Abstract

Although batch processes are “simple” in terms of equipment and operation design, it is often difficult to ensure consistently high product quality. The aim of this PhD project is the development of multivariate statistical methodologies for the realtime monitoring of quality in batch processes for the production of high value added products. Two classes of products are considered: those whose quality is determined by chemical/physical characteristics, and those where surface properties define quality. In particular, the challenges related to the instantaneous estimation of the product quality and the realtime prediction of the time required to manufacture a product in batch processes are addressed using multivariate statistical techniques. Furthermore, novel techniques are proposed to characterize the surface quality of a product using multiresolution and multivariate image analysis.

For the first class of products, multivariate statistical soft sensors are proposed for the real-time estimation of the product quality and for the online prediction of the length of batch processes. It is shown that, to the purpose of realtime quality estimation, the complex series of operating steps of a batch can be simplified to a sequence of estimation phases in which linear PLS models can be applied to regress the quality from the process data available online. The resulting estimation accuracy is satisfactory, but can be substantially improved if dynamic information is included into the models. Dynamic information is provided either by augmenting the process data matrix with lagged measurements, or by averaging the process measurements values on a moving window of fixed length. The process data progressively collected from the plant can be exploited also by designing time-evolving PLS models to predict the batch length. These monitoring strategies are tested in a real-world industrial batch polymerization process for the production of resins, and prototypes of the soft sensor are implemented online.

For products where surface properties define the overall quality, novel multiresolution and multivariate techniques are proposed to characterize the surface of a product from image analysis. After analyzing an image of the product surface on different levels of resolutions via wavelet decomposition, the application of multivariate statistical monitoring tools allow the in-depth examination of the product features. A two-level “nested” principal component analysis (PCA) model is used for surface roughness monitoring, while a new strategy based on “spatial moving window” PCA is proposed to analyze the shape of the surface pattern. The proposed approach identifies the abnormalities on the surface and localizes defects in a sensitive fashion. Its effectiveness is tested in the case of scanning electron microscope images of semiconductor surfaces after the photolithography process in the production of integrated circuits.