



Solving your Challenges using our Expertise






Services in analytical, material and environmental sciences

Expert Capability Center
Deventer

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Nouryon

Expert Capability Center Deventer

- Who?  Over 40 skilled, highly educated and experienced scientists
- What?  Services in analytical, material and environmental sciences
- Where?  Deventer, NL
- With?  Our unique capabilities and state of the art equipment
- What else? 
- Broad knowledge of chemical products and processes
 - Fast response
 - Collaboration with universities, knowledge institutes and Nouryon RD&I groups
 - REACH notification, GLP accreditation

Your partner in essential analysis and testing in the chemical industry

Expert Capability Center Deventer



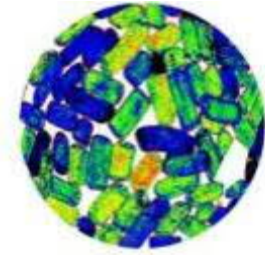
with over
50 years
of experience
in solving
challenges
in the
chemical industry

Expert Capability Center Deventer

Solving your challenges using our expertise

Your challenges:

- Developing new and improved products
- Developing and implementing new and optimized technologies and

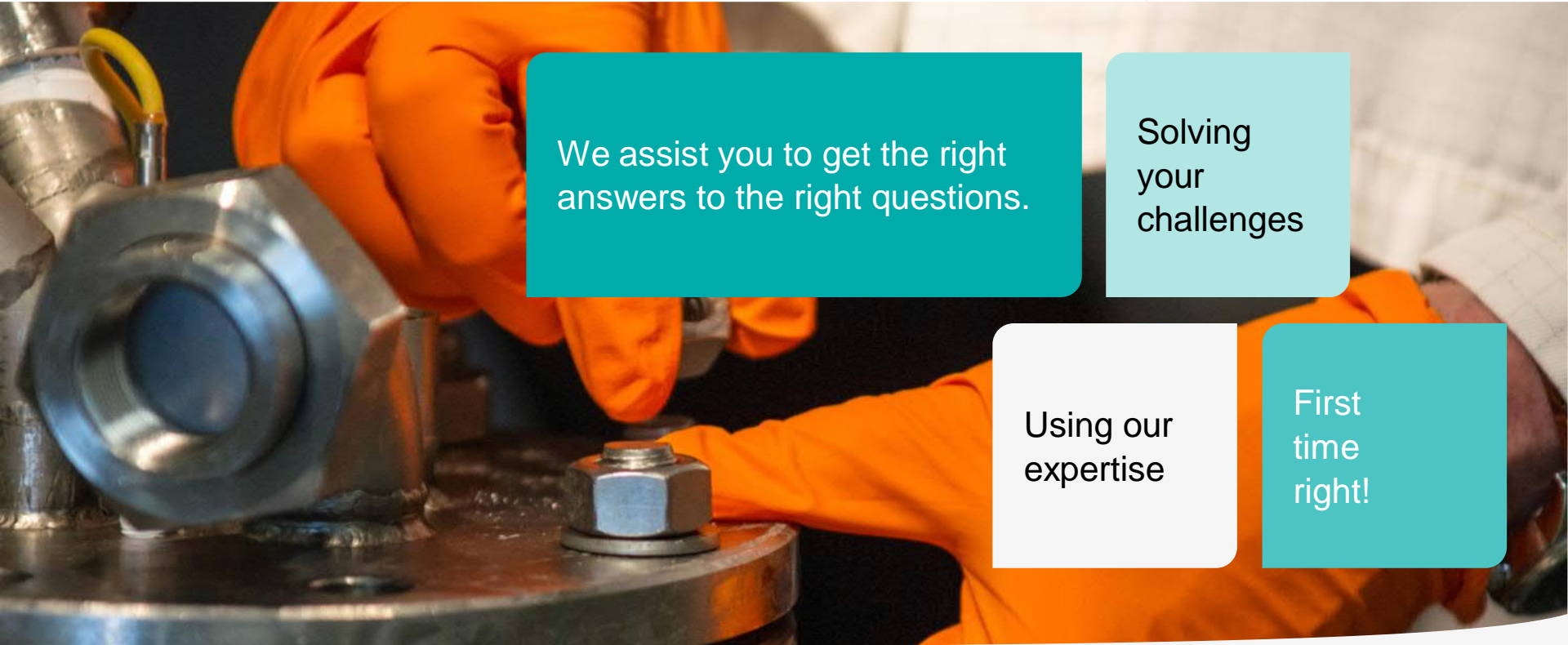


Our supporting role:

- Multi-disciplinary approach in R&D perspective
- Helping to optimize your products and processes
- Give better insight in your chemical reactions
- Analyzing in complex matrices and non-standard samples
- Failure analysis
- Method development, validation and transfer



Your center in essential chemistry

The background of the slide is a photograph of a person wearing bright orange protective gloves and clothing, working on a large, complex industrial metal component. The person's hands are visible, one holding a tool and the other supporting a part of the machinery. The scene is set in an industrial environment with various metal parts and machinery visible.

We assist you to get the right answers to the right questions.

Solving your challenges

Using our expertise

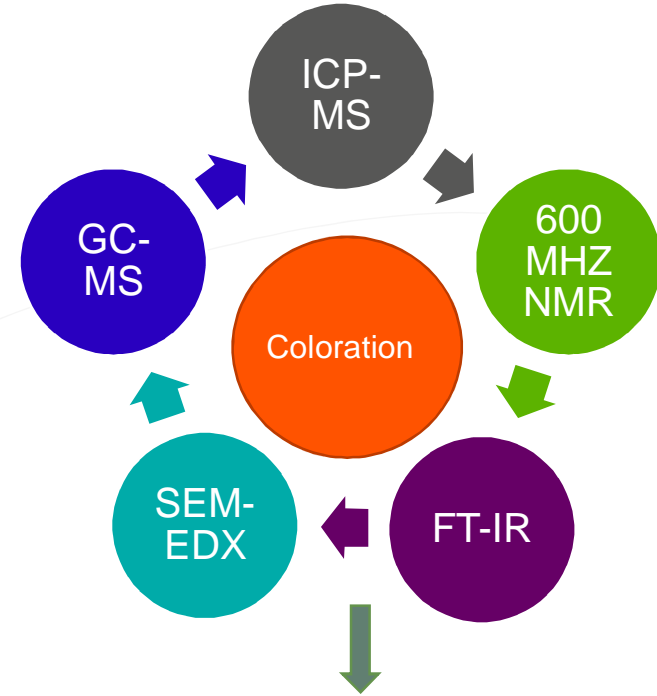
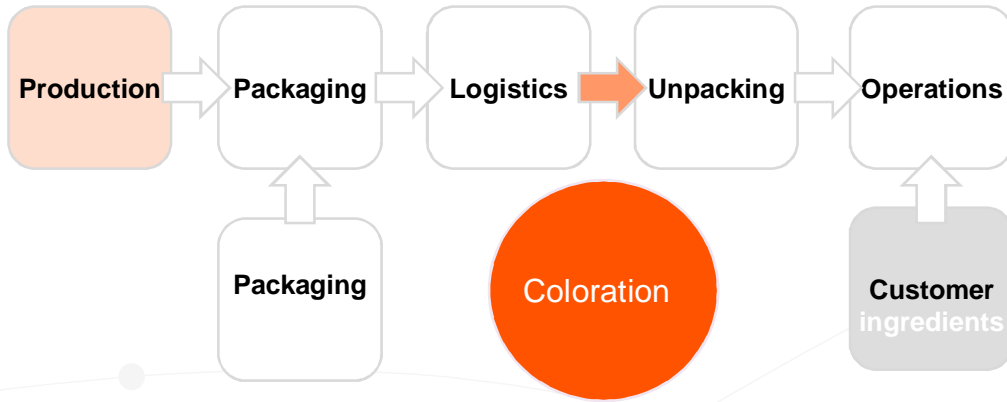
First time right!

Solving your Challenges using our Expertise

CASE STUDIES

Failure Analysis

Unwanted coloration of product

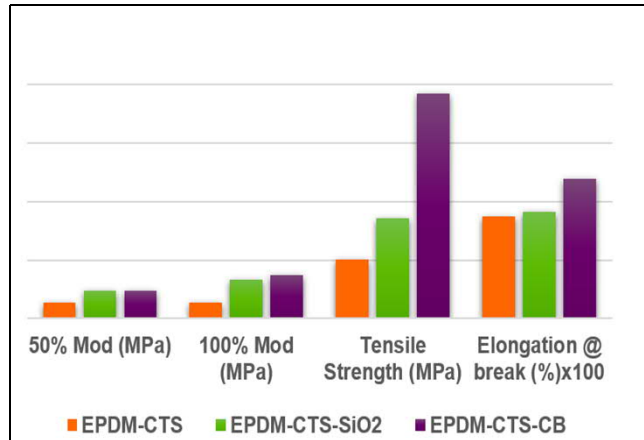


- Map out the entire process to identify possible causes
- Execute **multi-analytical** approach
- Extensive analysis until **parts per billion** level of impurities in product in every step
- **Root cause** determined

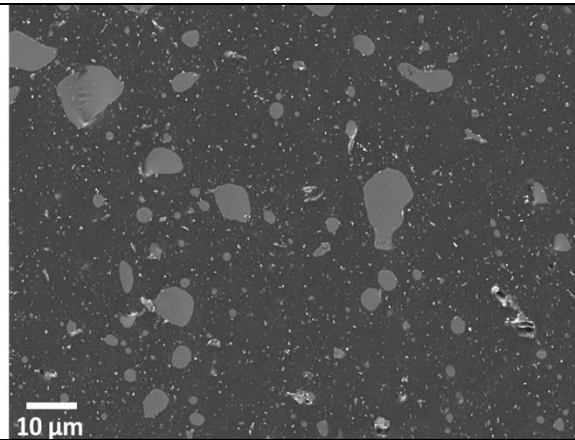
Improving Rubber Performance

structure ↔ property

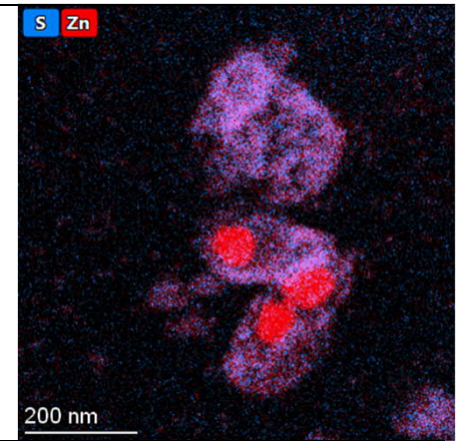
Mechanical performance



Polymer mixing



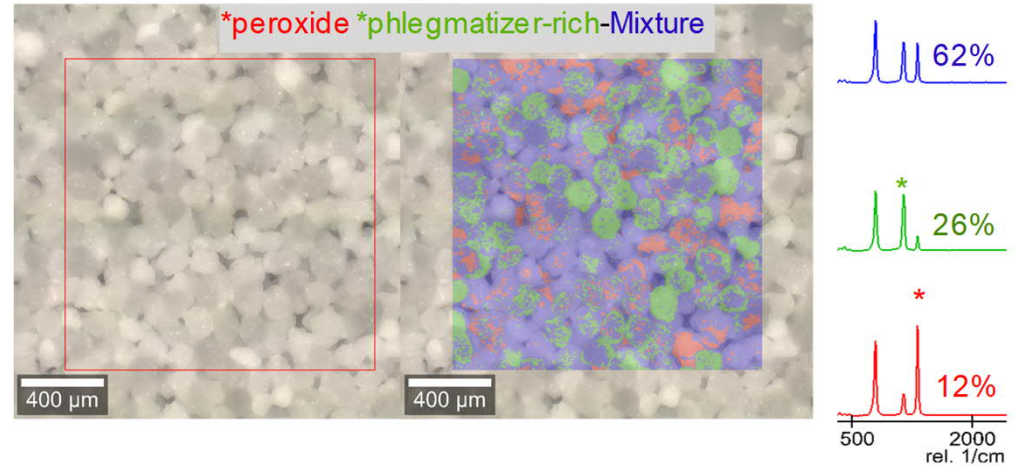
Reaction mechanism



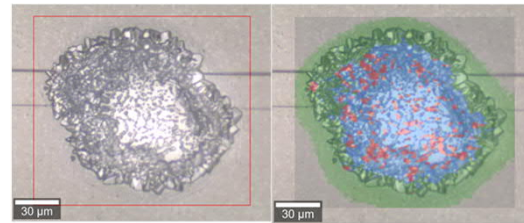
- Microscopy is an enabling technology to connect material performance with its microstructure
- Knowledge about the underlying chemistry helps enabling a focused development
- Combined with advanced sample preparation

Peroxide / phlegmatizer distribution

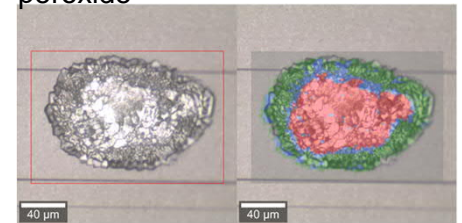
- Phlegmatizers are chemical components used to reduce the hazards of highly reactive peroxides during transport and while in storage.
- Raman imaging can be used to measure the homogeneity of a phlegmatizer / peroxide mixture.
- Blue indicates that the components are mixed well, red and green indicate that the components are **not** mixed well.



Phlegmatizer mixed well with peroxide

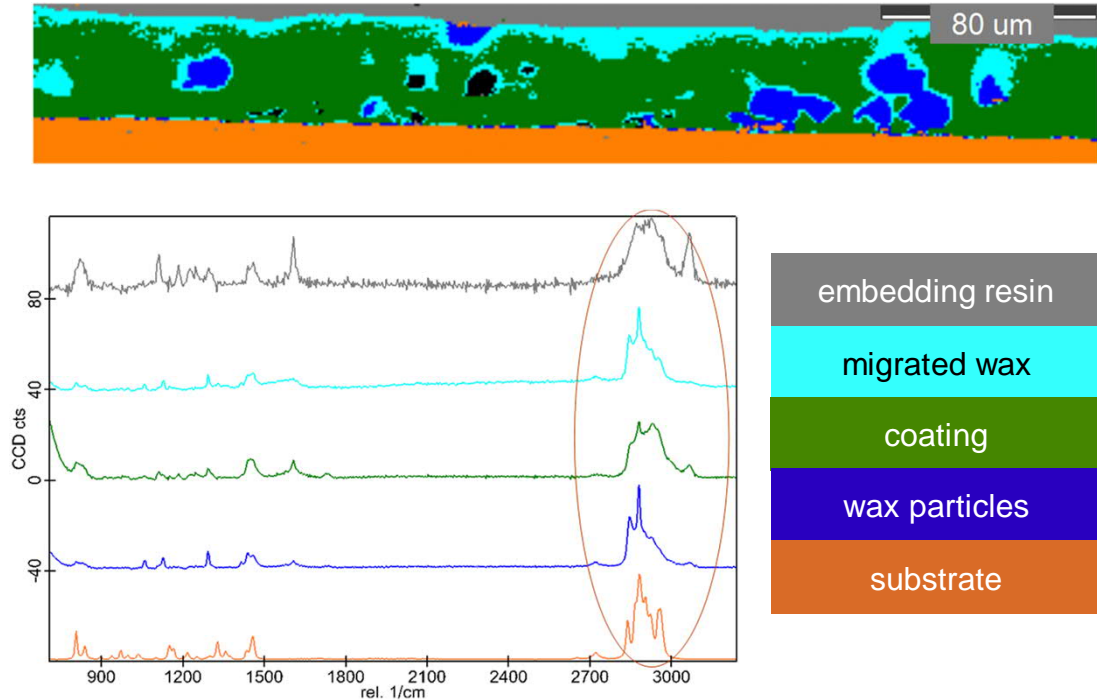


Phlegmatizer **not** mixed well with peroxide



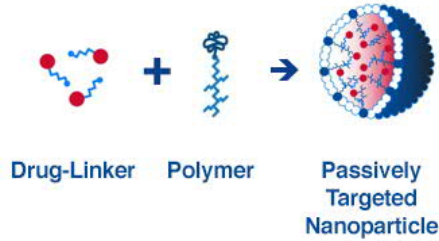
Migration properties of wax particles in a coating

- Wax migrates from small particles to the surface and forms a wax-enriched protective layer.
- The image shows a Raman map of a cross-section of a 40 μm thick coating.
- Multivariate cluster analysis is used to distinguish coating, wax particles and migrated wax.



Application research example

Nanomedicines analysis



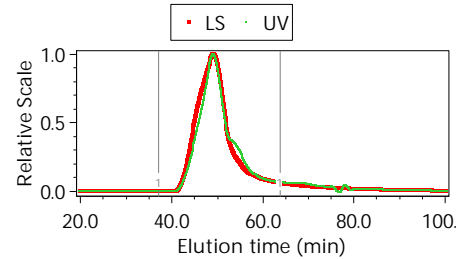
CriPec®-based nanomedicines*

- API attached to polymeric network in the core via hydrolysable linker

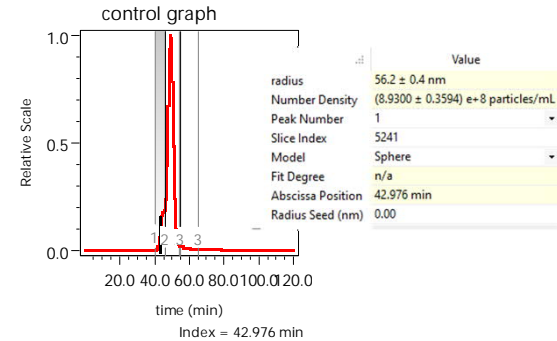
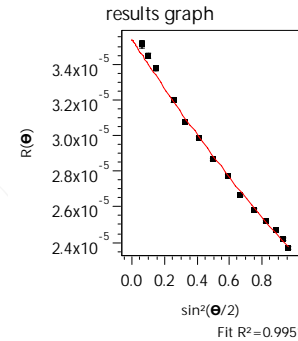
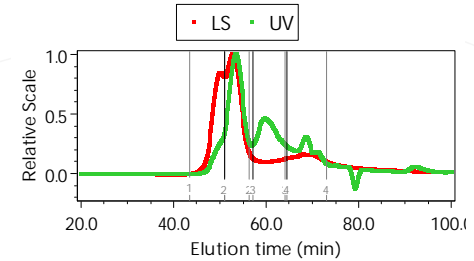
Information obtained

- API entrapment and release: reflected in **SEC-UV/LS traces**
- Nanoparticle size and count: can be derived from **LS intensity and angular dependence**
- Particle size distribution – **LS peak shape**

Entrapped API

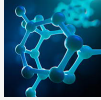


API not fully entrapped

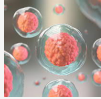


* <https://cristaltherapeutics.com/technology/cripec-technology-platform/>

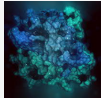
What materials and properties can you analyze with Triple Detection SEC



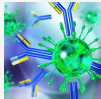
Synthetic, natural and hybrid polymers



Nanoparticles



Proteins



Drug delivery systems



Absolute molar mass and size



Branching, conformation, composition



Size distribution

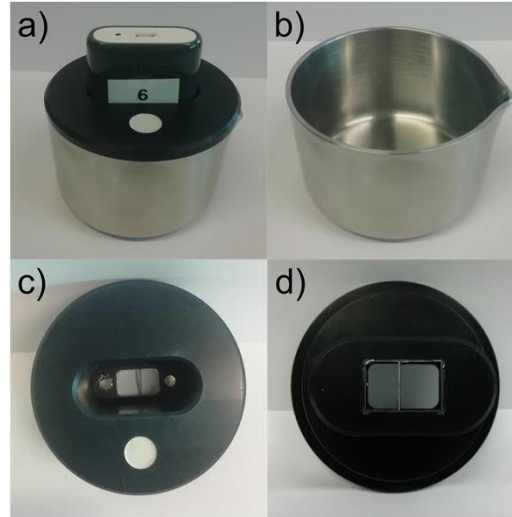
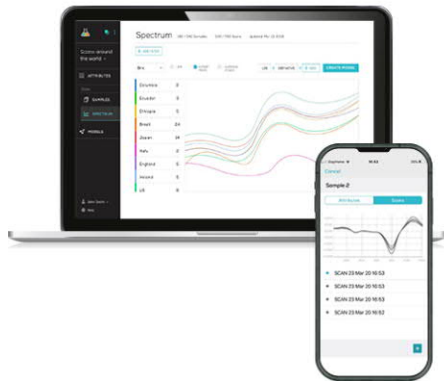


Conjugation

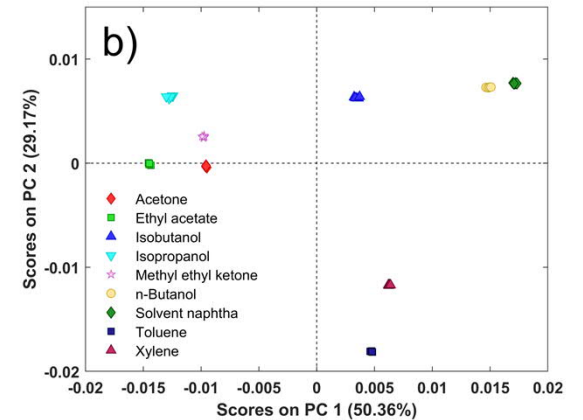
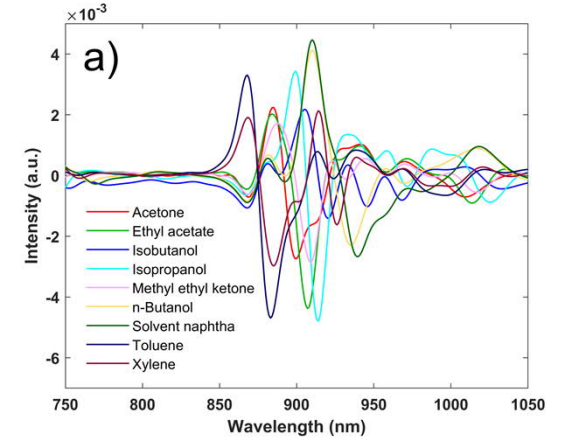


Aggregation

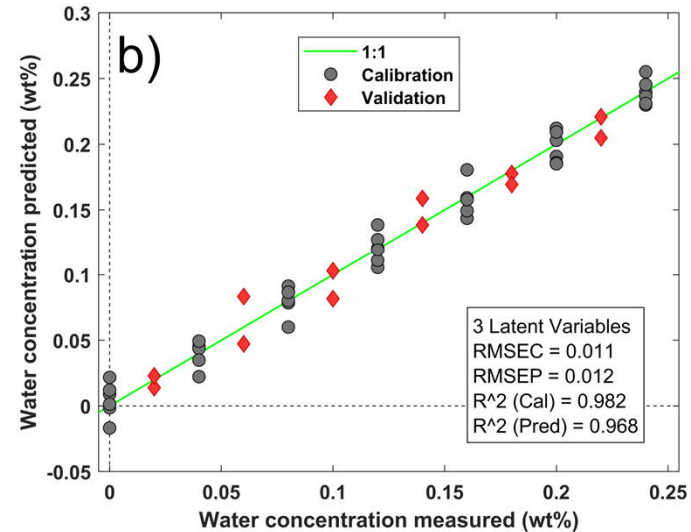
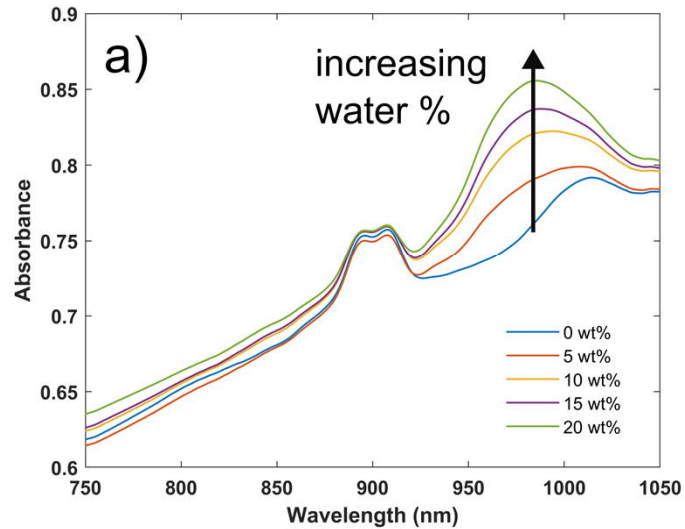
Handheld NIR for raw material analysis



Accessory for use with organic liquids developed in collaboration with **Radboud University**



Contamination testing using handheld NIR

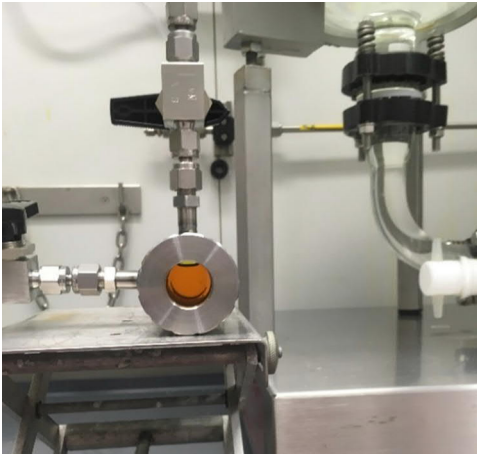


Van Kollenburg, Van Manen *et al.*, *Talanta* **2021**, 223, 121865.

Registration of chlorine for use as biocide

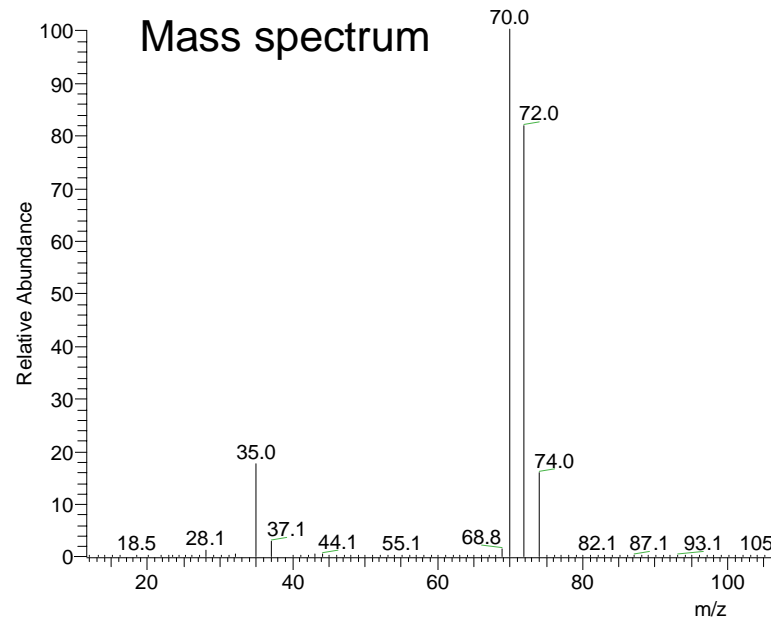
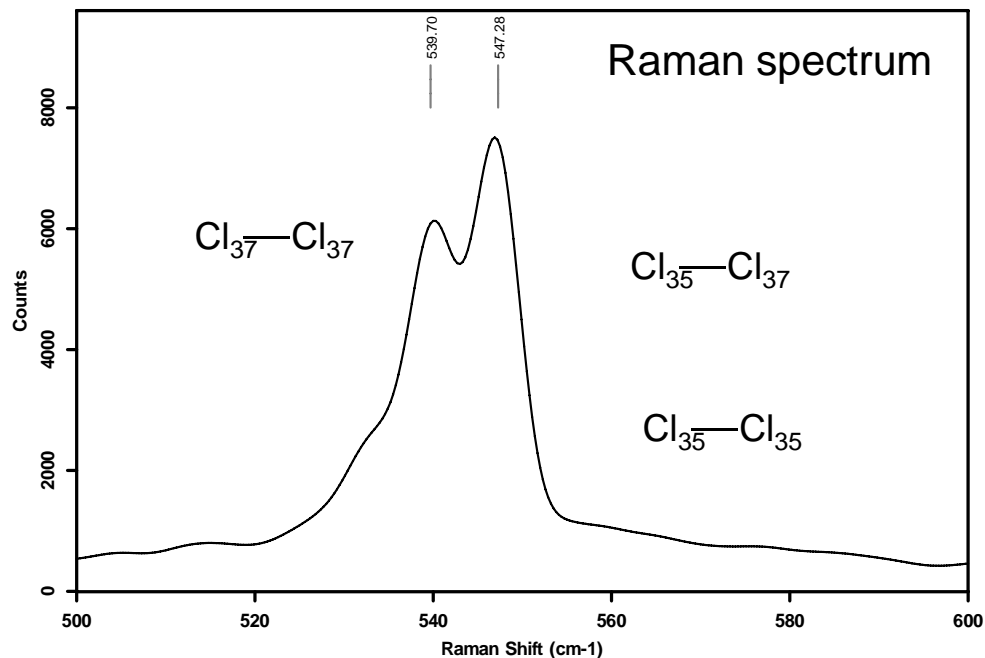
Multi-analytical approach required for Cl_2 identification and impurity assessment

- Dedicated setup for sample preparation and destruction (safety!)
- UV and Raman spectroscopy and MS spectrometry for identification
- GC, FT-IR, ICP-MS, ICP-OES, CVAFS for determination of impurities



Chlorine identification

Isotope patterns (^{35}Cl and ^{37}Cl) clearly observed in Raman and mass spectra



Expert Capability Center Deventer

ECCD in more detail
Available Expertise

Excellence in Analytical and Material Science

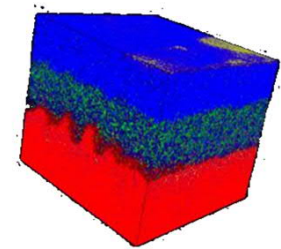
Competences

- Physical, chemical, and biological analysis
- Composition, structure, and materials performance
- Product analysis from trace level contaminants to bulk materials
- Analysis of Organic, Inorganic and Macromolecules
- Data Analysis
- In situ monitoring
- Environmental Testing



Technique areas

- Chromatography
- Resonance Spectroscopy
- Molecular Spectroscopy
- Elemental and Functional Group Analysis
- Surface Analysis, Microscopy and Diffraction
- Hyphenated Methods
- Physical Properties Analysis



Analytical Expertise Summary

- High performance liquid chromatography
- Size-exclusion chromatography
- Gas chromatography
- Capillary zone electrophoresis
- Gas/VOC analysis
- Olfactometry
- Safe handling of challenging samples

Separation techniques



- Nuclear magnetic resonance spectroscopy
- Mass spectrometry
- Vibrational spectroscopy
- UV/VIS
- Electron spin resonance spectroscopy
- Ion mobility spectrometry

Resonance & Optical Spectroscopies



- Carbon analysis
- Functional group analysis
- Ion analysis
- Main element analysis
- Trace element analysis
- Physical properties

Elemental & Functional Group Analysis



- Imaging
- Materials characterization
- Surface & interface analysis
- Crystallography
- Structure-property relationships
- Failure investigation
- 3D profiling
- Atomic Force Microscopy

Microstructure Analysis



- Biodegradation testing (GLP)
- Waste water treatment expertise
- Ecotoxicology testing
- Environmentally relevant physical-chemical properties
- Regulatory dossier strengthening & read-across acceptance

Environmental & Ecotox testing



- In-/on-/at-line analyses
- Physical property monitoring
- Consulting on Sensor development
- Specific real-time detection of chemicals
- Design of Experiments
- Chemometrics
- Thermal, rheological and mechanical analysis
- Particle sizing
- Electrochemical property characterization

Data and Materials Analysis



Curious?

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Thank you for your attention!

Questions?

Nouryon

Measurement & Analytical Science Detailed Overview

Elemental & Functional Group Quantification

Atomic Spectrometry

- Main & trace element analysis
- Inorganic and organic matrices
- From ppt until % level



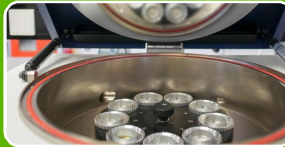
Sample Pretreatment

- Microwave medium & high pressure
- Fusion: borate, peroxide and carbonate
- Combustion and UV digestion



Fluorescence / Absorption

- Hydride Atomic Fluorescence Spectrometry (HAFS)
- Cold Vapor Atomic Fluorescence Spectrometry (CVAFS)
- Graphite Furnace Atomic Absorption Spectrometry (GFAAS)



X-Ray Fluorescence

- Energy Dispersive with secondary targets
- Wave length dispersive, high power



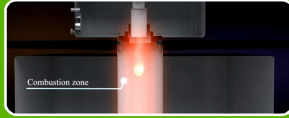
Inductively Coupled Plasma

- ICP-OES radial and axial view, 130 – 700 nm
- ICP-MS, quadrupole system including collision cell

Elemental & Functional Group Quantification

Wet Chemical Analysis

- Carbon and Nitrogen analysis
- Functional group analysis
- Ion analysis
- ppm - % level
- Inorganic- and organic matrices
- Physical properties



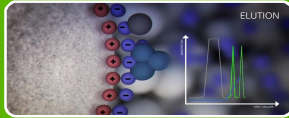
Organics

- TOC, TIC, NPOC analyzers
- C,H,N,S,O analyzer
- Kjeldahl nitrogen



Titration

- Karl Fischer and coulometric water titration
- Titration systems with redox, colorimetric, argentometric, pH detection
- Organic as well as inorganic systems



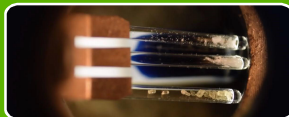
High Performance Ion Chromatography (HPIC)

- Conductivity detection
- UV, MS detection
- ICP-MS hyphenation, 2D system



Capillary Zone Electrophoresis

- Conductivity detection
- UV detection
- MS detection



Physical Properties & Spectrophotometry

- Melting point, refractive index, color analysis, density, pH
- UV-VIS

Separation Techniques

Separation Technology of Complex Systems

- Structure elucidation
- Organic impurity analysis
- Polymer characterization
- Odor and volatiles analysis
- Gas analysis



Liquid chromatography (LC) techniques

- HPLC – RI, UV, DAD, ELSD, CAD, Fluorescence, MS
- UHPLC – DAD, MS, RI, CAD
- Preconcentration by e.g. SPE, hydrolysis, derivatization, fractionation



Gas chromatography (GC) and related techniques

- GC – FID, ECD, HID, MSD, FPD, Olfactometry, in-line
- Split, splitless, on-column, headspace, pyrolysis, micro-GC
- SIFT-MS, thermal desorption GC-MS, SPME, SBSE, PTV, gas analysis



Size exclusion chromatography (SEC)

- Triple detection (LS, Viscosity, RI) & UV
- Water/Organic solvents (HFIP)
- Absolute MWD, Molecular Architecture



Capillary Zone Electrophoresis (CZE)

- Conductivity detection,
- UV (direct/indirect)
- MS

Microstructure Analysis

Visualize and analyze:

- Depth information by cross-sectioning and sputter profiling
- Local chemical specificity
- Focus on structure-properties relationships
- Imaging >1nm
- Surface sensitivity at 1nm-1 μ m



Microscopy

- SEM-EDX, WDX, FIB-SEM, Raman-AFM, FTIR imaging
- TEM, STEM-EDX, TEM-tomography, Optical microscopy



Diffraction

- X-ray Powder Diffraction
- Electron Diffraction (TEM)



Surface Analysis

- XPS, ToF-SIMS
- (Ar-cluster) depth profiling



Sample preparation

- (Cryo-)ultramicrotomy
- Ion milling; Polishing; Staining



External collaboration

- Cryo-SEM, SEM-EBSD, TEM-EELS,
- X-ray tomography, AFM-IR, XANES, EXAFS

Resonance & Molecular Spectroscopy

Spectroscopy

- Identification & quantification of chemicals
- Unknowns/competitor products analysis
- Side products in synthesis
- Chemical characterization
- Polymer characterization
- Formulation characterization



Resonance Spectroscopy

- Solution (including Cryoprobe) & Solid State capabilities
- Nuclear Magnetic Resonance: NMR up to 600 MHz (multinuclear & multidimensional)
- NMR 400 MHz open shop service (Deventer)
- Electron Spin Resonance (ESR)



Mass Spectrometry

- GC-MS including Curie Point Pyrolysis, Dynamic/Static Headspace, Thermal Desorption, SPME and open shop service (Deventer)
- LC-MS (+DAD and RID), LC-MS/MS (QToF, Orbitrap, Triple Quad), SEC-MS, CZE-MS, IC-MS, Direct Infusion-ESI-MS, Flow Injection-ESI-MS, IMS
- MALDI-ToF (external collaboration)



Vibrational Spectroscopy

- FTIR: ATR, gas, DRIFT (powders)
- FTIR Microscopy: ATR Imaging, transmission and reflection modes (<math>< 5 \mu\text{m}</math>)
- Raman Microscopy, Confocal Raman Imaging, AFM-Raman, Profilometry
- UV-Vis spectroscopy
- In-situ FTIR, NIR, Raman, UV

(Big) Data Analytics

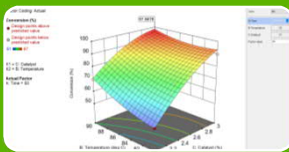
Data Analytics

- Objective conclusions from data
- Robust experimental design
- Extracting information from large data sets
- Reveal hidden patterns in data
- Tailored data analysis using self-developed software



Statistics

- Validation of analytical methods; sampling
- Reporting results
- Method performance studies (interlaboratory studies)



Design of Experiments (DoE)

- Experimental efficiency & robustness
- Screening and optimization
- Response surface methodology



Multivariate data analysis (*chemometrics*)

- Exploratory analysis; trends/pattern recognition (PCA)
- Clustering (*k*-means) and classification (PLS-DA, SIMCA)
- Quantitative calibration (PLS-R, MCR)



Data visualization & software development

- Automated data processing
- Data visualization creation and advice
- App (software) development, incl. Graphical User Interface

Environmental & Ecotoxicology Testing

Biodegradation & Ecotoxicology

- Environmental fate and Ecotoxicological data
- Physical-chemical properties & analytics
- Support hazard (PBT & vPvB) and risk assessment for registration (e.g. REACH)
- Waste water treatment effectiveness



Biodegradation testing (GLP)

- Ready biodegradability tests: Closed bottle (OECD 301D)
- Inherent Biodegradability & Simulation tests: (S)CAS (302A/B, 303, 309)
- Other tests: OECD 306, 311 & Toxicity tests with microorganisms (e.g. 209)



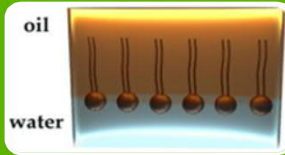
Waste water treatment

- Feasibility with biodegradability screening tests (aerobic and anaerobic) and toxicity tests with nitrifying bacteria
- Indication of the degradation potential, possible reduction of COD, BOD, etc



Ecotoxicology testing

- Acute and Chronic and In vitro studies with chemical analysis
- Daphnia, Algae, Fish embryo, Lumbriculus



Physical-chemical properties & Analytical support (GLP)

- Water solubility, Partition coefficient octanol/water, Hydrolysis, Adsorption/desorption
- LC-MS/MS, HPLC, GC, IC, TOC

Materials Characterization

Product properties:

- Characterization of physical-chemical properties
- Supporting Materials Science, product development, failure analysis and application R&D
- Focus on structure-properties relationships



Thermo(mechanical) Analysis

- TGA, (modulated) DSC, DMTA



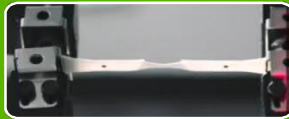
Rheology

- Rheometer with multiple geometries
- Stabinger Viscometer (density and viscosity simultaneously)



Characterization of Particles and Surfaces

- Laser Diffraction, Dynamic Light Scattering and Zeta Potential
- Surface and Interface Tension



Mechanical properties

- Tensile, compression and bending, up to 100 kN



Corrosion and Electrochemistry

- Electrochemical Impedance Spectroscopy