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Abstract

The surface of lignocellulosic pulp fibers was studied at microscopic level using Fourier transformed infrared imaging to obtain information regarding pattern distribution and concentration of the lignocellulosic components. As each pixel of the hyperspectral image contains a mixture of spectral information of all of the components present within, multivariate curve resolution-alternating least squares (MCR-ALS) analysis was performed to recover the pure spectra of the main components of lignocellulosic materials and determine their distribution on the surface of the fiber. Although MCR-ALS is not a quantitative analysis, the relative concentration profile obtained by MCR-ALS can be used to obtain real pixel-to-pixel quantitative information of the components. Some strategies have been described to transform the values obtained from MCR-ALS into real concentration units; however, they have been applied mostly to artificial mixtures, using available reference materials to create calibration models. In this work, two simple strategies are proposed to estimate single pixel concentration when no reference material is available. These strategies can be especially relevant for microscale quantitative analysis of natural, complex and heterogeneous samples.

Key Words: Infrared imaging; MCR-ALS; Lignin; Cellulose; pixel quantification; Concentration map