Classification and identification of oil samples and samples of oil pollution in environment by cluster analysis

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Oil Analysis

Technology

oil extraction
production
transportation
processing
petroleum products using

Data:
elemental composition
viscosity and density
fractional composition
group analysis
(SARA analysis)

General assessment of the
analysis metrology problem:

rather satisfactorily

Geochemistry & Environmental Chemistry

Objects:
dispersed and dissolved organic matter
in rocks, soil, water, atmosphere

Data: isomeric and homologous composition

Problems:
dynamic and spatially variable and
time-varying system with variability
under the influence of uncontrolled
exterior factors;
limited   precision of analytical procedures;
no standards (with the exception
of elemental and isotopic composition)

General assessment of the
analysis metrology problem:

absolutely unsatisfactorily

The purpose of our work:

Determine (to decide, to define):

is it possible to reliably identify oil samples,

if we take into account all the conditions

that complicate the work of the researcher:

– the limited accuracy of analyzes,

– the absence of standard samples
for assessing real not zero errors,

– the possibility of changing the composition of the
samples over time under the influence of uncontrolled
and often unknown external factors.

Samples:

Oil samples from three production wells (operating on two different productive geological horizons), sampling three times with an interval of ~ 2 months (9 samples)

Methods:

Crude oil samples SARA analysis with GC/MS study of the paraffin isomeric composition in saturated compounds fraction
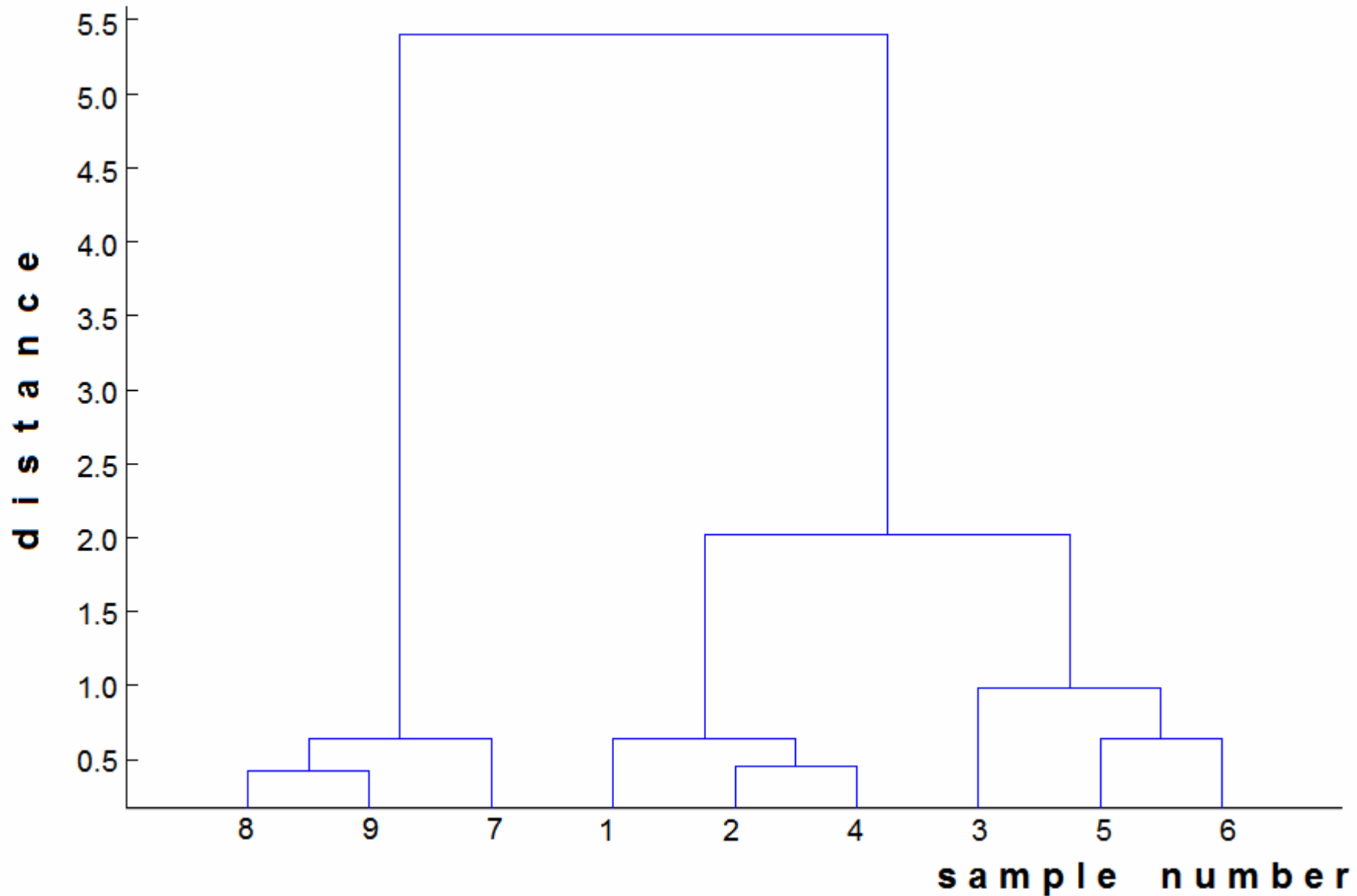
Data:

Relative contents of $C_{10}H_{22} \div C_{34}H_{70}$ paraffin, pristan and phytan in 9 samples

Data processing:

Cluster analysis using Euclidean measure for distances between object characteristics and Ward's algorithm for stepwise data clustering (MATLAB procedures)

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Results: dendrogram

Results of formal data clustering (see dendrogram):

1.According to the paraffin composition, 9 samples are divided into 3 clusters.

2. Each cluster groups the oil samples recovered from the same well.

3. The distance between the centers of two clusters is less than the center of the third.

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What does it mean:

1. The total errors in the analysis results allow to reliably distinguish the sources of oil samples.

2. Changes in the composition of recovered oil for 6 months of observations do not exceed the analysis errors.

3. Wells which operating on the same productive horizon have been identified.

4. The validity for using of statistical assessments of the reproducibility of the results of the samples composition analysis, as well as the values of geochemical indices, calculated from this composition was shown.

Conclusions

1. It has been shown that the root-mean-square deviations of the results of the analysis of the relative contents of paraffins (intralaboratory reproducibility) and the calculated geochemical indices do not exceed 5%.

2. This should be taken into account when comparing and interpreting the values of geochemical indices of various samples in organic geochemistry and environmental chemistry.

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Thank you for your attention!

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