

Title: Chemical Composition of LLDPE Using Raman Spectroscopy and Chemometrics

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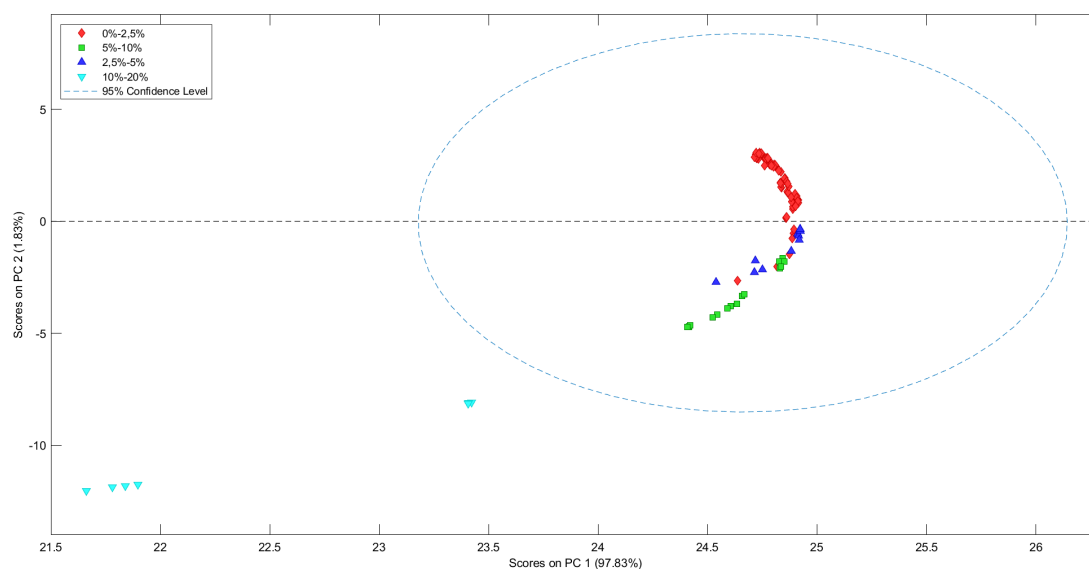
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References:

Reference 1: Macromolecular Chemistry and Physics (2019), 220(24), 1900376
Reference 2: Macromolecular Chemistry and Physics (2018), 219(11), 1700609
Reference 3:
Reference 4:
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Reference 7:
Reference 8:
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Abstract:

This work shows the interest of Raman spectroscopy associated with chemometrics methods to rapidly characterize the composition of linear low-density polyethylene (LLDPE). We have chosen to study hexene-based LLDPE in a wide range of content from 0 to 21 mol% comonomer. The LLDPEs used as a standard were produced using zirconocene catalysts activated with methylaluminumoxane to obtain polymers with a homogeneous composition. Each synthesized polymer was characterized by NMR to determine the composition value and then measured by Raman spectroscopy.

Regression methods to correlate the 1-hexene content in the copolymers with their Raman spectra were constructed. Multivariate calibration models were compared using Partial Least Squares Regression (PLSR) and Principal Component Regression (PCR) on pre-processed Raman data.

Finally, these models were tested and validated by comparing the obtained results with NMR results for some unknown ethylene-1-hexene copolymers.