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SMB-PLS for Expanding Multivariate Raw Material Specifications in Industry 4.0

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The advantages of being able to define precisely meaningful multivariate raw material specifications are enormous. They allow increasing the number of potential suppliers, by allowing a wider range of raw material properties, without compromising the Critical Quality Attributes (CQAs) of the final product. Despite their importance, specifications are usually defined in an arbitrary way based mostly on subjective past experience, instead of using a quantitative objective description of their impact on CQAs. Moreover, in many cases, univariate specifications on each property are designated, with the implicit assumption that these properties are independent from one another. Nevertheless, multivariate specifications provide much insight into what constitutes acceptable raw material batches when their properties are correlated (as usually happens) [1]. To cope with this correlation several authors suggest using multivariate approaches, such as Partial Least Squares (PLS) [2].

Besides, not only raw material properties influence the quality of the final product, but also process conditions. Thus, we propose a novel methodology, based on the Sequential Multi-block PLS (SMB-PLS), to identify the variation in process conditions uncorrelated with raw material properties, which is crucial to implement an effective process control system attenuating most raw material variations. This allows expanding the specification region and, hence, one may potentially be able to accept lower cost raw materials that will yield products with perfectly satisfactory quality properties.

[1] C. Duchesne and J. F. MacGregor, *J. Qual. Technol.*, 36, 78–94, 2004.

[2] J. Borràs-Ferrís, D. Palací-López, C. Duchesne, and A. Ferrer, *Chemom. Intell. Lab. Syst.*, 225, 2022.

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Classification

Both methodology and application

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