Exploring the particle size effect on the geochemical composition using experimental soil mixtures

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INTRODUCTION

- Fine fraction of sediment samples show higher element enrichment due to larger specific surface area (SSA)
- This assumption needs to be constantly examined and considered for fingerprinting studies because is often non-linear or more complex (Gaspar et al., 2022)
- Standard Particle Size Correction Factor (PSCF) is applied equally to all elements

OBJECTIVE

1. Explore in detail, and tracer by tracer, the effect of the particle size variation on geochemical composition to the correct estimation of source apportions
2. Analyse the effect of tracer selection methods in accurately estimating source apportionments in the presence of fine enrichment

METHODS

- Experimental mixture with known contribution of three experimental sources (33.3 % for each source) was created. Comparing different situations:
  - A. Like to like at 63 µ | Sources and mixture at <63 µ
  - B. Like to like at 20 µ | Sources and mixture at <2 µ
  - C. Fine enrichment | Sources at <63 µ and mixtures at <20 µ simulating the fine enrichment
  - D. Fine enrichment with PSCF particle size correction factor | Sources at <63 µ and mixtures at <20 µ but using the standard PSCF before unmixing

RESULTS

OBJECTIVE 1

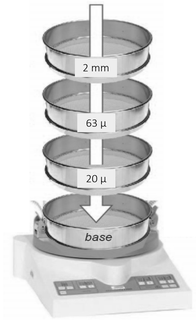
- Relationship between SSA and elemental geochemistry varies for each element and sample (different linearity, magnitude or direction)

OBJECTIVE 2

- Source apportionments estimated with unmixing models was sensitive to particle size variation on sources and mixtures
- Tracer selection was crucial in accurately estimating source contributions when there are differences in particle size between sources and mixture
- Using Conservativeness Index (CI) + Consensus Ranking (CR) + Consistent Tracer Selection (CTS) helps to minimize errors in source apportionments in scenarios of fine enrichment

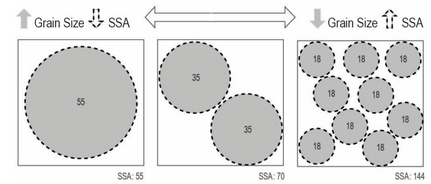
CONCLUSIONS

- Standard PSCF could negatively affect unmixing results when the element enrichment does not correspond to a higher SSA
- Alternative approaches are needed to improve the effectiveness of particle size correction factors in fingerprinting studies by avoiding uniform application for all elements
- Tracer selection method (CI+CR+CTS) identify tracers that fit the standard correction without having to measure individual behavior of each tracer with lab determinations in advance



PARTICLE SIZE EFFECT

Concentration VS Specific Surface Area (SSA)

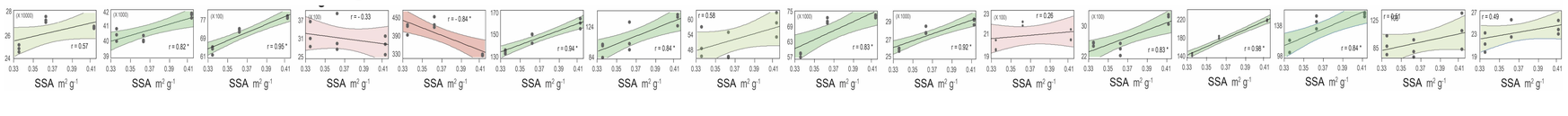


FingerPro
unmixing model

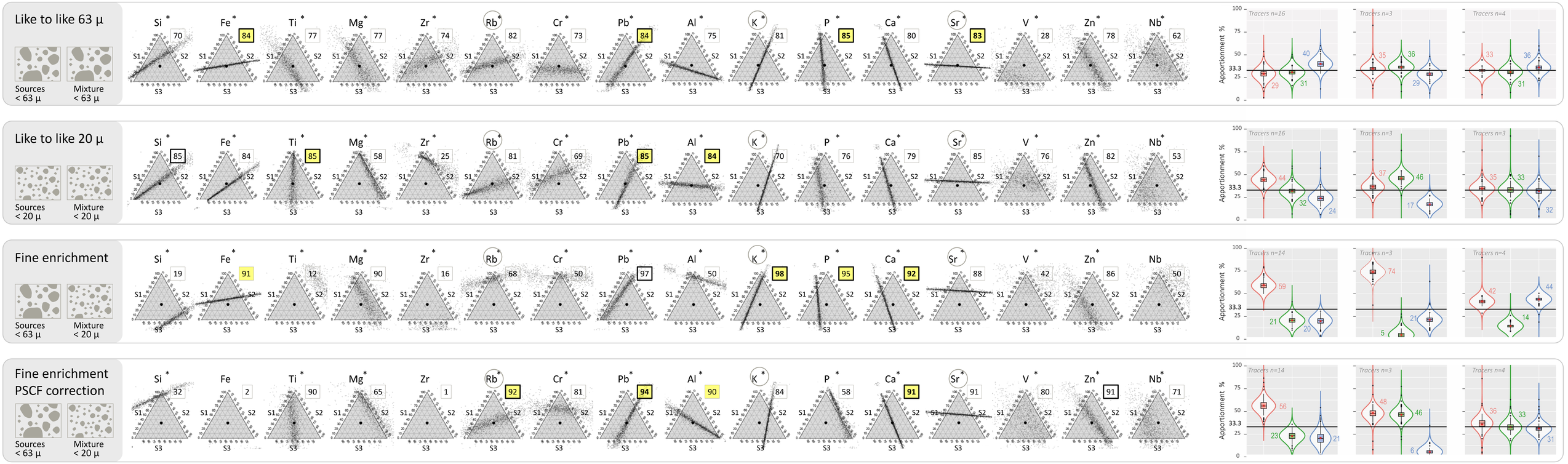
Experimental Mixture

- Source 1 33.3% S1
- Source 2 33.3% S2
- Source 3 33.3% S3

OBJECTIVE 1



OBJECTIVE 2



Range Test * KW + DFA ○ CI + CR + CTS CR

- **DFA** (*Discriminant Function Analysis*): method to discriminate sources without taking into account the mixture information
- **CI** (*Conservativeness Index*) + **CR** (*Consensus Ranking*) + **CTS** (*Consistent Tracer Selection*): methods to discriminate sources by taking into account the mixture information (CR) and with mathematical consistency (CTS)

* All tracer selection methods are avaible in Fingerpro. CI, CR and CTS Developed by EESA group (EEAD- CSIC)

- Gaspar, L., Blake, W.H., Smith, H.G., Lizaga, I., Navas, A., 2019. Testing the sensitivity of a multivariate mixing model using geochemical fingerprints with artificial mixtures. Geoderma 337, 498–510.
- Gaspar, L., Blake, W.H., Lizaga, I., Latorre, B., Navas, A., 2022. Particle size effect on geochemical composition of experimental soil mixtures relevant for unmixing modelling. Geomorphology, 403, 108178.
- Latorre, B., Lizaga, I., Gaspar, L., Navas, A., 2021. A novel method for analysing consistency and unravelling multiple solutions in sediment fingerprinting. Sci. Total Environ. 789, 147804.
- Lizaga, I., Latorre, B., Gaspar, L., Navas, A., 2020b. FingerPro: an R package for tracking the provenance of sediment. Water Resour. Manag. 34, 3879–3894.
- Lizaga, I., Latorre, B., Gaspar, L., Navas, A., 2020a. Consensus ranking as a method to identify non-conservative and dissenting tracers in fingerprinting studies. Sci. Total Environ. 720, 137537.

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