TOS variography – a missing link in MSPC and PAT

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Process monitoring and control in technology and industry is *incomplete* without full understanding of <u>all</u> sources of variation. It is not enough to be in command of Multivariate Statistical Process Control (MSPC) if the process data are affected by significant errors which have not been adequately identified, quantified and reduced to below a relevant a priori acceptance threshold. In fact process data are typically affected <u>both</u> by classical analytical measurement errors as well as sampling and/or PAT sensor acquisition errors. The latter categories can dominate over analytical errors by factors 10-20, or more when proper process sampling competence is not brought to bear in the design, maintenance and operation of the *total* process measurement system. These errors are often physical sampling errors associated with process sample- and/or reference sample extraction, but PAT signal acquisition gives rise to *identical* error types and magnitudes which therefore also contributes significantly (indeed often overwhelmingly) to the total process Measurement Uncertainty $MU_{(sampling+analysis)}$. All this is well understood and solutions abound in the Theory of Sampling (TOS). In science, technology and industry, in materials processing and in goods production and manufacturing it is essential to eliminate, or reduce maximally, all *unnecessary* contributions to $MU_{(sampling+analysis)}$ in order to perform *valid* chemometric multivariate monitoring and control (MSPC) in order to bring forth the process signals with maximum signal/noise enhancement. Variographic process description allows quantification of the sum-total effect of all unwanted, adverse sampling/sensor acquisition errors. Continuous variographic process characterisation, with application-dependent updating, is able to issue warnings that a particular process measurement system is not, or is no longer, fit-for-purpose representative and must therefore be rectified. The variographic approach works directly on the routine process data coming off the process, i.e. no extra measurements are needed than the existing process data. Variographics is a real-time, on-line self-controlling plug-in facility with a wide applicability potential. This workshop calls for a process monitoring *paradigm shift* in chemometrics: variographics constitutes a *missing link* in MSPC and PAT.

This workshop introduces the necessary-and-sufficient TOS specifics needed for these objectives, complete with extensive literature referrals [1-9]. TOS is outlined in a new compact didactic format and examples and case histories from selected industrial sectors will illustrate the above issues a.o. self-contradictionary FDA sampling demands for critical pharmaceutical mixing processes, EU GMO monitoring and control, and minerals processing pathways in a major European mining and value-added processing company. The workshop will allow participants to identify cases and problems in their own data, with a professional idea of what needs to be modified if/when necessary, with a particular focus how TOS can be used for improved development of spectroscopic calibration models.

Workshop literature

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