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Title: Mathematical Modeling of High Temperature Thermal Gradient and Solvent Gradient Interaction Chromatography (HT-TGIC and HT-SGIC) of Polyethylene and Ethylene/1-Olefin Copolymers

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Reference 8:
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Abstract:

Physical and mechanical characteristics of polyolefin end-products depend on their microstructures that can be broadly defined by molecular weight distribution (MWD) and chemical content distribution (CCD). Contrary to their relatively simple hydrocarbon building blocks, microstructures of polyolefin are so complicated because they are an incredibly complex mixture of molecules with similar chemical make-up. As aforementioned, advanced characterization techniques, as well as a deep understanding of their fractionation mechanism are essential to adequately characterize this complex mixture of molecules.

Recently, chromatography-based fractionation techniques for determining CCD of polyolefin, namely high temperature thermal gradient interaction chromatography (HT-TGIC) and high temperature solvent gradient interaction chromatography (HT-SGIC), have received considerable attentions because they allow for a wider working window of comonomer contents, while offer acceptable accuracy in comparison to crystallization-based methods.[1] HT-TGIC fractionation mechanism has been extensively studied and has an explicit mathematical model available.[2, 3] Unfortunately, HT-TGIC typically has a lower resolution than HT-SGIC, requires longer operating time (especially when high resolution is needed) and has a narrower operational window.[4] In contrast, the fractionation mechanism of HT-SGIC is also extensively studied, but lacks of a mathematical model because of the complexity of solvent gradients and semi-quantitative detector signals. Fortunately, due to the similarities between HT-TGIC and HT-SGIC, the previously proposed mathematical model of HT-TGIC can be further extended to describe the HT-SGIC fractionation mechanism.

In this work, non-equilibrium, multi-stage adsorption/desorption model for describing both HT-SGIC and HT-TGIC fractionation mechanisms in sizeable operating window was proposed. Instead of dealing directly with the complication of HT-SGIC model, the difficulties associated with it are overcome by extracting important thermodynamics parameters from HT-TGIC profiles of various ethylene/1-octene copolymers operated with multiple isocratic solvent compositions.[5] Additionally, the solvent pair was thoughtfully picked to minimize nonlinearity nature of evaporative light scattering detector (ELSD) signal.[6, 7] The proposed model was successfully validated with experimental HT-TGIC and HT-SGIC results of ethylene/1-olefin copolymers with different compositions over different operating conditions.