Contribution ID: **41** Type: **not specified**

Establishing Multivariate Specification Regions for Incoming Raw Materials –a QbD approach

Friday, 30 May 2025 09:00 (45 minutes)

Establishing multivariate specification regions for selecting raw material lots entering a customer's plant is crucial for ensuring smooth operations and consistently achieving final product quality targets. Moreover, these regions guide the selection of suppliers. By meeting these specifications, suppliers contribute to customer satisfaction, which can, in turn, enhance market share. Latent Variable Methods, such as Partial Least Squares regression (PLS) and the more recent Sequential Multi-block PLS (SMB-PLS), have proven to be effective data-driven approaches for defining multivariate specification regions. These methods model the relationships between raw material properties (Critical Material Attributes –CMA), process variables (Critical Process Parameters –CPP), and final product quality (Critical Quality Attributes –CQA), enabling the identification of a lower-dimensional latent variable subspace that captures quality-relevant variations introduced by raw materials and process conditions. This subspace is central to the methodology.
Within this latent variable space, several statistical limits are defined to ensure final product quality and guarantee data compliance with the latent variable model, collectively forming the multivariate specification region. After providing historical context on the early development of these methods, this presentation will cover several key topics. These include the data requirements for constructing latent variable models and how to organize them into distinct blocks. The techniques used to define the limits (in terms of shape and size) within the latent variable subspace—via direct mapping and latent variable model inversion—will be discussed, along with methods for addressing uncertainties. Particular attention will be given to how process variations generate different scenarios and approaches for establishing meaningful specification regions. Case studies using both simulated and industrial data will illustrate these methods. It will be demonstrated that the proposed framework aligns with the principles of Quality by Design (QbD), with notable similarities to the Design Space (DS) concept. The presentation will conclude by exploring potential future developments, including the establishment of multivariate process capability indices based on specification regions.

Type of presentation

Invited Talk

Primary author: DUCHESNE, Carl (Université Laval (Canada))

Presenter: DUCHESNE, Carl (Université Laval (Canada))

Session Classification: Keynote

Track Classification: Spring Meeting