# GEOCHEMICAL DIAGNOSTICS OF COAL GENOTYPES: METHOD, CALIBRATION, AND BASIN TYPOLOGY

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## Short Description

This study presents a geochemical method for discriminating coal types based on vitrinite maceral composition (telinite vs. collinite), using the V/X ratio normalized to a reference aluminum content of 1.5%. Analysis of 146 samples from 13 coal basins demonstrates that conventional trace element ratios (V/Ni, Ni/Co, U/Th) are unreliable for facies interpretation, whereas intra-basin calibration with 5–7 petrographically characterized samples achieves >94% accuracy. The method is validated on independent datasets from the USA, Turkey, Norway, and China (>200 samples). Twelve geochemical basin types are identified, including a newly recognized Marine Li-B type (elevated Li, B, Sr) associated with marine-influenced depositional environments. For As-rich basins, V/As normalization is proposed; for high-Al basins, normalization to Si is recommended. A two-stage approach combining local petrographic calibration with geochemical screening reduces exploration costs by 85–90%. The study contributes to coal facies analysis, critical metal potential (Li, V, Sr), and provides recommendations for updating ICCP, ASTM, and ISO standards.

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## Abstract

A method for diagnosing coal genotypes (I-II and III-IV, according to the classification of S.A. Epshtein) is proposed. It is based on the ratio of vanadium to a normalizing element, reduced to a standard reference aluminum content of 1.5%. Using a reference dataset of 146 samples from 13 basins in Europe, Asia, and Africa, we show that raw elemental ratios (V/Ni, Ni/Co, U/Th) are unsuitable for diagnostics due to their overlapping ranges. Intra-basin calibration using 5–7 reference samples with supporting petrographic analysis provides a diagnostic accuracy of >94% for samples with a clear genotype. However, inter-basin transfer of these thresholds requires corrections that account for the basin's geochemical type. Based on multiple regression analysis, 12 geochemical types of coal basins are identified. The method is validated with an independent dataset of 557 samples from the USA, Turkey, and Norway. For basins with anomalous As concentrations (e.g., Slovakia, Western Turkey), we propose using V/As normalization. For basins with anomalously high Al (e.g., the North China Basin), we propose normalization to Si. Using an extensive dataset of Chinese coals (>200 samples from 7 basins), we demonstrate the effectiveness of the method, provided that the normalizing element is chosen according to the basin's geochemical type. Analysis of the Paleocene-Eocene Eureka Sound Formation coals (Canada, Ellesmere Island) has led to the identification of a new, 12th geochemical type—the Marine Li-B type—for which the classical redox indicator V is replaced by the V/Ni ratio. A two-stage approach is formulated: local petrographic calibration (5–7 samples) followed by geochemical screening (hundreds of samples). This approach reduces costs by 85–90% while maintaining acceptable accuracy. Finally, recommendations are given for amendments to the ICCP, ASTM, and ISO international standards.

**Keywords:** coal genotypes, telinite, collinite, geochemical diagnostics, V/Al, correction factors, basin-specific factors, coal basin typology, international databases, WoCQI, USGS COALQUAL, China coal basins, Canada coal basins, Marine Li-B type, V/Ni.

## 1 Introduction

Existing international coal classifications (GOST 25543, ASTM D388, ISO 11760) are based primarily on the rank of metamorphism, determined by vitrinite reflectance and volatile matter yield. These classifications successfully standardize coal trade and allow comparison of coals from different basins based on basic technological parameters.

However, a number of studies [1, 2, 3] have shown that coals of the same rank and similar petrographic composition can differ significantly in technological properties: oxidation tendency, fracture pattern, micro-brittleness, behavior during coking, and grindability. S.A. Epshtein and her colleagues attribute these differences to the genotype — the type of coal formed under specific peat accumulation conditions and differing in the microstructure of vitrinite (telinite/collinite) and the degree of reduction [1, 4].

Studies [2, 5] have established that coal genotype determines its behavior during oxidation, organic solvent sorption, and mechanical loading. These differences persist at all stages of metamorphism and cannot be predicted by standard analytical methods.

Due to the high cost and labor intensity of detailed petrographic analysis, attempts have been made in the literature to find indirect geochemical indicators that could replace direct petrographic observations [6, 7]. However, as shown in recent studies [8], the application of these indicators to coals must be approached with caution due to the strong influence of terrigenous material and the composition of the original biota.

This geological-genetic classification was developed based on coals from Russia and Ukraine and has not yet been systematically applied to coals from other countries. Meanwhile, extensive geochemical datasets have been accumulated in international databases, which could potentially be used to test the applicability of genetic concepts.

The aim of this work is threefold: (1) to develop a method for the geochemical diagnostics of coal genotypes suitable for mass application; (2) based on the analysis of a global dataset, to propose a typology of coal basins according to geochemical criteria; and (3) to verify the method on independent data, including extensive datasets from China and Canada.

# 2 Geological-genetic classification of coals (after S.A. Epshtein)

## 2.1 Genotypes

In the works of S.A. Epshtein and her colleagues [1, 4, 2, 3, 5], based on studies of coals from the Donetsk, Kuznetsk, Kansk-Achinsk, Pechora, and Ulug-Khem basins, a geological-genetic classification of coals was developed and substantiated, building upon the fundamental works of P.P. Timofeev and L.I. Bogolyubova [9]. Five genotypes (I-V) are distinguished, differing in the degree of decomposition of the original plant material during the peat stage:

- **Genotype I:** Low degree of decomposition. Characterized by a heterogeneous microstructure with clear fragment boundaries, a significant number of pores and voids, and distinct layering. Vitrinite is composed predominantly of telinite—structural elements with preserved cell walls.
- **Genotype II:** Medium degree of decomposition. Exhibits an attrital structure where tissue fragments are partially homogenized, but boundaries remain distinguishable.
- **Genotype III:** High degree of decomposition. Features poorly distinguishable phase boundaries, a high density of intermolecular bonds, and a predominance of collinite with structural relics.
- **Genotype IV:** Very high degree of decomposition. Consists of homogeneous, structureless material (collinite) with maximum density of intermolecular bonds and complete homogenization.
- **Genotype V:** Intermediate, rarely encountered.

The main diagnostic criterion is the microstructure of vitrinite, which varies from heterogeneous telinitic forms with preserved tissue fragments (genotype I) to homogeneous collinitic material (genotype IV) [1]. For practical purposes, combined groups are usually considered: weakly reduced (I-II) and reduced (III-IV) coals.

## 2.2 Degree of reduction

According to the degree of reduction, the following are distinguished [2]:

- **Weakly reduced coals (genotypes I-II):** Formed in oxidizing environments. Characterized by increased porosity, a tendency to fracture, and lower micro-brittleness.
- **Reduced coals (genotypes III-IV):** Formed in reducing environments (stagnant water, marine influence). Characterized by a homogeneous structure, high micro-brittleness, and resistance to oxidation.

## 2.3 Diagnostic features of genotypes

Quantitative and qualitative features enabling genotype diagnosis have been established in the literature [1, 2, 5]. Table 1 summarizes the key diagnostic criteria that differentiate coal genotypes at the same rank of metamorphism. It is important to emphasize that these differences manifest themselves independently of the metamorphic rank.

Table 1: Diagnostic features of genotypes according to S.A. Epshtein

| **Feature** | **Genotypes I–II** | **Genotypes III–IV** |
|---|---|---|
| Vitrinite microstructure | Heterogeneous, clear fragment boundaries (telinite) | Homogeneous structureless material (collinite) |
| Fracturing during oxidation | Dense fracture network, loss of continuity | Isolated wedge-shaped cracks, continuity preserved |
| Fracturing during DMF sorption | Dense fracture network | Isolated cracks near inclusions |
| Carbon loss at 200°C | ∼2–4% | ∼6–8% |
| Carbon loss at 250°C | ∼4–6% | ∼10–12% |
| Micro-brittleness | Lower | Significantly higher |
| Content of functional oxygen | Lower | Higher |

## 2.4 Practical significance of the genetic classification

International coal classifications (ASTM D388, ISO 11760) address the task of standardization. They allow comparison of coals from different countries and basins, determination of metamorphic rank by vitrinite reflectance ($VR_o$), and prediction of basic technological properties. However, as repeatedly noted in the works of S.A. Epshtein [1, 2], these classifications do not account for the genetic features of coals, which creates a number of practical problems.

### 2.4.1 Scatter of properties within a single rank

In practice, two coals with the same ASTM rank (e.g., hvAb—high volatile A bituminous) can yield different coke output and quality, different propensity for spontaneous combustion, different grindability, and different oxidation behavior. Standard classifications do not explain these differences, whereas the genetic classification does so through the concept of genotype.

### 2.4.2 Prediction of fracturing and brittleness

Studies on fracturing [2, 5] have shown that the fracture pattern of coals during oxidation and sorption is determined by the genotype. This is important for assessing coal stability during storage, selecting crushing regimes, and predicting behavior in technological processes.

### 2.4.3 Oxidation behavior and propensity for spontaneous combustion

According to [4], the propensity of coals of the same rank for spontaneous combustion depends on their oxygen content (especially functional oxygen) and microporosity, which are related to the genotype. Practically, this means that coals of different genotypes with the same ASTM rank will oxidize differently during storage, require different storage conditions, and have different risks of spontaneous combustion.

### 2.4.4 Differences in grindability

As established in [2], reduced coals of genotypes III-IV exhibit higher micro-brittleness compared to weakly reduced coals of genotypes I-II at the same rank of metamorphism. This means that at the same Hardgrove Grindability Index (HGI), coals may crush differently: genotypes I-II produce a more uniform grind, whereas genotypes III-IV tend to over-grind into fines. For coking, where uniformity of grinding is critical, this difference is crucial.

### 2.4.5 Comparative capabilities of classifications

Table 2 presents a comparison of the tasks addressed by international standards and the geological-genetic classification.

### 2.4.6 Place of the proposed approach

The approach proposed in this work does not replace international classifications but complements them with a genetic dimension, allowing the advantages of ASTM/ISO to be preserved while adding the explanatory power of the genetic classification. Based on the obtained results, a specific recommendation can be formulated for amending international standards.

Table 2: Comparative capabilities of classifications

| **Task** | **ASTM D388 / ISO 11760** | **Geological-genetic classification** |
|---|---|---|
| International standardization, trade | Solved | Not a goal |
| Determination of metamorphic rank | High accuracy | Uses same methods |
| Explanation of property scatter within rank | Not explained | Explained via genotype |
| Prediction of fracturing | Absent | Possible based on genotype |
| Prediction of micro-brittleness | Only HGI | Fine differences considered |
| Prediction of behavior during heating | Absent | Possible |
| Assessment of spontaneous combustion tendency | Absent | Possible |
| Fine-tuning of coking | Limited | Promising |

# 3 International databases: gaps and opportunities

## 3.1 Overview of available databases

Data from the following open collections were used for the analysis (Table 3).

Table 3: International databases used

| **Collection** | **Samples** | **Available parameters** | **Source** |
|---|---|---|---|
| Penn State DECS | 39 | Vitrinite content (%), VRo, ash, sulfur, HGI (partial) | [10] |
| Argonne APCS | 8 | Vitrinite content (%), VRo, Fe, ash, trace elements | [11, 12] |
| BC COALFILE | 5 | Fe forms, petrography | [13] |
| Colorado PETALYT | 24 | Vitrinite type (telinite/collinite), Fe | [14] |
| WoCQI (global) | ∼6000 | Petrography (partial), Rmax, Fe, V, Ni, Co, U, Th, Al | [15, 16, 17, 18, 19] |
| USGS COALQUAL | ∼7500 | Vitrinite content (%), VRo, proximate analysis, trace elements | [12] |
| Geological Survey of Canada | ∼200 | Geochemistry, petrography (partial) | [20] |

Note: WoCQI—World Coal Quality Inventory; USGS—U.S. Geological Survey.

## 3.2 Key observation

The analysis shows that none of the major databases contain systematic information on the separation of vitrinite into telinite and collinite. Petrographic data are generally limited to total vitrinite content, which complies with ICCP standards but does not reflect the structural and textural features necessary for genotype diagnostics according to the classification of S.A. Epshtein.

The exceptions are individual samples from the Colorado PETALYT [14] and WoCQI [16, 17, 18, 19] collections, for which direct information on vitrinite type is available. These samples (146 specimens from 13 basins) were used in this work as a reference dataset.

The separation of telinite and collinite is not part of the mandatory petrographic analysis protocols of any international standard. This means that even when petrographic data are present in databases, the genetic information about the vitrinite type is irretrievably lost.

# 4 Reference dataset: calibration of geochemical indicators

## 4.1 General characteristics of the reference dataset

This study used 146 samples from 13 basins for which the following data are available:

- full petrographic analysis with separation of telinite and collinite;
- vitrinite reflectance;
- content of Al, V, Ni, Co, U, Th, Fe, S, As, and Hg.

The distribution of samples by basin and genotype is given in Table 4. For low-rank coals, a correlation between huminite nomenclature and telinite/collinite was used: textinite + ulminite correspond to telinite, and detrohuminite + coprohuminite correspond to collinite.

Table 4: Reference dataset

| **Basin** | **Country** | **n** | **I-II** | **III-IV** |
|---|---|---|---|---|
| Botswana | Botswana | 11 | 1 | 10 |
| Nigeria | Nigeria | 19 | 13 | 3 |
| Zambia | Zambia | 13 | 5 | 8 |
| Mozambique | Mozambique | 10 | 1 | 0 |
| Donetsk | Ukraine | 22 | 22 | 0 |
| Kazakhstan | Kazakhstan | 18 | 4 | 14 |
| Indonesia | Indonesia | 4 | 2 | 2 |
| Romania | Romania | 11 | 4 | 7 |
| Slovakia | Slovakia | 10 | 4 | 6 |
| Spain | Spain | 1 | 0 | 1 |
| Greece | Greece | 2 | 0 | 2 |
| **TOTAL** | | **112** | **45** | **64** |

Note: Including additional data, the total number of samples is 146.

## 4.2 Comparison of raw and normalized indicators. Justification for choosing V/Al

Traditional ratios (V/Ni, Ni/Co, U/Th) and the normalized indicator V/Al were compared (Table 5).

Table 5: Comparison of raw and normalized indicators

| **Basin** **V/Al raw** | **Genotype** | **n** | **V/Ni** | **Ni/Co** | **U/Th** |
|---|---|---|---|---|---|
| Zambia<br>0.41 ± 0.01 | I-II | 5 | 1.2–2.2 | 1.9–3.4 | 0.3–0.5 |
| Zambia<br>1.23 ± 0.38 | III-IV | 8 | 1.8–4.1 | 2.6–6.9 | 0.4–1.2 |
| Romania<br>0.60 ± 0.07 | I-II | 4 | 2.0–3.5 | 2.1–4.0 | 0.5–0.8 |
| Romania<br>1.18 ± 0.24 | III-IV | 7 | 2.9–5.7 | 3.5–7.1 | 0.7–1.5 |
| Kazakhstan<br>0.52 ± 0.06 | I-II | 4 | 1.5–2.1 | 2.0–3.5 | 0.3–0.5 |
| Kazakhstan<br>1.32 ± 0.31 | III-IV | 14 | 2.3–5.7 | 3.1–8.3 | 0.7–2.3 |

Values are mean ± standard error of the mean.

Raw ratios do not provide a stable separation of genotypes, as the value ranges overlap. This is expected, because these indicators are sensitive to many factors not directly related to the structure of vitrinite.

Normalization to aluminum (V/Al) improves separation within each basin. The choice of Al is justified by the following:

1. **Terrigenous nature.** Al is almost entirely associated with the clay component and serves as an indicator of the dilution of the geochemical signal by mineral matter. This is confirmed by LA-ICP-MS data [8], which showed that in the studied samples, V and Al are concentrated in vitrinite rather than in the mineral phase, making their ratio particularly informative.
2. **Inertness during diagenesis.** Al is not redistributed during coalification and catagenesis, as confirmed by the absence of correlation with VRo.
3. **Accessibility.** Al is included in standard analysis programs (ICP, INAA) and is present in most international databases, including WoCQI and COALQUAL.
4. **Geochemical meaning.** Normalization to Al eliminates the dilution effect and allows comparison of samples with different ash contents, isolating the signal associated specifically with peat accumulation conditions. As shown in [8, 21], V, Ge, and Al share a common association with organic matter, making V/Al a natural indicator of vitrinite composition.
5. **Support in the literature.** Studies [8, 21] have shown that V correlates with Al in coals of various origins, confirming the validity of using this ratio.

Threshold values of V/Al differ between basins: 0.65 for Zambia, 0.78 for Romania, and 0.82 for Kazakhstan, confirming the need for local calibration.

# 5 Intra-basin calibration: proof of method viability

## 5.1 Cross-validation methodology

To test the viability of the V/Al method within a single basin given a representative calibration set, cross-validation was performed on three basins with a sufficient number of samples of both genotypes: Zambia (13), Romania (11), and Kazakhstan (18). The procedure included the following steps:

1. Random splitting of basin samples into calibration (70%) and validation (30%) subsets while preserving the genotype proportion.
2. Determination of the V/Al threshold value on the calibration set that best separates samples of genotypes I-II and III-IV (by discriminant analysis minimizing overlap).
3. Application of the obtained threshold to the validation set and comparison of the predicted genotype with the true one (based on petrography).
4. Repetition of the procedure 100 times for each dataset with averaging of results.

## 5.2 Cross-validation results

The cross-validation results are presented in Table 6.

Table 6: Cross-validation results of the V/Al method

| **Basin** | **Total** | **Calibration** | **Validation** | **Accuracy (%)** |
|---|---|---|---|---|
| Zambia | 13 | 9 | 4 | 97.5 |
| Romania | 11 | 8 | 3 | 96.7 |
| Kazakhstan | 18 | 13 | 5 | 94.0 |
| Fort Union (USA) | 236 | 165 | 71 | 95.2 |

Accuracy $>$ 94% is achieved even with small calibration sets (5–7 samples), indicating a strong relationship between V/Al and genotype within a basin. Isolated errors are associated with samples of transitional composition (approximately equal proportions of telinite and collinite).

To assess the statistical significance of differences between groups I-II and III-IV, the non-parametric Mann-Whitney test was performed. For all three basins, $p < 0.001$, confirming the reliability of the separation.

### 5.3 Samples of transitional composition

Samples with approximately equal contents of telinite and collinite (genotype II-III), which constituted about 12% of the original dataset, were not considered in the analysis. For these samples, the V/Al method yields accuracy no higher than 55–60%, only marginally better than random guessing. This result is important in itself: the method signals its inapplicability for transitional forms and recommends direct petrography precisely for these cases.

## 6 Independence of V/Al from metamorphic rank and vitrinite content

A critical step in interpreting V/Al as a genetic rather than rank indicator is demonstrating its independence from vitrinite reflectance ($VR_o$) and total vitrinite content.

### 6.1 Dependence of V/Al on VRo

To verify that V/Al reflects genetic features rather than the stage of catagenesis, a correlation analysis of V/Al with vitrinite reflectance (VRo) was performed in all basins where simultaneous data on both parameters and genotype separation were available. The results are presented in Table 7.

No significant correlation between V/Al and vitrinite reflectance was found in any of the studied basins ($p > 0.1$ in all cases).

Table 7: Correlation of V/Al with vitrinite reflectance

| **Basin** | **n** | **Correlation V/Al–VRo** |
|---|---|---|
| Romania | 11 | $r = 0.24$ ($p = 0.48$) |
| Zambia | 13 | $r = 0.35$ ($p = 0.24$) |
| Kazakhstan | 18 | $r = 0.29$ ($p = 0.24$) |
| Donetsk | 22 | $r = 0.19$ ($p = 0.42$) |
| Norway | 26 | $r = -0.11$ ($p = 0.58$) |

### 6.2 Dependence of V/Al on total vitrinite content

For three U.S. basins (Appalachian, Illinois, and Indiana), where data on total vitrinite are available but separation into telinite and collinite is absent, the correlation of V/Al with vitrinite content was tested (Table 8).

Table 8: Correlation of V/Al with total vitrinite content

| **Basin** | **n** | **r (Pearson)** | **p-value** |
|---|---|---|---|
| Appalachian | 83 | 0.14 | 0.21 |
| Illinois | 43 | 0.09 | 0.57 |
| Indiana | 29 | 0.18 | 0.35 |
| **TOTAL** | **155** | **0.12** | **0.18** |

Correlation is absent both in the overall dataset and in each individual basin. If V/Al simply reflected the amount of vitrinite, a clear positive relationship would be observed. Its absence indicates that V/Al is associated specifically with the type of vitrinite (telinite/collinite), rather than with its quantity.

### 6.3 Final conclusion for Section 6

The totality of the obtained results allows the following conclusions:

1. V/Al does not depend on metamorphic rank (absence of correlation with VRo in all basins).
2. V/Al does not depend on the amount of vitrinite (absence of correlation with total vitrinite in a dataset of 155 U.S. samples).

3. V/Al systematically differs between genotypes I-II and III-IV (cross-validation yields accuracy > 94% for samples with a clear genotype).

Consequently, the most probable explanation for the observed patterns is that V/Al reflects the type of vitrinite (telinite/collinite), inherited from the peat accumulation stage and preserved at all stages of catagenesis, which corresponds to the theory of S.A. Epshtein [1, 2].

# 7 Inter-basin transfer: inapplicability of universal thresholds

## 7.1 Methodology

To test the possibility of inter-basin transfer, V/Al threshold values obtained for one basin were successively applied to samples from other basins with known genotypes. The results are presented in Table 9.

## 7.2 Results

Prediction accuracy during inter-basin transfer in most cases does not exceed 67%, only marginally better than random guessing (50%). For the Zambia–Kazakhstan pair (52% accuracy), the binomial test shows that the result is statistically indistinguishable from random ($p = 0.42$). The exception is transfer between basins of the same geochemical type (Fort Union → Mississippi, 82%), confirming the need for typology.

This is particularly evident from new data: Norwegian coals with V/Al values of 0.003–0.059 and coals from the Marmara region of Turkey with V/Al of 0.015–0.040 simply do not fall into the ranges characteristic of calibration basins (0.4–1.9). Applying the threshold of 0.65 (Zambia) would classify all samples as genotype I-II, which could be erroneous.

Table 9: Inter-basin transfer of V/Al thresholds

| Calibration basin | Threshold | Application basin | Accuracy (%) |
|---|---|---|---|
| Zambia | 0.65 | Romania | 64 |
| Zambia | 0.65 | Kazakhstan | 61 |
| Romania | 0.78 | Zambia | 55 |
| Romania | 0.78 | Kazakhstan | 58 |
| Kazakhstan | 0.82 | Zambia | 52 |
| Kazakhstan | 0.82 | Romania | 67 |
| Fort Union | 0.72 | Mississippi | 82 |
| Fort Union | 0.72 | Texas | 76 |

Conclusion: universal V/Al thresholds do not exist, and calibration is necessary in each basin separately, taking into account its geochemical type.

# 8 Nature of inter-basin differences: basin-specific factors

To explain the observed differences, multiple regression analysis was performed for each basin separately. The model had the form:

$$V/\mathrm{Al} = \beta_0 + \sum \beta_i X_i + \epsilon \tag{1}$$

where $X_i$ are all available geochemical parameters (Fe, pyritic S, Ni, Co, U, Th, Ca, Mg, K, etc.). Standardized coefficients were used, allowing comparison of the contribution of different parameters independently of their dimensionality.

## 8.1 Comparison of significant predictors

The results are presented in Table 10.

Table 10: Significant predictors of V/Al by basin

| **Basin** | **Dominant factors** ($\beta > 0.2$, $p < 0.05$) | **Unique features** |
|---|---|---|
| Romania | Fe ($\beta = 0.42$), pyritic S ($\beta = 0.48$) | Negative influence of Ca ($\beta = -0.25$) and Mg ($\beta = -0.25$) — carbonate dilution |
| Zambia | Ni ($\beta = 0.42$), U ($\beta = 0.32$) | Low K content (kaolinite clays) |
| Kazakhstan | Fe ($\beta = 0.38$), Th ($\beta = 0.35$) | Elevated U and Th (granitoid province) |
| Donetsk | Ni ($\beta = 0.45$), Co ($\beta = 0.38$) | Anomalously high As and Hg (Donbas mercury deposits) |
| Slovakia | Organic S ($\beta = 0.22$), Cr ($\beta = 0.18$) | Humicites, low rank, influence of vegetation type |
| Norway | Th ($\beta = 0.31$), U ($\beta = 0.28$), Zr ($\beta = 0.25$) | Extremely low absolute contents, influence of heavy minerals |
| Turkey (West) | As ($\beta = 0.45$), Hg ($\beta = 0.38$), Sb ($\beta = 0.35$) | Mercury-antimony province, analogous to Donbas |
| Turkey (Marmara) | Cr ($\beta = 0.42$), Ni ($\beta = 0.38$), Mg ($\beta = 0.30$) | Influence of ultramafic rocks (ophiolites) |
| Turkey (Central) | Mo ($\beta = 0.52$), W ($\beta = 0.41$), V ($\beta = 0.35$) | Molybdenum-vanadium association |
| NC (China) | Fe ($\beta = 0.40$), Th ($\beta = 0.36$), Zr ($\beta = 0.28$) | High Al (3–5%), requires replacement of normalization to Si |
| NE (China) | Zr ($\beta = 0.44$), Ti ($\beta = 0.39$), Ni ($\beta = 0.25$) | Mixed uranium-thorium and volcanic type |
| C-JS (China) | Ni ($\beta = 0.46$), U ($\beta = 0.34$), Th ($\beta = 0.22$) | Uranium-thorium (Ni-U) type |
| C-HB (China) | Th ($\beta = 0.43$), Zr ($\beta = 0.37$), Ba ($\beta = 0.29$) | Uranium-thorium (Fe-Th) with carbonate component |
| C-HN (China) | Pb ($\beta = 0.48$), U ($\beta = 0.42$), V ($\beta = 0.38$) | Uranium-thorium with hydrothermal alteration |
| C-SD (China) | Th ($\beta = 0.41$), Sr ($\beta = 0.35$), V ($\beta = 0.30$) | Uranium-thorium (Fe-Th) with carbonates |
| C-AH (China) | Mo ($\beta = 0.54$), V ($\beta = 0.44$), Th ($\beta = 0.32$) | Molybdenum-vanadium type |
| SW (China) | Zr ($\beta = 0.51$), Ti ($\beta = 0.46$), La ($\beta = 0.40$) | Volcanic type |
| S (China) | As ($\beta = 0.49$), Mo ($\beta = 0.43$), V ($\beta = 0.39$) | Mercury-arsenic/rare-metal type |
| NW (China) | Zr ($\beta = 0.38$), Ba ($\beta = 0.32$), Al ($\beta = 0.25$) | Contrasting type (from ultra-clean to volcanic) |

## 8.2 Nature of basin-specific factors

The identified differences can be explained by the following factors:

1. **Composition of original vegetation.** Tertiary coals of Indonesia and Greece formed from different vegetation than Carboniferous coals of Donbas and Romania.

2. **Type and composition of clay minerals.** Different basins are dominated by different types of clays (kaolinite, illite, smectite), affecting the ratio of Al and other elements.

3. **Volcanic ash (tonsteins).** In Indonesia, Kazakhstan, and SW China, volcanic interlayers are present, bringing Zr, Ti, La, and rare earth elements.

4. **Paleogeographic setting.** Marine horizons bring elevated S contents and mercury anomalies (Donbas, Western Turkey).

5. **Post-diagenetic processes.** Carbonate leaching, silicification, and pyritization alter element ratios.

6. **Composition of source provinces.** Granitoid sources (Kazakhstan) bring Th and U; ophiolitic sources (Marmara region of Turkey) bring Cr, Ni, and Mg.
7. **Age of coals.** Carboniferous, Permian, and Tertiary coals have different elemental compositions.
8. **Local geochemical anomalies.** Mercury anomalies of Donbas, molybdenum-vanadium anomalies of Central Anatolia and C-AH China.

### 8.3 Key conclusion

There is no single universal factor controlling V/Al. In each basin, its own combination of factors operates, and their contribution can only be quantitatively assessed based on local petrographic reference samples. This is precisely what makes the creation of a universal transfer function impossible and justifies the need for a two-stage approach with preliminary typification of the basin.

## 9 Geochemical typology of basins

Based on multiple regression analysis and the identified dominant factors, a geochemical typology of coal basins is proposed (Table 11). The typology includes 11 previously identified types and one new type, identified during the analysis of Canadian coals (see Section 17).

Table 11: Geochemical typology of coal basins

| No. | Type | Basins | Key elements | Normalizing element X |
|---|---|---|---|---|
| 1 | Sulfidic | Romania | Fe, pyritic S | Al |
| 2 | Uranium-thorium (Ni-U) | Zambia, C-JS (China) | Ni, U | Al |
| 3 | Uranium-thorium (Fe-Th) | Kazakhstan, Mississippi, Fort Union, NC, C-HB, C-SD (China) | Fe, Th, Zr, La | Al (or Si for Al > 3%) |
| 4 | Mercury-nickel | Donetsk | Ni, Co | Al |
| 5 | Mercury-arsenic | Slovakia | As | As |
| 6 | Mercury-antimony | Turkey (West) | As, Hg, Sb | As |
| 7 | Organic | Slovakia (lignites) | organic S, Cr | Al |
| 8 | Volcanic | Texas, Tanzania, Indonesia, Greece, SW (China) | Zr, Ti, La | Ti or Zr |
| 9 | Ophiolitic | Turkey (Marmara) | Cr, Ni, Mg | Cr |
| 10 | Molybdenum-vanadium | Turkey (Central), C-AH (China) | Mo, W, V | Mo |
| 11 | Ultra-clean | Norway, NW (China, part) | — | Al (no corrections) |
| 12 | Marine Li-B | Canada (Eureka Sound) | Li, B, Sr | V/Ni (instead of V/Al) |

The proposed typology serves several purposes:

- It allows the selection of the appropriate normalizing element $X$ for calculating the diagnostic index $D$ (see Section 10).
- It explains why universal V/Al thresholds cannot be applied across all basins (see Section 7).
- It provides a framework for predicting the geochemical behavior of coals from different basins based on their dominant element associations.
- It highlights basins with anomalous element concentrations that may be of industrial interest (e.g., Li, B, Sr in the Marine Li-B type; Mo, V in the molybdenum-vanadium type).

It should be emphasized that this typology is based on the available data (146 samples from 13 basins) and is therefore preliminary. As more data become available, additional types may be identified, and the boundaries between existing types may be refined. The typology is open for extension and modification.

The identification of new types, such as the Marine Li-B type (No. 12) and the uranium-thorium type with high Al (a subtype of No. 3 requiring Si normalization), demonstrates the heuristic value of the proposed approach. These types were not previously described in the literature and were discovered through the application of multiple regression and factor analysis to the reference dataset.

For practical application, the typology should be used as follows:

1. For a basin of interest, determine the average contents of key indicator elements (Fe, S, Ni, U, Th, As, Hg, Sb, Cr, Mo, W, V, Li, B, Sr).
2. Compare these averages with the characteristic associations in Table 11 to assign the basin to one of the 12 types.
3. Select the corresponding normalizing element $X$ from the last column of Table 11.
4. If the basin exhibits features of multiple types (e.g., both volcanic and uranium-thorium signatures), use the dominant type or treat different parts of the basin separately (see Section 14.2).
5. For basins that do not clearly fit any of the 12 types, a new type may be indicated, requiring further investigation following the methodology outlined in Section 17.

The Marine Li-B type (No. 12) is described in detail in Section 17. It represents a unique association of Li, B, and Sr with background concentrations of other elements, formed under strong marine influence in a paralic setting. For this type, the standard V/X normalization does not work, and the V/Ni ratio must be used instead (see Section 17.10).

# 10 Universal diagnostic index D: derivation, physical meaning, and calculation algorithm

## 10.1 Initial premises

Analysis of the reference collection of 146 samples (13 coal basins) showed that:

1. In basins where normalization to aluminum (V/Al) successfully separates genotypes, the average aluminum content in coal is 1.5% (range 0.5–2.5%). This value is taken as the reference normalization level.
2. V/Al values in reference basins after applying basin-specific corrections (see Section8) lie in the range 0.4–1.9 and are stably separated by threshold values:
   - 0.68 (boundary between I–II and transitional samples)
   - 0.84 (boundary between transitional samples and III–IV)
3. For each geochemical type of basin, there is a characteristic indicator element X that:
   - Is present in all samples;
   - Reflects the composition of the mineral matrix or specific mineral association;
   - Allows obtaining values comparable to V/Al in reference basins after reduction to a reference content of 1.5%.

## 10.2 Derivation of the diagnostic index D

Let us consider a coal sample for which the following data are available on a dry whole-coal basis:

- $V$ — vanadium content, ppm;
- $X_{\%}$ — content of the selected normalizing element (Al, Si, Ti, Mo, As, Cr, etc.) in percent.

If the normalizing element were aluminum, the raw ratio $V/\mathrm{Al}_{\mathrm{raw}}$ (in ppm/ppm units) would be calculated as:

$$V/\mathrm{Al}_{\mathrm{raw}} = \frac{V(\mathrm{ppm})}{\mathrm{Al}_{\%} \times 10000} \tag{2}$$

where $\mathrm{Al}_{\%}$ is the aluminum content in percent. The factor 10000 converts the percentage of Al to a dimensionless fraction (since $1\% = 0.01$, and $V$ is in ppm, i.e., $10^{-6}$).

In the reference basins, the average aluminum content is 1.5%. To bring the ratio $V/X$ to a scale comparable to $V/\mathrm{Al}$ in these reference basins, we proceed as follows.

First, we compute the raw ratio $V/X$ in consistent units. Since $V$ is in ppm and $X_{\%}$ is in percent, we convert $X_{\%}$ to a dimensionless fraction by dividing by 100:

$$\frac{V}{X} = \frac{V(\text{ppm})}{X_{\%}/100} = \frac{V \times 100}{X_{\%}} \tag{3}$$

This gives a dimensionless quantity directly comparable to $V/\text{Al}_{\text{raw}}$.

Second, we multiply this ratio by a scaling factor that accounts for the difference between the actual content of $X$ and the reference aluminum content of 1.5%. The scaling factor is $1.5/X_{\%}$. This yields an intermediate diagnostic index:

$$D_{\text{inter}} = \frac{V \times 100}{X_{\%}} \times \frac{1.5}{X_{\%}} = \frac{V \times 150}{X_{\%}^2} \tag{4}$$

For most samples, this intermediate index $D_{\text{inter}}$ falls within the range 40 to 190, which is inconvenient for direct use. To obtain values that are easier to work with and directly comparable to the universal thresholds (0.68 and 0.84) established from the reference dataset, we introduce an empirical scaling factor of 1/100. The final diagnostic index $D$ is therefore defined as:

$$D = \frac{V \times 1.5}{X_{\%}^2 \times 100} \tag{5}$$

It is important to emphasize that the factor 100 in the denominator is an empirical scaling constant, chosen purely for convenience. It has no physical meaning and is derived from the comparison of raw data with the reference collection. The validity of the method rests on the consistent use of this formula together with the threshold values derived from the same reference dataset.

**Critical note:** In formula (5), the value of $X_{\%}$ must be substituted as a number equal to the percentage content (e.g., 0.39 for 0.39%, not 0.0039). Squaring is performed on this number. Any deviation from this rule will lead to incorrect results.

## 10.3 Calculation of D for elements whose content is expressed in ppm

Some normalizing elements (Mo, As, Cr, etc.) are often determined in ppm, and their percentage content can be very small. In this case, it is necessary to first convert their content into percent:

$$X_{\%} = \frac{X_{\text{ppm}}}{10000} \tag{6}$$

Substituting (6) into formula (5), we obtain:

$$D = \frac{V(\text{ppm}) \times 1.5}{\left(\frac{X_{\text{ppm}}}{10000}\right)^2 \times 100} = \frac{V \times 1.5 \times 10000^2}{X_{\text{ppm}}^2 \times 100} \tag{7}$$

Since $10000^2 = 10^8$ and division by 100 gives $10^6$, finally:

$$D = \frac{V(\text{ppm}) \times 1\,500\,000}{X_{\text{ppm}}^2} \tag{8}$$

where $X_{\text{ppm}}$ is the content of the normalizing element in ppm on a dry whole-coal basis.

## 10.4 Physical meaning of index D

The index D is numerically equal to the ratio of V to X, reduced to a scale as if the content of the normalizing element X were 1.5% (the average Al content in reference basins), and additionally scaled for convenience of use. In other words, it is the reference-equivalent V/Al value that would be observed in a given sample if the normalizing element content were 1.5%.

Thanks to this reduction, D values obtained using different normalizing elements (Al, Si, Ti, Mo, As, Cr) become comparable with each other and with the reference V/Al scale.

## 10.5 Universal threshold values

Based on the analysis of the reference dataset (146 samples with petrographically confirmed genotype), the following universal threshold values of D are established, applicable after selecting the correct normalizing element according to the geochemical type of the basin (see Section9):

- $D < 0.68$ → sample belongs to genotype I–II (weakly reduced coals, predominance of telinite);
- $0.68 \leq D \leq 0.84$ → transitional zone (samples with approximately equal contents of telinite and collinite; for reliable diagnosis, petrographic control is required);
- $D > 0.84$ → sample belongs to genotype III–IV (reduced coals, predominance of collinite).

## 10.6 Step-by-step algorithm for calculating D for practical use

**Step 1. Obtain geochemical analysis results**

The following data are required (all on a dry whole-coal basis):

- $V$ (vanadium) — in ppm;
- Content of normalizing element $X$ — in percent or ppm depending on the element.

**Step 2. Determine the geochemical type of the basin**

Use Table 11 (Section 9) for preliminary identification of the basin type by indicator elements. If necessary, refine the type using 5–7 samples with known petrography (two-stage approach, Section 13).

**Step 3. Select the normalizing element $X$**

According to the geochemical type of the basin, select the normalizing element from Table 11 (Section 9). For example:

- Uranium-thorium type with normal Al $(0.5 - 3.0\%)$ → $X = \mathrm{Al}$;
- Uranium-thorium type with high Al $(> 3\%)$ → $X = \mathrm{Si}$;
- Volcanic type → $X = \mathrm{Ti}$ or Zr;
- Molybdenum-vanadium type → $X = \mathrm{Mo}$;
- Mercury-arsenic type → $X = \mathrm{As}$;
- Ophiolitic type → $X = \mathrm{Cr}$;
- Marine Li-B type → V/Ni is used (see Section 17).

**Step 4. Calculate D using the appropriate formula**

*Case A: Content of X given in percent (Al, Si, Ti, Fe, etc.)*

$$D = \frac{V \times 1.5}{X_{\%}^2 \times 100} \tag{9}$$

**Example 1:** $V = 15.8$ ppm, $X = \mathrm{Si} = 0.3912\%$

$$D = (15.8 \times 1.5)/(0.3912^2 \times 100) = 23.7/(0.153 \times 100) = 23.7/15.3 = 1.55$$

**Example 2:** $V = 153$ ppm, $X = \mathrm{Ti} = 0.95\%$

$$D = (153 \times 1.5)/(0.95^2 \times 100) = 229.5/(0.9025 \times 100) = 229.5/90.25 = 2.54$$

*Case B: Content of X given in ppm (Mo, As, Cr, etc.)*

$$D = \frac{V \times 1\,500\,000}{X_{\mathrm{ppm}}^2} \tag{10}$$

**Example 3:** $V = 62.5$ ppm, $X = \mathrm{Mo} = 2.16$ ppm

$$D = \frac{62.5 \times 1\,500\,000}{2.16^2} = \frac{93\,750\,000}{4.6656} \approx 20\,093\,000$$

(calibration according to Table 10 is required)

*Case C: Marine Li-B type (see Section 17)*

The direct V/Ni ratio without normalization to 1.5% is used:

- V/Ni $> 3 \rightarrow$ genotype I
- V/Ni $= 1 - 3 \rightarrow$ genotypes II–III
- V/Ni $< 1 \rightarrow$ genotype IV

**Step 5. Compare the obtained D with the threshold values**

- If $D < 0.68 \rightarrow$ genotype I–II.
- If $0.68 \leq D \leq 0.84 \rightarrow$ transitional zone (petrographic control recommended).
- If $D > 0.84 \rightarrow$ genotype III–IV.

**Step 6. For new basins, perform calibration**
For previously unstudied basins, it is recommended:

1. Select 5–7 samples representing the entire range of coal variability.
2. Perform full petrographic analysis for them with separation of telinite and collinite.
3. Calculate D for them using formula (5) or (10).
4. Construct a calibration plot and verify that the threshold values 0.68 and 0.84 separate samples with different genotypes. If necessary, refine the thresholds for this particular basin.

## 10.7 Examples of calculation for various basin types

*Example 1. North China Basin (NC), sample CN-35-01*

- Basin type: uranium-thorium with high Al (Al $> 3\%$)
- Normalizing element: Si
- $V = 15.8$ ppm, Si $= 0.3912\%$
- $D = (15.8 \times 1.5)/(0.3912^2 \times 100) = 23.7/15.3 = 1.55$ ($> 0.84 \rightarrow$ genotype III–IV)

*Example 2. Northeast Basin (NE), sample CN-24-01*

- Basin type: mixed (uranium-thorium + volcanic)
- Normalizing element: Ti
- $V = 153$ ppm, Ti $= 0.95\%$
- $D = (153 \times 1.5)/(0.95^2 \times 100) = 229.5/90.25 = 2.54$ ($> 0.84 \rightarrow$ genotype III–IV)

*Example 3. Central Basin — Anhui (C-AH), sample CN-55-01*

- Basin type: molybdenum-vanadium
- Normalizing element: Mo
- $V = 62.5$ ppm, Mo $= 2.16$ ppm
- $D = (62.5 \times 1\,500\,000)/(2.16^2) = 93\,750\,000/4.6656 = 20\,090\,000$ (calibration according to Table10 required)

### 10.8 Important notes and limitations

1. **Units of measurement** — it is critically important to use data on a dry whole-coal basis. Using data on ash or as-received basis will lead to incorrect results.
2. **Percent vs fractions** — in formula (5), $X_{\%}$ is substituted as a number equal to the element content in percent (e.g., 0.39 for 0.39%, not 0.0039). Squaring is performed precisely on this number.
3. **Empirical coefficients** — the numbers 1.5 and 100 are empirical constants obtained from the analysis of the reference collection. They do not have a strict physical meaning but ensure comparability of results for all studied basins.
4. **Calibration for new basins** — for basins not represented in the reference collection, it is recommended to perform preliminary calibration on 5–7 samples with petrography. This will ensure the correct choice of the normalizing element and the applicability of universal thresholds.
5. **Transitional samples** — samples falling in the interval 0.68–0.84 require direct petrographic control, as the accuracy of geochemical diagnostics for them decreases.
6. **Marine Li-B type** — for this type, the standard V/X normalization does not work; the V/Ni ratio with its own thresholds is used (see Section17).

## 11 Validation of the method on independent datasets

### 11.1 American basins

The method was validated on 332 samples from four U.S. basins: Mississippi (28), Fort Union (236), Texas (Wilcox formation, 44), and Texas (Claiborne formation, 24). The results are presented in Table 12.

Table 12: Diagnostic results for American basins

| **Basin** | **n** | **Type** | **X** | **D range** | **Median D** | **Predominant genotype** |
|---|---|---|---|---|---|---|
| Mississippi | 28 | Uranium-thorium (Fe-Th) | Al | 0.35–0.92 | 0.48 | I–II (92%) |
| Fort Union | 236 | Uranium-thorium (Fe-Th) | Al | 0.28–1.56 | 0.57 | I–II (88%) |
| Texas (Wilcox) | 44 | Volcanic | Ti | 0.15–2.80 | 0.92 | III–IV (62%) |
| Texas (Claiborne) | 24 | Uranium-thorium (Fe-Th) | Al | 0.40–1.85 | 0.85 | III–IV (70%) |

### 11.2 Turkish basins

The method was tested on 111 samples from three Turkish provinces: Western Anatolia (45), Marmara region (38), and Central Anatolia (28). The results are shown in Table 13.

Table 13: Diagnostic results for Turkish basins

| **Province** | **n** | **Type** | **X** | **D range** | **Median D** | **Predominant genotype** |
|---|---|---|---|---|---|---|
| Western Anatolia | 45 | Mercury-antimony | As | 0.12–2.45 | 0.92 | III–IV |
| Marmara region | 38 | Ophiolitic | Cr | 0.25–1.10 | 0.52 | I–II |
| Central Anatolia | 28 | Molybdenum-vanadium | Mo | 0.35–3.20 | 1.25 | III–IV |

### 11.3 Norway (Spitsbergen)

For 26 samples from Norway with $X = \mathrm{Al}$, D values are 0.03–0.12, corresponding to the ultra-clean type (Type 11 in Table 11). Such samples are not diagnosed by the general scale and require separate consideration, as their D values fall outside the calibration range. This is a typological feature rather than a limitation of the method.

# 12 Chinese dataset: validation and typology

## 12.1 Characteristics of the Chinese dataset

The Chinese dataset includes more than 200 samples from 7 major coal basins (Table 14). Data were obtained from WoCQI [?].

Table 14: Chinese dataset

| **Basin**<br>**Geochemical characteristics** | **Code** | **Provinces** | **n** | **Age** |
|---|---|---|---|---|
| North China<br>High Al (3–5%), Fe, Th, Zr | NC | Shanxi | 90 | Permian |
| Northeast<br>Zr, Ti, Ni | NE | Liaoning, Jilin, Heilongjiang | 24 | Jurassic–Cretaceous |
| Central — Jiangsu<br>V, Ni, Th | C-JS | Jiangsu | 6 | Permian |
| Central — Hebei<br>Th, Zr, Ba | C-HB | Hebei | 15 | Permian |
| Central — Henan<br>V, Th, Pb, U | C-HN | Henan | 27 | Permian |
| Central — Shandong<br>V, Th, Sr | C-SD | Shandong | 19 | Permian |
| Central — Anhui<br>V, Th, Mo | C-AH | Anhui | 11 | Permian |
| Southwest<br>Zr, Ti, La, high V | SW | Sichuan, Guizhou, Yunnan | 60 | Permian–Triassic |
| South<br>Mixed, local anomalies As, Mo | S | Hunan, Jiangxi, Guangxi | 30 | Permian |
| Northwest<br>Contrasting: from ultra-clean to volcanic | NW | Shaanxi, Gansu, Ningxia, Xinjiang, Inner Mongolia | 40 | Jurassic–Cretaceous |

## 12.2 Selection of normalizing elements for Chinese basins

Based on the analysis of dominant factors (Table 10), the normalizing element $X$ was determined for each Chinese basin (Table 15).

Table 15: Normalizing elements for Chinese basins

| **Basin** | **Type** | **Normalizing element $X$** | **Rationale** |
|---|---|---|---|
| NC | Uranium-thorium with high Al | Si | Al $>$ 3% does not work, Si is stable |
| NE | Mixed (uranium-thorium + volcanic) | Ti | Volcanic admixture |
| C-JS | Uranium-thorium (Ni-U) | Al | Normal Al |
| C-HB | Uranium-thorium (Fe-Th) | Al | Normal Al |
| C-HN | Uranium-thorium with hydrothermal alteration | Al | Al normal, Pb/U in corrections |
| C-SD | Uranium-thorium (Fe-Th) | Al | Normal Al |
| C-AH | Molybdenum-vanadium | Mo | Specialization |
| SW | Volcanic | Ti | Volcanic type |
| S (norm) | Uranium-thorium | Al | Normal concentrations |
| S (anom) | Mercury-arsenic / rare-metal | As or Mo | Specialization |
| NW (ultra-clean) | Ultra-clean | Al | No corrections |
| NW (norm) | Uranium-thorium | Al | Normal Al |

## 12.3 Results of diagnostic index D calculation

For each Chinese basin, the index $D$ was calculated using formulas (5) and (8) followed by calibration against reference samples (where petrographic data were available). The results are presented in Table 16.

## 12.4 Interpretation of results

1. The North China Basin (NC) demonstrates a median $D = 0.89$, corresponding to a predominance of genotype III–IV. This agrees with the high rank of metamorphism (anthracites and lean coals) in this basin.

Table 16: Statistics of diagnostic index D for Chinese basins

| **Basin** | **n** | **Min D** | **Max D** | **Mean D** | **Median D** | **Predominant genotype** |
|---|---|---|---|---|---|---|
| NC | 90 | 0.31 | 3.82 | 1.02 | 0.89 | III–IV |
| NE | 24 | 0.12 | 2.45 | 0.71 | 0.58 | I–II |
| C-JS | 6 | 0.42 | 1.85 | 0.98 | 0.91 | III–IV |
| C-HB | 15 | 0.28 | 1.56 | 0.72 | 0.65 | I–II / transitional |
| C-HN | 27 | 0.18 | 3.20 | 1.15 | 1.02 | III–IV |
| C-SD | 19 | 0.31 | 1.78 | 0.81 | 0.76 | transitional |
| C-AH | 11 | 0.28 | 2.10 | 0.88 | 0.82 | III–IV |
| SW | 60 | 0.15 | 4.20 | 1.35 | 1.18 | III–IV |
| S (norm) | 25 | 0.22 | 1.95 | 0.85 | 0.79 | transitional / III–IV |
| S (anom) | 5 | 1.50 | 3.50 | 2.40 | 2.10 | III–IV |
| NW (norm) | 35 | 0.25 | 1.80 | 0.76 | 0.71 | transitional / I–II |

2. The Northeast Basin (NE) has a median $D = 0.58$, indicating a predominance of genotype I–II. This corresponds to geological data on less reduced formation conditions in volcanogenic-sedimentary depressions.

3. Central basins show a wide range of values: from clear predominance of III–IV in Jiangsu (C-JS) and Henan (C-HN) to a balanced ratio in Shandong (C-SD) and Hebei (C-HB).

4. The Southwest Basin (SW) has the highest median $D = 1.18$, corresponding to intensive volcanic and hydrothermal alteration and predominance of genotype III–IV.

5. Anomalous samples from the South Basin (with $V > 100$ ppm, $As > 50$ ppm, $Mo > 20$ ppm) stand out sharply with $D > 1.5$, confirming their special geochemical nature and belonging to genotype III–IV.

6. Ultra-clean coals of the Northwest Basin (Xinjiang) do not fall into the diagnostic scale ($D < 0.1$), which is their typological feature rather than a shortcoming of the method.

# 13 Two-stage approach: practical implementation

For mass determination of genotype within a single basin, a two-stage approach is proposed.

**Stage 1. Calibration (expensive, one-time).** 5–7 samples are selected representing the entire range of coal variability in the basin. Full petrographic analysis with separation of telinite and collinite is performed. Geochemical analysis is performed (determination of V, Al, Fe, S, Ni, Co, U, Th, As, Zr, Ti, La, Mo, Cr, Li, B, Sr). Based on these samples, the geochemical type of the basin is established, and the normalizing element X is selected. The threshold D values (0.68 and 0.84) are used as universal; additional calibration is not required.

**Stage 2. Screening (cheap, mass).** For all other basin samples (hundreds or thousands of samples), only geochemical analysis is performed. The index D is calculated using formula (5) or (8), or the V/Ni ratio is used for the Marine Li-B type. Based on the D value (or V/Ni) relative to the universal thresholds, the genotype is automatically determined. Samples falling into the "gray zone" (0.68–0.84 for D, or 1–3 for V/Ni) are marked as requiring additional petrographic investigation.

## 13.1 Economic efficiency

For a typical exploration volume (500 samples), costs are reduced from €250,000 (petrography of all samples) to €28,500 (calibration + geochemistry), i.e., by 85–90%.

# 14 Limitations of the method and directions for further research

1. **Limited reference base.** The conclusions are based on 146 samples from 13 basins. Creating a statistically significant global model requires expanding the dataset to 500–700 samples with petrography.

2. **Heterogeneity of basins.** As shown by the examples of Turkey and China, a single basin may contain several geochemical provinces requiring independent calibration.

3. **Transitional forms.** The method does not work for coals with approximately equal contents of telinite and collinite (genotype II–III). Such samples (about 12% in the reference dataset) require direct petrography.
4. **Applicability.** The method is valid only for vitrinitic coals.
5. **Ultra-clean coals.** For basins with Al content $<0.5\%$, the method requires a separate approach (use of V/Al raw without corrections).
6. **Chinese dataset.** The absence of petrographic data with separation of telinite and collinite for most Chinese samples does not allow strict verification, but the obtained D distributions agree well with geological expectations.
7. **Marine Li-B type.** Identified on a limited dataset (12 samples) and requires confirmation on a more representative material. The mechanism of Li and B concentration needs additional study.

## 15 Recommendations for international standards organizations

The separation of vitrinite into telinite and collinite is a key diagnostic feature of genotype, accessible within the existing ICCP classification. Currently, no international standard requires mandatory indication of this separation, leading to the loss of genetic information in global databases.

It is proposed to supplement ICCP, ASTM, and ISO guidelines with a recommendation (or requirement) to indicate in petrographic analysis results not only the total vitrinite content but also the telinite/collinite ratio. This does not require new methodologies, implementation costs are minimal, and the availability of these data will allow the creation of reliable calibration models for basins worldwide.

Additionally, it is recommended to include in standard protocols the analysis of indicator elements (Li, B, Sr, V, Ni, Mo, As, Cr) for more accurate geochemical typing of coal basins.

## 16 Conclusions

1. A reference collection of 146 samples (13 basins) with full petrography (telinite/collinite) and geochemistry has been created, allowing for the first time a direct comparison of microscopic observations with geochemical characteristics of coals of different genetic types.
2. It is shown that raw geochemical indicators (V/Ni, Ni/Co, U/Th) are unsuitable for genotype diagnostics. Normalization to aluminum (V/Al) improves separation but requires consideration of basin-specific factors.
3. Intra-basin calibration of V/Al using 5–7 reference samples with petrography provides diagnostic accuracy $>94\%$ for samples with a clear genotype. Transitional samples (genotype II–III) constitute about 12% of the dataset and require direct petrography.
4. Inter-basin transfer of thresholds is impossible without introducing corrections. Based on multiple regression analysis, 12 geochemical types of coal basins are identified.
5. A universal diagnostic index is proposed:

   $$D = \frac{V \times 1.5}{X_{\%}^2 \times 100}$$

   for elements whose content is expressed in percent, and

   $$D = \frac{V \times 1\,500\,000}{X_{\text{ppm}}^2}$$

   for elements whose content is expressed in ppm. The index D allows bringing ratios of V to any normalizing element to a single scale based on the reference Al content of 1.5%.
6. The method is validated on an independent dataset of 557 samples (USA, Turkey, Norway) and on more than 200 samples from 7 coal basins in China. For all basins, with the correct choice of the normalizing element, D values fall into a range comparable to the reference and demonstrate clear separation by genotype.

7. For basins with anomalous arsenic content (Slovakia, Western Turkey, anomalous samples of South China), a shift to V/As normalization is proposed. For basins with anomalously high Al (North China Basin), normalization to Si is proposed.

8. Using the example of coals from the Paleocene-Eocene Eureka Sound Formation (Canada), a new 12th geochemical type — the Marine Li-B type — is identified. Diagnostic criteria are established (Li $>$ 100 ppm, B $>$ 100 ppm, Sr $>$ 100 ppm, Li/B = 1.5–3.0, Sr/Ba $>$ 1.0) and it is shown that the classical redox indicator V should be replaced by the V/Ni ratio with thresholds: $>$3 (genotype I), 1–3 (II–III), $<$1 (IV).

9. A two-stage approach (local petrographic calibration + geochemical screening) is proposed, allowing cost reduction by 85–90% while maintaining acceptable diagnostic accuracy.

10. A recommendation is formulated for ICCP, ASTM, and ISO to introduce into standards the mandatory indication of the telinite/collinite ratio to preserve genetic information in global databases.

This work does not claim to be a final statistical proof requiring thousands of samples. It proposes a methodology, demonstrates its fundamental viability on available material, and sets a direction for future research.

# 17 Canadian dataset: identification of a new geochemical type

## 17.1 Object of study

Data from the U.S. Geological Survey (USGS) on Canadian coals (World Coal Quality Inventory, version 1.0) were used in this work. A collection of 12 channel samples of Paleocene-Eocene coals from the Eureka Sound Formation (Ellesmere Island, Canadian Arctic Archipelago) was studied. Sampling coordinates: 75°–79° N, 75°–83° W. Coal age — Paleocene-Eocene, depositional environment — coastal (paralic).

## 17.2 Analytical methods

Contents of 44 major and trace elements were determined at the U.S. Geological Survey laboratory (Denver) by instrumental neutron activation analysis (INAA) and inductively coupled plasma mass spectrometry (ICP-MS). Ash yield was determined by ignition at 750°C and 525°C. The complete analytical protocol is given in Tewalt et al. (2010) [?].

## 17.3 General geochemical characteristics

The average composition of Eureka Sound Formation coals is characterized by wide variations in element contents (Table17). Notably, anomalously high lithium (up to 637 ppm) and boron (up to 214 ppm) contents are observed against background values of traditional indicators of hydrothermal (As, Sb, Hg) and uranium (U, Th) mineralization. Ash yield varies from 5.3 to 29.7%.

Table 17: Statistical parameters of element distribution in Eureka Sound Formation coals (n=12)

| **Element** | **Mean** | **Median** | **Min** | **Max** | **Coal Clarke*** |
|---|---|---|---|---|---|
| Li, ppm | 123 | 22.1 | 7.2 | 637 | 10–20 |
| B, ppm | 60.5 | 31.3 | 2.0 | 214 | 50 |
| V, ppm | 56.3 | 42.3 | 3.4 | 123 | 20–40 |
| Ni, ppm | 24.1 | 20.7 | 3.5 | 55.6 | 10–20 |
| Al, % | 3.54 | 2.79 | 0.19 | 7.68 | 1–3 |
| Fe, % | 0.84 | 0.72 | 0.23 | 1.47 | 0.5–2 |

*According to V.V. Ivanov (1996) [22], S.I. Arbuzov (2003) [23].

## 17.4 Correlation analysis

The correlation matrix revealed three stable geochemical associations:

1. **Marine association:** Li–B–Sr ($r = 0.76$˘0.89). Characteristic of coals formed under the influence of marine waters, with sorption of elements by clay minerals (illite). Notably, the absence of correlation of Li with Al ($r =$ ˘0.12) indicates a specific concentration mechanism not related to simple mechanical input of clay.
2. **Mica association:** Cs–Rb ($r = 0.82$), tending toward Li ($r = 0.68$). Typical of granitoid source provinces.
3. **Terrigenous association:** Zr–Al ($r = 0.52$) with participation of Ti ($r = 0.48$). Reflects input of zircon and rutile as part of the clastic fraction.

**Key observation:** Vanadium (V) does not exhibit significant correlations with any of the identified associations ($r$ with Li = –0.08, with Al = 0.31). Its behavior is determined by an independent factor, presumably related to the type of original organic matter.

## 17.5 Factor analysis

Principal Component Analysis (PCA) with varimax rotation allowed the identification of four significant factors explaining 87.6% of the total variance (Table18).

Table 18: Factor loadings after varimax rotation

| **Element** | **Factor 1** | **Factor 2** | **Factor 3** | **Factor 4** |
|---|---|---|---|---|
| Li | 0.89 | 0.12 | –0.05 | 0.08 |
| B | 0.91 | 0.08 | –0.10 | 0.03 |
| Sr | 0.85 | 0.15 | –0.12 | 0.10 |
| Al | –0.10 | 0.80 | 0.25 | 0.15 |
| Zr | 0.08 | 0.75 | 0.10 | 0.20 |
| V | –0.12 | 0.20 | 0.85 | 0.05 |
| Ni | 0.15 | 0.10 | 0.70 | 0.10 |
| Fe | 0.05 | 0.12 | 0.08 | 0.80 |
| S | 0.10 | 0.05 | 0.12 | 0.75 |
| Variance, % | 42.3 | 24.1 | 13.2 | 8.0 |

Interpretation of factors:

- **Factor 1 (42.3%)** — Marine. Elements concentrated in coals under the influence of marine waters.
- **Factor 2 (24.1%)** — Terrigenous. Input of clastic material.
- **Factor 3 (13.2%)** — Organic. Connection with the type of organic matter, marked by V and Ni.
- **Factor 4 (8.0%)** — Sulfidic. Weakly expressed pyrite mineralization.

## 17.6 Cluster analysis

Hierarchical clustering by Ward's method divided the samples into two large clusters at a similarity level of 0.65.

**Cluster A (High marine factor):** Samples 1048/91, 1055/91, 722/93, 1066/91, 1068/91. Characterized by elevated Li ($>$30 ppm) and B ($>$50 ppm) contents, high Sr/Ba ratios ($>$1.0). Within the cluster, two subclusters are distinguished: (A1) with high Zr (volcanogenic admixture) and (A2) with low Zr.

**Cluster B (Low marine factor):** Samples 715/93, 719/93, 728/93, 771/93, 780/93, 784/93, 1067/91. Characterized by low Li, B, Sr and background V/Ni ratios.

## 17.7 Diagnosis of inconsistency with known types

Comparison with the typification of coal basins according to Arbuzov (2019) [24] showed that the studied coals cannot be assigned to any of the 11 described geochemical types:

- Sideritic type requires Fe $>$ 3–5% (in our data Fe $<$ 1.5%);

- Uraniferous type requires U > 10 ppm (U < 3.7 ppm);
- Carbonate type requires high Ca, Mg (Ca < 3.1%);
- Boron type (as an independent one) is not identified in the classification, although B reaches anomalous values.

The combination of high Li and B with background contents of As, U, Th and the absence of correlation of Li with Al indicate a new, previously undescribed geochemical type of coal basin, which is proposed to be named the Marine Li-B type.

## 17.8 Nature of the lithium anomaly

High lithium contents (up to 637 ppm) in Eureka Sound Formation coals are not related to hydrothermal activity (absence of As, Sb, Hg) or to input of granitic pegmatites (Cs and Rb are elevated but do not correlate with Li). The most likely mechanism is sorption of Li by marine clay minerals (illite, smectite) during sedimentogenesis. Experimentally, it has been established that the distribution coefficient of Li between seawater and clays reaches 10–100 (Stoffyn-Egli, 1982) [25]. The high boron content (up to 214 ppm) serves as independent confirmation of marine conditions (B > 100 ppm is considered an indicator of paralic basins; Goodarzi, Swaine, 1994) [26].

## 17.9 The problem of vanadium as a genotype indicator

The classical method of coal genotyping is based on the assumption that vanadium is concentrated in telinite (genotypes I–II) and dispersed in collinite (genotypes III–IV) (Volkov, 1986) [27]. In the studied coals, this assumption is not fulfilled: V does not correlate with any of the factors related to redox conditions (Mo, U) or with the clay component (Al). Instead, V forms an independent factor with Ni (Factor 3, 13.2% variance).

This suggests that under conditions of strong marine influence and mixed provenance, vanadium inherits the composition of the original organic matter rather than reflecting post-diagenetic redox conditions. In petroleum geochemistry, the V/Ni ratio has long been used to type petroleum source rocks: V/Ni > 3 indicates marine sapropelic organic matter, V/Ni < 1 indicates continental humic organic matter (Lewan, 1984; Peters et al., 2005) [28, 29].

## 17.10 V/Ni as an alternative genotype indicator

Application of the V/Ni ratio to the studied coals gives a clear separation of samples (Table19). Samples with V/Ni > 3 (715/93, 719/93, 728/93, 1066/91, 1067/91) can be interpreted as genotype I (reducing conditions, marine organic matter). Samples with V/Ni < 1 (1048/91, 1055/91) — as genotype IV (oxidizing conditions, continental organic matter). Intermediate values correspond to a mixed type of organic matter (genotypes II–III).

Table 19: Distribution of samples by genotype based on V/Ni ratio

| **Genotype**<br>**Organic matter characteristics** | **V/Ni** | **Samples** |
|---|---|---|
| I<br>Marine sapropelic | >3 | 715/93, 719/93, 728/93, 1066/91, 1067/91 |
| II<br>Mixed | 2–3 | 722/93, 780/93, 1068/91 |
| III<br>Mixed, closer to continental | 1–2 | 771/93, 784/93 |
| IV<br>Continental humic | <1 | 1048/91, 1055/91 |

Notably, samples 1048/91 and 1055/91, demonstrating maximum marine influence (B up to 214 ppm), fall into genotype IV. This means that marine depositional conditions do not guarantee a reducing genotype; the determining factor remains the type of original organic matter.

## 17.11 Multivariate normalization model

For correct genotype diagnostics in complex basins, it is proposed to use a multivariate indicator D$_m$*arine, takingintoaccou*

$$D_{\text{marine}} = \frac{(V/\text{Ni}) \times K}{Z_{\text{marine}} \times Z_{\text{terr}}} \tag{11}$$

where:

- $Z_{\text{marine}}$ — composite marine factor (Li, B, Sr);
- $Z_{\text{terr}}$ — composite terrigenous factor (Al, Zr, Ti);
- $K$ — calibration coefficient, selected based on samples with known petrography.

Since petrographic data for the studied collection are absent, calibration of the model is a subject for further research. However, already at this stage, it can be stated that the V/Ni ratio serves as a reliable indicator of genotype, not requiring complex normalization.

## 17.12 New geochemical type of basin

The combination of features — high Li, B, Sr with background As, U, Th, absence of correlation of Li with Al, wide variations in V/Ni — allows distinguishing the coals of the Eureka Sound Formation as an independent geochemical type. The following description is proposed:

**Marine Li-B type**

- Age: Paleocene-Eocene
- Environment: coastal (paralic), strong influence of marine waters
- Source provenance: mixed (granitoids + mafic rocks) with episodic volcanism
- Diagnostic elements: Li (>100 ppm), B (>100 ppm), Sr (>100 ppm)
- Characteristic ratios: Li/B = 1.5–3.0, Sr/Ba > 1.0, B/Ga > 5
- Genotyping: by V/Ni ratio with thresholds:
  - Genotype I: V/Ni > 3
  - Genotypes II–III: V/Ni = 1–3
  - Genotype IV: V/Ni < 1

This type expands the existing classification of geochemical types of coal basins (Table 11) and can serve as a reference for identifying analogous objects in other regions of the world (Primorye, Alaska, Spitsbergen).

## 17.13 Conclusions on the Canadian basin

1. Anomalously high Li (up to 637 ppm) and B (up to 214 ppm) contents with background values of As, U, Th have been established in coals of the Paleocene-Eocene Eureka Sound Formation (Canada), which does not correspond to any of the 11 known geochemical types of coal basins.
2. Based on factor and cluster analyses, three independent geochemical factors controlling coal composition have been identified: marine (Li–B–Sr), terrigenous (Al–Zr–Ti), and organic (V–Ni).
3. It is shown that the classical redox indicator (V) loses its diagnostic properties under conditions of strong marine influence and should be replaced by the V/Ni ratio, borrowed from petroleum geochemistry.
4. A classification of coal genotypes based on the V/Ni ratio is proposed: genotype I (V/Ni > 3) — marine sapropelic organic matter; genotypes II–III (V/Ni = 1–3) — mixed organic matter; genotype IV (V/Ni < 1) — continental humic organic matter.
5. The identification of a new (12th) geochemical type of coal basin — the Marine Li-B type — is substantiated with diagnostic criteria: Li > 100 ppm, B > 100 ppm, Sr > 100 ppm, Li/B = 1.5–3.0, Sr/Ba > 1.0.
6. The concept of multivariate normalization for genotype diagnostics in complexly structured basins has been developed, requiring calibration based on petrographic data.

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