Modelling and Identification of Individual Stage Contributions in an Industrial Pharmaceutical Process by Multiblock PLS

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Abstract
In this paper, multiblock partial least squares (MBPLS) was applied to model a multi-stage pharmaceutical process producing an active pharmaceutical ingredient (API) by fermentation. The aim is to model the final API’s chromatographic purity in terms of each operating variable, establishing the relative contribution of each process stage. A balanced bootstrap algorithm was used to choose the best set of variables from each stage to obtain a model with the highest predictive capability. Seven variables from the original twenty-eight were selected and a two-latent variable MBPLS model was found to minimize the prediction residuals ($Q^2_Y = 64.3\%$). The multiblock methodology revealed that the fermentation stage has a prominent role in the description of the final API’s chromatographic purity.

Keywords: multivariate data modelling, multiblock PLS, pharmaceutical production

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