

Impact of Metallocene Catalysts on Polyolefins (91S4)

Chem Systems' Process Evaluation/Research Planning program has recently published a report which covers the rapidly developing field of polyolefins, primarily polyethylene, produced with single site or constrained geometry catalysts. The report "***Impact of Metallocene Catalysts on Polyolefins***" (91S4) covers the chemistry, current commercial technology, economics, and markets for these materials.

By developing "second generation" LLDPE technologies, polyolefin producers are responding to the technology-driven market to enhance growth and profitability. Currently, a variety of technological options achieve property improvements that result in intrapolyolefin and interpolymer competition.

Since the late 1970s considerable research has been expended on a new class of Ziegler-Natta catalysts, usually referred to as metallocene catalysts. These catalysts can be varied in structure and designed to give atactic, isotactic, or syndiotactic polymers from alpha-olefins such as propylene.

The chief difference between metallocene catalysts and conventional Ziegler-Natta catalysts is in the distribution of active sites. Ziegler-Natta catalysts are heterogenous and have many active sites. Only some of these sites are stereospecific, and some are more accessible to monomers for coordination and subsequent polymerization. On the other hand, the metallocene catalysts are believed to be homogeneous. Each catalyst molecule has the same activity and each has essentially the same accessibility to monomer. This results in a very uniform product, and with the appropriate catalysts, in a highly stereoregular product with alpha-olefins. These catalysts are referred to as single site catalysts (SSC).

Constrained geometry catalyst technology (CGCT) is based on homogeneous, single-site catalysts that allow for property design and optimization, and are capable of preparing homogeneous polyolefin copolymers. The catalyst technology is based on a constrained geometry ligand attached to a transition metal catalyst center. Strong Lewis acid systems are used to activate the catalyst to a highly efficient form. The catalyst activity is based on Group IV transition metals (e.g. titanium) that are covalently bonded to a monocyclopentadienyl group bridged with a hetero atom. The three components are connected in such a way that a constrained cyclic structure is formed with the transition metal center.

The success of metallocene-based resin will ultimately depend on the cost/performance relationship of the fabricated end products. Therefore, in addition to tailoring the molecular structure of the polymer to enhance properties, producers are optimizing the

process and catalyst systems to reduce overall resin production costs.

The single-site catalysts allow a more uniform distribution of comonomers along the polyethylene backbone resulting in two areas of savings: 1) the total amount of comonomer consumed (the incorporation efficiency), leading to reduction in the comonomer required to give a designated density, and 2) recovery efficiency (a reduction in the amount of comonomer lost in the recycle purge stream).

Dow Chemical and Exxon Chemical are the notable leaders with respect to metallocene/single-site catalyst commercialization. While this report focuses on these producers as representative of market trends, a number of other key global polyolefin producers including Fina, Chisso, Phillips, Mobil, BASF, BP, Shell, Hoechst, Mitsui Toatsu, Idemitsu Kosan, and Mitsubishi are also developing metallocene single-site catalyst technologies to produce polyethylene, polypropylene, and various ethylene-propylene copolymers.

The growth of future metallocene-based resin capacity will most likely occur as a result of modifications to existing LLDPE plants and these resins will then become another family of resins produced in "swing" LLDPE/HDPE plants. Therefore, it is probable that grass-roots metallocene-based polyolefin plants will not be built and capacity expansions will be driven by overall LLDPE market growth for the next seven years.

Given the limited commercial availability of these new polymers, it is too early to accurately determine their impact on the marketplace in terms of specific numbers. It is likely that by 2000, these new metallocene catalyst systems will be employed by several polyolefin producers, each probably with a different target market and strategy.