



## Comprehensive Analysis of Metallocene Catalyst Utilization

Subita Bhagat<sup>1</sup>, Nikhil Prakash<sup>2</sup>  
Assistant Professor<sup>1</sup>, Assistant Professor<sup>2</sup>  
Department of Chemical Engineering  
SLIET, Longowal

---

**Abstract:** *Polymers like olefins, diolefins and Styrene are formed with the help of highly active catalyst like Metallocene. It was discovered at University of Hamburg 25 years ago. Polymers which have high defined microstructure, tacticity and stereoregularity and some other unique properties like film clarity, tensile strength and lower extractables. If one is able to understand the concept of olefin polymerization correctly, they may find new catalyst site bindings.*

*Increase in the production of metallocene has indicated a growth in polyolefin industry. With the introduction of new technologies the polyolefin industry has reached new heights. These technologies tend to provide environmentally green products.*

**Keywords:** *Polymers, Metallocene Catalyst, polyolefin, green products*

---

### I. INTRODUCTION

Metallocene has presented a lot of challenges and opportunities for the catalyst chemist and polyolefin industry. The chemical used in polymerization of polyolefin is EXXON. And the technology used is known as EXXPOL technology (Kuklin et al., 2015).

The high yield of polymer is obtained from this catalyst which has narrow molecular weight distribution. The broader polymers provide better melt processing. Metallocene has a diverse property of single site, inter compatibility and diverse molecular weights through which they can produce both narrow and broad weight distributions (Velthoen et al., 2018).

These days metallocene produced propylene is easily available. Metallocene catalyst have identical active site and their properties like molecular weight and stereo structure can be altered according to the need of the application. The production of Syndio-tactic propylene is carried out by metallocene catalyst which was not possible with Ziegler catalyst (Credendino et al., 2015).

Metallocene's are organic-metal compounds which have a spatial arrangement between them and spaces are filled with a transition element (iron, titanium etc.). Ferrocene was the first ever metallocene to be discovered. This valuable discovery was done by Geoffrey Wilkinson and Ernst O. Fischer for which they even received a Nobel prize. Titanocene dichloride and an aluminum alkyl was first metallocene to be used for Polymerization but due to its poor activity it stayed limited to scientific studies only. In 1975 water was accidentally introduced in a test tube containing metallocene. This reaction caused increase in ethylene and polymerization rate 1000 times. As a result methylalumoxane (MAO) was formed due to partial hydrolysis of trimethylaluminum (Kissin et al., 2005).

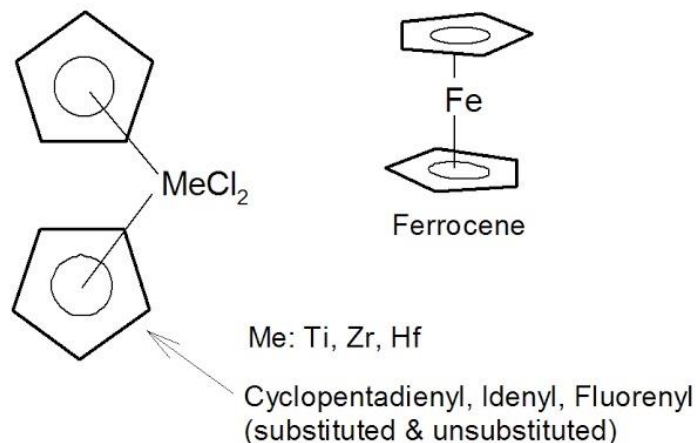


Figure 1: metallocene catalyst

## II. STRUCTURE OF METALLOCENE CATALYST:

A zirconium (Zr) atom is bounded to two chlorine atoms and an alkyl group. Inside the cleft created by alkyl group a complex name ZrCl<sub>2</sub> is located. The polymerization reaction occurs in this cleft (Zakharov et al., 2008).

The molecule has three dimensions: The dotted lines tells us that one chlorine is located behind the plane of paper and heavy bold line indicated the location of chlorine atom on front side of plane of paper (Matsko et al., 2009).

The stereo-selective polymerization of propylene into isotactic polymerization was firstly done in 1980 by introducing chiral, bridged metallocene and then zirconium.

A molecular bridge connects two organic compounds of metallocene in a bridged metallocene. The chiral atom can not be superimposed upon its mirror image. Syndiotactic propylene was formed using zirconium metallocenes in 1988 (Rahaman et al., 2014).

Today almost all metallocene has zirconium chloride (ZrCl<sub>2</sub>) as the transitional metal complex.

Different complexes can be used to form propylene resins of different microstructure, molecular weight and other chemical properties.

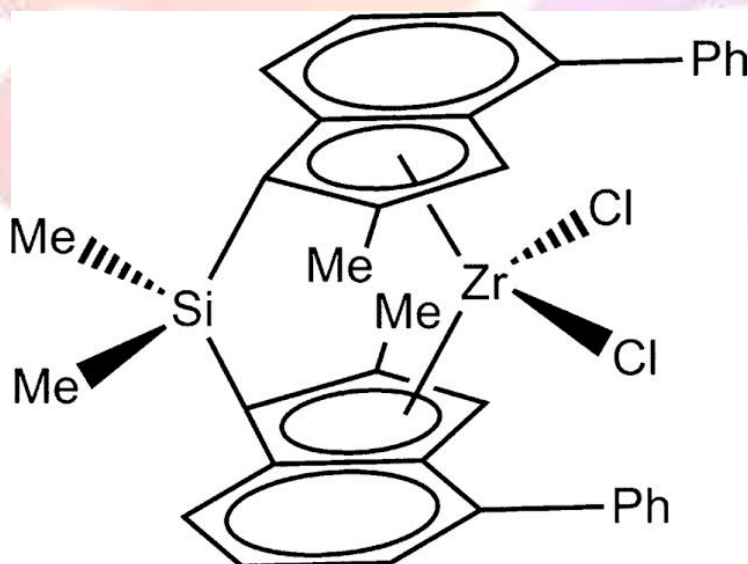


Figure 2: Structure of a metallocene catalyst

Homogenous catalysis is used in the laboratory for metallocene polymerization in which catalyst and reacting materials are kept in solution. For large scale production metallocene is supported on powdery insoluble substrates like SiO<sub>2</sub>, Al<sub>2</sub>O<sub>3</sub>, OR MgCl<sub>2</sub>. On each grain of powder a polypropylene chain is synthesized. As the active sites are identical the chain formed is of uniform length(Sun et al., 2006).

### III. PREPERATION OF METALLOCENE CATALYST:

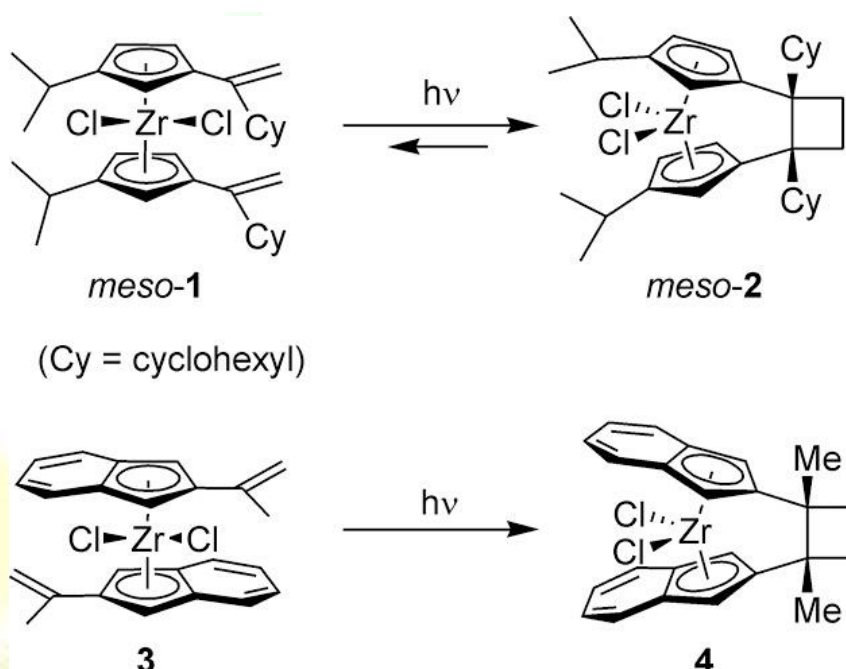


Figure 3: Reaction showing preparation of metallocene catalyst

### IV. CONCLUSION

Metallocene catalysts have proved to bring a evolution in the polymer industry. It's easy to produce and is cheaply available and alters the speed of reaction at a high rate. Due to it's unique properties the products formed are eco- friendly. Syndiotactic propylene one of the best quality of polymer is created with the help of metallocene catalysts. Zirconium metal complexes are used in metallocene catalyst which help in easy reactions. Metallocene catalyst have completely changed the face of polypropylene polymerization. Thus we can conclude that Metallocene catalyst are more effective and efficient than Ziegler-natta catalyst in the field of Polymer polymerization.

### REFERENCES

1. Credendino, R., Liguori, D., Fan, Z., Morini, G., & Cavallo, L. (2015). Toward a Unified Model Explaining Heterogeneous Ziegler-Natta Catalysis. *ACS Catalysis*, 5(9), 5431–5435. <https://doi.org/10.1021/ACSCATAL.5B01076>
2. Kissin, Y. v., Mirabella, F. M., & Meverden, C. C. (2005). Multi-center nature of heterogeneous Ziegler-Natta catalysts: TREF confirmation. *Journal of Polymer Science, Part A: Polymer Chemistry*, 43(19), 4351–4362. <https://doi.org/10.1002/POLA.20875>
3. Kuklin, M. S., Hirvi, J. T., Bochmann, M., & Linnolahti, M. (2015). Toward Controlling the Metallocene/Methylaluminoxane-Catalyzed Olefin Polymerization Process by a Computational Approach. *Organometallics*, 34(14), 3586–3597. <https://doi.org/10.1021/ACS.ORGANOMET.5B00394>
4. Matsko, M. A., Echevskaya, L. G., Zakharov, V. A., Nikolaeva, M. I., Mikenas, T. B., & Vanina, M. P. (2009). Study of multi-site nature of supported Ziegler-Natta catalysts in ethylene-hexene-1 copolymerization. *Macromolecular Symposia*, 282(1), 157–166. <https://doi.org/10.1002/MASY.200950816>
5. Rahaman, M., Parvez, M. A., Soares, J. B. P., & Hussein, I. A. (2014). Effect of polymerization conditions on thermal and mechanical properties of ethylene/1-butene copolymer made with Ziegler-Natta catalysts. *International Journal of Polymer Science*, 2014. <https://doi.org/10.1155/2014/654260>



6. Sun, T., Wang, L., Dong, X., Wang, W., & Wang, L. I. (2006). An insight into the chain-propagation mechanism of propylene polymerization catalyzed by traditional Ti-based Ziegler-Natta catalysts in view of recently developed catalysts. *Designed Monomers and Polymers*, 9(2), 117–127. <https://doi.org/10.1163/156855506776382691>
7. Velthoen, M. E. Z., Muñoz-Murillo, A., Bouhmadi, A., Cecius, M., Diefenbach, S., & Weckhuysen, B. M. (2018). The Multifaceted Role of Methylaluminoxane in Metallocene-Based Olefin Polymerization Catalysis. *Macromolecules*, 51(2), 343–355. <https://doi.org/10.1021/ACS.MACROMOL.7B02169>
8. Zakharov, V., Echevskaya, L., Mikenas, T., Matsko, M., Tregubov, A., Vanina, M., & Nikolaeva, M. (2008). Supported ziegler-natta catalysts for ethylene slurry polymerization and control of molecular weight distribution of polyethylene. *Chinese Journal of Polymer Science (English Edition)*, 26(5), 553–559. <https://doi.org/10.1142/S0256767908003266>

