Effect of Metallocene Structures on their Performance in Ethene Polymerisation

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Metallocene/MAO catalysts have been studied intensively the past 20 years for olefin polymerisation. By modifying the catalyst structure it is possible to control the composition of the formed polymer. Despite there are hundreds of complexes with different ligand structures synthesised, there is still much to learn on how an individual substituent or small difference in complex structure influence the polymerisation behaviour or polymer structure. [1]

Four (Cp)(4-phenyl-indenyl)MCl₂ (A) and four (Cp)(1-phenyl-indenyl)MCl₂ (B) (M=Zr/Hf) based complexes have been used as such and modified by adding methyl substituents, a bridge and by changing the metal. All complexes have been studied carefully in ethene homo- and copolymerisation in different polymerisation conditions to explain how these differences in the complex structure affect the polymerisation process and the formed polymer.

With both type of complexes, the zirconocene is more active and produces higher molecular weight than the corresponding hafnocene. Comparing the zirconocene form of A and B, the latter has better activity, but the both complexes produce same molecular weight. Three methyl substituents in the Cp ligand increase the copolymerisation capability of the complex. Complexes based on structure B are more sensitive to the variations of aluminium concentration. All unbridged complexes have good hydrogen response.