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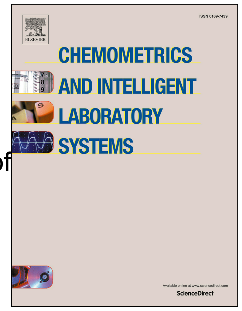

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A COMPUTATIONAL APPROACH TO PARTIAL LEAST SQUARES MODEL INVERSION IN THE FRAMEWORK OF THE PROCESS ANALYTICAL TECHNOLOGY AND QUALITY BY DESIGN INITIATIVES

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Abstract

In the context of the paradigms founding the Quality by Design and Process Analytical Technology initiatives, the work herein presents a computational approach to support the decision-making process, in particular, about the feasibility of a product defined for some a priori given quality characteristics.

The approach is based on the computation of the pareto-optimal front when simultaneously minimizing the expected differences between the predicted and the desired characteristics. Thus, the feasibility is tackle as an optimization problem with the novelty of doing so simultaneously for all the characteristics, preserving the correlation structure, but by handling each individual characteristic separately.

With data from a low-density polyethylene production process, with fourteen process variables and five measured characteristics of the final polyethylene, solutions are found to define the Design Space for targeted quality characteristics on the product, and without the need of explicitly inverting the PLS (Partial Least Squares) prediction model fitted to the process.

Keywords: Process Analytical Technology; Quality by Design; Partial Least Squares; Pareto optimality; process decision making; industrial processes

1. Introduction

The need of more organised approaches to process and product development with the aim of consistently guaranteeing quality and value to processes and products has been formally identified [1] by the pharmaceutical industry as the Quality by Design (QbD) initiative, but the concept can be extended to any industrial process, in particular, chemical processes.

In any case, the implementation of these concepts requires the quantitative characterization of process and product performance and, also, some modelling techniques that support decision-making, usually, multivariate models that relate the input variables (process parameters, material properties, etc.) and product quality (measured characteristics of the final product), which is the setting of the so-called Process Analytical Technology (PAT). In fact, in [2] it is already stated that the identification of optimal operating conditions for large

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