# Improvement of the bimodal parameterization of particle size distribution using laser diffraction

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# Soil texture

Soil texture

Used for soil classification

Soil properties:

- Thermal
- Biological
- Hydraulic (water retention curve and hydraulic conductivity)
- Soil dielectric properties (TDR, FDR)

Textural triangle is insufficient for soil characterization.

Mathematical models are commonly used to represent the PSD.

PSD parameters are used for pedotransfer functions

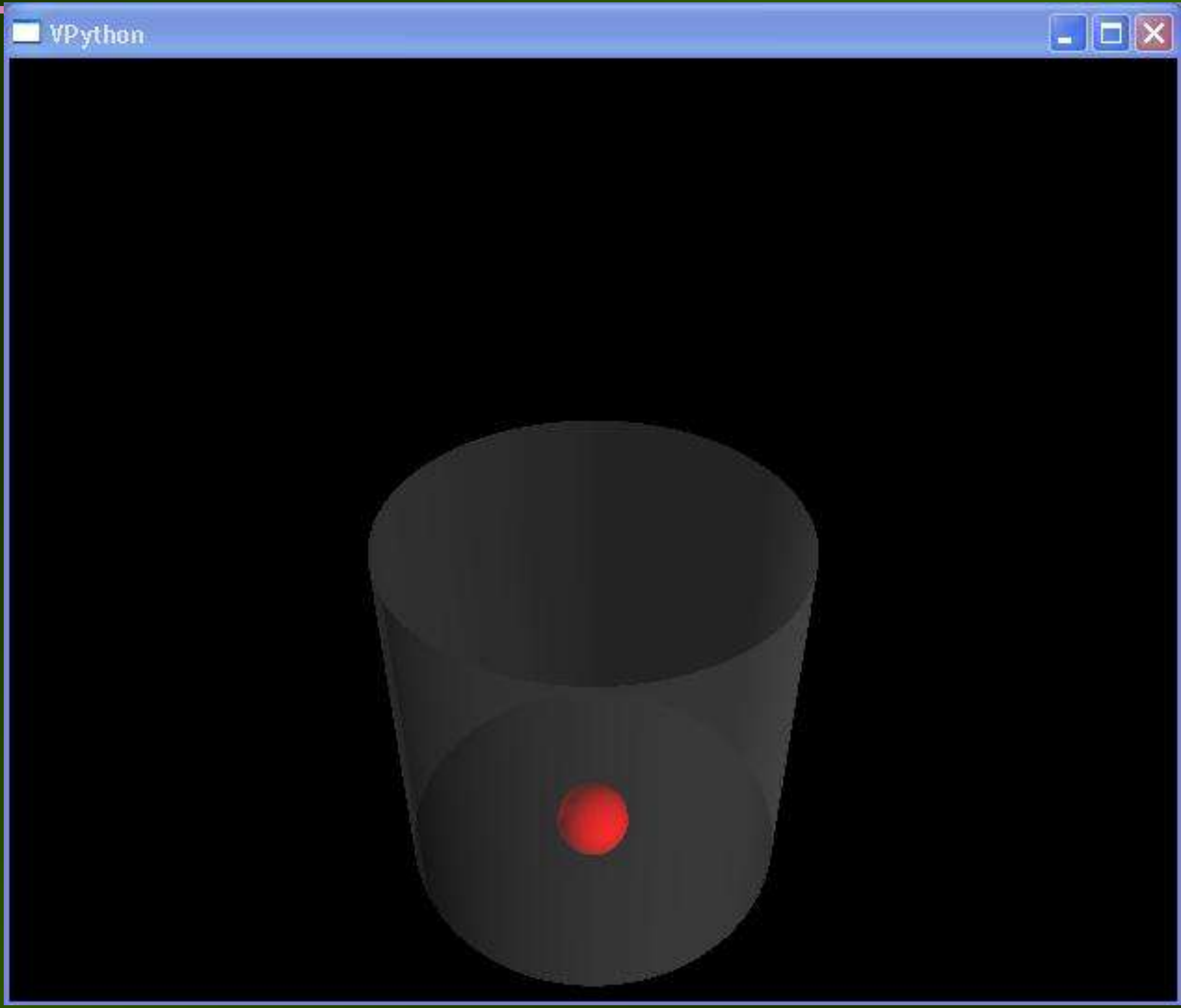
# Soil textural analysis

- Sedimentation is based on Stokes law and it computes an equivalent diameter based on the settling times.
- Laser diffraction is based on light diffraction. The angle of diffraction depends on particle size.
- Image analysis is based on a direct measurement by microscope observations and use of image analysis software. The surface area is measured.

# Sedimentation (mass based)

Assumptions and limitations:

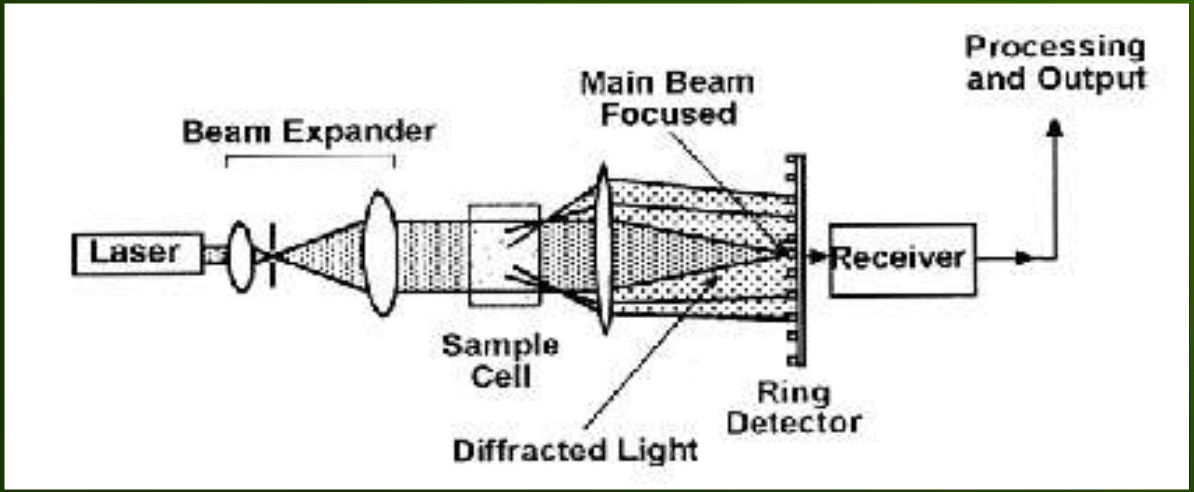
1. spherical particles
2. uniform density
3. uniform viscosity
4. laminar flow (upper limit)
5. Brownian motion (lower limit)

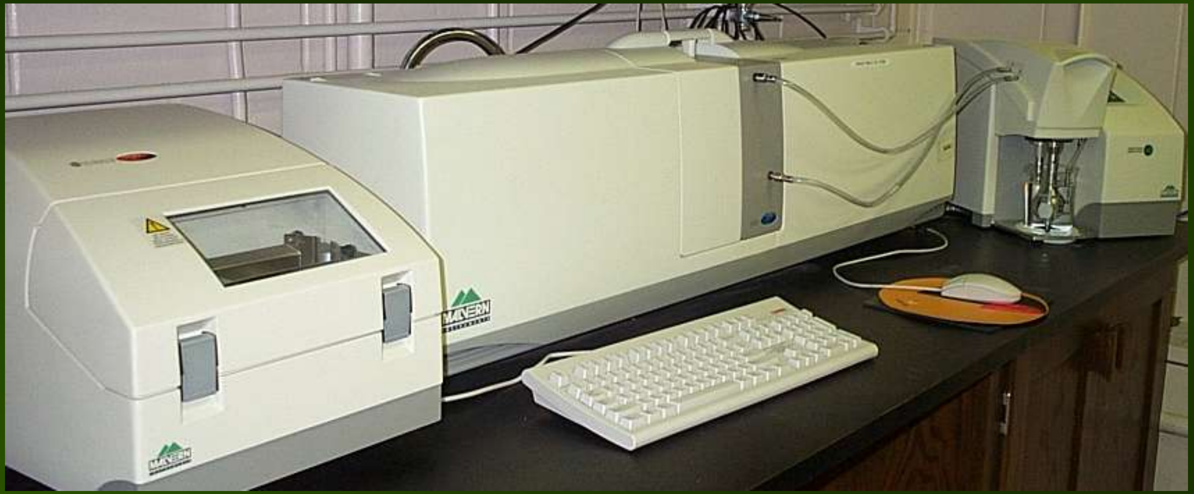


# Laser diffraction (volume based)

Assumptions and limitations:

1. spherical particles
2. known or assumed diffraction parameters (real and imaginary part)
3. $n_r$= 1.5-1.7 (1.53)
4. $n_i$= 0.1-0.3



# Refractive index

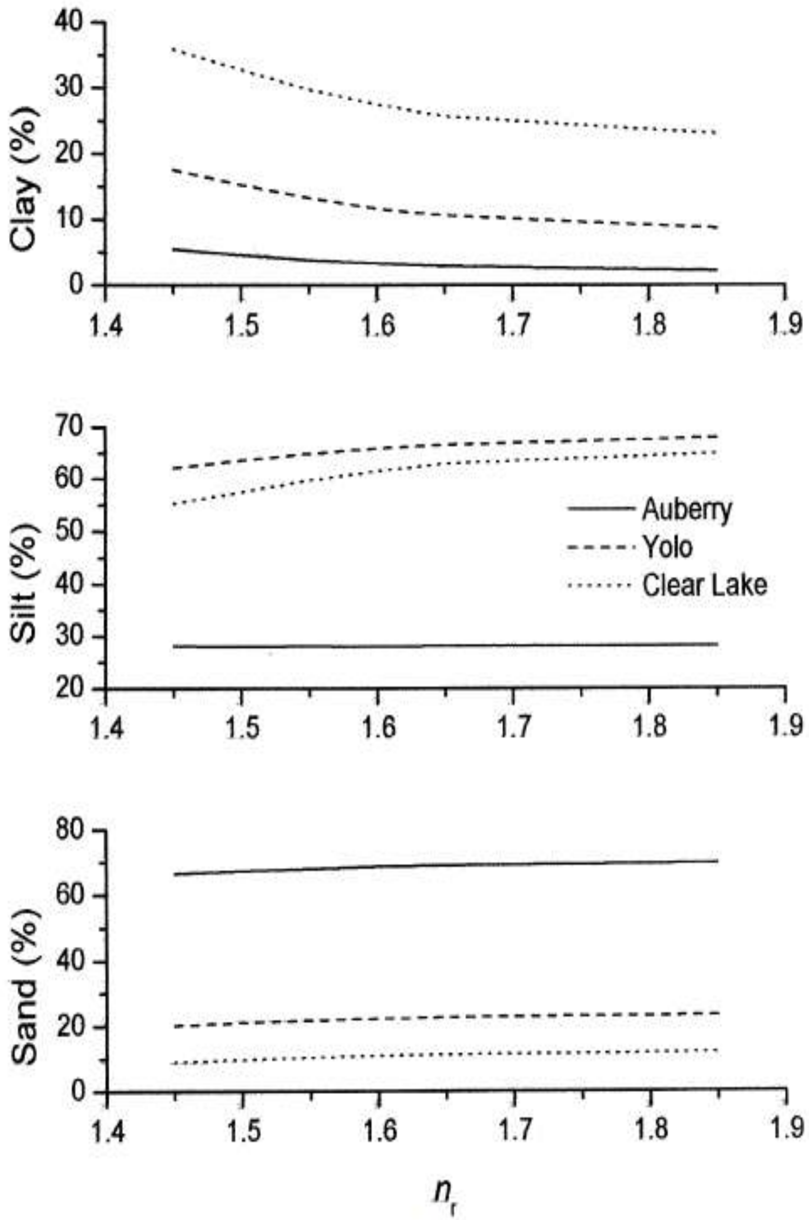



Fig. 1. Effects of the real part of the refractive index ($n_r$) on the volume percent of (a) clay, (b) silt, and (c) sand in the Auberry, Yolo, and Clear Lake soils.

Table 2. The real part of the refractive index ($n_r$) and particle density of common soil minerals. Unless stated otherwise, data were taken from the Handbook of chemistry and physics (CRC Press, 2002).

| Minerals | $n_r$ | Particle density |
|---|---|---|
| | 589 nm | Mg $m^{-3}$ |
| Albite (Na feldspar) | 1.525–1.536 | 2.61–2.64 |
| Andesine | 1.549–1.556 | 2.647–2.69 |
| Anorthite | 1.575–1.588 | 2.703–2.763 |
| Apatite | 1.65–1.648 | 3.1–3.3 |
| Calcite | 1.48–1.66 | 2.7 |
| Feldspars | 1.525† | 2.5–2.8‡ |
| Gibbsite | 1.566–1.587 | 2.3–2.4 |
| Gypsum | 1.52–1.53 | 2.32 |
| Hematite | 2.91–3.19 | 4.9–5.3 |
| Humus | | <1.5‡ |
| Illite | 1.56–1.59 | 2.8 |
| Kaolinte | 1.549–1.565 | 2.65 |
| Micas | 1.53–1.7† | 2.7–3.3‡ |
| Microcline (K feldspar) | 1.522–1.53 | 2.54–2.57 |
| Montmorillonite | 1.55–1.57 | 2.5 |
| Quartz | 1.544–1.553 | 2.65 |

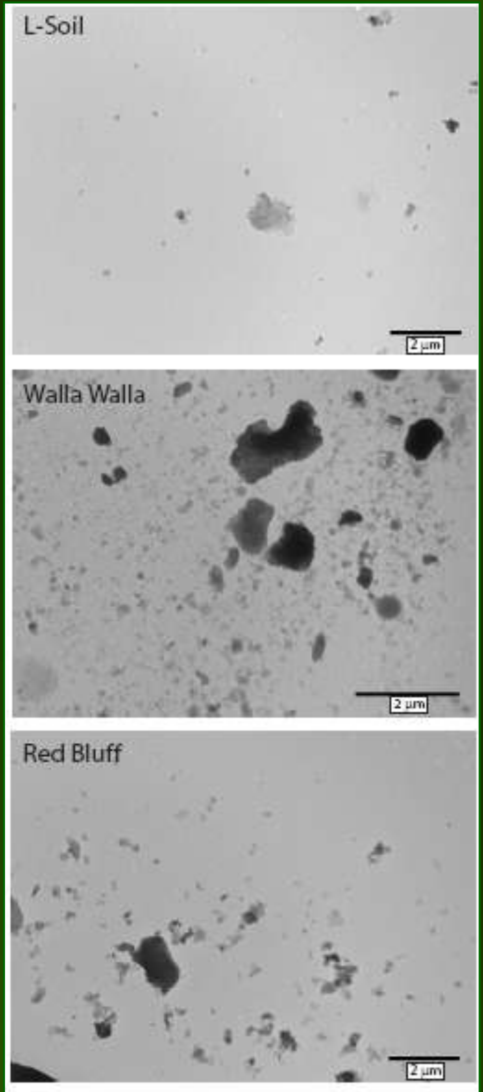
† Beckman Coulter (1999).
‡ Gee and Bauder (1986).

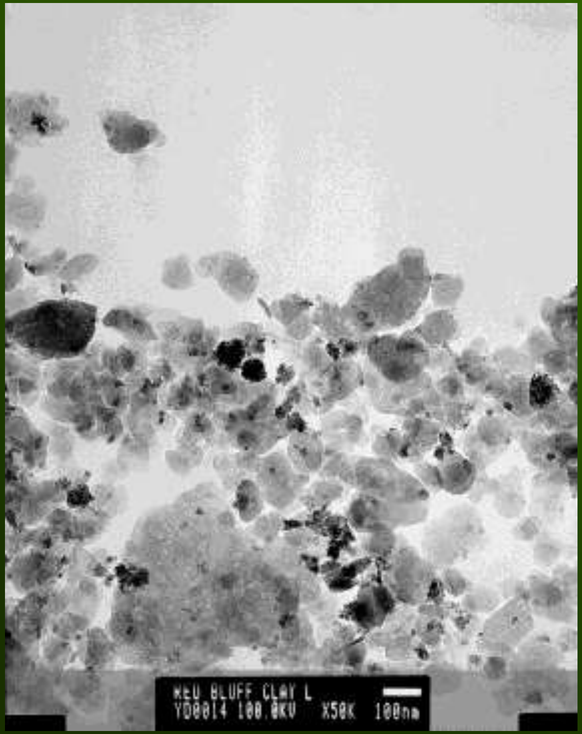
# Image analysis (volume based)

## from Transmission Electron Microscopy (TEM)

Assumptions and limitations:

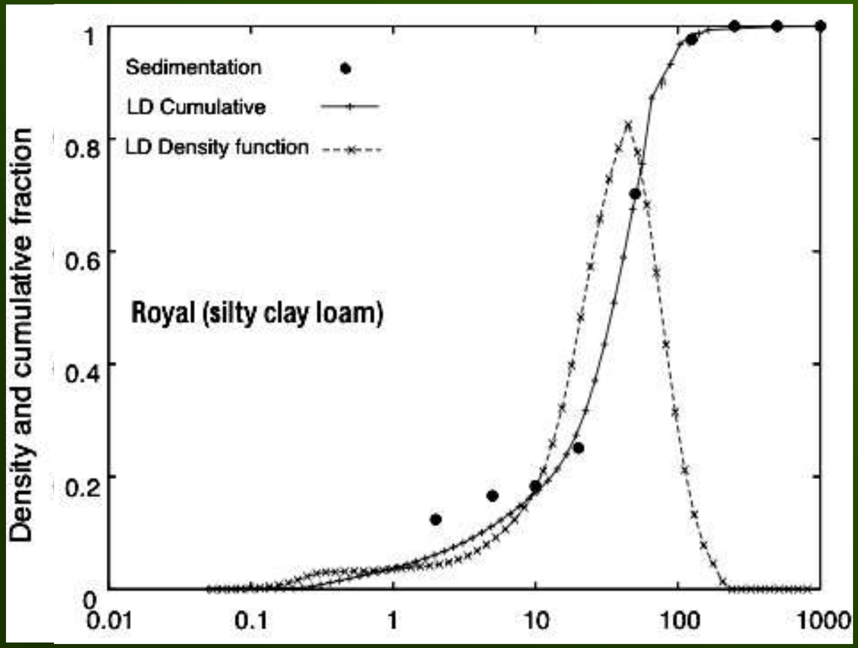
1. 2D-image
2. uniform density
3. pixel size
4. high number of samples
5. particle aggregation
6. geometrical analysis



# Models for PSD

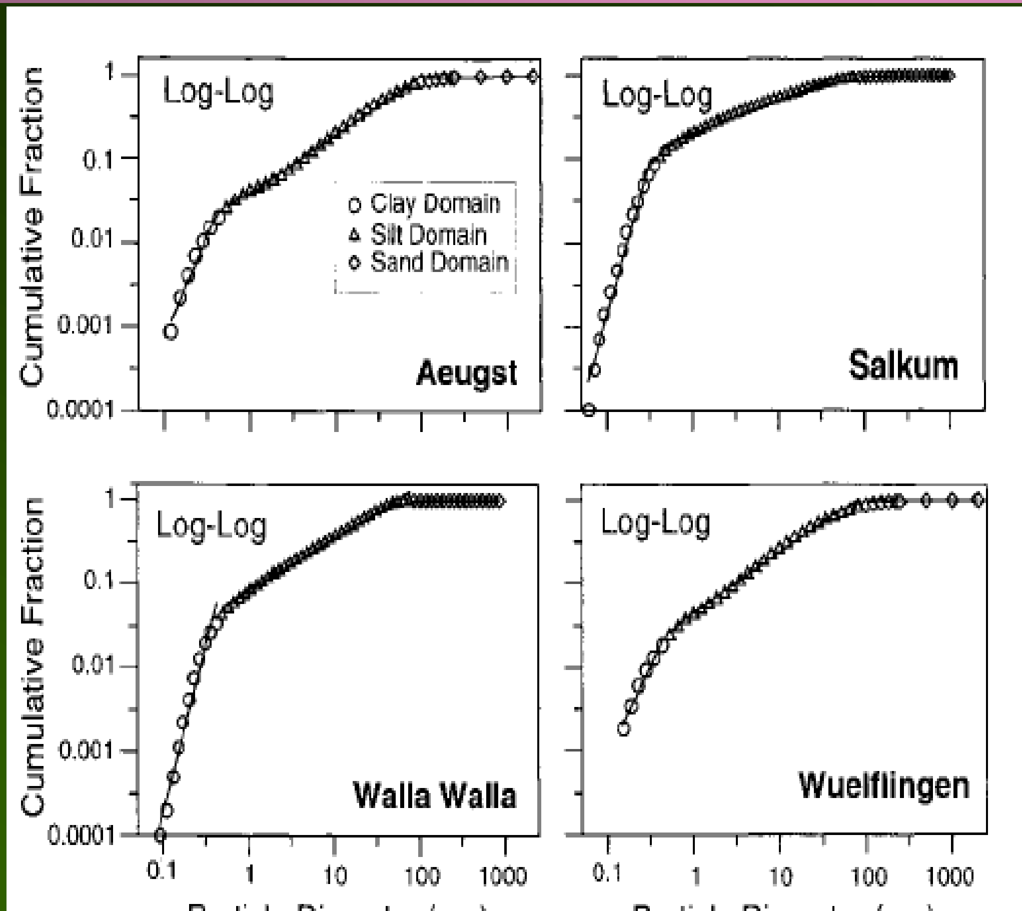
- Logistic (Arya and Paris, 1991)
- Bimodal (Shiozawa and Campbell, 1990)
- Fractal (Wu et al., 1993; Bittelli et al., 1999)




Comparisons:

Buchan,G.D., K.S.Grewal, andA.B. Robson. 1993. Improved models of particle-size distribution: An illustration of model comparison techniques. Soil Sci. Soc. Am. J. 57:901–908.

# Are PSDs scale-invariant ?

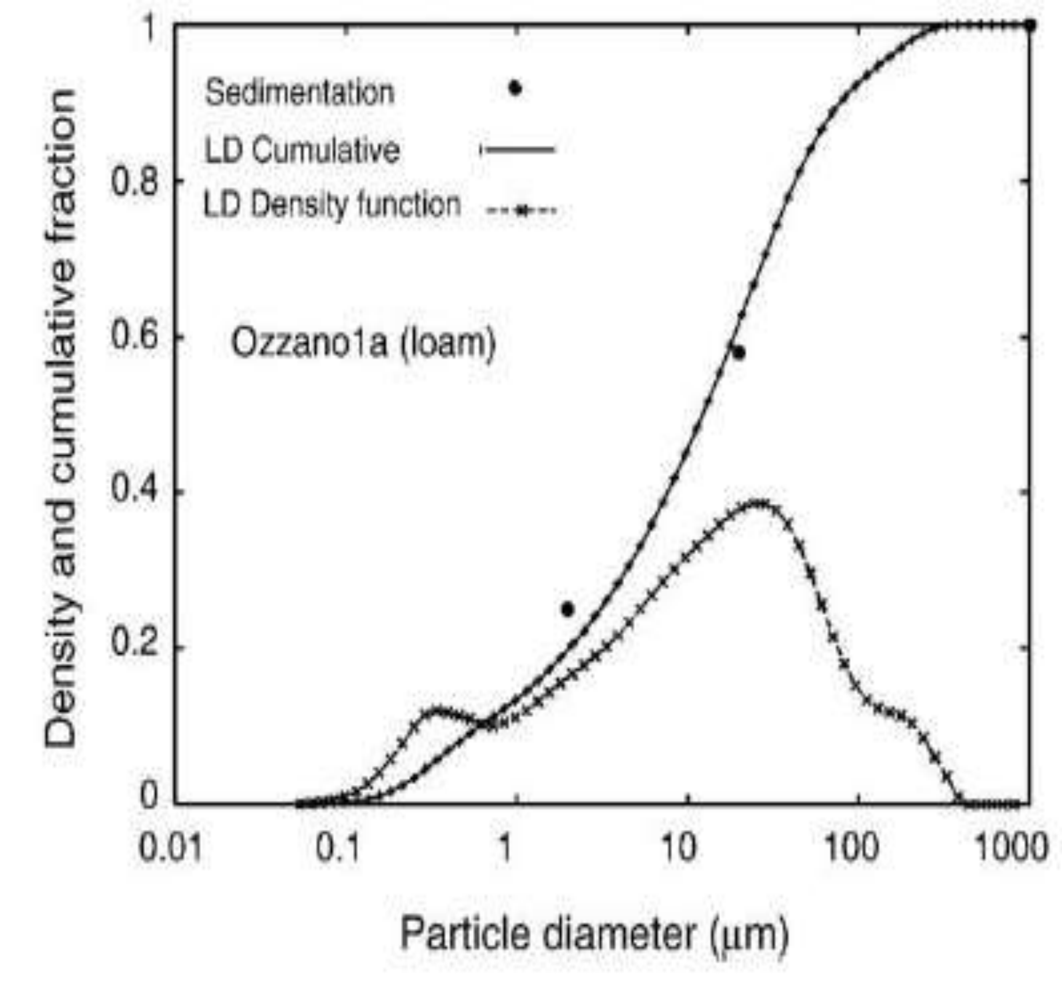



$$N(r > R) = CR^{-D}$$

$$\frac{M(r < R)}{M_T} = \left(\frac{R}{R_{L,upper}}\right)^{v}$$

Bittelli M., G.S. Campbell and M. Flury, 1999. Characterization of PSD using a fragmentation model. SSSAJ, 63: 782-788

# bimodal Gaussian




$$F(x) = \varepsilon F_1(x) + (1-\varepsilon) F_2(x)$$

F2(x): primary minerals (sand and silt)
F1(x): secondary minerals (clay)
ε: clay fraction (or fitting parameter)

$$F(x) = \frac{1}{2}\left\{1 + \operatorname{erf}\left[\frac{(x-\mu)}{\sigma\sqrt{2}}\right]\right\} \quad \text{for } (x > \mu)$$

$$F(x) = \frac{1}{2}\left\{1 - \operatorname{erf}\left[\frac{(x-\mu)}{\sigma\sqrt{2}}\right]\right\} \quad \text{for } (x \leq \mu)$$

# Derive mean and standard deviation from three fractions only

Computation of $\mu$ and the $\sigma^2$ from the **three fractions** only:

$$\ln\mu = m_y \ln d_y + m_t \ln d_t + m_d \ln d_d$$

$$\ln\sigma^2 = m_y (\ln d_y)^2 + m_t (\ln d_t)^2 + m_d (\ln d_d)^2 - (\ln \mu)^2$$

**m** = **mass fraction**

**d** = **geometric mean**, which were calculated from set limits:

$d_y$ = clay diameter = $(0.01 \quad 2)^{1/2}$ = 0.141 μm

$d_t$ = silt diameter = $(2 \quad 50)^{1/2}$ = 10 μm

$d_d$ = sand diameter = $(50 \quad 2000)^{1/2}$ = 316.2 μm

# Objectives

1. Testing the bimodal model by using more accurate PSD (laser diffraction technique and image analysis)

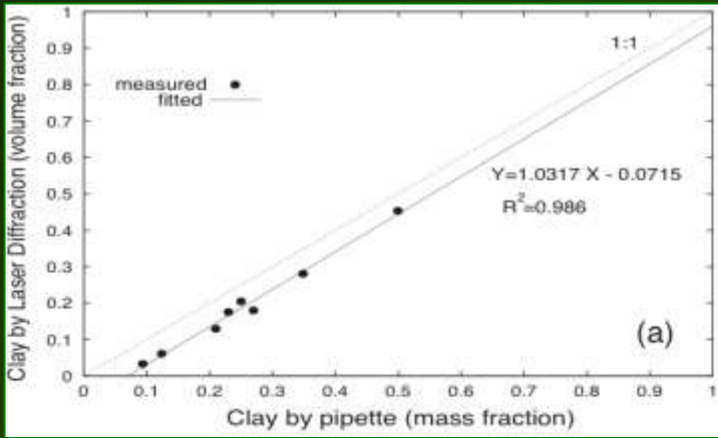
2. Improve the parameterization

3. Comparing the LD methods with other methodologies

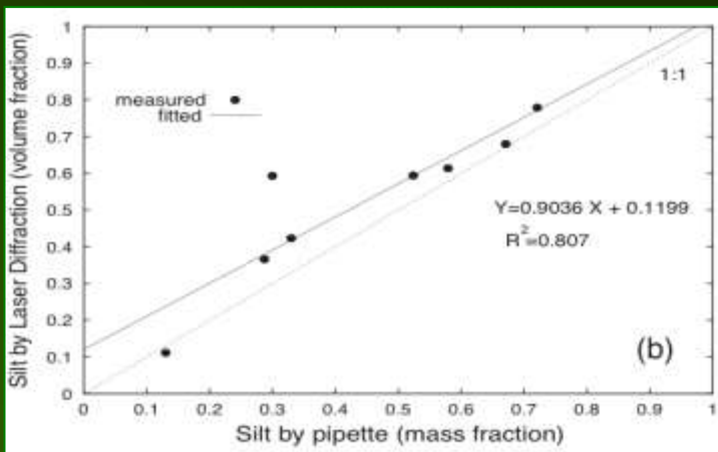
# Materials and methods

- Eight soil samples with different textural compositions and parent material
- Three experimental techniques (sedimentation, laser diffraction and image analysis)

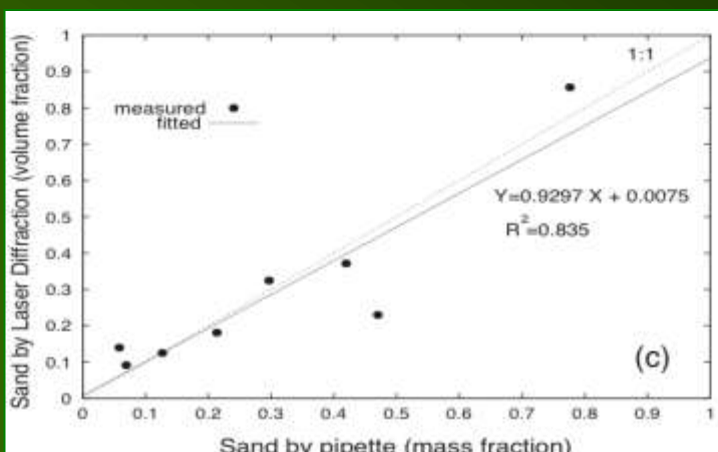
# Results: LD *vs* Pipette




**CLAY:**
LD measured a smaller clay fraction

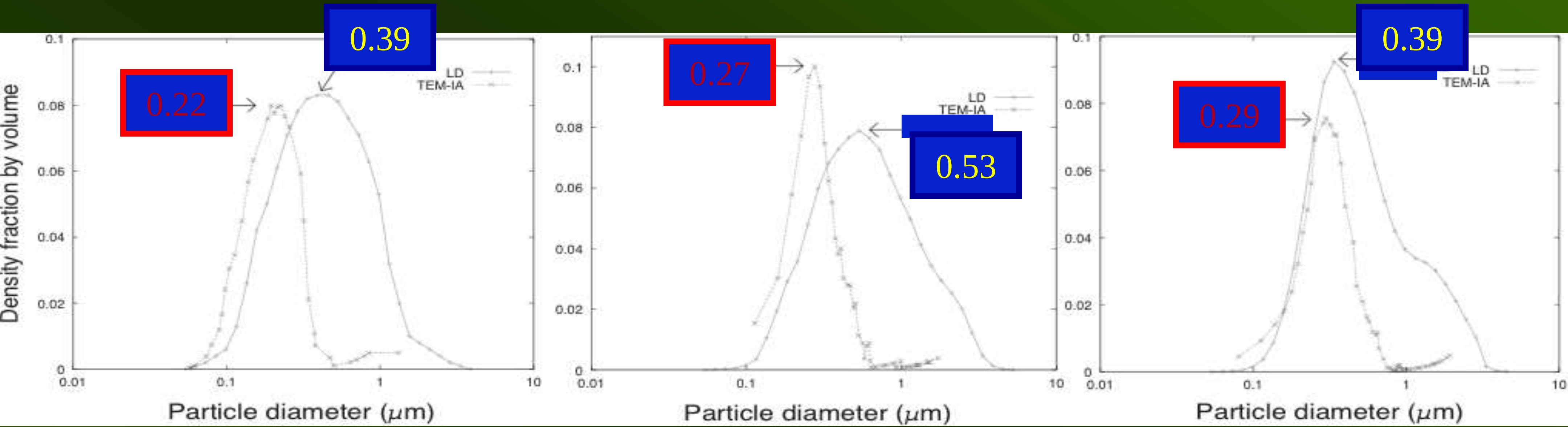



**SILT:**
LD measured a larger silt fraction




**SAND:**
good agreement

# Results: Comparison between **LD** and **IA**

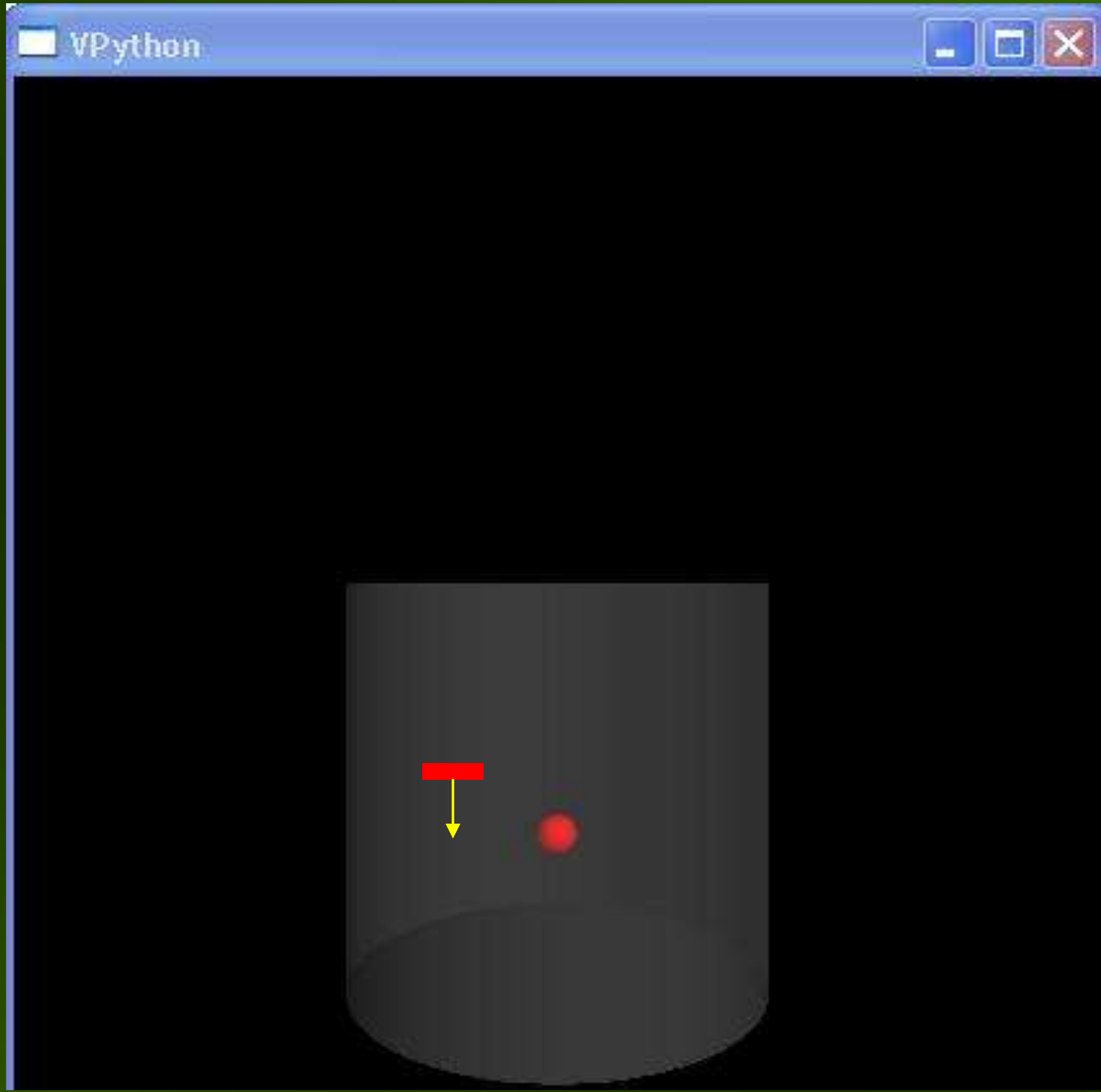



**LD** means in the clay fractions are higher than **TEM**

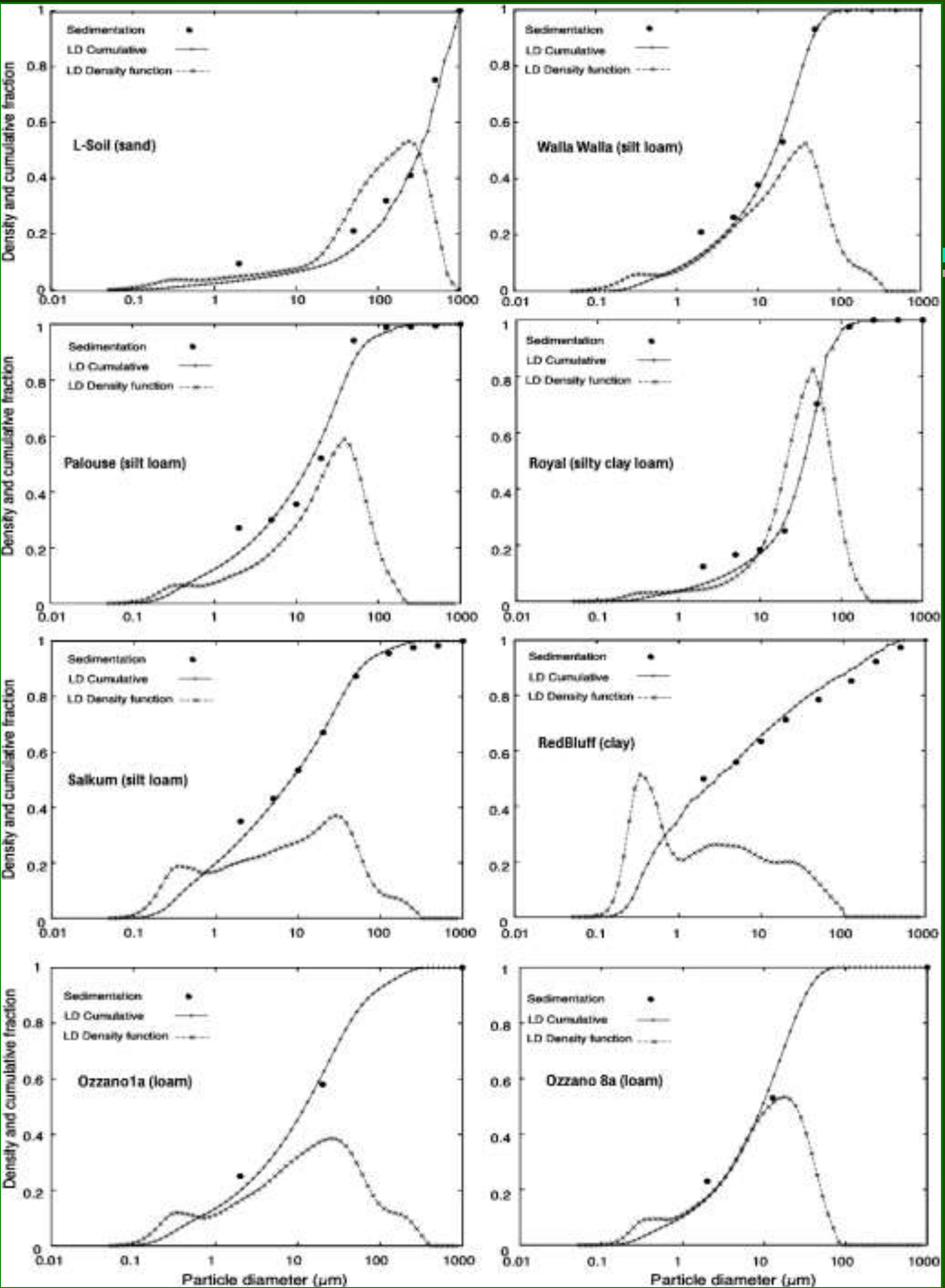
LD particles are represented as spheric-shaped

# Results:

- LD method tends to under-estimate the clay fraction (over estimate the mean diameter), when compared to the traditional sedimentation techniques. This result was confirmed by image analysis.
- The mean diameter for the sedimentation method is not measured, because only a single point at 2 µm is obtained.
- The differences are due to the assumption about spherical particles.



# Results: bimodal Gaussian model




**8 soils with different textural composition**

Density and cumulative distribution fractions of the eight soils, obtained by laser diffraction (LD) and sieving-pipette (Sedimentation) techniques.

# Improved equations for mean and standard deviations from mass of clay, silt and sand

$$\ln \mu = m_y (0.0049) + m_t (2.3) + m_d(5.76)$$

$$\ln \sigma^2 = my\, (0.0049)^2 + mt\, (2.3)^2 + md\, (5.76)^2 - (\ln \mu)^2$$

221 µm

| Texture | $m_d$ | $m_t$ | $m_y$ | $\mu$ | $\sigma$ |
|---|---|---|---|---|---|
| Sand | 0.92 | 0.05 | 0.03 | 5.40 | 1.21 |
| Loamy sand | 0.81 | 0.12 | 0.07 | 4.93 | 1.75 |
| Sandy loam | 0.65 | 0.25 | 0.1 | 4.31 | 2.05 |
| Loam | 0.42 | 0.40 | 0.18 | 3.33 | 2.20 |
| Silt loam | 0.08 | 0.79 | 0.13 | 2.27 | 1.28 |
| Silt | 0.06 | 0.87 | 0.07 | 2.34 | 1.03 |
| Sandy clay | 0.60 | 0.13 | 0.27 | 3.75 | 2.54 |
| Clay loam | 0.32 | 0.34 | 0.34 | 2.62 | 2.34 |
| Silty clay loam | 0.08 | 0.58 | 0.34 | 1.79 | 1.57 |
| Sandy clay | 0.53 | 0.07 | 0.40 | 3.21 | 2.75 |
| Silty clay | 0.10 | 0.45 | 0.45 | 1.61 | 1.75 |
| Clay | 0.20 | 0.20 | 0.60 | 1.61 | 2.25 |

Fractions of sand ($m_d$), silt ($m_t$) and clay ($m_y$) were chosen within a textural class.

5 µm

With respect to the original Shiozawa and Campbell formulation these equations are based on a measured mean in the clay fraction instead of arbitrary limits

# Results

- Sedimentation: because of non-spherical particles the method “over-estimates” the clay fraction
- Light diffraction: because of non-spherical particles the method “under-estimates” the clay fraction
- Optical methods: they are considered the most precise because they observe the particles. However they provide a 2D image, so errors may also be introduced by the unknown vertical dimensions (although they are often considered vary small with comparison to the horizontal dimensions).

# Conversion equations

- Van Dongen (1989) (68 samples) — $clay_{LD} = 0.185\ clay_{SED} + 0.662$
- Konert and Vanderberghe (1997) (158 samples) — $clay_{LD} = 0.361\ clay_{SED} - 0.232$
- Eshel et al. (2004) (42 samples) — $clay_{LD} = 0.345\ clay_{SED} + 2.69$
- This study (8 samples) — $clay_{LD} = 1.0317\ clay_{SED} - 0.0175$
- ……………………..

# Conclusions

- The bimodal model provides a good characterization of PSD for six of the eight samples analyzed, revealing that more complex distributions are required for soils where multimodal modes were found.

- The laser diffraction allowed to improve the parameterization by obtaining data in the clay fraction.

- Three techniques for the PSD determination have been compared: laser diffraction (LD), sedimentation, transmission electron microscopy (TEM) and image analysis:

  » LD method tends to underestimate the clay fraction when compared to the traditional sedimentation techniques;

  » LD method tends to overestimate the clay fraction when compared with TEM, when particles are assumed to be represented as spheres;

  » LD presents several advantages.

# What is needed

- Reliable mathematical relationships to convert from traditional sedimentation techniques to the laser techniques and vice-versa.
- Standardization of sample preparation and pre-treatment for laser diffraction (not present yet in most *methods of soil analysis*).
- Test and standardization of optical methods to overcome the limitations of particle shape assumptions.
- Better understanding of relationships between PSD information and structural information of the solid-pore matrix obtained from experimental methods such as x-ray tomography.

# Thank you for your attention