Self-Modeling Curve Resolution Analysis of On-line Near Infrared Spectra Measured during the Melt-Extrusion Transesterification of Ethylene/Vinylacetate Copolymer

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The transesterification of molten ethylene/vinylacetate (EVA) copolymers by octanol as a reagent and sodium methoxide as a catalyst in an extruder has been monitored by on-line near infrared (NIR) spectroscopy. A total of 60 NIR spectra were acquired for 37 minutes with the last spectrum recorded 31 minutes after the addition of octanol and catalyst was stopped. The experimental spectra show strong baseline fluctuations which are corrected for by multiplicative scatter correction (MSC). The chemometric methods of orthogonal projection approach (OPA) and multivariate curve resolution (MCR) were used to resolve the spectra and to derive concentration profiles of the species. The detailed analysis reveals the absence of completely pure variables that leads to small errors in the calculation of pure spectra. The initial estimation of a concentration that is necessary as an input parameter for MCR also presents a non-trivial task. We obtained results that were not ideal but applicable for practical concentration control. They enable a fast monitoring of the process in real-time and resolve the spectra of the EVA copolymer and the ethylene/vinyl alcohol (EVAL) copolymer to be very close to the reference spectra. The chemometric methods used and the decomposed spectra are discussed in detail.

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