PROGRAM

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Ultrasonic particle manipulation approaches in on-line ATR FTIR

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The electromagnetic spectrum

**Introduction**

**ATR FTIR**  
**USW in ATR FTIR**  
**The End**

**Mid-IR**: 2.5 – 25 µm (4000 - 400 cm⁻¹)
Mid-IR vs. Raman-Spectroscopy

$\Delta E = \frac{h^*c}{\lambda}$

Introduction

ATR FTIR    USW in ATR FTIR    The End
Introduction

Fourier Transform InfraRed spectrometry

Interferometer

Monochromatic light source

Polychromatic light source
Information contained in Mid-IR and Raman spectra

- Functional groups, fingerprint
  Identification of analytes
  Simultaneous determination of several analytes

- Inter- and intramolecular Interactions
  Determination of secondary structure of Proteins

- Information on latent variables
  Octane number, wine varieties, cancer
Transmission FTIR spectroscopy

Spectrum Acquisition

\[ I_0 = f(\lambda) \]

\[ I = f(\lambda) \]

\[ A = \log \frac{I_0}{I} \]  Lambert-Beer
Identification of analytes

Measurement of natural emissions

**Attenuated Total Reflection FTIR**

**Spectrum acquisition**

\[
E(z) = E_0 \exp\left(-\frac{z}{d_p}\right)
\]

\(d_p\): penetration depth
Determination of latent variable

Classification of red wines

Solid Phase Extraction

1. Conditioning
2. Sample loading
3. Washing
4. Elution

FTIR Spectroscopy (Attenuated Total Reflection)

Introduction ATR FTIR USW in ATR FTIR The End
Classification of red wines: result

Spectra of phenolic extracts

Hierarchical clustering

ZW: Zweigelt, SL: St. Laurent, BF: Blaufränkisch
ME: Merlot, CS: Cabernet Sauvignon, PN: Pinot Noir
Assessment of cells in suspension

Operation in the stopped flow mode

Flow “on”

Measurement of dissolved reactants

Measurement of cells

Flow “off”
Is PHB in the E.coli amorphous or crystalline?

![Absorbance vs Wavenumber, 1/cm graph]

- PHB amorphous
- PHB crystalline
- E. coli with PHB settling
ATR FTIR for fermentation control

Experimental set-up

Fermentor

Peristaltic pump

Syringe pump

Holding Cell

Sagittarius V2

FTIR ATR

F

Acetate buffer

NaHCO₃

H₂O

Waste

Waste
Stopped flow spectra during fermentation
Problem: biofilm formation

ATR FTIR

USW in ATR FTIR
USW reduces biofilm formation

without US field

[Graphs showing absorbance versus wavenumber for data with and without US field]
Ultrasound Enhanced ATR FTIR flow cell

- Aggregation of cells in the nodes of the US field
- Application of standing 2 MHz US field before settling and rinsing

Introduction

ATR FTIR
USW in ATR FTIR
The End
Pictures of Experimental Set-up
USW reduces biofilm formation

without US field

with US field
Increased settling by application of USW

without US field

with US field
Settling speed

increased about 2.5 fold (185 vs. 70s)
Conclusions

**USW enhanced ATR FTIR spectroscopy**

Significant improvements in terms of

- Measurement speed, and
- Robustness

could be made.

Still sterility issues and flexibility demand in-line set-up
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