

L1. Representative sampling in PAT and environmental/geological work: Theory of Sampling (TOS) — a missing link

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Representative sampling is a critical success factor for PAT, in the geo-sciences and for environmental characterisation. Many instrumental analytical methods are based on "analysis by proxy", for which the representativity of the reference data is critical w.r.t. the underlying multivariate calibrations.

Both X-data as well as Y-data need to be fully representative, in themselves but also w.r.t. intercalibrations. Although TOS has been known for >25 years, it is still only very little known or implemented in today's analytical chemistry, even though sampling errors form the by far most dominant part of what is all too loosely termed "measurement errors". This presentation presents a theoretical as well as practical framework of seven sampling unit operations (TOS) with which to approach all types of sampling issues in the field or plant, in industry; the laboratory as well as for PAT purposes.