Measurement of Catalyst Activity and Stability in Metallocene-Catalyzed Olefin Polymerization: An Engineering Approach

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ABSTRACT

An engineering approach has been presented that simultaneously calculates the activity and stability of the metallocene catalyst systems polymerizing ethylene or propylene in a semi-batch reactor interfaced with a data acquisition system. The methodology is based on a developed model that uses polymerization temperature, pressure, and the olefin feed rate as the input variables. Using the given temperature and pressure, the model first predicts the olefin solubility in toluene/solvent, the usual polymerization solvent, using the concept of phase equilibrium and Redlich-Kwong-Soave (R-K-S) equation of state. The model prediction agrees well with the experimental solubility values at and below 10 atm and 50 °C.

Next, the model converts the monomer volumetric feed rate into the mass flow rate. Finally, it calculates the normalized catalytic activity, expressed as *(g polyolefin formed)/{(mol metallocene) (hr) (concentration of monomer)}*, from the mass flow rate and plots the same as a function of time. From this plot, the catalyst stability can be determined and the region of superactivity can be identified. The above approach has been implemented using some literature data related to ethylene polymerization by the Cp_2ZrCl_2/MAO system. Determining the catalyst stability and identifying the region of superactivity using discrete batch polymerization studies is an exhaustive task which the above model remarkably simplifies. The model equally applies to solution and slurry olefin polymerization processes.

Int'l Conf. 2