

Three major problems of grain size measurements: (1) grain, (2) size, and (3) measurement

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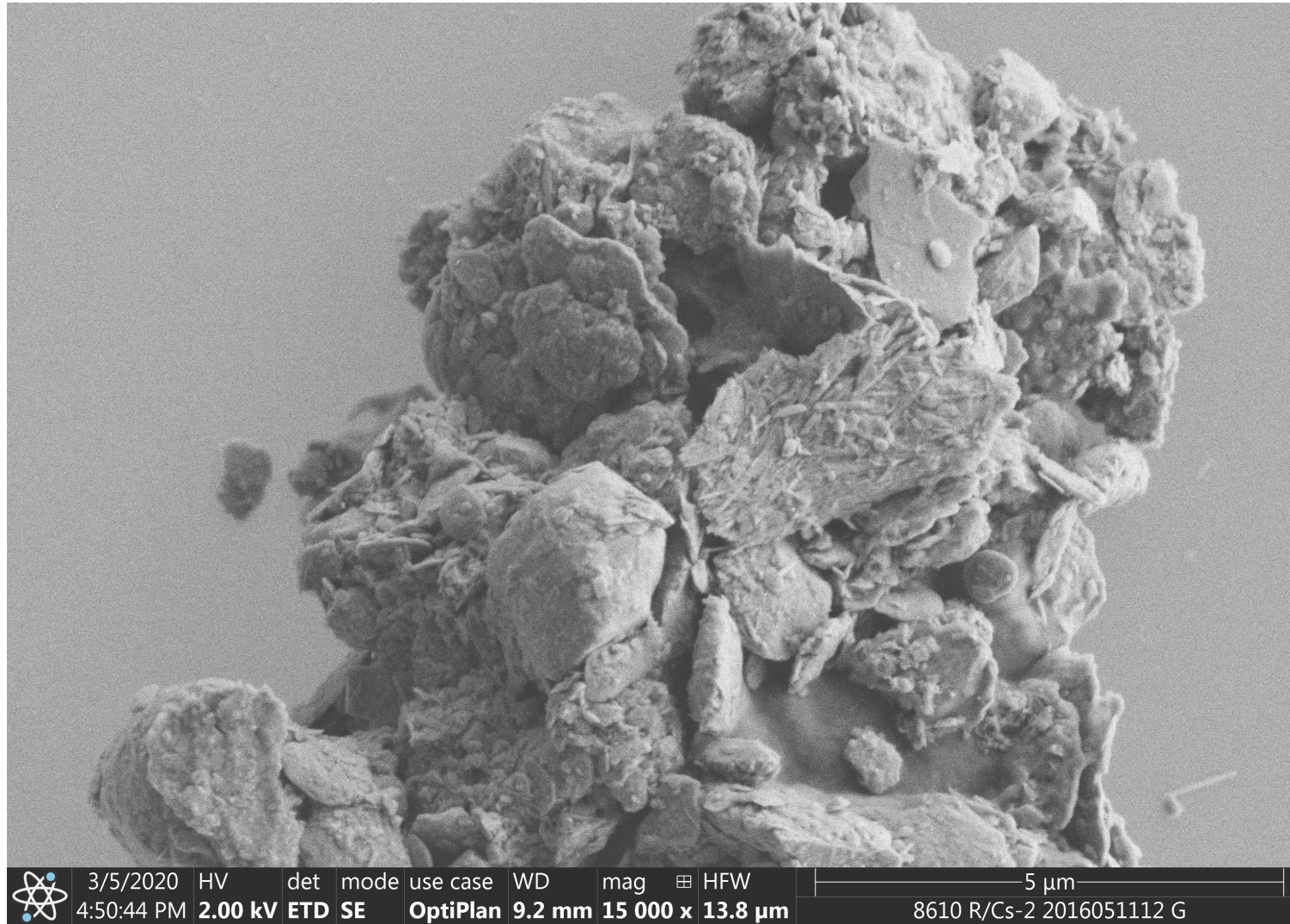
(1) Grain

Single grains vs aggregates

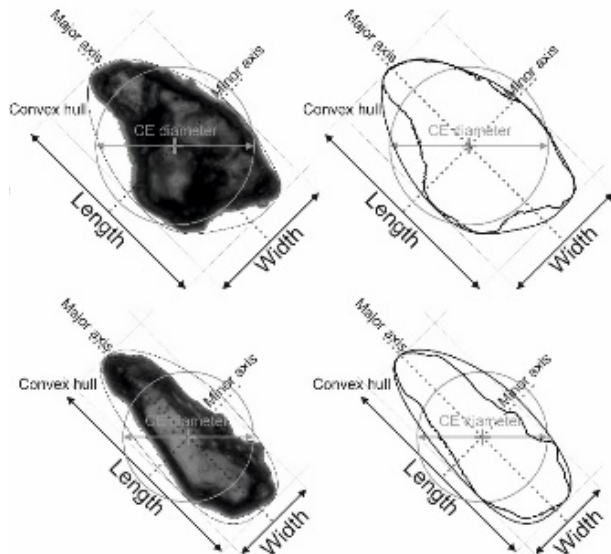
Should we disaggregate the particles?

Why? Why not?
And how?

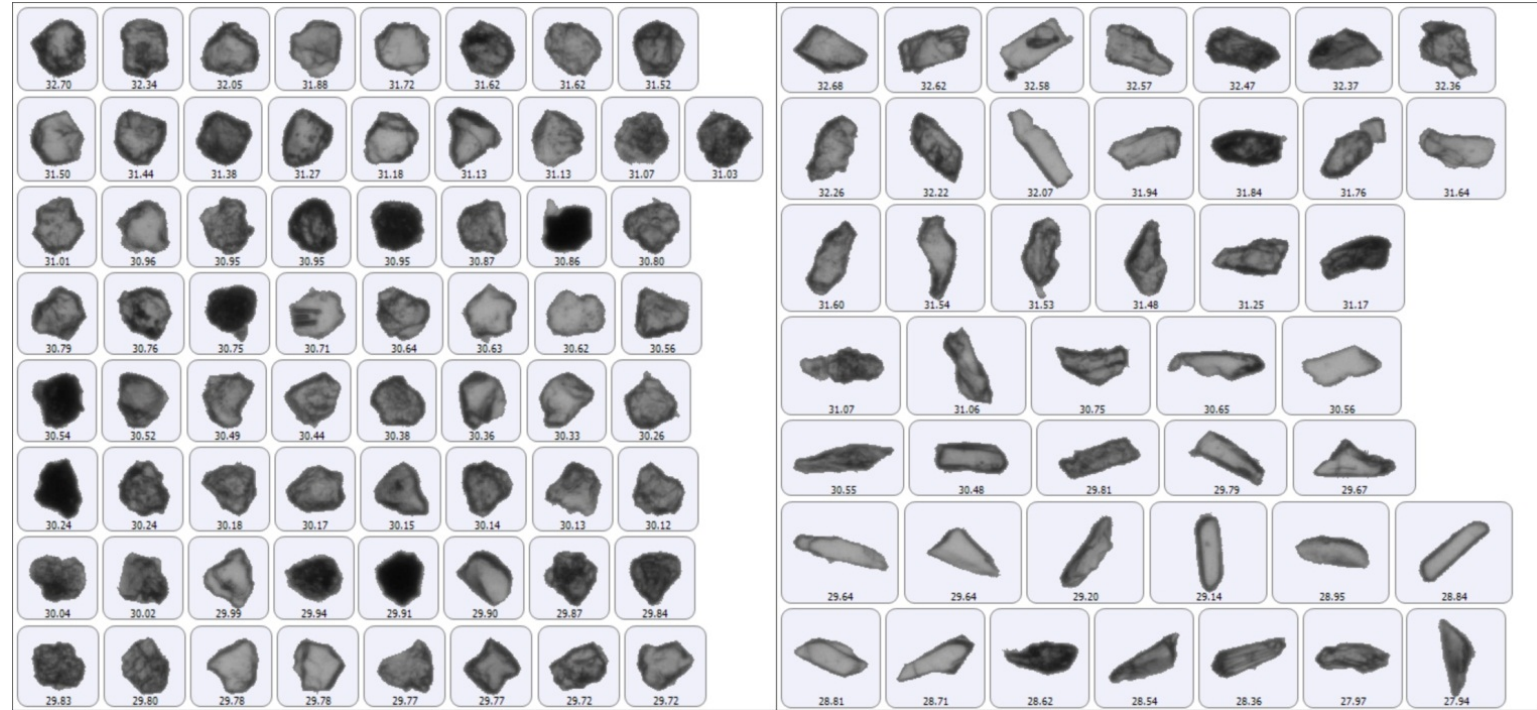
Depends on YOU!



- single grain or aggregates: **non-spherical**
- a real complex, **irregular 3D particle shape and size is transformed** into a simple and standardized shape (e.g. sphere)
- a given particle is replaced with an **imaginary sphere** that has one of the properties (surface-area, volume) identical with the particle: equivalent diameter



(2) Size and (3) measurements

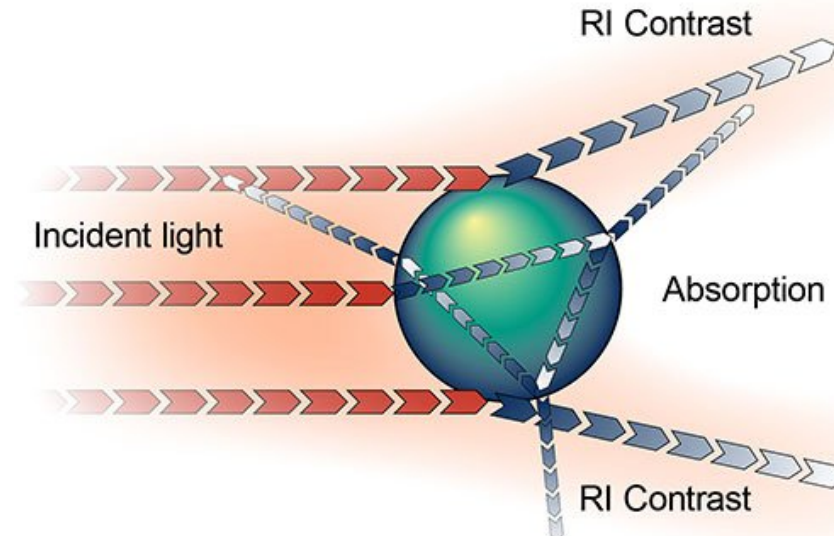


- **laser diffraction:** indirect estimation of grain size by measuring the angular variation in intensity of light scattered as a laser beam passes through a dispersed particulate sample
- **automated (static) image analysis** provides particle size and shape information from direct observations (2D images of particles)

(3) Measurements... Laser diffraction

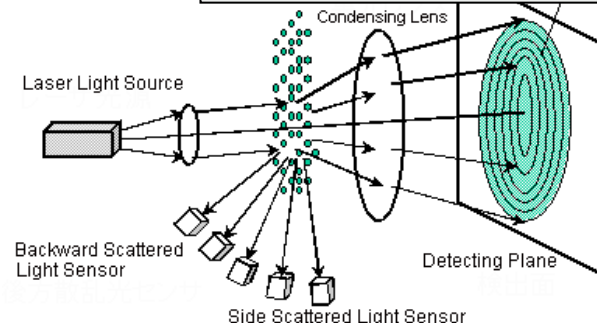
Effects of optical settings in laser diffraction measurements

- Fraunhofer vs. Mie optical theories
- Mie:
 - prior information is needed to solve the Maxwell's electromagnetic field equations
- 68 different optical settings:
 - refractive index: 1.2-2 [1.45-1.6]
 - absorption coefficient: 0.01-1
- Laser scattering** is known to be a robust method for determination of particle sizes. However, you **do not obtain a „direct” measure** of the particles:



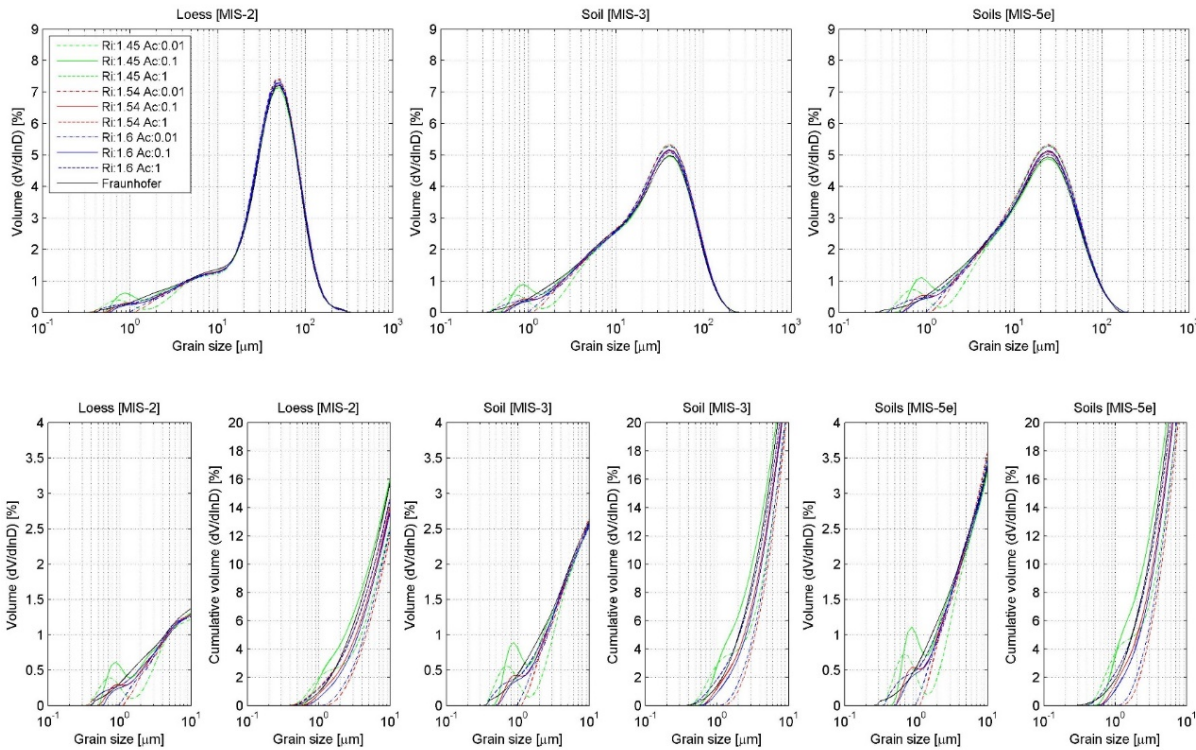
$$I(\theta) = |D(\theta)|^2 = r^2 \left[2J_1(kr \sin \theta) \right]^2$$

$$\begin{pmatrix} E_{||s} \\ E_{\perp s} \end{pmatrix} = \begin{pmatrix} S_1(\theta) & 0 \\ 0 & S_2(\theta) \end{pmatrix} \frac{e^{i(kr + k_2)}}{ikr} \begin{pmatrix} E_{||i} \\ E_{\perp i} \end{pmatrix}$$

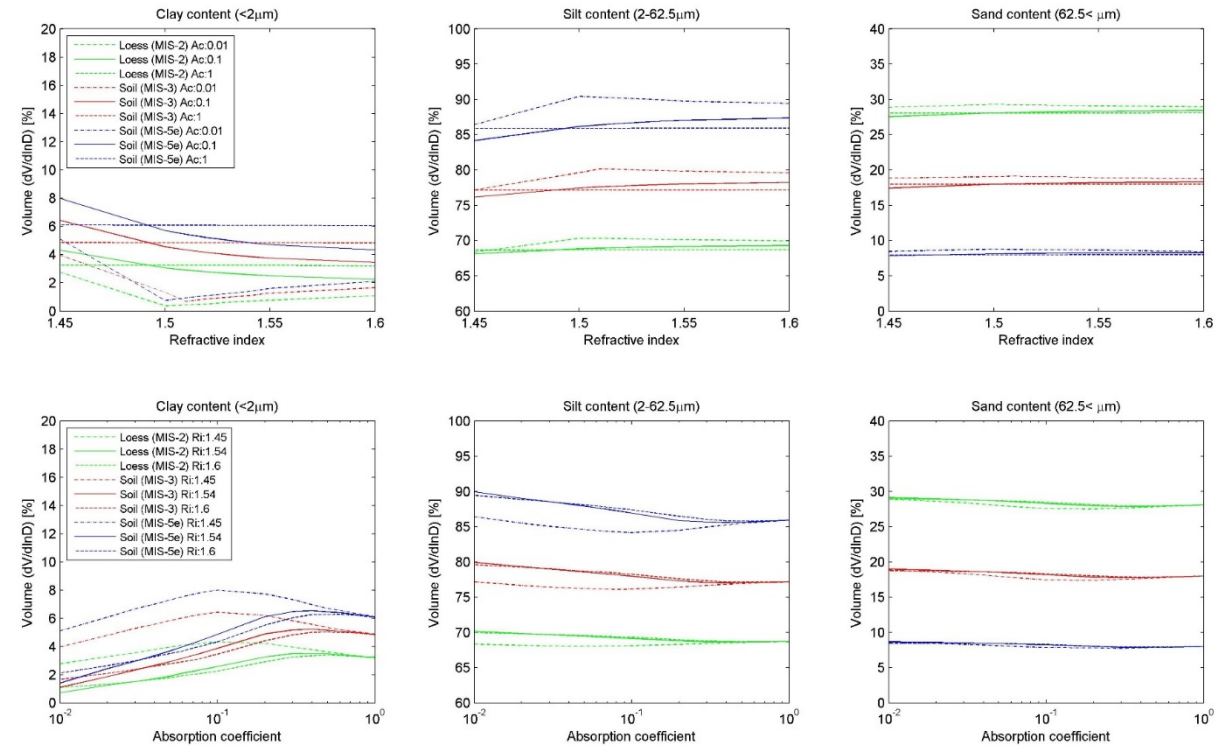


Minerals	Refractive Indices		
	Malvern (1993)	ISO 13320-1 (1999)	CRC Press (2008)
Albit (feldspar)	1.527–1.538	—	1.527–1.538
Andezin (feldspar)	1.544–1.563	—	1.550–1.557
Anortite (feldspar)	1.577–1.590	—	1.577–1.590
Apatite	—	1.63–1.67	1.645–1.648
Biotite (mica)	1.565–1.696	—	1.595–1.651
Brucite	—	1.56–1.60	1.575–1.590
Calcite	1.486–1.740	1.49–1.74	1.486–1.658
Chlorite	—	—	1.61–1.62
Dolomite	—	1.50–1.68	1.500–1.679
Fluorite	1.433–1.435	1.43–1.44	1.434
Gibbsite	—	1.56–1.60	1.57–1.59
Gypsum	1.519–1.531	1.52–1.53	1.52–1.53
Hematite	2.94–3.22	2.90–3.20	2.91–3.19
Illite	1.54–1.61	1.54–1.61	1.56–1.59
Kaolinite	1.533–1.570	1.53–1.57	1.549–1.565
Magnesite	1.563–1.700	1.51–1.78	1.536–1.741
Mica	1.53–1.70	1.53–1.70	—
Microcline (K feldspar)	1.514–1.539	—	1.522–1.530
Montmorillonite	1.48–1.64	—	1.55–1.57
Muscovite (mica)	1.552–1.616	—	1.563–1.602
Olivine	—	—	1.73–1.78
Opal	—	1.41–1.46	1.44
Orthoclase	1.518–1.539	1.52–1.54	1.523–1.531
Quartz	1.544–1.553	1.54–1.55	1.544–1.553
Serpentine	—	1.53–1.57	1.55–1.56
Talc	1.589	1.54–1.60	1.545–1.595
Topaz	—	1.61–1.64	1.618–1.627
Vermiculite	—	—	1.542–1.556

(3) Measurements... Laser diffraction



Grain size distribution curves of different sedimentary units by using different optical setting of the laser scattering device.



Separate effects of refractive index and absorption coefficient settings on different grain size fractions of loess and paleosol samples.

(3) Measurements... Laser diffraction

Sample pre-treatment (after Konert – Vandenberghe, 1997):

- 10 ml, 30% H_2O_2 (organic matter removal)
- 10 ml, 10% HCl (carbonate removal)
- 10 ml of 3.6% $\text{Na}_4\text{P}_2\text{O}_7 \cdot 10\text{H}_2\text{O}$ (dispersion)

3 state-of-the-art laser scattering instruments:

- Fritsch Analysette 22 Microtec (IR 850 nm [532 nm])
- Horiba Partica La-950 v2 (650 nm [LED 405 nm])
- Malvern Mastersizer 3000 Hydro LV (633 nm [LED 405nm])

68 different optical settings:

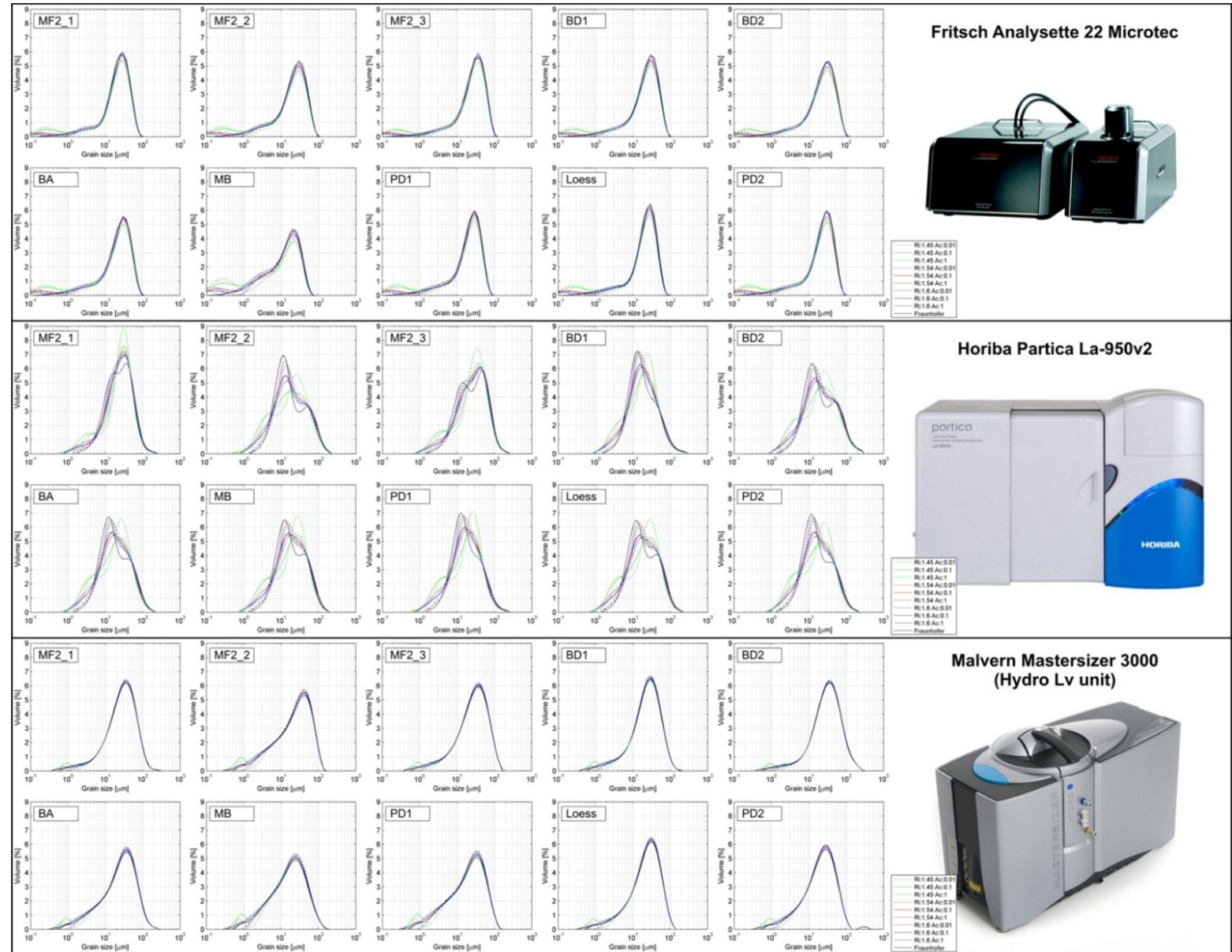
- refractive index: 1.2-2 [1.45-1.6]
- absorption coefficient: 0.01-1

2040 particle size distributions for the 10 samples



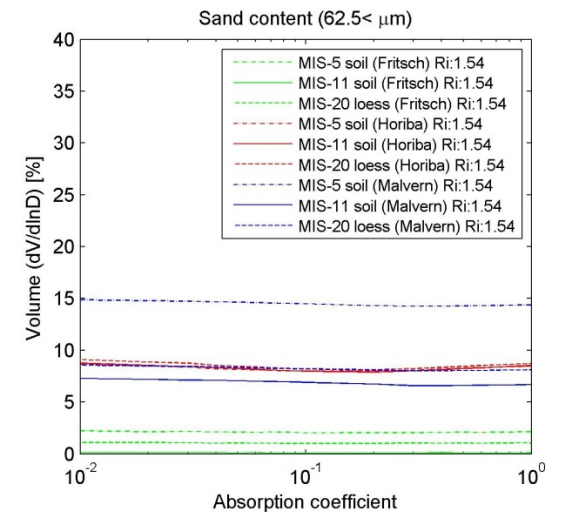
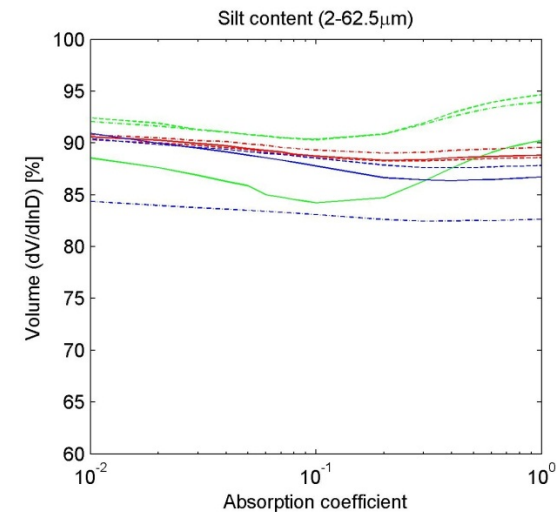
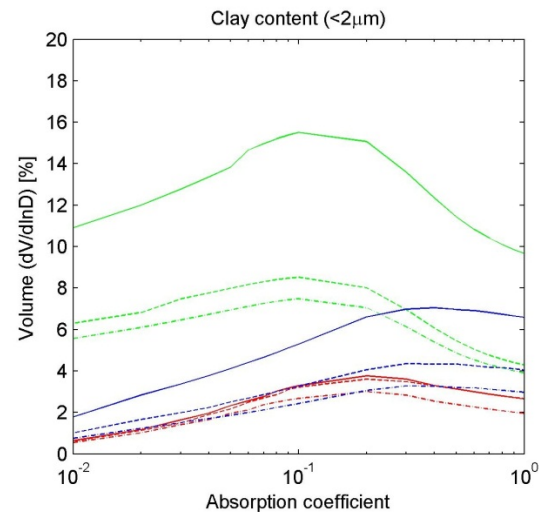
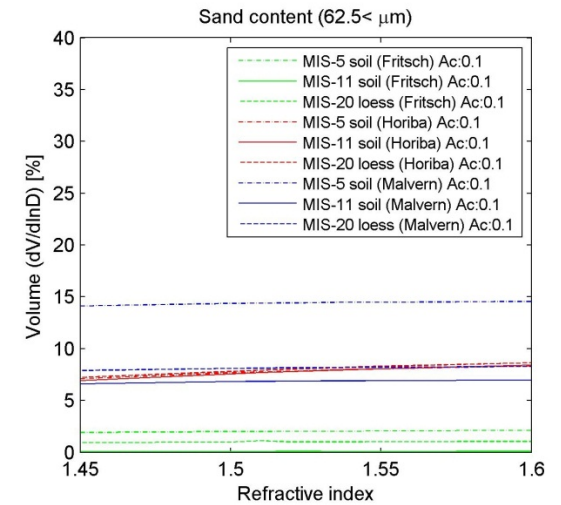
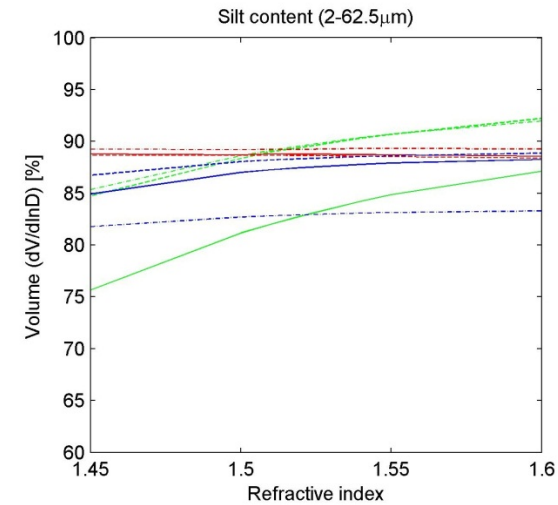
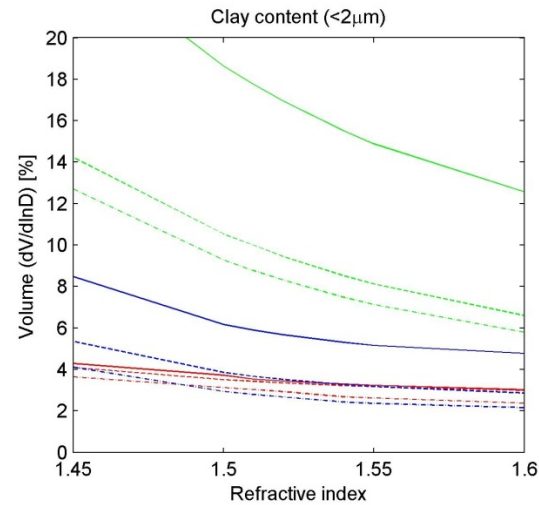
(3) Measurements... Laser diffraction

Effects of applied devices
in laser scattering
measurements



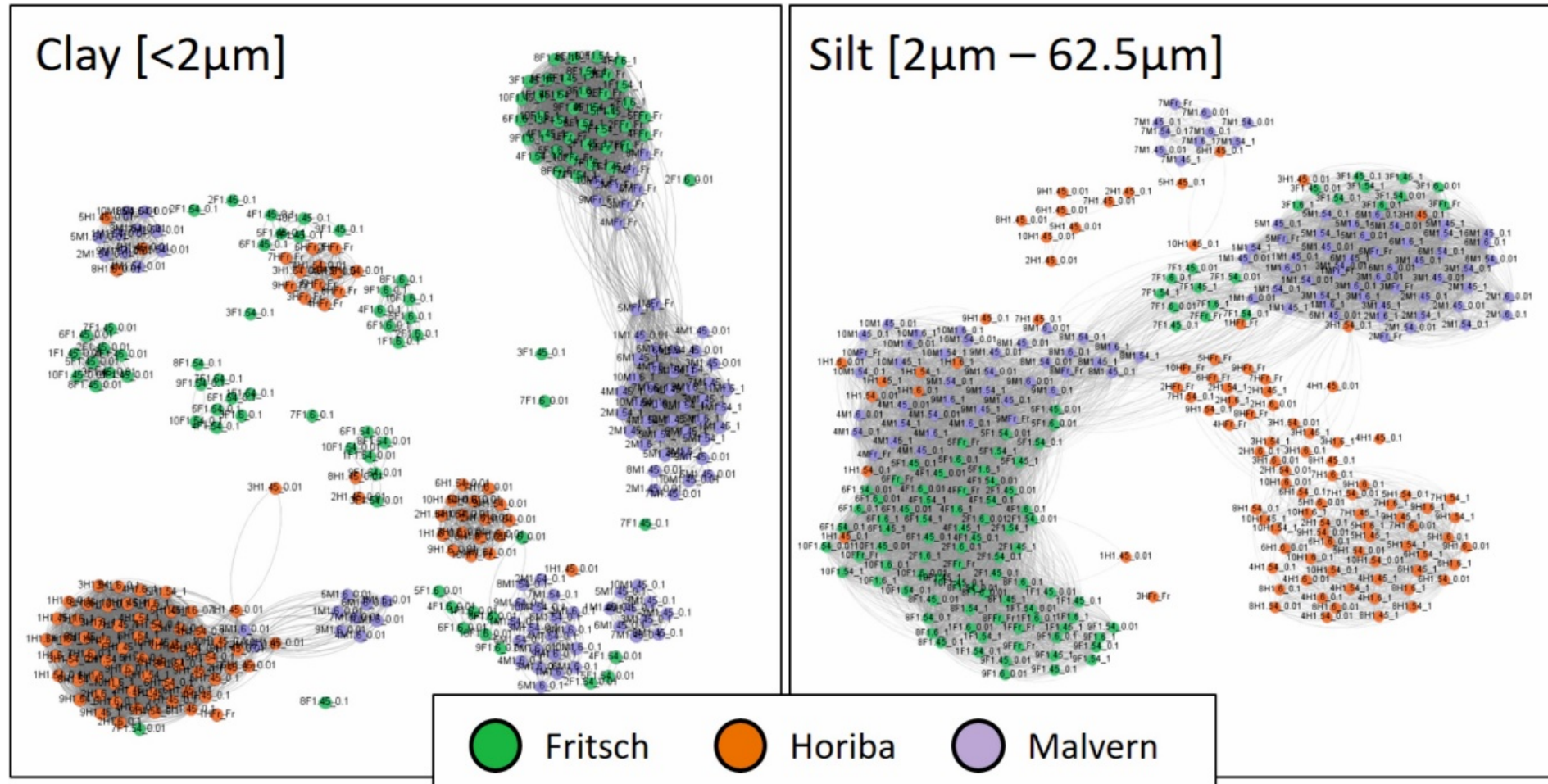
(3) Measurements... Laser diffraction

Effects of applied devices in laser scattering measurements



(3) Measurements... Laser diffraction

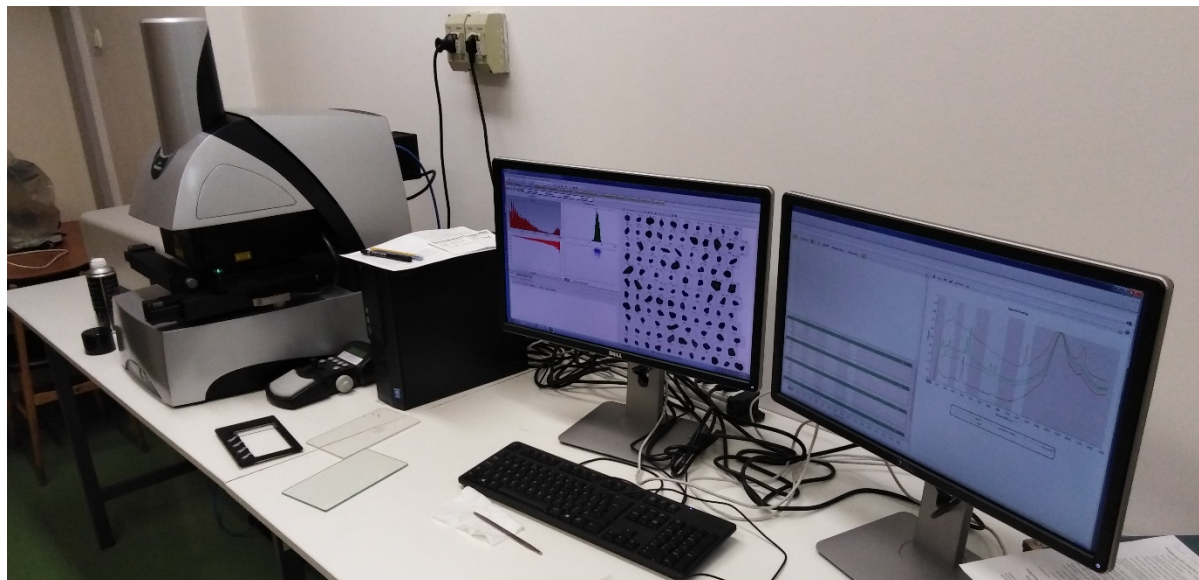
Effects of applied devices in laser scattering measurements



(3) measurements... automated static image analysis

Malvern Morphologi G3-ID

- granulometric data obtained from the captured 2D images of the individual particles
 - direct information
 - size
 - shape parameters

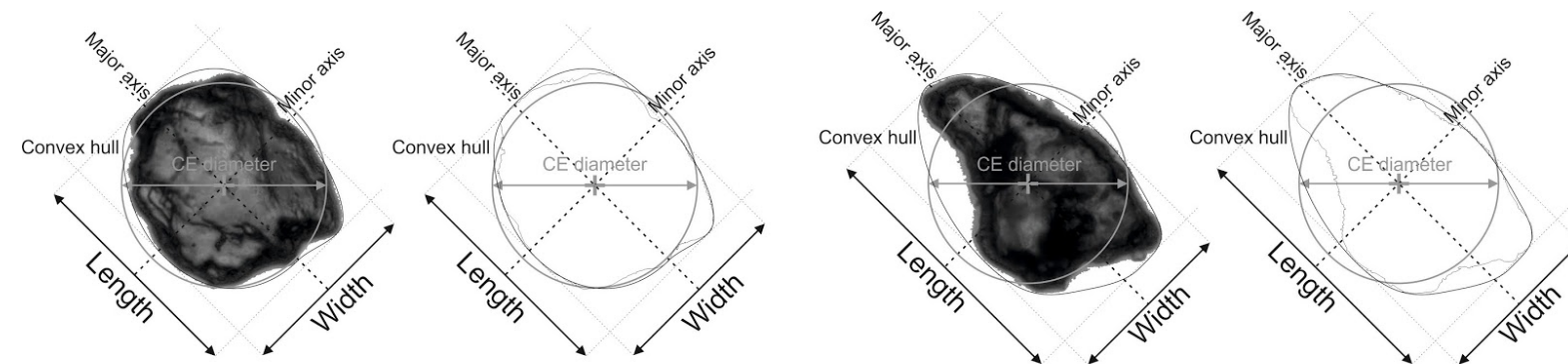


Automated imaging provides a unique technique to gather direct information on granulometric characteristics of particles. Granulometric data obtained from automatic image analysis of **Malvern Morphologi G3-ID** is a rarely applied new technique for **particle size and shape analyses** in sedimentary geology.

Size and shape data of **10^4 - 10^6 individual particles** are automatically recorded for each sample from the captured high-resolution images.

Raman-spectroscopy (at 785 nm wavelength with $3\mu\text{m}$ spot) was also applied to directly **identify the quartz** grains (as an indicator of Saharan dust contribution).

The acquired spectra of targeted particles were compared to Raman spectral reference libraries using **KnowItAll®** software from Bio-Rad to identify the minerals present.



Aspect Ratio = Width/Length

CE Diameter: diameter of a circle with the same area as the projected 2D particle image

Circularity = $(2 \times \pi^{0.5} \times \text{Area}^{0.5}) / \text{Perimeter}$

Convexity = $\text{Perimeter}_{\text{Convex hull}} / \text{Perimeter}$

Elongation = $1 - (\text{Width}/\text{Length}) = 1 - \text{Aspect Ratio}$

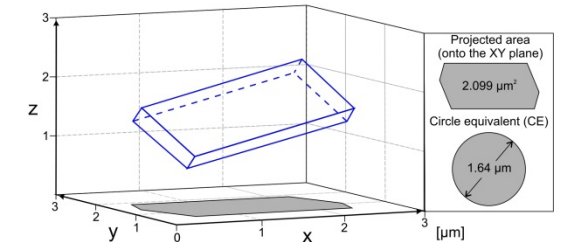
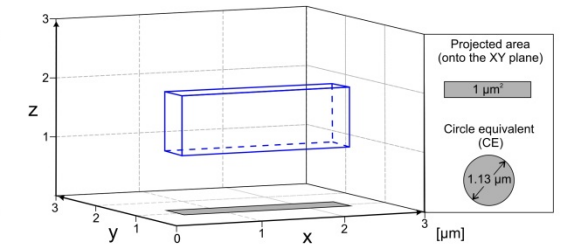
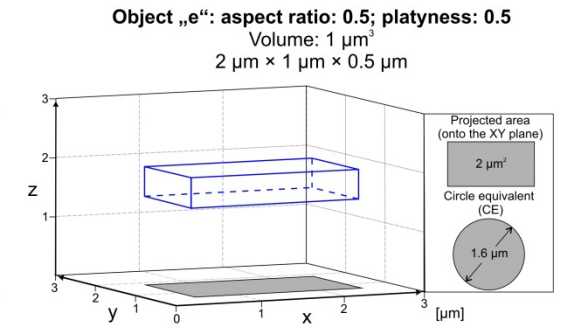
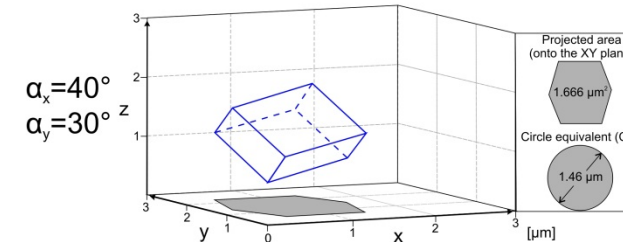
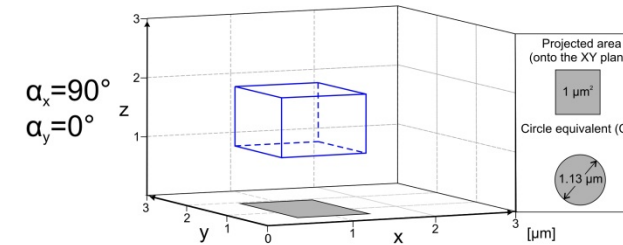
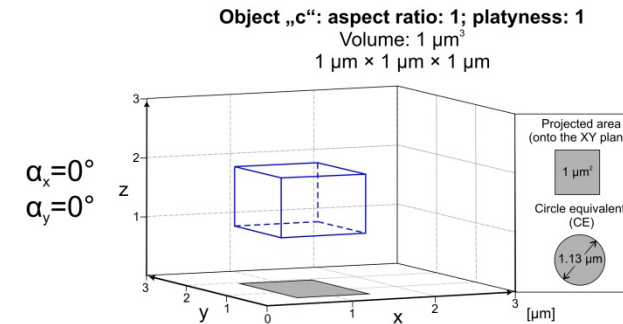
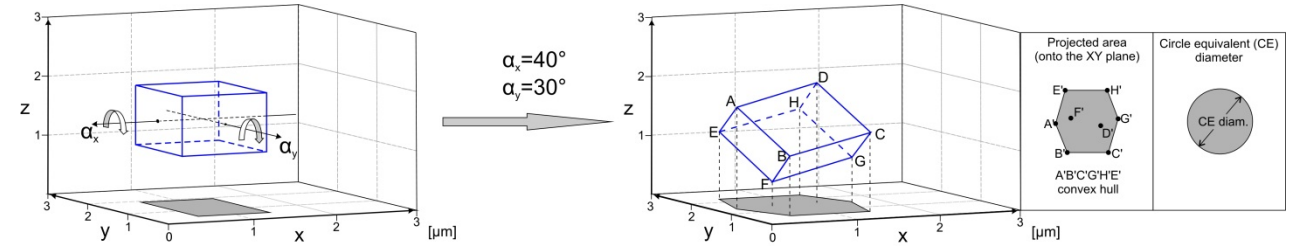
SE Volume: volume of a sphere with the same CE Diameter as the projected 2D particle image

Solidity = $\text{Area}_{\text{Convex hull}} / \text{Area}$

(3) measurements... automated static image analysis

Underestimation of fine-grained fractions

- the CE diameter is calculated from the acquired **2D image** of particle
- the instantaneous pulse of compressed air disperse the particles onto the glass slide with a **consistent orientation with their largest area** facing to camera
 - only one outcome of infinite possible 2D projections of a 3D object
 - is it representative?



(4) Interpretation... particles size data -> information

Data: What kind of data?

THREE MAJOR PROBLEMS...

- Pretreatment
- measurement techniques
 - laser diffraction
 - image analysis
- instruments:
 - Fritsch Analysette 22 Microtec
 - Horiba Partica La-950 v2
 - Malvern Mastersizer 3000...
- Fraunhofer vs. Mie optical theories
- Mie:
 - prior information is needed to solve the Maxwell's electromagnetic field equations
 - refractive indices
 - absorption indices (coefficients/imaginary refractive indices)
 - polymineral agent...

Information: On what?

THE 4TH MAJOR PROBLEM...

- wind pattern:
 - wind strength/speed
 - direction
 - gustiness
 - and the temporal distribution of these
- distance(s) from the dust source area(s)
- transport and sedimentation modes
- post depositional alterations

Grain size data records the combined effects of several environmental factors
-> proper interpretation is needed.

Thank you very much for your kind attention!

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