COST Action TD1105 - European Network on New Sensing Technologies for Air Pollution Control and Environmental Sustainability - *EuNetAir*

Action Start date: 01/07/2012 - Action End date: 30/06/2016 - Year 2: 2013-2014 (*Ongoing Action*)

Management Committee and Working Groups meeting, Queens College, University of Cambridge, UK, December 17th - 20th, 2013

THE USE OF REFLECTANCE SPECTROSCOPY FOR THE ANALYSIS OF AIR-BORNE DUST

Agricultural University of Iceland

LANDBÚNAÐARHÁSKÓLI ÍSLANDS

- Arngrímur Thorlacius
- MC Member
- Iceland

COST is supported by the EU Framework Programme

EUROPEAN SCIENCE FOUNDATION ESF provides the COST Office through a European Commission contract

Introduction

- The use of reflectance spectra in the near-infrared and visible regions has proven to be a very useful tool in projects on source-appointment of particulate air pollution in Iceland.
- Reflectance spectra have provided valuable data in addition to results from conventional wet-chemical element determinations.
- In this lecture, the focus is on further applications of this technique for the characterization and quantification of components in air-borne particulate matter

Previous utilization

- In our previous COST TD1105 meeting in Copenhagen (October 2013) I described the utilization of reflectance spectra to supply quantitative information that is used in multivariate modeling of source contribution to air-borne particles or dust.
- These quantitative variables that we extract from the reflectance spectra are of an unknown nature i.e. we don´t know what chemical constituents that are being quantified.
- The identity of these “analytes” is not really of great concern for the outcome of the source appointment.

Extended use of reflectance spectra for air-quality monitoring

- For other purposes it may be of significant help to be able to use such spectra to quantify more real analytes or even chemical compounds.
- To realize this, the problem of variable contributions from the background spectrum, produced by the filter material, has to be solved without iteration.
- I expect that this technique may have a much wider applicability for the characterization and quantification of components in air-borne particulate matter.

The Near-InfraRed or NIR spectral region

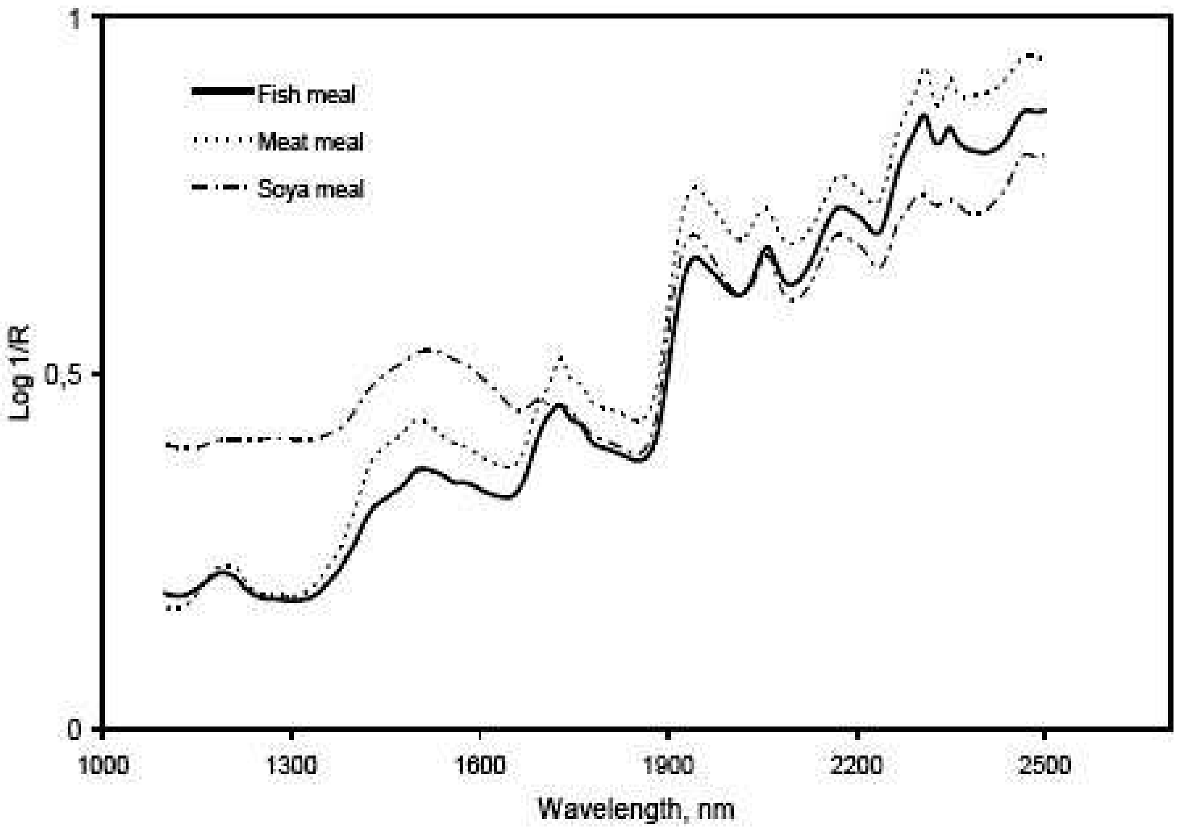
- Traditionally, the near infrared spectral region has been avoided by spectroscopists, as everything organic exhibits complex infrared reflectance with poor resolution. Inorganic constitutents as well, albeit less severely.
- A reflectance spectrum is thus a complex mix with contributions from most or all major sample constituents
- This lack of specificity is in fact the strength of infrared spectroscopy when it is teamed up with multivariate mathematical analysis.

Utilization of NIR-spectroscopy within other fields

- Infrared reflectance spectra have been widely used for quantitative analysis especially within the fields of food and feed analysis, respectively and more recently pharmaceutical analysis.

- This is now a mature analytical technique with a large number applications published in thousands of scientific papers and with many commercial instruments available, bundled with multivariate-mathematical calibration software packages, tailored to the task.

Agricultural applications



Some NIR analytes

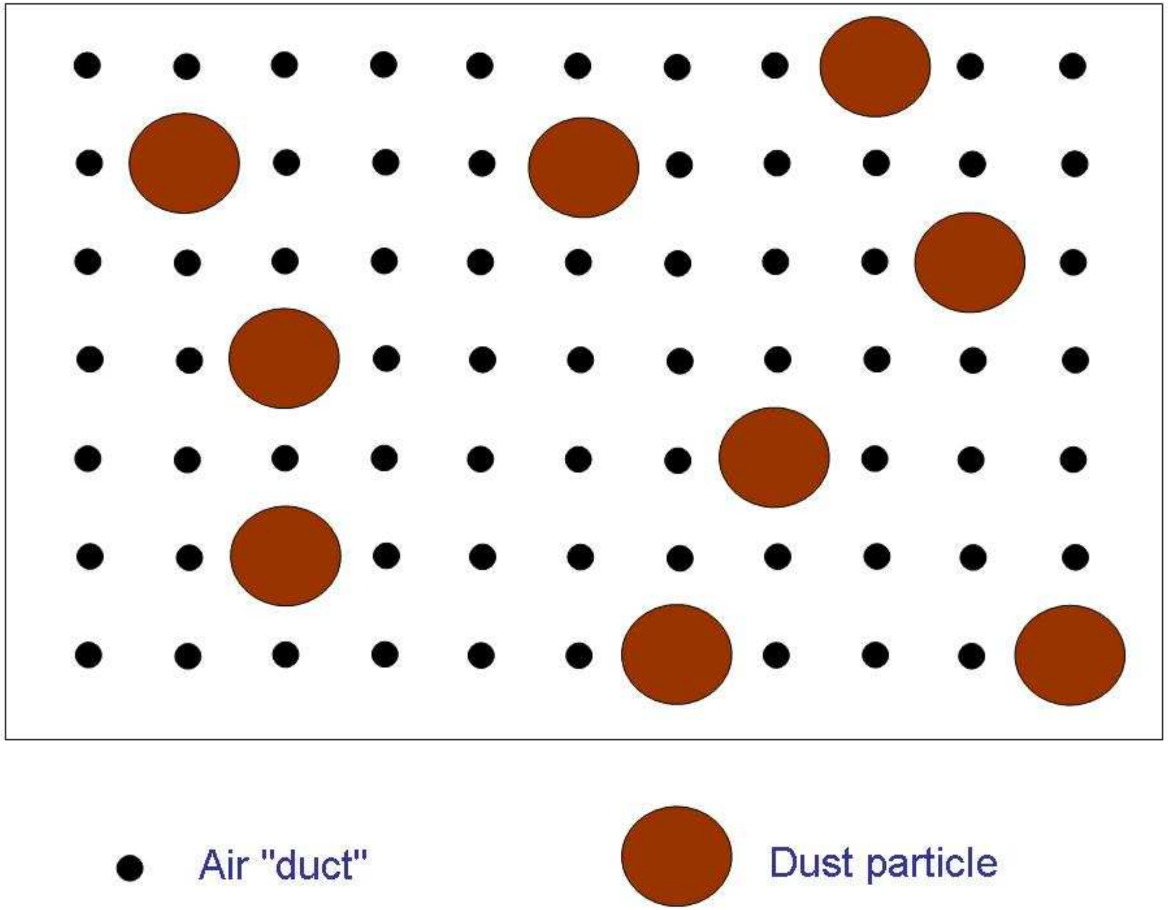
- Protein
- Dry matter
- Fat
- Starch
- Cellulose
- Digestibility
- Crude fiber

The problem of variable filter background

Filter materials exhibit a significant reflectance over the entire wavelength range. This background can not be easily subtracted as it varies with the amount of dust collected (dust particles cover a portion of the filter surface and thus shield the background reflectance. This has, in my previous work, been handled with an iterative procedure during modeling

Reflectance from filter surface varies with the amount of collected particles

A collected particle will cover a part of the filter surface and thus reduce the background reflectance. This reduction will at first be linear with number (or mass) of collected particles and then the effect will level off with increased overlap



A simple shielding model

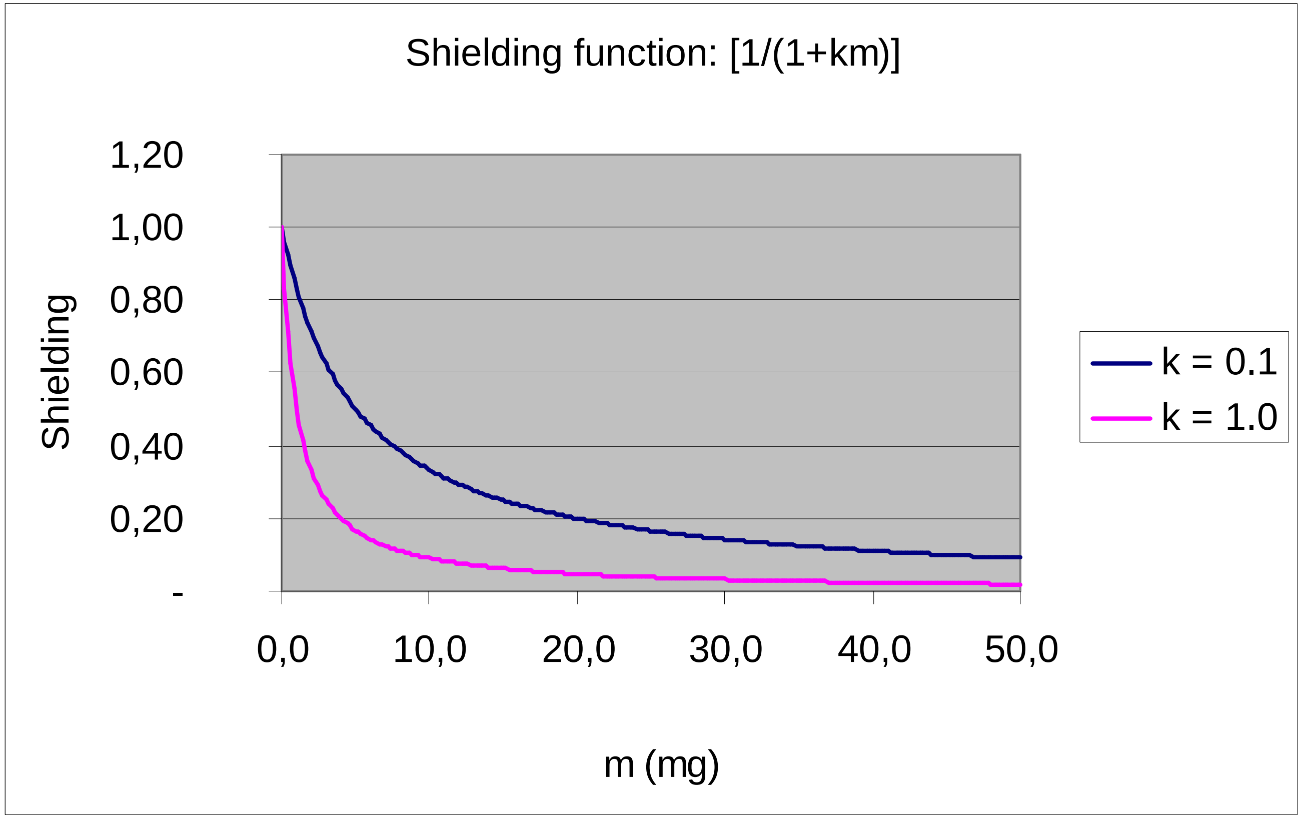
The following relationship can be used to mimic the reduced background reflectance caused by particles from one source, Si :

$R_{background} = R_{blank} \cdot [1/(1 + ki \cdot mi)]$ ki : a shielding constant for Si

mi : the collected mass of Si

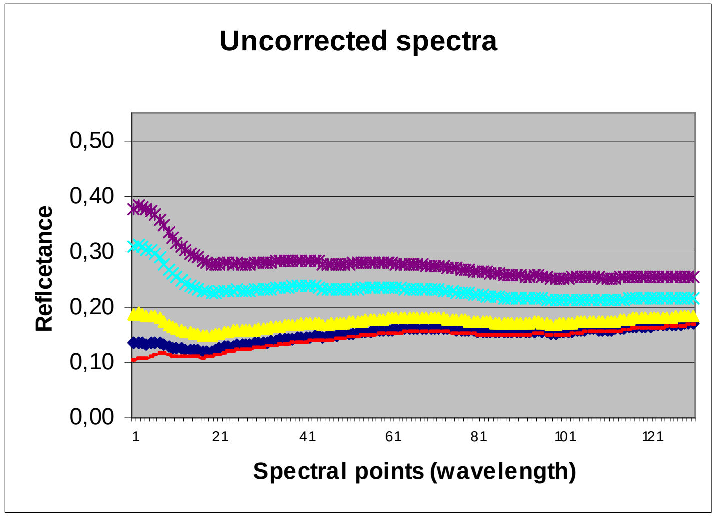
(Note that the relation within the brackets returns a value ≤ 1)

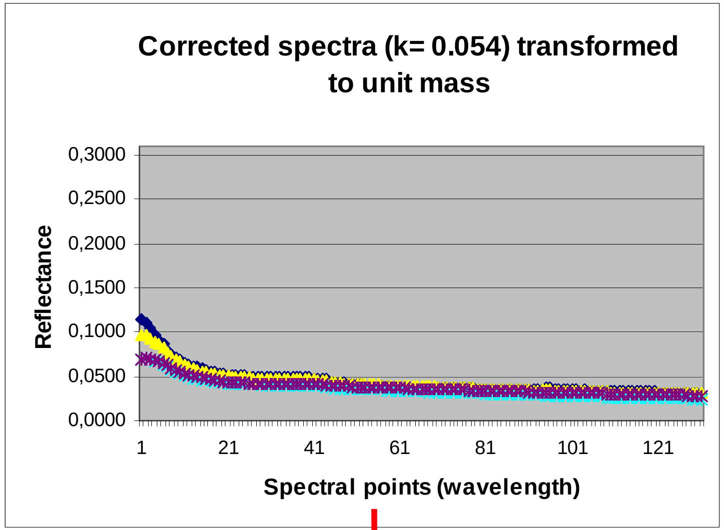
The overall shielding effect is obtained by summing over all sources

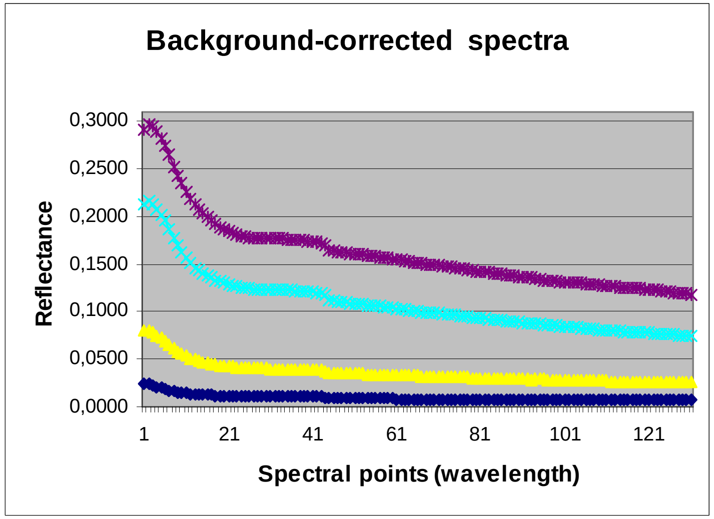


If a source material is effective in shielding the background reflectance (large k-value), relatively less mass is needed to produce an effect.

Correcting for variable background







Visible range:	400-1100 nm
Near-InfraRed range:	1100-2500 nm

Background correction without iteration

Collecting duplicate samples, different in weight, from each sampling stream, would enable background-correction of spectra from unknown (mixed-source) samples in the same manner as used for the source spectra.

It should be a reasonably simple task to construct a sampling arrangement for this by using separate channels with different flow resistance for the two samples

Future developments

I plan to test this approach in an attempt to quantify polycyclic aromatic hydrocarbons (PAH) using reflectance spectra with multivariate calibration against liquid chromatographic measurements (HPLC).

Should this turn out to be somewhat successful, it would more than compensate for the added efforts needed to collect duplicate dust samples.

THANK YOU !!