

# المجلة العربية للعلوم والهندسة

## ZIRCONOCENE-CATALYZED OLEFIN POLYMERIZATION: MODELING OF CATALYST STABILITY, NONISOTHERMAL MODE OF OPERATION, AND SUPPORTED CATALYST CHARACTERIZATION

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## ABSTRACT

This paper summarizes (a) an engineering approach to calculation of catalytic activity and stability profile, (b) influence of nonisothermal polymerization mode, (c) and characterization of supported zirconocene catalysts by X-ray photoelectron spectroscopy (XPS) and micro-proton induced X-ray spectroscopy (micro-PIXE).

The engineering approach is based on modeling the solubility of ethylene in the polymerization diluent as a function of temperature and pressure.

Under the nonisothermal mode of polymerization, a change in stirring level from diffusion-controlled regime to nondiffusion-controlled, external gas-liquid mass transfer resistance-free one, increased the reaction exotherm and the run time-average catalytic activity. The copolymer composition distribution and soluble fraction generated by  $\text{Et}(\text{Ind})_2\text{ZrCl}_2$  was sensitive to mixing conditions and thermal perturbations. Incorporation of 1-hexene significantly decreased the average molecular weights and density but increased the average catalyst activity, the peak melting temperatures and the weight- and number-average solution crystallization temperatures. Thermal perturbations broadened the polydispersity index.

XPS results showed that heterogenization of  $\text{Et}(\text{Ind})_2\text{ZrCl}_2$  on silica in the presence of MAO generated two types of zirconocenium cations (Cations 1 and 2), irrespective of the heterogenization procedures. Cation 1 is presumed to be in the form of an ion-pair  $[\text{SiO}]^-[\text{Et}(\text{Ind})_2\text{ZrCl}]^+$  while Cation 2, a trapped multi-coordinated crown complex of MAO. In absence of MAO, only Cation 1 is formed.

Trace element impurities such as K, Ca, Ti, Fe, Ni, Cu, and Zn detected by micro-PIXE may be the potential sources of poisoning the heterogenized catalyst.