

Mathematical Model of High Temperature Thermal Gradient Interaction Chromatography (HT-TGIC) for Ethylene/1-Octene Copolymers.

Nantiya Inwong¹, Siripon Anantawaraskul¹, João B. P. Soares², Abdulaal Alkhazaal³

¹Department of Chemical Engineering, Faculty of Engineering, Kasetsart University (Thailand)

²Department of Chemical and Materials Engineering, Faculty of Engineering, University of Alberta (Canada)

³Department of Chemical Engineering, Faculty of Engineering, University of Waterloo (Canada)

High temperature thermal gradient interaction chromatography (HT-TGIC) with a graphitic carbon column has been developed in order to characterize chemical composition distribution of ethylene/1-olefin copolymer over a wide range of comonomer composition. HT-TGIC is interactive liquid chromatography technique; polymer molecules are fractionated based on their interaction with surface of graphitic carbon packing material under a temperature gradient. HT-TGIC not only can characterize sample over a wider comonomer composition and but also take shorter analysis time compared to other crystallization based techniques. As a new technique, quantitative details on fractionation mechanism of HT-TGIC are still largely under investigation.

In this work, a mathematical model of HT-TGIC is developed based on population balance in multi-stage adsorption/desorption combined with adsorption/desorption kinetic in order to describe its fraction mechanisms. Effect of chain microstructures and operating conditions (i.e., cooling rate, heating rate, solvent flow rates during adsorption and desorption periods) on the resulting chromatograms were also investigated. The simulated results from the proposed model shown a good agreement with the experimental results of ethylene/1-octene samples with different comonomer fractions over various operating conditions.

References:

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