Understanding Polyolefin Processes: Fact 2

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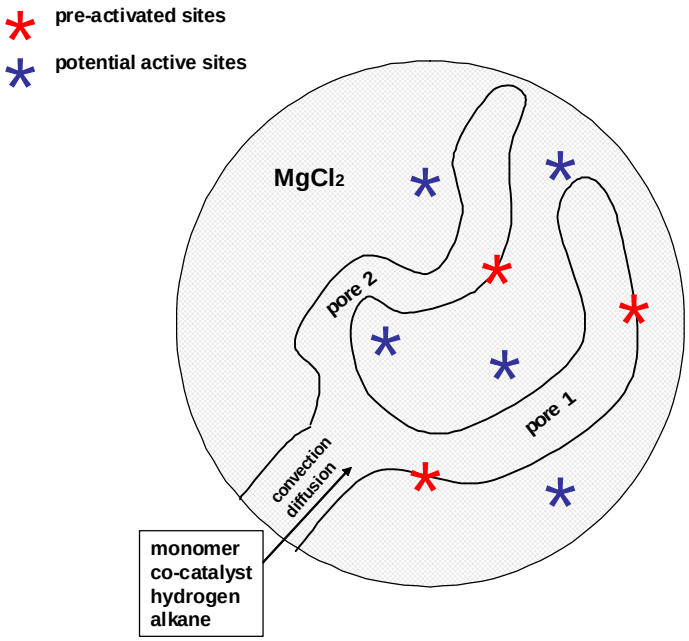
How does a catalyst particle look like at time zero?

We observe a Ziegler-Natta catalyst particle that was pre-activated by contacting with a co-catalyst. It has been injected into a olefin polymerization reactor just at this moment:

Two pores with 3 activated sites and 5 potentially active sites
time = 0 s: catalyst injection; monomer, co-catalyst, hydrogen, alkane...start entering the pores



Our particle has a representative size of 20 µm and consists of 90% porous $MgCl_2$ and 10% of $TiCl_4$. The particle volume is 4.2 10^{-21} m^3. With a density of 1800 kg/m3 (depends on porosity!), the mass of the particle is 7.54 10^{-15} g. Therefore, our catalyst contains 7.54 10^{-14}g $TiCl_4$ or 3.975 10^{-16} mol[1] or 2.4 10^{10} Ti atoms. Let us assume that 1% of all Ti atoms is "potentially active" – thus we have 2.4 10^8 potentially active sites in our catalyst particle. Only part of it can be pre-activated, because:

Activation is possible under two conditions: 1.the Ti atom must be located at the surface of the $MgCl_2$ carrier and 2. there must be sufficient co-catalyst near this site

One can assume an activation equilibrium: Potential active site + CoCat **ó** Active site

Therefore: access of co-catalyst is required to form active sites.

The figure above shows only a very small part of our particle containing 3 pre-activated sites and 5 potentially active sites – therefore, this part represents only a weight fraction of 3.3 10^{-8} of the 20 µm particle. Of course, within this small part, two "normal" pores (30 nm) cannot exist – the figure above is very schematic – or can be seen as a catalyst with extreme low loading…

[1] molar mass of $TiCl_4$ is 189.7 g/mol