LECTURE

NIR hyperspectral imaging spectroscopy and chemometrics in pharmaceutical analysis

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Near-infrared hyperspectral imaging (NIR-HI) has been increasingly employed as a new analytical tool for the study and characterization of pharmaceuticals. The main advantage of this technique is the possibility to obtain spatial distribution information about the sample, differently of traditional NIR spectroscopy that provides information about the bulk of the sample and reflects an average composition.

In NIR-HI, a given monitored area is split in pixels and a spectrum is recorded in each pixel. The spectrum of each pixel must be processed by chemometric tools to extract the distribution of each compound in the surface, obtaining the chemical images. The possibility to obtain information about the distribution of chemical species in the monitored area enables information about the degree of chemical and/or physical heterogeneity within a given sample.

In this lecture, three applications will be presented, in which the NIR-HI coupled with chemometrics was able to solve different problems in analytical chemistry applied to the pharmaceutical field.

In the first aplication, NIR-HI and multivariate methods such as PLS and MCR-ALS were applied to quantify compounds presented in polymeric films loaded with paracetamol, highlighting the properties like homogeneity and chemical affinity among the compounds within the sample. In second application, the homogeneity of distribution of a drug dispersed in polymeric transdermal films was studied using NIR-HI by combining the macropixel analysis concept with split-plot experimental design. In the last application, solid-state physical transformation of pharmaceuticals, in time and temperature series, due to loss of water in pharmaceutical hydrates and transitions of amorphous-crystalline type were studied on the surface of pharmaceutical samples using the chemometric approaches MCR-ALS, PARAFAC and PARAFAC2.