ÅBO AKADEMI
PROCESS CHEMISTRY CENTRE

EQUIPMENT LIST
SOFTWARE AND EXPERTISE

Collected by Kalle Arve, Markus Engblom, Kim Granholm, and Robin Manelius
Checked and edited by T. Salmi
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WOOD AND PAPER CHEMISTRY (Trä- och papperskemi)
Gadolinia Building, Porthansgatan 3, FI-20500 ÅBO, Finland

INORGANIC CHEMISTRY (Oorganisk kemi)
Axelia II Building, Biskopsgatan 8, FI-20500 ÅBO, Finland

INDUSTRIAL CHEMISTRY AND REACTION ENGINEERING (Teknisk kemi och reaktionsteknik)
Axelia Building, Biskopsgatan 8, FI-20500 ÅBO, Finland

ANALYTICAL CHEMISTRY (Analytisk kemi)
Axelia Building, Biskopsgatan 8, FI-20500 ÅBO, Finland

WOOD AND PAPER CHEMISTRY
Trä- och papperskemi, Gadolinia

Contact person: Jarl Hemming

MAIN EQUIPMENT

- **GC-MS, gas chromatography mass spectrometers** (2) (Markku Reunanen)
- **Py-GC-MS, pyrolysis unit** (Pyrola) for use with GC-MS (Markku Reunanen)
- **GC-FID, gas chromatographs** (6) with auto injectors and flame ionization detectors (Jarl Hemming)
- **Analytical HPLC, High Performance Liquid Chromatographs** (2) with RI, UV-Vis diode array, MALLS and ELSD detectors (Andrey Pranovich, Jarl Hemming)
- **Preparative HPLC** with gradient pumps, and RI and UV detectors (Jarl Hemming, Annika Smeds)
- **Particle charge detector** (Mütek PCD 03) (Anders Strand, Lari Vähäsalo)
- **Flow cytometer** (Lari Vähäsalo)
- **TOC, total organic carbon analyzer** (Leif Österholm)
- **UV-Vis spectrophotometer** (Anders Strand, Jarl Hemming)
- **Large-scale Soxhlet extractors** (2) (Leif Österholm, Christer Eckerman)
- **ASE extractors** (3) (Andrey Pranovich, Song Tao , Jarl Hemming)
- **Freeze-drying equipment** (2) (Leif Österholm)
- **Flash chromatography** (2) (Christer Eckerman)
- **Xenotester** (Leif Österholm)
- **Wood mills** (3) (Leif Österholm)
- **Hand sheet equipment** (Hanna Lindqvist)
- **DDA**, dynamic drainage analyzer (Lari Vähäsalo)

- **TOF-SIMS**, Time-of-Flight Secondary Ion Mass Spectrometry (Sylwia Bialczak, Elena Tokareva)
- **XPS**, X-ray photoelectron spectroscopy (Sylwia Bialczak, Elena Tokareva)

MAIN EXPERTISE

Auer, Markku, TkD, Professor
- Biorefinery, wood as raw material
- Papermaking chemistry
- Polymer chemistry

Holmbom, Bjarne TkD, Professor Emeritus
- Wood- and paper chemistry
- Processes and products in the wood industry
- Analytical chemistry

Krogell, Jens DI, PhD student
- Extraction
- Analysis of wood components, carbohydrates and lignin

Manelius, Robin PhD, researcher
- Starch chemistry
- Organic fillers

Pranovich, Andrey Ph.D., Docent
- Chemi-mechanical pulping processes
- Lignin chemistry
- Wood chemistry
- Analytical techniques

Smeds, Annika PhD, Docent
- Chemical characterizations of products from agriculture and wood
- Quantification of lignans in biological samples
- Isolation and identification of polyphenols in wood extracts

Sundberg, Anna TkD, Docent
- Wood- and paper chemistry
- Analysis techniques for carbohydrates
- Wood extractives

Vähäsalo, Lari TkD, Researcher
- Wet end chemistry in paper making
- Deposition mechanisms
- Wood extractives
- Coated Broke and White Pitch
- Flow Cytometry
- Chemometrics

Willför, Stefan TkD, Docent, Professor
- Wood chemistry
- Bio-chemicals
- Chemistry of biomaterials
- Analysis techniques (biorefinery, wood industry)

INORGANIC CHEMISTRY
Oorganisk kemi, Axelia

Laboratory manager: Kaj Fröberg

MAIN EQUIPMENT

Scanning Electron Microscopes

- Cambridge Instruments scanning electron microscope type Stereoscan 360. Secondary and Backscattered electrons detectors. Energy Dispersive X-ray analyser and Image processing system, IMIX, by Princeton Gamma Tech.
- S360 A LEO (former Cambridge Instruments) scanning electron microscope type Stereoscan 360 equipped with a Energy Dispersive X–ray analyzer and image processing system, IMIX, by Princeton Gamma Tech.
- LEO1530 A FEG–SEM, equipped with an energy dispersive X–ray analysis system, Vantage, by ThermoNoran. It also has some image analysis possibilities.
- For more demanding image analysis, we have a very versatile package called "microGOP" from ContextVision. We have found much use for it's powerful programming (scripting) capabilities.
- Contact person: Kaj Fröberg

Atomic Force Microscope (AFM) / Scanning Tunnelling Microscope (STM)

- JEOL SPM 4200 Environmental AFM and STM microscope
  - Scanners: x,y : 10 micrometre, z: 3 µm
  - xy : 80 micrometre, z: 7 µm
- AFM modes: contact mode, non–contact mode and AC–mode, Phase contrast, Friction mode
- Sample size: 10x10x3 mm^3
- Resolution(x,y,z): atomic
- Electrochemical cell for in situ measurements
- Contact person: Mikael Bergelin

Atomic Force Microscope (AFM) NanoSurf Mobile S

- Scanners: x,y: 110 micrometre, z: 22 µm
- AFM modes: contact mode, non–contact mode and AC–mode, Phase contrast, Force modulation, Spreding resistance mode
- Sample size unlimited (mobile scan head)
- Resolution: x,y: 1,7 nm, z: 0.3 nm
- Contact person: Mikael Bergelin

Confocal Microscope (NanoFocus µSurf)

- Scan ranges (x, y): 160 m to 10 cm
- Resolution (z): 2 nm to 30nm
- Sample size: approximately 1*1 mm to 10*10 cm
- Wet lens for imaging in non-aggressive transparent liquids
- Contact person: Mikael Bergelin

Biopotentiostat and Electrode Rotator for Hydrodynamic Electrochemistry

- Pine instrument
- AFCBP1 biopotentiostat
- AFMSRX rotator
- RDE-electrodes: Pt and glassy carbon

- RRDE-electrodes: Pt/Pt and glassy carbon/Pt
- Software: PineChem
- Contact person: Mikael Bergelin

Computercontrolled Potentiostats/Galvanostats
Electrochemical Impedance Measurement Units
Ivium Iviumstat, for use with static, flow and IJFC cells
Contact person: Mikael Bergelin

X–ray Diffractometer
Phillips "X´pert" X–ray diffractometer with powder and high temperature attachment (1600°C).
Contact person: Kaj Fröberg

Heating Microscope/ Hot Stage Microscope (HSM)
Misura 3.0, with programmable heating ramps.
For imaging sample form changes during heating.
Tmax =1600°C)
Contact person: Kaj Fröberg

Hot Stage Microscope – Optical Dilatometer (HSM-ODHT)
Misura 3 HSM-ODHT, with programmable heating ramps.
For acquiring the complete sintering curve of the material, the expansion and contraction, the coefficient of expansion, the glass transition temperature and the dilatometric softening temperature.
Heating rate up to 50°C/min.
Tmax =1600°C
Contact person: Kaj Fröberg

Thermogravimetric Analyzer (Mettler Toledo TG/SDTA 841)
Tmax = 1600°C).
Heating rate: 5–20°C/min
Controlled gas atmosphere (N_2) (Others as H_2O, SO_2, HCl, etc. can be applied)
Sample weight up to 5g
Accuracy 0.1µg
Automated sample robot with room for 34 samples.
Contact person: Kaj Fröberg

Thermogravimetric Analyzer
Tmax = 1500°C
Heating rate: 5–100°C/min
Controlled gas atmosphere (H_2O, SO_2, HCl, etc)
Sample weight up to 500 mg
Contact person: Kaj Fröberg

Pressurized Thermogravimetric Analyzers
pmax = 60 bar, Tmax = 1000°C
Controlled gas atmosphere (H_2O, SO_2, HCl, etc)
Sample weight up to 500 mg
Contact person: Kaj Fröberg

Furnaces
High temperature furnaces (air), 1100 – 1550°C
Contact person: Kaj Fröberg

Pressurized Grid Heater
Temperature 25-1000°C
Heating rate 1000°C/s
Pressure 1-40 bar
Contact person: Nikolai DeMartini

Single Particle Furnace
Tmax = 1100°C
Controlled gas atmosphere (O_2, CO_2, N_2)
Contact: Nikolai DeMartini

Gas Analyzers for CO and CO_2
Non–Dispesive InfraRed (NDIR)
CO, 0–5000 ppm, 0-10%
CO_2, 0–5000 ppm, 0-10%
Contact person: Nikolai DeMartini

Gas Analyzers for NO
Chemiluminescence NO analyzer
0–5 ppm, 0–10 ppm, 0–15 ppm, 0–60 ppm, 0–200 ppm
Contact person: Nikolai DeMartini

Gas Analyzers for SO_2
IR
0-100 pm, 0-600 ppm
Contact person: Nikolai DeMartini

Gas Analyzers for O_2
Paramagnetic
0-25%
Contact person: Nikolai DeMartini

Catalyst Reactor with Carbon-Molybdenum for oxidizing NH3 and reduced sulphur gases
Contact person: Nikolai DeMartini

SOFTWARE
Contact person: Anders Brink

Computational Fluid Dynamics
Fluent

Thermodynamic Equilibrium
HSC Chemistry
Fact Sage
ChemApp

Chemical Kinetics
CHEMKIN II
CHEMKIN 4

Multiphysics
COMSOL

INDUSTRIAL CHEMISTRY AND REACTION ENGINEERING
Teknisk kemi och reaktionsteknik, Axelia

Laboratory manager: Kari Eränen

MAIN EQUIPMENT

Reactor equipment

Parallel high-throughput catalyst and reaction screening system with gas chromatography-mass spectrometry (**GC-MS**) and liquid chromatography (**LC**)
(Kari Eränen)
Spinning basket reactor system (Autoclave Engineers) (Kari Eränen)
Minireactor systems (aromatization, dearomatization, hydrocarbon conversion, de-NO_x, isotopic exchange) (Kari Eränen, Kalle Arve)
High-pressure autoclaves (Parr and Autoclave Engineers) (Kari Eränen)
Special autoclave for structured catalysts (Pasi Virtanen, J.-P. Mikkola)
Shaking reactor for liquid-solid-gas systems (Parr) (Kari Eränen, Anton Tokarev)
Autoclaves for catalyst preparation (Kari Eränen, Narendra Kumar)
Quartz reactor (oven) for catalyst preparation (Kari Eränen, J.-P. Mikkola)
Liquid-phase and liquid-solid test reactor system (Kari Eränen)
Test reactor system for liquid-liquid reaction kinetics (Kari Eränen)
Column reactor for liquid-liquid reactions and extraction (Kuhni) (Kari Eränen)
Ultrasonic reactor equipment for enhancement of chemical reactions (two devices; horn and high-power cavity)) (Kari Eränen, J.P. Mikkola, Mats Rönnholm)
Microwave test reactor system (2 kW, designed in collaboration with Sairem) (Kari Eränen, J.-P. Mikkola)
Microreactor and millireactor systems for gas and liquid phases, separate 3-phase microreactor (Kari Eränen, Mats Rönnholm, José Hernandez Carucci))
Equipment for pyrolysis of biomass (Atte Aho)

Equipment for characterization of solid materials

Wicke-Kallenbach diffusion cell for determination of diffusion coefficients (Kari Eränen)
He-pycnometer (Micromeritics) (Kari Eränen)
Microbalance for sorption and kinetic studies (Cahn) (Kari Eränen)
Sorptometer for physisorption and chemisorption studies (Carlo Erba Sorptomatic 1900) (Kari Eränen, Narendra Kumar)
Mass spectrometers for TPD, TPSR and transient kinetic studies (Carlo Erba QTMD and Balzers) (Kari Eränen)
Catalyst testing and characterization unit (Autochem sorptometer, TPD, pulse chemisorption, Micromeritics) (Kari Eränen)
On-line catalyst potential measurement system (Kari Eränen, Anton Tokarev)
On line and off line mass spectrometers (3 pcs) (Kari Eränen)
Fourier Transformed Infrared Spectrometer for catalytic studies (Ati Mattson) (Kari Eränen)
X-ray fluorescence metal analyzer (Outokumpu X-met) (Kari Eränen)

Equipment for chemical analysis

UV-VIS and IR spectrophotometers (Kari Eränen)
Several gas chromatographs (FI, EC and TC detectors) (Kari Eränen, Päivi Mäki-Arvela)
Micro gas chromatograph (Kari Eränen, José Hernandez Carucci)
Gas chromatography – mass spectrometry (GC-MS) (Kari Eränen, Päivi Mäki-Arvela)
High Pressure Liquid Chromatographs (Hewlett Packard) (Kari Eränen, J.-P. Mikkola, Jyrki Kuusisto)
Gas analyzers for hydrocarbons, NOx and oxygen (IR, chemiluminescence and paramagnetic) (Kari Eränen, Kalle Arve)

Other equipment
Measurement system for gas solubilities (Fugatron) (Kari Eränen)
Densitometer (A. Paar) for the measurements of liquid and gas densities (Kari Eränen)
Liquid viscosity measurement (Kari Eränen)
Melting point measurement apparatus (Büchi) (Kari Eränen)
Potentiometers and conductometers (Kari Eränen)
On line potential measurement of solid surfaces (Anton Tokarev)
Particle size analyzer (MTS) (Kari Eränen)
Sieving devices (Kari Eränen)
Rotavapor equipment (Kari Eränen, J.-P. Mikkola)

SOFTWARE

Modelling and parameter estimation
MODEST - a simulation, optimization and parameter estimation package (ProfMath/H. Haario) (Johan Wärnå, J.-P. Mikkola, Mats Rönnholm, Andreas Bernas, Henrik Grénman, Teuvo Kilpiö)
Matlab (Johan Wärnå)
ATHENA Visual Studio (Johan Wärnå)
Process simulation
Pro/II (Simsci 7.0) (José Hernandez Carucci)
Flowbat (Johan Wärnå)
Flow modelling -CFD
Fluent (Johan Wärnå)
Reactor modelling and kinetics
Chemkin III – Chemical kinetics simulator (Reaction Design) **(**Timo Petteri Suominen, José Hernandez Carucci)
KINSIM - a program package for simulation of homogeneous reactors (Tapio Salmi, Johan Wärnå)
CATSIM - a program package for simulation of heterogeneous catalytic reactors (Tapio. Salmi and Johan Wärnå)
Molecular modelling
Quantum chemical software (Dmitry Murzin)
Chemometrics
Chemometric software (Mats Rönnholm)
Neural network software (Mats Rönnholm)

EXPERTISE IN CATALYSIS AND CHEMICAL PROCESSES

Catalyst preparation and characterization

- Supported metal catalysts (P. Mäki-Arvela, J.-P. Mikkola, D. Murzin)
- Exhaust catalysts (K. Eränen, K. Arve, D. Murzin)
- Zeolites, micro and mesoporous materials (Narendra Kumar, D. Murzin)
- Structural catalysts (monoliths, cloths, carbon nanotubes, catalytic packings (J.-P. Mikkola, T. Salmi, D. Murzin)
- Catalyst and solid material characterization (K. Eränen, N. Kumar, P. Mäki-Arvela; see the equipment list above)

Catalytic and other chemical processes

- Environmental catalysis and catalytic combustion (K. Arve, K. Eränen, D. Murzin)
- Hydrocarbon transformations; isomerization, ring opening, dearomatization (N. Kumar)
- Catalytic hydrogenation (P. Mäki-Arvela, J.-P. Mikkola, A. Bernas, H. Bernas)
- Catalytic oxygenation (A. Tokarev, D. Murzin)
- Biofuels (P. Mäki-Arvela, A. Bernas, D. Murzin)

- Enantioselective catalytic processes; asymmetric catalysis (P. Mäki-Arvela, T. Salmi, D. Murzin)
- Hydroformylation (A. Bernas, P. Mäki-Arvela, T. Salmi, D. Murzin)
- Fine chemicals (P. Mäki-Arvela, J.-P. Mikkola, T. Salmi, D. Murzin)
- Sugar chemistry (J.-P. Mikkola, T. Salmi)
- Chemicals from wood (A. Bernas, H. Bernas, P. Mäki-Arvela, J.-P. Mikkola, R. Sjöholm, D. Murzin, T. Salmi)
- Boron chemistry (A. Bernas, P. Mäki-Arvela, D. Murzin, T. Salmi)
- Decomposition of organics in liquid phase (S. Leveneur, J. Wärnå, T. Salmi)
- Water purification chemicals (M. Rönnholm)
- Metallurgical processes (S. Fugleberg)

EXPERTISE IN CHEMICAL THERMODYNAMICS, KINETICS AND TRANSPORT PHENOMENA

Kinetic and thermodynamic experiments

- Kinetic experiments in batch and continuous reactors (A. Bernas, H. Bernas, J. Wärnå)
- Thermogravimetric experiments (K. Eränen)
- Solubility measurements (K. Eränen)

Modelling of thermodynamics, chemical kinetics and mass transfer

- Thermodynamic calculations (J. Wärnå, S. Fugleberg, J. Hernandez Carucci, D. Murzin, T. Salmi)
- Batch process modelling (J. Wärnå, J.-P. Mikkola, D. Murzin, T. Salmi)
- Continuous process modeling (J. Wärnå, M. Rönnholm, T. Salmi)
- Complex reaction systems (D. Murzin, T. Salmi)
- Kinetics of transient systems (D. Murzin, T. Salmi)
- Coupled kinetics and diffusion incl. porous media (J. Wärnå, T. Salmi, T. Kilpiö)

EXPERTISE IN CHEMICAL REACTOR MODELLING

Batch and semibatch reactors

- Homogeneous reactors and multiphase reactors (incl. catalytic reactors, gas-liquid reactors and reactive solids) (J. Wärnå, J.-P. Mikkola, A. Bernas, S. Leveneur, H. Grénman, D. Murzin, T. Salmi)

Continuous reactors

- Gas-phase reactors (J. Wärnå, D. Murzin, T. Salmi)
- Multiphase reactors (J. Wärnå, M. Rönnholm, T. Kilpiö, T. Salmi)
- Residence time distributions (J. Wärnå, T. Salmi)
- Transient phenomena (D. Murzin, T. Salmi)

Computational fluid dynamics

- General applications (J. Wärnå)
- Combustion applications (J. Hernandez Carucci)

EXPERTISE IN CHEMOMETRICS AND MOLECULAR MODELLING

Chemometrics (M. Rönnholm)
Molecular modelling (D. Murzin)

EXPERTISE IN REACTION INTENSIFICATION AND NEW REACTION MEDIA

Reaction and process intensification

- Reaction intensification by ultrasound and microwave technologies (J.-P. Mikkola, M. Rönnholm, E. Murzina, D. Murzin, K. Eränen, T. Salmi)

- Reaction intensification by reactor structures (monoliths, catalyst nets, microreactors) (J-P. Mikkola, M. Rönnholm, J. Hernandez Carucci, A. Bernas, D. Murzin, T. Salmi)

Ionic liquids synthesis, characterization and applications

- (J.-P.Mikkola, P. Virtanen, P. Damlin)

EXPERTISE AND EQUIPMENT VIA COLLABORATION

- Separation technology (E. Paatero, Lappeenranta University of Technology)
- Pilot reactor technology (I. Turunen, Lappeenranta University of Technology)
- Catalytic monoliths (TU Delft)
- Ionic liquids (L. Kustov, Zelinsky Institute of Organic Chemistry, Moscow)
- NMR, incl. solid-state (ÅA/Organic chemistry and Tallinn Technical Univ.)
- Ion mass spectrometry (ÅA/Organic chemistry)
- SEM, scanning electron microscopy PCC/Combustion and material chemistry
- TEM – high resolution transmission electron microscopy (TU Delft, University of Lund)
- XRD (University of Turku, Department of Physics, Mikko Tenho)
- AFM, Atomic force microscopy (PCC/Combustion and material chemistry, ÅA/Physical chemistry)
- DCP and ICP/MS (PCC/Analytical chemistry)
- Ion chromatography MS (PCC/Analytical chemistry)
- Special viscosity measurements (ÅA/Physical chemistry)
- Particle size measurement (ÅA/Physical chemistry)
- Measurement of dielectric constants (ÅA/Physical chemistry)
- Melting point & freezing point determination (ÅA/Polymer technology)
- Mercury porosimetry (ÅA/Paper coating and converting)

ANALYTICAL CHEMISTRY
Analytisk kemi, Axelia

Laboratory manager: Paul Ek

MAIN EQUIPMENT

- **Computer-controlled high resolution Leica microscope** (*contact persons / main expertise*: Paul Ek)
- **Computer-controlled Metrohm 16-channel 711 Liquino (+700 Dosino) titrator** (Johan Bobacka, Tomasz Sokalski)
- **Computer controlled Mettler Toledo titrator** (Paul Ek, Kim Granholm)
- **Conductometer** (Paul Ek, Pia Sjöberg-Eerola, Tom Lindfors)
- **DCP** (Paul Ek)
- **Deionized water equipment**, **ELGA** (Paul Ek)
- **Flame AAS** (Paul Ek, Kim Granholm, Tom Lindfors, Pia Sjöberg-Eerola)
- **FTIR** spectrophotometer (Pia Damlin, Rose-Marie Latonen)
- **High performance microwave digestion unit** (Paul Ek)
- **ICP-MS with laser ablation** and equipment for the sample pretreatment (Paul Ek)
- **Impedance analyzers** (2) (Johan Bobacka)
- **Ion chromatographs** (2) (Pia Sjöberg-Eerola, Paul Ek, Leo Harju)
- **Photometer with an optical fiber probe**; λ=400-700 nm (Pia Sjöberg-Eerola, Tom Lindfors)
- **Potentiometers with 10 channels** (4); the potential of 10 working electrodes can be measured simultaneously (Johan Bobacka, Tom Lindfors)
- **Potentiostats and galvanostats** (5) (Johan Bobacka, Pia Damlin, Rose-Marie Latonen, Tom Lindfors, Fredrik Sundfors)
- **Quartz crystal microbalance** (Pia Damlin and Rose-Marie Latonen)
- **Raman spectrometer**; λ_{exc}=514, 633 and 780 (Pia, Damlin, Rose-Marie Latonen, Tom Lindfors)
- **Sequential injection analyzers** (3) (Paul Ek, Kim Granholm, Tom Lindfors, Tomasz Sokalski)
- **Ultrasonic bath,** small: V≅ 3 l (Paul Ek)
- **UV-vis spectrophotometers** (2); λ=190-1100 nm (Pia Damlin, Rose-Marie Latonen and Tom Lindfors)

MAIN EXPERTISE

- **Chemical sensors** (in general): Johan Bobacka, Ari Ivaska, Andrzej Lewenstam, Tomasz Sokalski
- **Complexation of metals**: Leo Harju, Ari Ivaska
- **Conducting polymer based ion sensors**: Johan Bobacka, Pia Sjöberg-Eerola, Ari Ivaska, Tom Lindfors, Andrzej Lewenstam
- **Development of new ICP-MS analysis methods**: Paul Ek
- **Electrosynthesis of conducting polymers**: Pia Damlin, Rose-Marie Latonen
- **Flow injection analysis**: Kim Granholm, Ari Ivaska, Tomasz Sokalski, Tom Lindfors
- **Mathematical modeling of potential formation processes in ion-selective electrode membranes**: Andrej Lewenstam, Tomasz Sokalski
- **Metals in wood**: Kim Granholm, Leo Harju, Ari Ivaska
- **Potentiometric measurements**: Johan Bobacka, Tom Lindfors
- **Soluble conducting polymers**: Johan Bobacka, Tom Lindfors
- **Spectroscopic measurements**: Johan Bobacka, Ari Ivaska
  - *UV-vis*: Pia Damlin, Rose-Marie Latonen, Tom Lindfors
  - *Raman*: Pia Damlin, Rose-Marie Latonen, Tom Lindfors
  - *FTIR*: Pia Damlin, Rose-Marie Latonen
  - *Impedance*: Johan Bobacka

MATERIALS SCIENCE EXPERTISE

See above for the experts

- **Conducting polymers and functionalized thin films**
- **Electroactive materials and fullerenes**
- **Ion-selective membranes**
- **Metals in wood fibres**

COMPUTING AND SOFTWARE EXPERTISE

- Tomasz Sokalski