

Selected Topics in Experimental Design and Chemometrics

Prof. Tadeusz Górecki

Department of Chemistry, University of Waterloo, Waterloo, Ontario, Canada

Experimentation is one of the foundational pillars of science. Any theoretical hypothesis that is formulated must ultimately be proved or disproved by experiments. While the scientific method is generally intuitively understood by researchers, not all of them fully realize how various controllable and uncontrollable factors might affect their results. Also, the approach to experimentation is often far from optimal. The course will try to fill these voids by exploring the areas mentioned above. It will begin by introducing the tools needed to evaluate the sources of variation in data through the analysis of variance (ANOVA). This will be followed by a discussion of calibration approaches, method ruggedness and sensitivity. Once these issues are understood, the focus will shift towards experimental designs that allow gaining a multitude of insights in a minimum number of experiments. Approaches discussed will include block designs with all their variants (randomized block designs, Latin square designs, Graeco-Latin squares, etc.), factorial and fractional factorial designs, composite designs, mixture designs and Plackett-Burman designs. In the last part of the course issues related to experimental optimization will be discussed. Approaches ranging from sequential “one-factor-at-a-time” through evolutionary operation to response surface methods will be covered. Finally, purely experimental simplex optimization will be introduced.

References:

G.E.P. Box, J.S. Hunter, W.G. Hunter, “Statistics for Experimenters”, 2nd Ed., Wiley Interscience, 2005

D.L. Massart, B.G.M. Vandeginste, S.M. Deming, Y. Michotte, L. Kaufman, “Chemometrics: a textbook”, Elsevier, 2003

R.G. Brereton, “Applied Chemometrics for Scientists”. J. Wiley & Sons, 2007

Termin	Dzień tygodnia	Godzina	Miejsce
27.05.2019	poniedziałek	13.15 – 16.00	Minicentrum Konferencyjne (Luwr)
28.05.2019	wtorek	13.15 – 16.00	Minicentrum Konferencyjne (Luwr)
29.05.2019	środa	13.15 – 16.00	Minicentrum Konferencyjne (Luwr)
30.05.2019	czwartek	13.15 – 16.00	Minicentrum Konferencyjne (Luwr)
31.05.2019	piątek	12.15 – 15.00	Minicentrum Konferencyjne (Luwr)