AUTOMATION FOR ANALYTICAL CHEMISTRY

David J. Cocovi-Solberg

University of Natural Resources and Life Sciences (BOKU), Muthgasse 18, Vienna, Austria <u>david.cocovi-solberg@boku.ac.at</u>

Abstract

At the end of this module, students will have a panoramic view of the different current approaches for environmental and clinical analysis, as well as the importance of automating those workflows. They will be able to completely automate a simple analytical workflow, using flow techniques: Designing a proper fluidic manifold, controlling the components from a computer, basic troubleshooting, real-time data acquisition and data treatment. The opportunities of trending 3D printing manufacturing technique will be presented and discussed. Lectures and seminars on similar topics will be interleaved for the sake of enhanced understanding, as far as it suits the students schedules and needs.

Lectures (15h)

- EXPOSOME EVALUATION. Introduction to targeted and untargeted workflow approaches. Introduction to bioaccessibility, bioavailability and exposome evaluation. Importance of the sample preparation. Current instrumental workhorse and trends. Focus on the importance of automation. Instrumental challenges. (3h)
- FLOW TECHNIQUES. Fundamentals on laboratory automation and usual instrumentation. Fluidic principles. 1st generation Flow Injection Analysis (FIA). Peristaltic pumps, Injection valves. 2nd generation Sequential Injection Analysis (SIA). Syringe pumps, Selector valves. 3rd generation Lab-On-Valve (LOV). Sequential Injection Chromatography (SIC), Bead Injection (BI). Examples in the scientific literature. (3h)
- HYPHENATION TO INSTRUMENTAL ANALYSIS. Hyphenation of flow techniques to instrumental analysis equipment. Examples: ETAAS, ICPOES, ICPMS, HPLC. Tips and tricks for troublesome hyphenations. (3h)
- 3D PRINTING FOR ANALYTICAL CHEMISTRY. Basics of 3D printing. Technologies. Working principles. Use of 3D printed pieces in the analytical chemistry lab. Current trends. Main advantages, disadvantages and opportunities of the technique. (3h)

 (TRANSFER) TRENDS IN SAMPLE PREPARATION. Examples on different flow systems used for sample preparation. Performance of commercial products vs. taylor made systems. Review of commercial equipment and future trends. Commercial strategies. Strategies for publication, patenting, cooperation and transfer. (3h)

Seminars (15h)

- WORKING PRINCIPLES OF FLUIDIC MANIFOLDS. Mechanics, electronics, communications. Troubleshooting in automation through flow techniques. (3h)
- SETUP OF AN AUTOMATED METHOD. Setting up of an automated fluidic method for analysis based on available fluidic components. (3h)
- 3D PRINTING HANDS-ON. Use of CAD/CAM software for 3D printing: Autodesk 123D Design, Autodesk Fusion 360. Formlabs Preform. Design of simple models. Design of complex models. (3h)
- INTRODUCTION TO PYTHON. Introduction to computational thinking. Basic course on Python programming languaje. Installation of Python, choosing an Integrated Development Environment. (Students will need a computer with administrator rights) (3h)
- PYTHON FOR ANALYTICAL CHEMISTRY. Use of Python programming in the analytical chemistry lab: Control of instrumentation, data acquisition, data treatment, programming smart (unsupervised) methods. (3h)

Consulting (30h)

David J. Cocovi Solberg will be available to help students in automating analytical processes in their respective research lines, with both preparative or analytical aims: Design of fluidic manifolds, control or data processing. Also, to solve any question arisen during the material presentation or to expand the presented contents. Students should arrange the consulting hours by mail appointments, preferably but not mandatorily in the 10 to 14 February week: <u>dj.cocovi.solberg@gmail.com</u>

Termin	Dzień tygodnia	Godzina	Miejsce
27.01.2020	Poniedziałek	12.15 – 15.00	Minicentrum Konferencyjne WCH
28.01.2020	Wtorek	12.15 – 15.00	Minicentrum Konferencyjne WCH
29.01.2020	Środa	12.15 – 15.00	Minicentrum Konferencyjne WCH
30.01.2020	Czwartek	12.15 – 15.00	Minicentrum Konferencyjne WCH
31.01.2020	Piątek	13.15 – 16.00	Minicentrum Konferencyjne WCH
03.02.2020	Poniedziałek	12.15 – 15.00	Minicentrum Konferencyjne WCH
04.02.2020	Wtorek	12.15 – 15.00	Minicentrum Konferencyjne WCH
05.02.2020	Środa	12.15 – 15.00	Minicentrum Konferencyjne WCH
06.02.2020	Czwartek	12.15 – 15.00	Minicentrum Konferencyjne WCH
07.02.2020	Piątek	13.15 – 16.00	Minicentrum Konferencyjne WCH