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MODELING THE SOLUBILITY OF ETHYLENE AND PROPYLENE IN A TYPICAL POLYMERIZATION DILUENT: SOME SELECTED SITUATIONS

MUHAMMAD ATIQULLAH,* HASSAN HAMMAWA and HALIM HAMID

Petroleum and Gas Technology Division, The Research Institute, King Fahd University of Petroleum and Minerals, Dhahran, 31261, Saudi Arabia

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Abstract—The solubility of ethylene and propylene in toluene, which is mostly used as the diluent in metallocene-catalyzed olefin polymerization, was modeled as a function of temperature and pressure. Two selected slurry polymerization situations were considered: the early stage of a conventional slurry polymerization and the prepolymerized one. The phase equilibrium approach and the Prausnitz–Shair (P–S) correlation were used to independently develop the models. The former, unlike the latter, predicted the solubility which closely matched the experimental value. However, in the phase equilibrium approach, the type of the cubic equation of state affected the prediction. The Redlich–Kwong–Soave (R–K–S) equation, compared to the Peng–Robinson (P–R) one, showed better results. The overall prediction was more accurate at pressures below 5 atm. So far as the influence of temperature is concerned, the R–K–S equation also performed overall the best up to about 50°C. The above model-predicted solubility can be applied to calculate as a function of polymerization time the activity of metallocene catalyst systems polymerizing ethylene or propylene in a semi-batch computer-interfaced automated, laboratory-scale reactor. These activity values can be later used to model the kinetics of such olefin polymerization.