{Si}^{+4} / 4 \text{O}^-$  but the  $\text{AlO}_4$  results in a net negative charge:  $\text{Al}^{+3} / 4\text{O}^-$ . The net negative charge is

balanced by cations that are present during the synthesis. These cations are highly mobile and can be exchanged for other cationic species.

**Q7: How can zeolites framework be modified?**

**A7:** Zeolite modification implies an irreversible change, unlike ion exchange or adsorption. The framework of the zeolite can be modified by synthesizing zeolites with metal cations other than aluminum and silicon in the framework. The framework of the zeolites can be modified by dealumination to increase the silica and increase the hydrophobic nature of the zeolite. There are many proprietary methods to modify zeolites that impart unique characteristics to them.

**Q8: How Sticking Coefficients can be determined?**

**A8:** The most common method of determining the sticking coefficient is by measuring the uptake of a gas by a surface as a function of the dose to which the surface is exposed. In such experiments, great care should be taken to ensure that gas and surface are in thermal equilibrium. In addition, we need to determine the coverage, either by surface sensitive methods (XPS, AES, IR) or by thermal desorption and ensure that adsorption is not accompanied by desorption.

**Q9: What are the properties of zeolite?**

**A9:** Since silicon typically exists in a 4+ oxidation state, the silicon-oxygen tetrahedra are electrically neutral. However, in zeolites, aluminium typically exists in the 3+ oxidation state so that aluminium-oxygen tetrahedra form centres that is electrically deficient one electron. Thus, zeolite frameworks are typically anionic, and charge compensating cations populate the pores

to maintain electrical neutrality. These cations can participate in ion-exchange processes, and this yields some important properties for zeolites. When charge compensating cations are "soft" cations such as sodium, zeolites are excellent water softeners because they can pick up the "hard" magnesium and calcium cations in water leaving behind the soft cations. When the zeolitic cations are protons, the zeolite becomes a strong solid acid. Such solid acids form the foundations of zeolite catalysis applications including the important fluidized bed cat-cracking refinery process. Other types of reactive metal cations can also populate the pores to form catalytic materials with unique properties. Thus, zeolites are also commonly used in catalytic operations and catalysis with zeolites is often called "shape-selective catalysis".

**Q10:** a) What are the advantages of shell catalysts compared to bulk catalysts?

b) What is the preferred support material for shell catalysts?

**A10:** a) Short transport or diffusion paths; pore structure independent of the support; improved heat transfer in the catalyst layer; low coking.

b) Generally  $\gamma$ -Al<sub>2</sub>O<sub>3</sub> spheres; low specific surface area (1 m<sup>2</sup>/g).