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Chemical Mass Fluxes and Water Quality Assessment of the Transboundary Shu River, Central Asia

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Abstract

This study presents long-term background concentration estimates for hydrochemical parameters in the Shu River at the Kaynar transboundary section for 2002–2025 and assesses chemical mass transport across this section. Annual mean values for 31 hydrochemical parameters were analyzed; 533 annual values were processed, and 498 remained after statistical extremes were excluded from background-concentration calculations. Background concentrations were estimated as one-sided confidence limits of the mean at a 0.95 confidence level. The Shu River water is characterized by a bicarbonate-sulfate composition and moderately elevated mineralization. Background-level exceedances of the reference maximum permissible concentration (*MPC*) values were observed for sulfate, nitrite nitrogen (NO_2-N), and copper. Suspended solids were assessed separately because the applicable criterion is expressed relative to the background concentration rather than as a fixed *MPC* value. The comprehensive water pollution index (*CWPI*) indicated moderate pollution in most years, with high pollution levels in 2002, 2003, 2006–2008, and 2016. Annual mass transport of ionic constituents increased from 555.2 thousand metric tons in 2021 to 899.6 thousand metric tons in 2023, while nutrient mass transport ranged from 3.14 to 3.55 thousand metric tons per year. Nitrate nitrogen (NO_3-N) made the largest contribution to nutrient mass transport. The results support regional water-quality assessment and water-protection planning in arid transboundary river basins.

Keywords: Shu River; water quality; mass transport of chemicals; maximum permissible concentrations; *CWPI*; biogenic substances; heavy metals

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1. Introduction

Assessing the quality of surface waters in the context of increasing anthropogenic pressure requires scientifically sound criteria that enable a distinction to be made between natural variability in water chemistry and anthropogenic-induced deviations. The relevance of this issue is confirmed by current assessments of the status of water bodies worldwide [1–3]. According to data from the European Environment Agency, in 2021 only 37 percent of Europe's surface water bodies achieved good or high ecological status, whilst

29 percent achieved good chemical status [4]. In European environmental policy, a similar objective is pursued under the Water Framework Directive, which aims to prevent the deterioration of water bodies and to achieve good status for rivers, lakes and groundwater [5].

One of the key criteria for the ecological interpretation of hydrochemical data is the background concentration of pollutants, regarded as the reference level of a component's concentration in the natural environment and the basis for identifying anthropogenic anomalies [6–8]. The concept of geochemical background was originally developed in exploration geochemistry. In environmental research, it is used to distinguish the natural component from the effects of human activity [8,9]. That means approaches to determining background values remain ambiguous and depend on the natural conditions of the area [10], the density of the monitoring network [11], and the quality of the source data [6–12]. Accurate determination of background levels is of fundamental importance for assessing environmental risk and interpreting pollution in natural waters [13–15].

In international practice, alongside background concentration, the concept of a geochemical baseline is used, reflecting the actual state of the environment whilst taking into account existing diffuse anthropogenic influences [16–18]. Unlike the 'absolute' natural background, such a baseline may include both natural and anthropogenically modified components [11,18,19]. Current research considers data on surface waters, bottom sediments and suspended matter as the basis for establishing baseline levels, which are necessary for identifying sources of pollution, assessing spatial heterogeneity and planning monitoring [20–22]. This distinction is particularly important in river basins, where undisturbed conditions are virtually absent, and the long-term hydrochemical regime is shaped by both natural processes and human activities, including water regulation, irrigation, and transboundary water use [23,24], as in the Shu River basin.

For a comprehensive assessment of river water quality, a regulatory comparison of concentrations must be supplemented by integrated indices, an analysis of pollution sources and a calculation of the mass transport of chemical substances [25,26]. The use of the Comprehensive Water Pollution Index (*CWPI*) and adapted Water Quality Indices (WQI) makes it possible to identify priority pollutants and take into account the regional characteristics of river basins [27,28]. However, the concentration analysis does not reflect the actual quantity of a substance transported by the river flow. Therefore, for transboundary catchment areas, the calculation of mass transport becomes particularly important, as it allows the actual pollutant load passing through the calculation cross-section to be assessed [29]. Recent reviews show that the deterioration of water quality in river basins is most often linked to the combined impact of agricultural runoff, urban wastewater and industrial discharges [30].

This issue is of particular relevance to the Shu River basin, situated in the arid and sharply continental part of Central Asia. The Shu River is formed by the confluence of the mountainous tributaries Joonaryk and Kochkor in Kyrgyzstan. Its total flow depends to a large extent on high-altitude snow and glacial meltwater [23,31]. The basin is characterized by pronounced seasonal variations in flow, high sensitivity to water abstractions for water management, and the transboundary nature of its water resources [24,31]. Significant volumes of water are used for irrigation. The flow regulation by reservoirs alters the natural hydrological regime, the conditions for the dilution of pollutants, and the magnitude of their mass transport [31].

In arid river basins, water quality is shaped by a combination of natural hydrochemical processes and water management interventions that alter the flow regime. A reduction in water availability intensifies the evaporative concentration of dissolved substances and reduces the flow's diluting capacity, whereas in years of high-water flow, the total removal of dissolved and suspended solids may increase [32]. In the post-Soviet period, the moni-

toring network in the Shu River basin has been significantly reduced, which complicates the assessment of the current state of water bodies and the calculation of representative background concentrations [23,24,31]. Under these circumstances, reproducible statistical approaches take on particular importance, as they allow for emissions, the heterogeneity of observation series and varying data availability for individual hydrochemical parameters [33,34].

This study addresses the calculation of background concentrations of hydrochemical parameters in the Shu River at the Kaynar transboundary section, the first hydrological monitoring section within Kazakhstan, based on long-term observation data. The approach includes the compilation of annual mean concentration series, the identification and exclusion of unrepresentative extreme values, the calculation of statistical characteristics, and the estimation of background concentrations as one-sided confidence limits of the mean at a confidence level of 0.95 in accordance with RD 52.24.622-2001 [35]. In addition, the mass transport of chemical substances through the Kaynar transboundary section was calculated to complement the concentration-based assessment of water quality with information on the quantities of substances transported by river flow.

Despite the considerable number of studies devoted to assessing water quality with the help of background concentrations, approaches combining the calculation of regional background concentrations, normative assessment, integrated water quality indices and analyses of the mass transport of chemical substances remain underdeveloped, even for transboundary basins under arid and semi-arid climate in Central Asia [22–24,32]. The scientific novelty of this study lies in deriving long-term background concentration estimates for hydrochemical parameters in the Shu River over a multi-year observation period and supplementing these estimates with calculations of chemical mass transport across the transboundary section. This approach makes it possible to distinguish between a persistently elevated regional background, episodic pollution and the actual pollutant load carried by the river flow.

The aim of this study is to calculate and interpret the background concentrations of hydrochemical parameters in the Shu River at the Kaynar transboundary section and to assess the mass transport of chemical substances through this section.

To achieve this aim, the following tasks were undertaken: to compile and pre-process a multi-year hydrochemical dataset; to identify and exclude unrepresentative extreme values; to calculate background concentrations of the analyzed parameters; to compare the obtained values with the reference maximum permissible concentration (*MPC*) values and the Comprehensive Water Pollution Index (*CWPI*); to calculate the mass transport of the main groups of chemical substances through the Shu River at the Kaynar transboundary section; and to interpret the results considering hydrological conditions, water-management pressures, and the transboundary characteristics of the basin.

2. Materials and Methods

2.1. Study Area

The Shu River basin is located in Central Asia. It is part of the biggest inland drainage area on Earth between the Caspian Sea in the west and southern Mongolia and Northwest China in the east. It is drying up at the northern edge of the Moiykum Desert. Only in wet years does the Shu River flow into the endorheic salt lake Akzhaikyn in the Aschykol Depression [23]. The transboundary basin covers territories in Kyrgyzstan and Kazakhstan. The total area of the basin is approximately 186.8×10^3 km^2 [23,24], including the mountainous regions of the Tian Shan in the south and the vast plains in the north. The Shu River is formed by the confluence of the mountainous tributaries Joonaryk and Kochkor at an altitude of 1.7 km. After the confluence, the Shu River flows in a north-

eastern direction, approaching Issyk Kul Lake, but does not flow into the lake. Because of tectonic influences, it turns first in a western direction near Balykchy, then through the narrow Boom Gorge in a northern direction, and then in a west-northwestern direction, forming a broad valley along the state border between Kemin and Bishkek, which is used for irrigated agriculture on both sides of the river in the Kyrgyz and Kazakh parts of the river course [23]. Its length is approximately 1.186 km, of which about 800 km flow through the territory of Kazakhstan. The catchment area of the Shu—including the drainless lower reaches—extends to 67.500 km^2 [23,24]. The formation of the river's flow exhibits a distinct mountainous-lowland zonation. The main sources of the river's water supply are the melting of snow and glaciers in the mountains in spring and summer, as well as meltwater from the seasonal snow cover in the foothills. As a result, the river basin is characterized by a complex pattern of high-water periods and floods: in spring, water levels rise due to the melting of low-altitude snow with a long-term (1937–2017) average discharge of 20 m^3/s, whilst in summer a second wave of high water occurs due to the melting of high-altitude snow and glaciers with a long-term (1937–2017) average discharge of 27–30 m^3/s [24]. During the period between 2001 and 2017, the average discharge was higher than in the periods before, which can be interpreted as a consequence of more melting water caused by global warming [24]. The water resources of the Shu River are characterized by a significant proportion of transboundary inflow. Only 27 per cent of the long-term average total discharge originates within Kazakhstan, whilst the majority comes from Kyrgyzstan [30] (Figure 1).

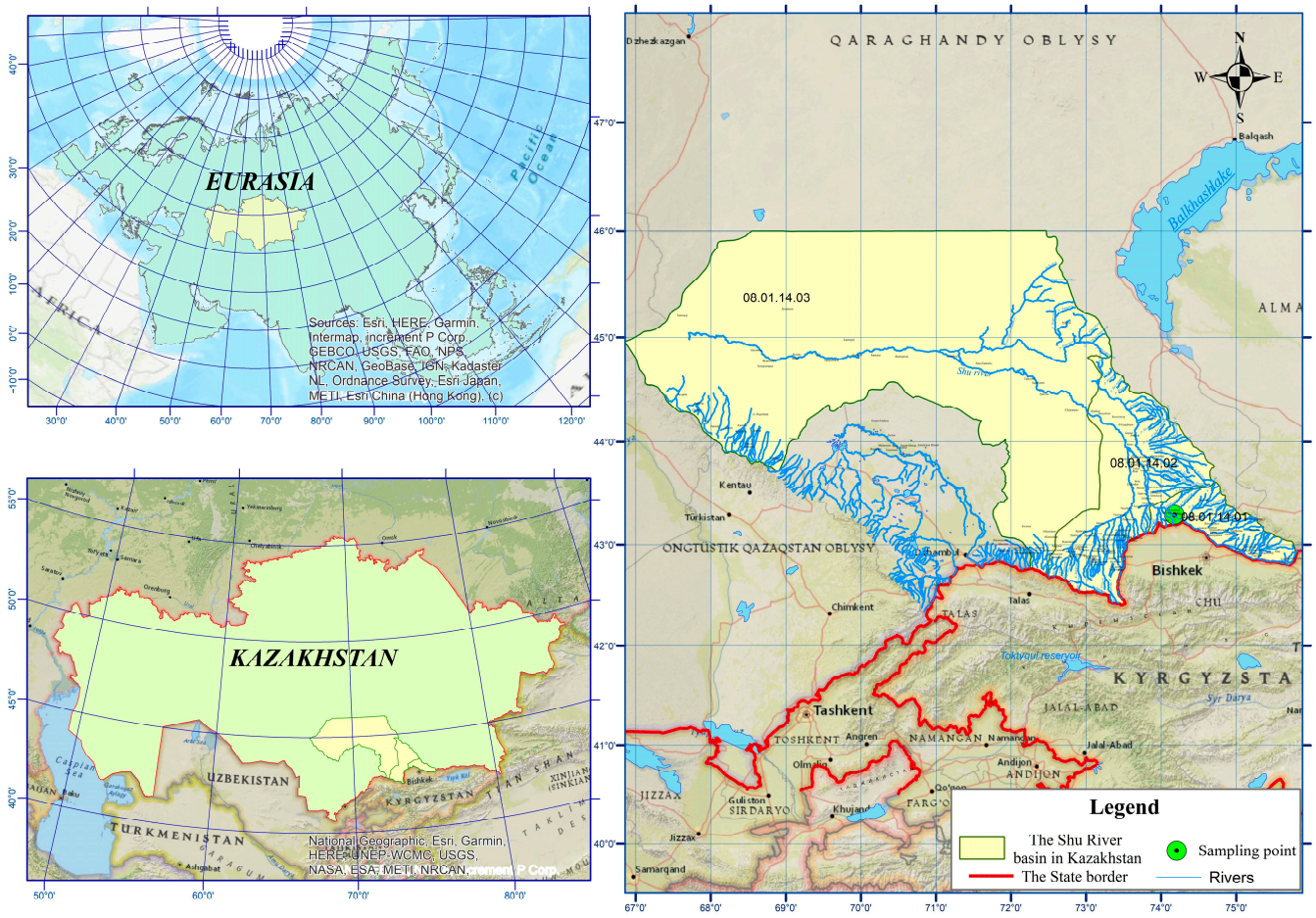


Figure 1. Location of the study area (Kazakhstan part of the Shu River catchment) within Kazakhstan and Eurasia.

2.2. Initial Data

From a methodological point of view, the determination of background concentrations must take into account the effects of water content, seasonal flow, dilution, washout from the catchment area and channel processes [34,35]. However, in the absence of reliable synchronous concentration–discharge data, statistical estimates based on long-term annual averages can be used, followed by an analysis of the mass transport of substances. For heavy metals, their association with suspended matter and bottom sediments is of particular significance, as these can act both as reservoirs and as secondary sources of pollution [36,37]. In regulated rivers, the processes of deposition, sorption and remobilisation of metals can significantly alter their migration and ecological availability [38,39].

Source data were obtained from the hydrochemical observations conducted within the state surface-water monitoring programme of the RSE 'Kazhydromet' at Kaynar gauging station for the period 2002–2025. The dataset includes indicators of ionic composition, physicochemical characteristics, biogenic substances, organic pollution indicators, and heavy metals.

Water sampling and laboratory analyses were performed within the national monitoring programme of RSE "Kazhydromet" and were not conducted by the authors of the present study. The archived dataset contained intra-annual observations and corresponding annual mean concentrations for the monitored parameters. Because the number and timing of observations were not uniform for all parameters and years, particularly for parameters introduced into the monitoring programme more recently, the present analysis was based on the annual mean values reported in the source monitoring dataset. Detailed information on individual analytical procedures, sampling frequency, and method-specific detection limits was not uniformly available in the archived dataset for the entire 2002–2025 period and therefore could not be reconstructed retrospectively for every parameter and year.

Background concentrations were calculated separately for each hydrochemical parameter. When data for individual years were missing, the actual calculation period was determined by the availability of annual mean values for the relevant parameter. The minimum number of annual values required for the calculation was set at three.

The methodological basis for the calculation followed RD 52.24.622-2001 [35], according to which the background concentration of a chemical substance is defined as a quantitative characteristic of its content at a specified cross-section of a watercourse under conditions influenced by both natural factors affecting water chemistry and upstream pollution sources. In accordance with this methodology, the background concentration was estimated as a one-sided confidence limit of the mean at a confidence level of 0.95.

Prior to the calculations, the source data were converted into a standard machine-readable format. The first stage involved the automatic identification of header rows, columns containing parameter names, units of measurement, and annual mean values.

During preliminary data processing, non-numeric entries, missing values, service symbols, and textual markers indicating the absence of data were excluded from the analysis. Values recorded with a decimal comma were converted to numerical format. For values reported in the source dataset as "<0.01" or similar censored entries, the stated threshold value was retained as a conservative upper-bound estimate of the actual concentration. This approach was used because uniform method-specific detection-limit information was not available for the entire 2002–2025 monitoring period. Importantly, these values remained below the corresponding regulatory thresholds and therefore did not affect parameter selection for the *CWPI* calculation or the resulting water-quality classification. This procedure provided a consistent series of annual mean concentrations for subsequent statistical processing.

The computer programme was written in Python (version 3.11.11) using the pandas (version 2.2.3), numpy (version 2.2.1) and openpyxl (version 3.1.5) libraries. The script was adapted to the structure of the original Excel dataset, in which substances are listed in rows. Monthly observations for each year are presented in columns, and the corresponding annual mean values are provided separately. The statistical calculations in the present study were based on these annual mean concentrations for the selected observation period.

Method-specific detection limits were not uniformly available in the archived dataset for the entire 2002–2025 period; therefore, they could not be reconstructed retrospectively for every parameter and year.

2.3. Exclusion of Outlier Extreme Values

For the estimation of long-term background concentrations, statistically identified extreme annual values were excluded from the series of annual averages. This procedure was carried out in accordance with [35] using the I_H criterion. For each indicator, the mean of the series, the standard deviation, and the normalised deviations of the maximum and minimum values were calculated:

$$I' = \frac{C_{max} - \overline{C}}{\sigma}, \quad (1)$$

$$I'' = \frac{\overline{C} - C_{min}}{\sigma}, \quad (2)$$

where C_{max} is—the maximum concentration value in the series, C_{min} is—the minimum concentration value, and $\overline{C}$ is– the mean value, σ—standard deviation.

If either of the calculated values I' or I'' exceeded the standard value I_H, the corresponding extreme value was excluded from the series. The procedure was repeated iteratively until the remaining series no longer contained any non-significant extremes. The limit values for I_H were taken from Table 1 [35].

Table 1. I_H value limits [35].

n	I_H	I_H	I_H	I_H	I_H	I_H	I_H
3	1.150	10	2.180	17	2.480	50	2.860
4	1.460	11	2.230	18	2.500	200	3.076
5	1.670	12	2.290	19	2.530	250	3.339
6	1.820	13	2.330	20	2.560	500	3.528
7	1.940	14	2.370	25	2.635		
8	2.030	15	2.410	30	2.696		
9	2.110	16	2.440	40	2.792		

Importantly, the annual values identified as statistical extremes by the (I_H) criterion were not considered erroneous measurements and were not removed from the original monitoring dataset. Their exclusion was applied only for the purpose of estimating long-term background concentrations, because the background value is intended to characterize long-term hydrochemical conditions rather than episodic extreme events.

The excluded annual values may reflect genuine hydrological events, short-term pollution episodes, or other atypical conditions. Therefore, they were retained in the annual time-series analysis and were also used in the *CWPI* and chemical mass-flux calculations whenever the corresponding monitoring and discharge data were available. Thus, the outlier procedure affected only the estimation of background concentrations and did not remove extreme events from the overall environmental assessment of the Shu River.

In the computer programme, this procedure was implemented by the function 'remove_outliers_rd', which sequentially compared the maximum and minimum deviations from the mean and excluded the extreme value that exceeded the tabulated I_H criterion.

The exclusion of statistically identified extreme annual values was applied only to background-concentration calculations. These values were not considered erroneous measurements and were retained in the original monitoring dataset. They were also retained in the annual time-series assessment and used in the *CWPI* and chemical mass-flux calculations whenever the corresponding monitoring data were available.

2.4. Calculation of Background Concentration

During the preliminary stage, the source data were checked: numerical values were standardised to a single format, decimal separators were harmonized. Empty cells and missing observations were excluded from the calculation dataset. Measurement units were retained in their original form: mg/L for major constituents and μg/L for trace elements. An individual time series was generated for each parameter:

$$C_1, C_2, \ldots, C_n,$$

where C_i is—the average annual concentration or hydrochemical parameter for the i-th year, and n is—the number of years actually used in the calculation after removing missing values and outliers.

After excluding outliers, the following statistical characteristics were calculated for each parameter:

$$\overline{C} = \frac{1}{n}\sum_{i=1}^{n} C_i, \tag{3}$$

$$\sigma = \sqrt{\frac{\sum_{i=1}^{n}\left(C_i - C_{cp}\right)^2}{n-1}}, \tag{4}$$

The background concentration of most chemical substances was defined as the upper one-sided confidence limit of the mean:

$$C_b = C_{average} + \frac{t_{St}\sigma}{\sqrt{n}}, \tag{5}$$

where C_b is—the calculated background concentration of the substance, t_{St} is—Student's t-value for a one-tailed confidence level of P = 0.95, n is—the number of values in the calculated sample. The values of the t_St coefficient were taken depending on the number of degrees of freedom $n - 1$, in accordance with Table 2 [35].

For dissolved oxygen in water, the calculation was carried out using the reverse logic, as it is not an elevated oxygen content but a reduced one that is considered unfavorable. Therefore, the lower confidence limit of the mean value was used for this parameter:

$$C_b = C_{average} - \frac{t_{St}\sigma}{\sqrt{n}}, \tag{6}$$

This approach is in line with the methodological guidelines, according to which, when determining the background concentration of dissolved oxygen, the 'plus' sign in the confidence interval is replaced by a 'minus' sign.

Where synchronous data on substance concentrations and water flow rates are available, the methodology provides for a preliminary assessment of the statistical relationship of the form $C = f(Q)$, where C is the substance concentration and Q is the water flow rate. The validity of such a relationship is determined by the correlation coefficient and the ratio of the root mean square error of the verification calculations to the standard deviation of the

original data series. If the relationship is deemed significant, the background concentration can be calculated using the regression equation for the design minimum water flow rate at the 95 percent confidence level. In this study, the main calculation was performed using a series of mean annual concentrations. Therefore, the regression model $C = f(Q)$ was not used as the primary method. It may be applied additionally where 'concentration–water flow' paired data are available for each sampling date.

Table 2. Values of Student's *t*-statistic (t_{St}) at a one-tailed confidence level of P = 0.95 [35].

$n-1$	t_{St}	$n-1$	t_{St}	$n-1$	t_{St}
5	2.02	20	1.72	40	1.68
6	1.94	21	1.72	42	1.68
7	1.90	22	1.72	44	1.68
8	1.86	23	1.71	46	1.68
9	1.83	24	1.71	48	1.68
10	1.81	25	1.71	50	1.68
11	1.80	26	1.71	55	1.67
12	1.78	27	1.70	60	1.67
13	1.77	28	1.70	65	1.67
14	1.76	29	1.70	70	1.67
15	1.75	30	1.70	80	1.66
16	1.75	32	1.69	90	1.66
17	1.74	34	1.69	100	1.66
18	1.73	36	1.69	120	1.66
19	1.73	38	1.69		

Note: when $n < 5$, $t_{St} = 1$.

2.5. Calculation of the Comprehensive Water Pollution Index (CWPI)

A comprehensive assessment of the water quality of the Shu River was carried out by calculating the comprehensive water pollution index (*CWPI*) using the mandatory list of regulated parameters that are measured most regularly. Given the nature of the actual concentrations of hydrochemical and toxic parameters available in the database, the methodological approaches developed under the guidance of Professor M. Zh. Burlibayev [40–43] are the most appropriate for calculating the *CWPI*.

The *CWPI* was calculated separately for each group of indicators in order to improve the informativeness of the assessment. The pollution index for the *j*-th group was determined based on the exceedance ratio of pollutant concentrations relative to their corresponding maximum permissible concentrations (*MPCs*, Table 3):

$$CWPI_j = \frac{\sum_{i=1}^{n} C_i/MPC_i}{n}, \quad (7)$$

where $CWPI_j$—water pollution index for the *j*-th indicator group; C_i—concentration of the *i*-th pollutant within the *j*-th group (mg/L); *MPCi*—maximum permissible concentration corresponding to *Ci* (mg/L); *n*—number of pollutants with concentrations equal to or exceeding the corresponding *MPC* ($C_i/MPC_i \geq 1$) within the *j*-th group.

The integrated Comprehensive Water Pollution Index (*CWPI*) was calculated as the average value across all indicator groups:

$$CWPI = \sum_{j=1}^{m} CWPI_j/m, \quad (8)$$

where m—number of indicator groups included in the calculation for the respective year. Each indicator group was assigned equal weight in the integrated *CWPI*.

Table 3. Reference maximum permissible concentrations (*MPCs*) used for regulatory comparison and, where applicable, *CWPI* calculations [44].

Pollutants	Unit	Maximum Permissible Concentration (*MPC*)
BOD_5	mg O_2/L	3.0
SO_4^{2-}	mg/L	100
Ca^{2+}	mg/L	180
Mg^{2+}	mg/L	40.0
Cl^-	mg/L	300
Ammonium nitrogen (NH_4-N)	mg N/L	0.39
Nitrite nitrogen (NO_2-N)	mg N/L	0.02
Nitrate nitrogen (NO_3-N)	mg N/L	9.1
Mineral phosphorus (as P)	mg P/L	0.10
Cu	mg/L	0.001
Zn	mg/L	0.010
Pb	mg/L	0.010
Cd	mg/L	0.005
Co	mg/L	0.005
Ni	mg/L	0.01
Petroleum products	mg/L	0.050
Phenols	mg/L	0.001

Missing annual values were not imputed and were not treated as zero. For each year, the *CWPI* calculation was based only on the annual mean concentrations actually available for the corresponding regulated parameters. If a value for an individual parameter was unavailable in a given year, that parameter was omitted from the calculation for that year. If no monitoring data were available for an entire indicator group, that group was excluded from the integrated *CWPI* calculation for that year, and the value of m was adjusted accordingly. Thus, the annual *CWPI* values were calculated using the monitoring data actually available for each respective year.

The resulting *CWPI* values were classified as follows: $CWPI \leq 1.0$, normatively clean; 1.1–3.0, moderate contamination; 3.1–10.0, high contamination; and $\geq$10.1, extremely high contamination [40].

The monitored parameters were assigned to the following methodological groups: major ions, biogenic substances, heavy metals, toxic compounds, organic substances, and organochlorine pesticides [40–43]. However, only groups for which appropriate monitoring data were available were considered in the present study.

In accordance with the applied methodological approach, the ionic-saline composition was not included in the *CWPI* calculation for the Shu River because concentrations of major ions are strongly influenced by the natural climatic, hydrogeological, and hydrological characteristics of the catchment. Therefore, the *CWPI* calculation was based on the available regulated non-saline hydrochemical and toxicological parameters.

The maximum permissible concentrations (*MPCs*) used for regulatory comparison and *CWPI* calculations were adopted from the reference values established for fishery water bodies [44]. In the original RSE "Kazhydromet" monitoring dataset, the nitrogen parameters are reported as ammonium nitrogen, nitrite nitrogen, and nitrate nitrogen. Therefore, their concentrations and the corresponding *MPC* values are expressed as nitrogen (NH_4-N, NO_2-N, and NO_3-N, respectively).

The list of ingredients included in the *CWPI* calculations is divided into the following categories: major ions, biogenic elements, heavy metals, toxic compounds, organic substances and organochlorine pesticides. Among these groups of hydrochemical and toxicological parameters, the Kazakh national monitoring database contains long-term data on four groups: major ions, biogenic substances, heavy metals and organic substances.

In accordance with the requirements of existing methods, the ionic-saline composition of natural waters should not be included in the calculation of the Shu River's *CWPI*, as its content depends on soil and climatic, hydrogeological, and other natural and genesis characteristics of the catchment, as well as on the hydrological regime of water bodies.

2.6. Calculation of Mass Transport of Chemical Substances

To assess the mass transport of dissolved and particulate chemical substances, the mass flux through the transboundary section of the Shu River near Kaynar village was additionally calculated. Unlike concentration analysis, this approach makes it possible to assess not only the concentration of a substance in the water but also its actual quantity transported by river flow over the calculation period.

The mass flux was calculated from the annual mean concentration of each chemical parameter and the corresponding water-flow volume for the calculation period according to Equation (9) and the methods described in [45,46]:

$$G = \sum_{i=1}^{m} C_i W_i, \quad (9)$$

where G is the mass of the substance transported during the calculation period; m is the number of intervals within the calculation period; C_i is the mean concentration of the substance during the i-th interval; and Wi is the corresponding water-flow volume, km^3. When C_i is expressed in mg/L and W_i in km^3, the numerical result $C_i \times W_i$ is expressed in thousand metric tons (10^3 t), because 1 mg/L × 1 km^3 = 10^3 t. For trace elements expressed in μg/L, the corresponding result is expressed in metric tons (t), because 1 μg/L × 1 km^3 = 1 t.

Mass-transport calculations were performed for major ions, total dissolved solids, nutrients, heavy metals, and selected organic pollutants. For parameters with incomplete observation series, the analysis was restricted to periods for which synchronous concentration and water-flow data were available.

3. Results

The calculated background concentrations were interpreted as long-term regional reference levels for the hydrochemical characteristics of the Shu River at the Kaynar gauging station. Since annual mean values were used, the influence of short-term seasonal peaks and episodic fluctuations was reduced, although intra-annual variability in water chemistry was also smoothed. Thus, the results primarily characterize long-term regional hydrochemical conditions over the observation period. Background concentrations were calculated for 31 hydrochemical parameters. In total, 533 annual values were processed, and 498 values remained after the exclusion of statistically identified extreme annual values. The general characteristics of the processed dataset are presented in Table 4.

Table 4. General characteristics of the results.

Indicator	Value
Number of calculated parameters	31
Total number of annual values used before data cleaning	533
Remaining values after excluding extreme values	498
Excluded extreme annual values	35
Parameters with $n \geq 20$ (long observation series)	16
Parameters with $10 \leq n < 20$ (intermediate-length series)	7
Parameters with $n < 10$ (short observation series)	8

The statistical reliability of the calculated background concentrations varies depending on the length and completeness of the available observation series. Parameters represented by long-term series ($n \geq 20$) provide a stronger basis for characterizing the long-term hydrochemical conditions of the Shu River. Estimates based on intermediate-length series ($10 \leq n < 20$) should be interpreted with greater caution, whereas background concentrations derived from short series ($n < 10$), particularly those based on only three or four annual observations, should be regarded as preliminary and indicative for the available observation period. For each parameter, Table 5 reports the number of observations retained after data processing, allowing the reliability of individual background estimates to be assessed directly.

Table 5. Final background concentrations.

No.	Parameter	N After Data Cleaning	Mean	Sigma	Background Concentration	Excluded Years
1	Transparency, cm	24	4.998	1.650	5.574	-
2	Suspended solids, mg/L	22	127.058	38.067	141.018	2010, 2016
3	pH	22	7.843	0.087	7.875	2009, 2025
4	Dissolved oxygen, mg/L	24	9.483	0.434	9.331	-
5	CO_2, mg/L	18	8.827	1.599	9.483	2021, 2009
6	Total hardness, mg-eq/L	18	5.416	0.293	5.536	2009, 2013, 2024, 2016, 2002, 2003
7	Ca^{2+}, mg/L	24	73.048	9.764	76.456	-
8	Mg^{2+}, mg/L	22	23.329	2.910	24.396	2008, 2002
9	$Na^+ + K^+$, mg/L	16	41.013	27.392	52.996	-
10	Cl^-, mg/L	24	24.013	5.742	26.017	-
11	HCO_3^-, mg/L	22	239.733	18.419	246.488	2016, 2005
12	SO_4^{2-}, mg/L	23	133.197	30.373	144.090	2002
13	Mineralization, mg/L	20	544.077	70.410	571.315	2005, 2002, 2009
14	Ammonium nitrogen (NH_4-N), mg N/L	22	0.329	0.085	0.360	2010, 2021
15	Nitrite nitrogen (NO_2-N), mg N/L	23	0.0417	0.0130	0.0464	2016
16	Nitrate nitrogen (NO_3-N), mg N/L	24	2.490	0.882	2.798	-
17	Mineral phosphorus (as P), mg P/L	21	0.0281	0.0116	0.0325	2016, 2022, 2005
18	Cu, µg/L	23	3.147	1.334	3.626	2002
19	Zn, µg/L	23	6.552	1.837	7.211	2002
20	Pb, µg/L	17	2.612	1.524	3.259	2021
21	Ni, µg/L	14	1.059	0.390	1.244	2011, 2017
22	Co, µg/L	11	0.0537	0.1008	0.1087	2009
23	Cd, µg/L	10	0.000	0.000	0.000	2009, 2010
24	Total phosphorus	3	0.0411	0.0066	0.0449	2022
25	BOD_5, mg O_2/L	4	2.476	0.127	2.540	-
26	COD, dichromate method	4	26.256	1.927	27.220	-
27	Anionic surfactants/synthetic surfactants	4	0.0276	0.0052	0.0302	-
28	Volatile phenols, mg/L	4	0.000649	0.000441	0.000869	-
29	Petroleum products, mg/L	4	0.0436	0.00925	0.0482	-
30	Dry residue, mg/L	4	638.979	42.620	660.289	-
31	Total iron, mg/L	4	0.0929	0.00654	0.0962	-

3.1. Mineralization and Salt Composition

The analysis of the background concentrations of major ions shows a bicarbonate-sulphate composition of the Shu River with a significant presence of calcium, magnesium and the sum of sodium and potassium. The background mineralization is 571.315 mg/L, and the dry residue is 660.289 mg/L. Among the anions, the highest background values were recorded for bicarbonates—246.488 mg/L—and sulfates—144.090 mg/L, whilst the concentration of chlorides is significantly lower at 26.017 mg/L. Among the cations, cal-

cium predominates at 76.456 mg/L, followed by the sum of sodium and potassium at 52.996 mg/L and magnesium at 24.396 mg/L.

The annual average values for total salinity and the major ions show interannual variability. For certain parameters, extreme values were excluded from the calculations: for total salinity—2002, 2005 and 2009; for bicarbonates—2005 and 2016; for sulfates—2002; and for magnesium—2002 and 2008. The trends in average annual concentrations and the calculated background levels are shown in Figure 2.



Figure 2. Background concentrations of (**a**) water mineralization; (**b**) dry residue; and salt composition indicators: (**c**) bicarbonates; (**d**) sulfates; (**e**) calcium; (**f**) magnesium; (**g**) chlorides; (**h**) sodium and potassium of the Shu River.

3.2. Suspended Solids

The background concentration of suspended solids is 141.018 mg/L, with an average value after data cleaning of 127.058 mg/L. The concentration of suspended solids is characterized by marked interannual variability. The highest annual average values were observed in 2010—around 399 mg/L—and in 2016—around 272 mg/L. Both values were excluded from the calculation as outliers.

After 2017, the annual average concentrations are below the calculated background level in most years. The lowest values were recorded in 2022–2023. The trends in annual average concentrations of suspended solids and the calculated background concentration are shown in Figure 3.

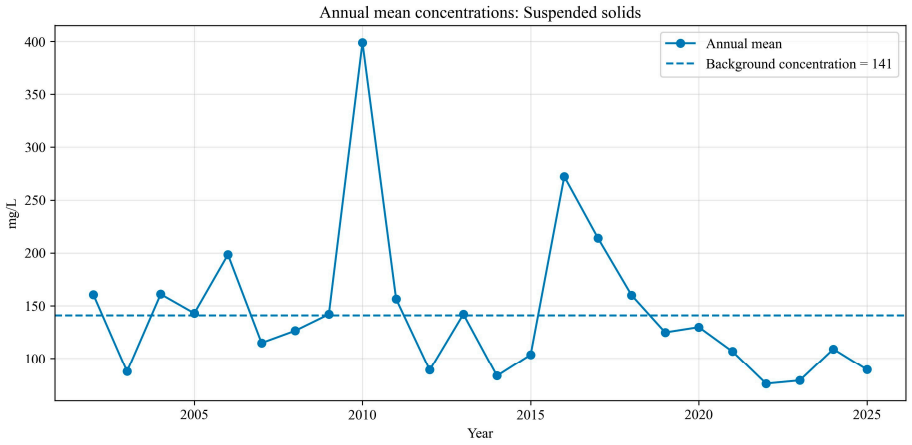


Figure 3. Trends in average annual concentrations of suspended solids and the estimated background concentration in the water of the Shu River for 2002–2025.

3.3. Biogenic Substances

For ammonium nitrogen (NH_4-N), the calculated background concentration is 0.360 mg N/L. The annual average values are characterized by interannual fluctuations, with elevated values in 2006, 2010, and 2019–2021. The extreme values from 2010 and 2021 were excluded from the calculation of the background concentration.

The background concentration of nitrite nitrogen (NO_2-N) is 0.0464 mg N/L. In most years, the values are close to the calculated background level. However, for 2016, a sharp peak of around 0.195 mg N/L was recorded. This value was excluded from the calculation as an outlier.

For nitrate nitrogen (NO_3-N), the background concentration is 2.798 mg N/L. At the beginning of the observation period, particularly between 2002 and 2010, nitrate nitrogen concentrations were higher than the calculated background level. After 2011–2012, a decline was observed, and in 2013–2025 the values were generally below the background concentration.

The background concentration of mineral phosphorus (as P) is 0.0325 mg P/L. For this parameter, the extreme values from 2005, 2016 and 2022 were excluded. The interannual dynamics of ammonium nitrogen, nitrite nitrogen, nitrate nitrogen, and mineral phosphorus are presented in Figure 4. Total phosphorus was calculated based on only a short series of observations. It is characterized by a background concentration of 0.0449 mg P/L.

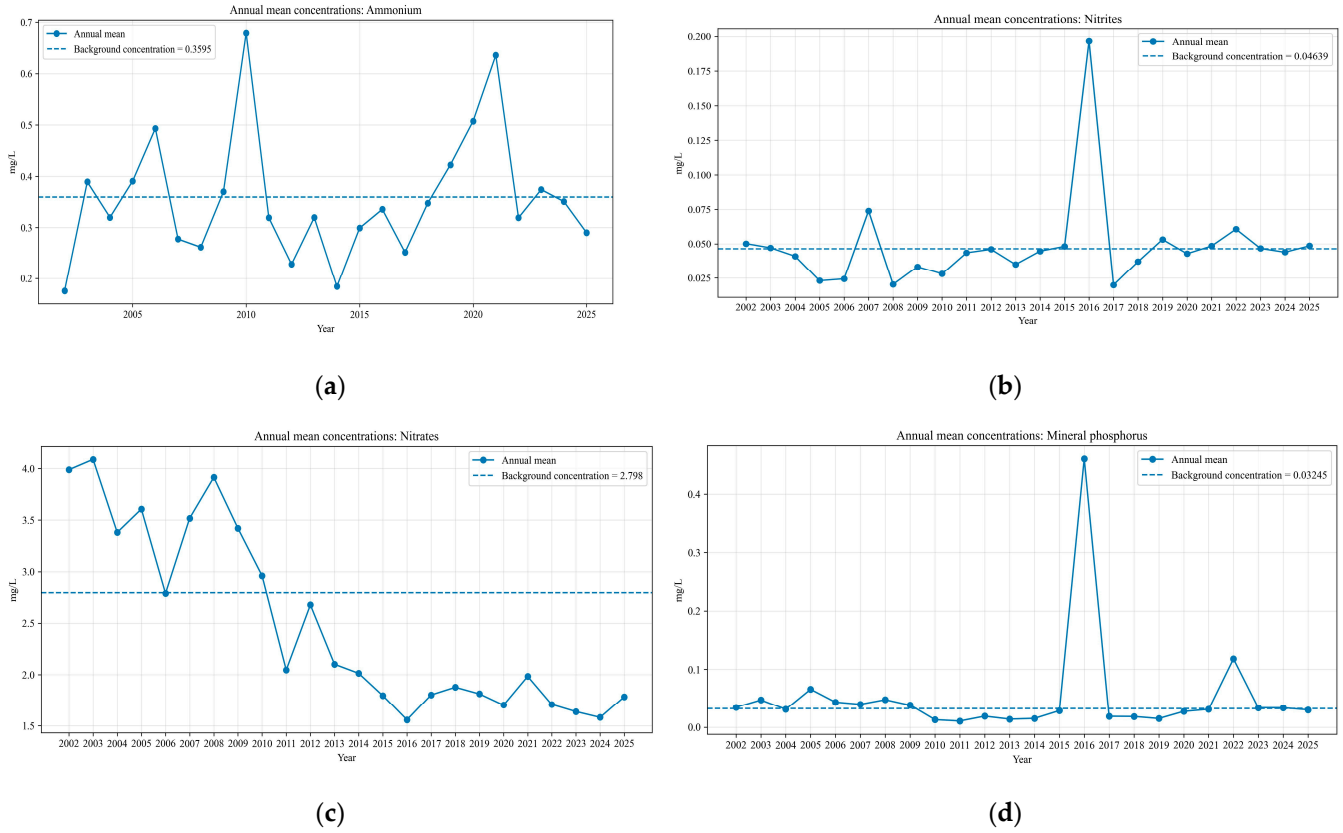


Figure 4. Dynamics of average annual concentrations of nutrients in the Shu River water for 2002–2025 and the calculated background concentrations: (**a**) NH_4-N; (**b**) NO_2-N; (**c**) NO_3-N; (**d**) P_{min}.

3.4. Organic Parameters

The background concentrations of organic water pollution indicators in the River Shu for the period 2022–2025 are as follows: BOD_5—2.540 mg/L, COD—27.220 mg/L, petroleum products—0.0482 mg/L, surfactants—0.0302 mg/L, volatile phenols—0.000869 mg/L. As these indicators are represented by only four annual average values, the figures obtained should be regarded as preliminary background estimates for the current observation period.

The ratio between the independently calculated background concentrations of BOD_5 and COD was approximately 0.09; this value is presented only as a descriptive comparison of the two background estimates. Among specific organic pollutants, the highest background values are characteristic of petroleum products and surfactants, whilst phenols are characterized by the lowest absolute concentrations.

3.5. Heavy Metals

Background concentrations of heavy metals are as follows: copper—3.626 µg/L, zinc—7.211 µg/L, lead—3.259 µg/L, nickel—1.244 µg/L, cobalt—0.1087 µg/L, cadmium—0 µg/L.

For copper and zinc, higher concentrations are observed at the start of the monitoring period, particularly between 2002 and 2009. After 2010, copper concentrations decline in most years and remain below the calculated background level. Zinc is characterized by marked interannual variability, with isolated increases in 2002, 2006, 2018, 2019 and 2024.

Lead concentrations are generally below background levels between 2008 and 2019. However, an increase is observed between 2020 and 2024, peaking in 2021. The most pronounced nickel peaks are observed in 2011 and 2017. Cobalt and cadmium are characterized by low values in most years. The zero value for the background concentration of cadmium is due to the prevalence of zero values in the source data and should not be taken as evidence of the complete absence of the element in the water. The interannual dynamics of heavy metal concentrations and their calculated background levels are presented in Figure 5.

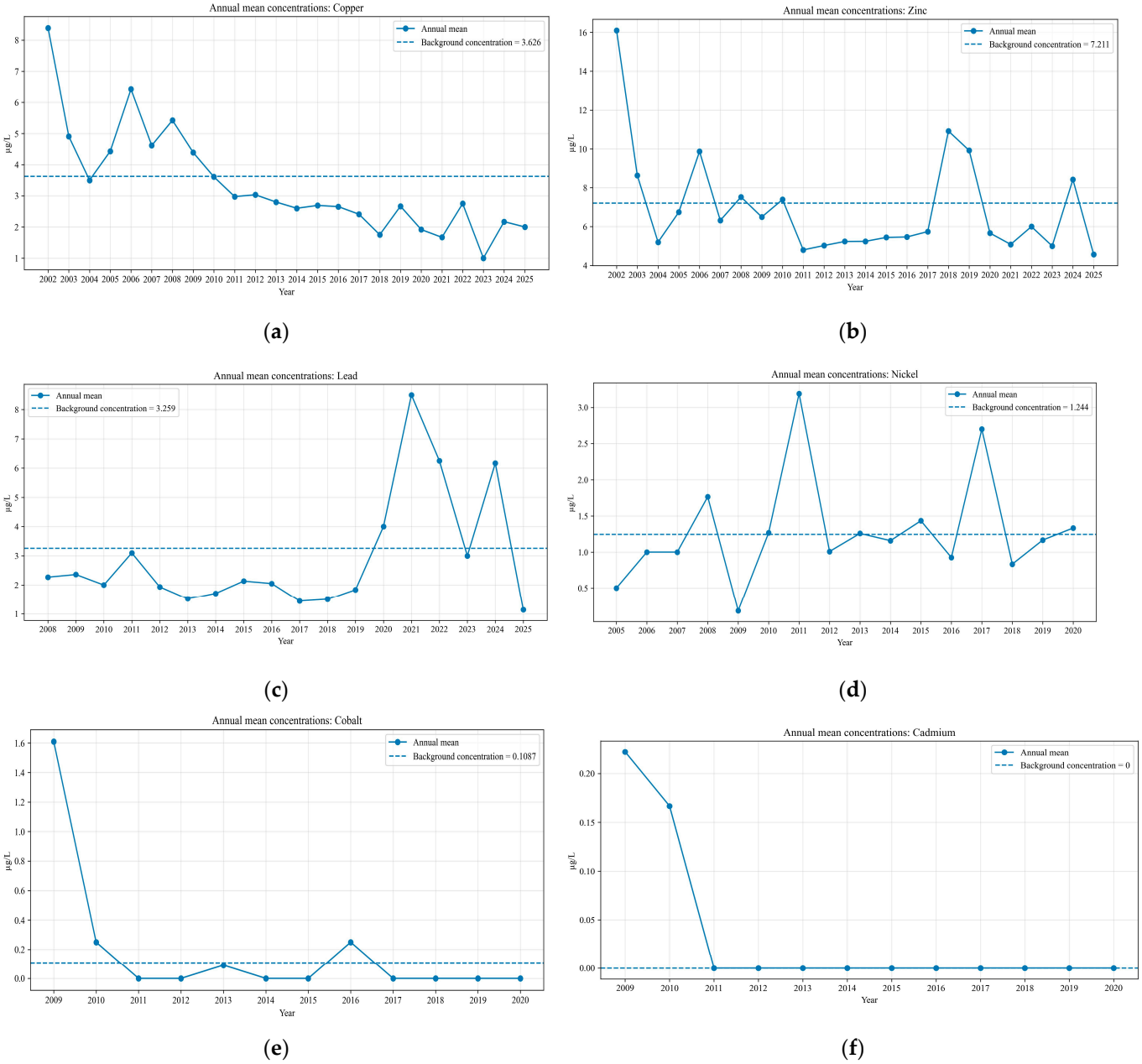


Figure 5. Dynamics of average annual heavy metal concentrations and the calculated background concentrations (dotted line) in the Shu River water for 2002–2025: (**a**) Cu; (**b**) Zn; (**c**) Pb; (**d**) Ni; (**e**) Co; (**f**) Cd.

3.6. Comprehensive Assessment of the Water Quality

A comparison of the calculated background concentrations with the reference maximum permissible concentrations (MPC_s) shows that exceedances at the background-concentration level were observed for sulfates, nitrite nitrogen, and copper. The corresponding Cb/*MPC* ratios were 1.44 for sulfates, 2.32 for nitrite nitrogen (NO_2-N), and 3.63 for copper.

Suspended solids were assessed separately because the applicable regulatory criterion is expressed relative to the background concentration rather than as a fixed *MPC*. Therefore, suspended solids were not included in the *C*/*MPC* comparison or *CWPI* calculation.

For ammonium nitrogen (NH_4-N), mineral phosphorus (as P), zinc, petroleum products, and phenols, exceedances of the corresponding MPC_s were predominantly episodic. For calcium, magnesium, chlorides, nitrate nitrogen (NO_3-N), lead, nickel, cobalt, cadmium, and BOD_5, the calculated background concentrations did not exceed the corresponding reference MPC_s. The annual concentration-to-*MPC* ratios for selected water-quality parameters are presented in Figure 6.

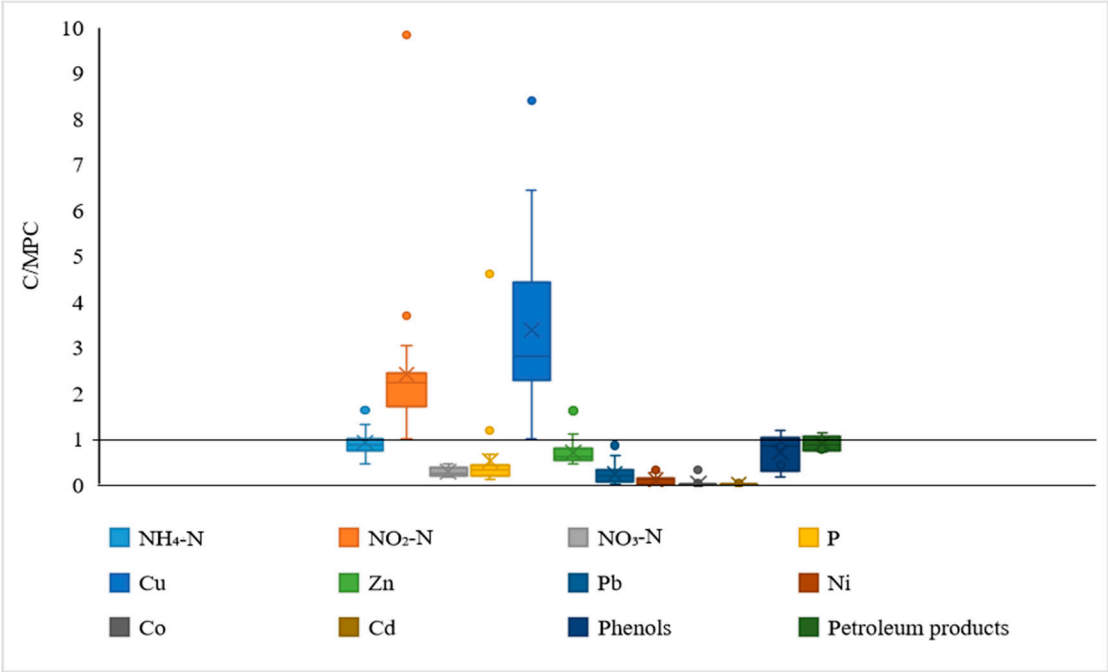


Figure 6. Distribution of annual concentration-to-MPC ratios (*C*/*MPC*) for selected water-quality parameters of the Shu River during 2002–2025. The horizontal line at *C*/*MPC* = 1 indicates the regulatory threshold.

Calculations of the *CWPI* show that, in most years, the water quality of the Shu River corresponded to a moderate level of pollution. High pollution levels were recorded in 2002, 2003, 2006–2008, and 2016, with the highest *CWPI* value observed in 2016. After 2017, the *CWPI* generally remained within the moderate pollution range. No cases of extremely high pollution were recorded during the study period. The long-term dynamics of the *CWPI* are presented in Figure 7. The annual concentration-to-*MPC* ratios and corresponding *CWPI* values are presented in Table 6.

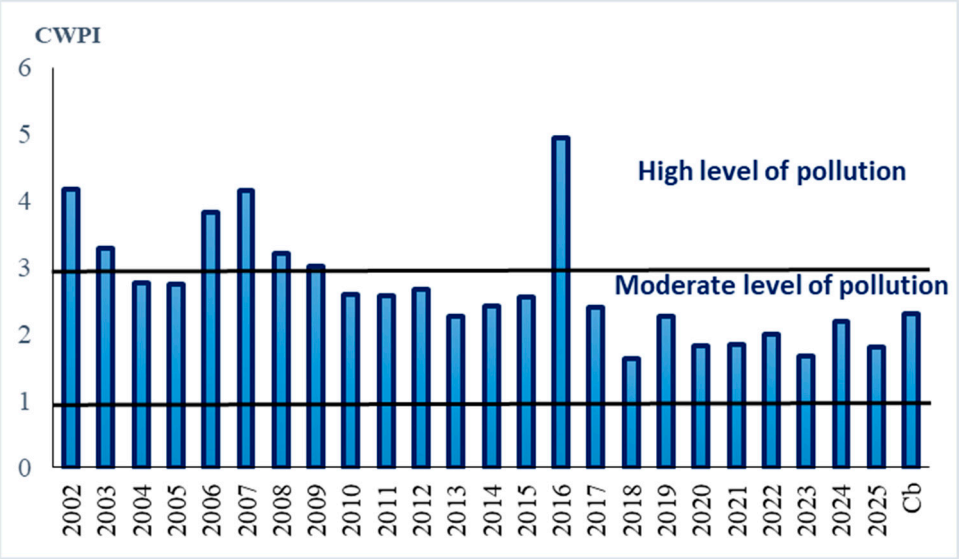


Figure 7. Long-term trends of the Comprehensive Water Pollution Index (*CWPI*) for the Shu River.

Table 6. Annual concentration-to-*MPC* ratios (C_i/MPC_i) and Comprehensive Water Pollution Index (*CWPI*) values for the Shu River at the Kaynar monitoring section, 2002–2025.

Year	NH_4-N	NO_2-N	NO_3-N	P	Cu	Zn	Pb	Ni	Phenols	Petroleum Products	*CWPI*
2002	0.45	2.51	0.44	0.35	8.39	1.61	n/d	n/d	n/d	n/d	3.75
2003	1.00	2.35	0.45	0.47	4.91	0.86	n/d	n/d	n/d	n/d	3.29
2004	0.82	2.05	0.37	0.31	3.50	0.52	n/d	n/d	n/d	n/d	2.78
2005	1.00	1.15	0.40	0.66	4.43	0.67	0.00	0.05	n/d	n/d	2.79
2006	1.26	1.22	0.31	0.44	6.43	0.99	0.00	0.10	n/d	n/d	3.83
2007	0.71	3.70	0.39	0.40	4.62	0.63	0.00	0.10	n/d	n/d	4.16
2008	0.67	1.02	0.43	0.48	5.43	0.75	0.23	0.18	n/d	n/d	3.22
2009	0.95	1.66	0.38	0.38	4.39	0.65	0.24	0.02	n/d	n/d	3.03
2010	1.74	1.40	0.33	0.13	3.61	0.74	0.20	0.13	n/d	n/d	2.59
2011	0.82	2.18	0.22	0.11	2.98	0.48	0.31	0.32	n/d	n/d	2.58
2012	0.59	2.30	0.29	0.19	3.03	0.50	0.19	0.10	n/d	n/d	2.67
2013	0.82	1.75	0.23	0.14	2.80	0.52	0.15	0.13	n/d	n/d	2.27
2014	0.47	2.23	0.22	0.15	2.60	0.52	0.17	0.12	n/d	n/d	2.42
2015	0.77	2.41	0.20	0.29	2.69	0.54	0.21	0.14	n/d	n/d	2.55
2016	0.86	9.84	0.17	4.61	2.65	0.55	0.21	0.09	n/d	n/d	4.94
2017	0.65	1.00	0.20	0.19	2.41	0.57	0.14	0.27	n/d	n/d	1.70
2018	0.89	1.85	0.21	0.19	1.75	1.09	0.15	0.08	n/d	n/d	1.64
2019	1.08	2.66	0.20	0.15	2.67	0.99	0.18	0.12	n/d	n/d	2.27
2020	1.30	2.14	0.19	0.27	1.92	0.57	0.40	0.13	n/d	n/d	1.82
2021	1.63	2.42	0.22	0.31	1.67	0.51	0.85	0.00	n/d	n/d	1.85
2022	0.82	3.03	0.19	1.18	2.75	0.60	0.63	0.00	1.17	1.13	2.00
2023	0.96	2.33	0.18	0.34	1.00	0.50	0.30	0.00	0.83	0.87	1.67
2024	0.90	2.20	0.17	0.34	2.17	0.84	0.62	0.00	0.17	0.72	2.18
2025	0.74	2.43	0.20	0.30	2.00	0.46	0.11	0.00	0.43	0.77	2.21

Notes: Values for individual parameters represent annual concentration-to-MPC ratios (C_i/MPC_i). "n/d" no monitoring data. *CWPI* classification: ≤1.0, normatively clean; 1.1–3.0, moderate contamination; 3.1–10.0, high contamination; ≥10.1, extremely high contamination.

3.7. Mass Transport of Chemicals Through the Shu River–Kaynar Village Section

Calculations of the mass transport of chemical substances made it possible to estimate the actual quantity of substances carried by river flow through the section of the River Shu at the village of Kaynar. The analysis was carried out for mineral salts, major ions, biogenic substances, heavy metals and certain specific organic pollutants.

A positive relationship was observed between mineral-salt mass flux and river discharge (r = 0.73; Figure 8). However, this correlation should be interpreted with caution because the river discharge is itself a component of the mass-flux calculation. Therefore, the observed relationship partly reflects the mathematical dependence of mass flux on water discharge and should not be considered independent evidence of hydrological control.

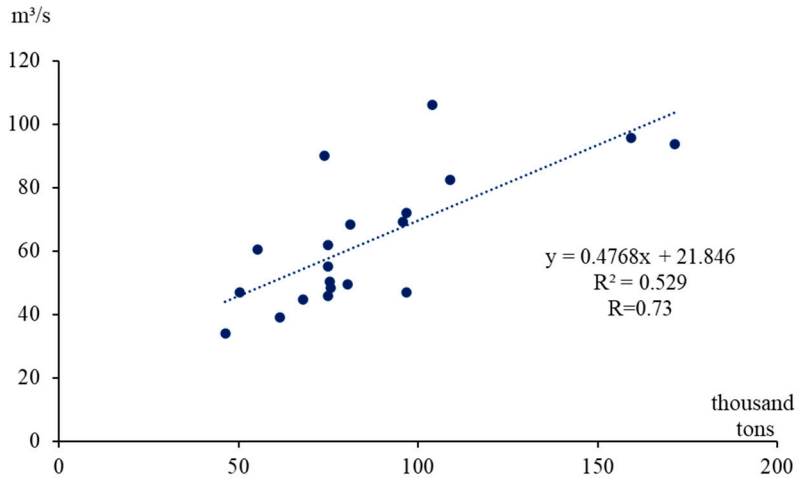


Figure 8. Relationship between the flux of mineral salts and water discharge of the Shu River at the transboundary hydrological station Kaynar.

The average monthly mass transport of mineral salts was highest at the beginning of the study period: 171.6 thousand metric tons per month in 2002 and 159.2 thousand metric tons per month in 2003. The lowest value was recorded in 2021, at 46.3 thousand metric tons per month. In 2022–2023, the average monthly mass transport increased to 67.9–75.0 thousand metric tons per month (Figure 9).

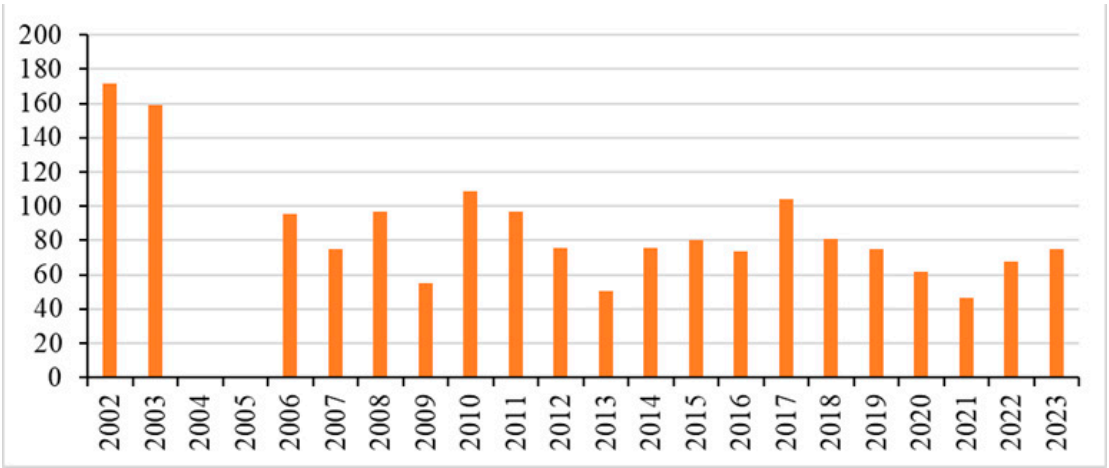


Figure 9. Dynamics of the transboundary mass transport of mineral salts in the Shu River (based on monthly averages in thousand metric tons).

The total annual removal of ionic constituents was calculated for 2021–2023. It amounted to 555.2 thousand tons per year in 2021, 815.2 thousand tons per year in 2022, and 899.6 thousand tons per year in 2023. Bicarbonates, sulfates and calcium made the main contribution to the composition of ionic removal (Table 7).

Table 7. Total ion flux of the Shu River at the transboundary section near Kaynar village.

Year	Ca^{2+}	Mg^{2+}	$Na^{+} + K^{+}$	Cl^{-}	HCO_3^{-}	SO_4^{2-}	Mineralization	Water Volume, km^3
	Thousand Tons							
2021	74.4	24.1	42.8	24.2	249.4	129.5	555.2	1.1
2022	97.3	34.7	90.7	35.6	349.3	216.7	815.2	1.4
2023	109.5	34.7	88.4	30.1	366.6	228.3	899.6	1.4

The analysis of average monthly nutrient mass transport shows that nitrate nitrogen (NO_3-N) was the dominant component, whereas ammonium nitrogen (NH_4-N), nitrite nitrogen (NO_2-N), and mineral phosphorus contributed much less. The mass transport of nitrate nitrogen was highest during 2002–2005 (0.74–1.05 thousand metric tons per month), peaking in 2003, and then declined, stabilizing at 0.18–0.23 thousand metric tons per month during 2019–2023 (Figure 10).

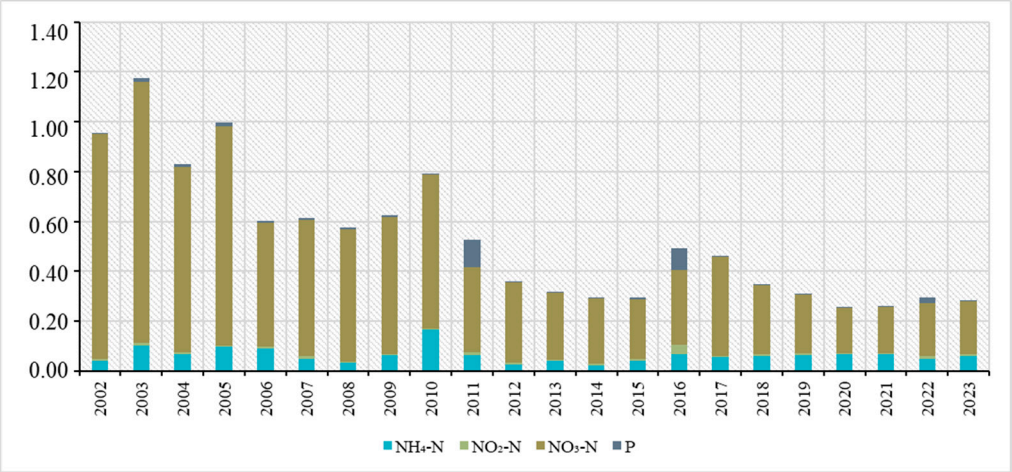


Figure 10. Dynamics of the transboundary nutrient mass transport in the Shu River (based on monthly averages in thousand metric tons).

The total annual nutrient mass transport was 3.14 thousand metric tons in 2021, increased to 3.55 thousand metric tons in 2022, and slightly declined to 3.40 thousand metric tons in 2023. The increase in 2022 was mainly associated with higher mineral phosphorus transport, whereas its contribution decreased in 2023. Overall, nitrate nitrogen (NO_3-N) accounted for the largest contribution to nutrient mass transport, while ammonium nitrogen (NH_4-N), nitrite nitrogen (NO_2-N), and mineral phosphorus accounted for much smaller shares (Table 8).

Table 8. Annual total nutrient mass transport in the Shu River at the transboundary section near Kaynar village (thousand metric tons per year).

Parameter	2021	2022	2023
Ammonium nitrogen (NH_4-N)	0.79	0.60	0.71
Nitrite nitrogen (NO_2-N)	0.07	0.10	0.08
Nitrate nitrogen (NO_3-N)	2.24	2.58	2.55
Mineral phosphorus (as P)	0.04	0.26	0.06
$\Sigma_{nutrients}$	3.14	3.55	3.4

The average monthly mass transport of heavy metals showed pronounced interannual variability. The highest values for copper and zinc were recorded at the beginning of the

study period in 2002, amounting to 2.16 and 4.04 metric tons per month, respectively. In subsequent years, copper mass transport generally declined, whereas zinc showed greater variability. For lead, average monthly mass transport increased to 0.86–0.99 metric tons per month during 2020–2022, followed by a decline in 2023 (Figure 11).

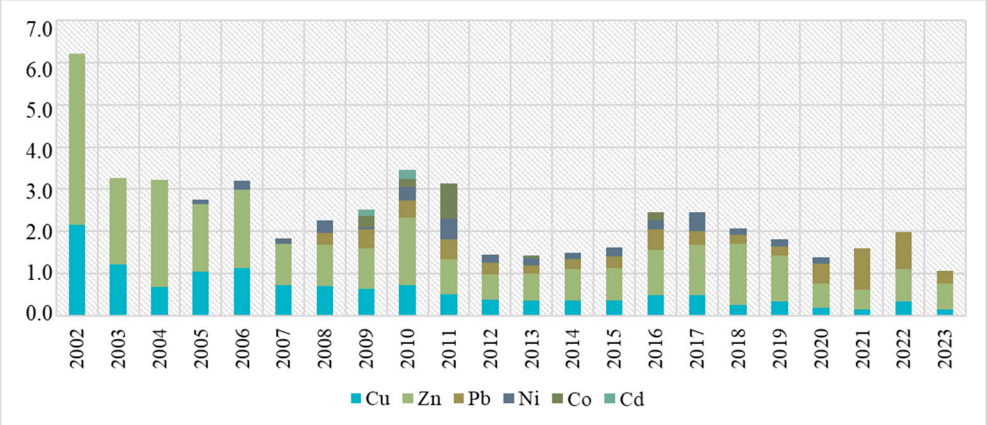


Figure 11. Dynamics of the transboundary mass transport of heavy metals in the Shu River (based on monthly averages in metric tons).

The combined annual mass transport of the major heavy metals considered in this analysis (Cu, Zn, and Pb) was 19.23 metric tons per year in 2021, increased to 23.44 metric tons per year in 2022, and decreased to 12.87 metric tons per year in 2023. Lead and zinc accounted for the largest shares of the combined heavy-metal mass transport during this period. Other heavy metals were not included in this calculation because corresponding monitoring data were not available for the same period. Total iron mass transport amounted to 0.08 thousand metric tons per year in 2022 and 0.15 thousand metric tons per year in 2023 (Table 9).

Table 9. Annual mass transport of heavy metals in the Shu River at the transboundary section near Kaynar village (metric tons per year).

Parameter	2021	2022	2023
Cu	1.76	3.41	1.80
Zn	5.59	8.18	7.46
Pb	11.88	11.85	3.61
$\Sigma_{(Cu+Zn+Pb)}$	19.23	23.44	12.87

For specific organic pollutants, the calculation was limited to the period 2022–2023. Annual fluxes of petroleum products, surfactants, and phenols decreased from 82.47 to 65.92 t/year, from 53.48 to 32.37 t/year, and from 1.77 to 1.25 t/year, respectively (Table 10).

Table 10. Average monthly and annual total flux of specific organic pollutants at the transboundary section of the Shu River near Kaynar village (in tons).

Parameter	Average Monthly Flux, t		Total Flux, t	
	2022	2023	2022	2023
Surfactants	4.46	2.70	53.48	32.37
Phenols	0.15	0.14	1.77	1.25
Petroleum products	6.87	5.49	82.47	65.92

4. Discussion

The results show that the background concentrations of hydrochemical parameters in the Shu River reflect not only the natural conditions governing the formation of its chemical composition, but also the long-term cumulative impact of water management activities in the catchment. This is in line with the methodological provisions of RD 52.24.622-2001 [35], according to which the background concentration is determined for a specific section of a watercourse. It characterises the concentration of a substance under unfavorable conditions, caused by both natural factors and the impact of pollution sources located upstream of the observed section [35]. Therefore, the calculated Cb values should be regarded not as an 'absolutely natural' background, but as a regionally determined background level, formed under the current conditions of the catchment [35,46].

This approach is consistent with studies in which background water quality indicators are used not only as statistical values but also as regional benchmarks for assessing the condition of water bodies, comparing sections of watercourses, and justifying water protection measures [47]. For transboundary and managed river basins, this interpretation is particularly important, as there are no completely undisturbed conditions, and water quality is shaped by natural processes, flow regulation, irrigation and return flows.

The background salt composition of the Shu River is characterised by a bicarbonate-sulfate type, which is consistent with the conditions under which the river flow is formed in mountainous and foothill regions. The predominance of bicarbonates and calcium reflects the interaction of water with carbonate and terrigenous rocks, whereas the increased role of sulfates is associated with sulfate-containing minerals, soil salinity, and the characteristics of an arid watershed [48].

The exceedance of the *MPC* for sulfates even at the background concentration level indicates the regional specificity of the water's salt composition. This situation cannot be explained solely by a local source of pollution. Arid basins are characterized by evaporation-caused concentrations of dissolved substances. In areas with extensive irrigation, return-flowing irrigation water and drainage-collector water are of additional significance. Therefore, mineralization, sulfates, dry residue, and the sum of Na^+ and K^+ should be considered as indicators of the combined influence of natural mineralization and water management pressures.

The difference between mineralization and dry residue also requires a comprehensive interpretation. Mineralization characterizes the total content of dissolved ions, whereas dry residue may additionally reflect the contribution of sparingly soluble and suspended components, as well as the specifics of the analytical determination. Therefore, it is advisable to consider these indicators together.

A high background concentration of suspended solids is one of the most important indicators of the hydrochemical status of the Shu River. Even after excluding the extreme values from 2010 and 2016, the average concentration of suspended solids remained high. This indicates the persistent role of erosion runoff, channel processes, and sediment transport in shaping water quality [48].

The ecological significance of suspended solids is not limited to water turbidity. Fine-grained material can transport heavy metals, phosphorus-containing compounds, and organic pollutants, and subsequently contribute to the formation of bottom sediments [36,37]. Therefore, high concentrations of suspended solids can enhance the spatial migration of pollutants and create conditions for secondary contamination of the aquatic environment.

Biogenic substances demonstrate a distinction between concentration risk and mass load. Nitrite nitrogen (NO_2-N) is the most problematic indicator in terms of the multiple by which the *MPC* is exceeded, whereas nitrate nitrogen (NO_3-N) accounts for the main

contribution to the mass load of biogenic substances. This shows that the interpretation of nitrogen compounds should not be limited solely to comparison with regulatory standards.

Elevated nitrite nitrogen (NO_2-N) concentrations may be associated with incomplete oxidation of ammonium nitrogen, the inflow of domestic and agricultural runoff, and changes in the oxygen regime of the water. Current studies of river systems also consider nitrite nitrogen and phosphorus compounds as sensitive indicators of the effects of urban runoff, agricultural inputs, and insufficiently treated wastewater [27,31].

The decline in nitrate nitrogen (NO_3-N) concentrations after 2011–2012 may reflect changes in runoff formation, hydrological conditions, and the input of nitrogen-containing substances from the catchment. However, in terms of mass transport, nitrate nitrogen (NO_3-N) remained the dominant nitrogen form because its concentrations were substantially higher than those of nitrite nitrogen (NO_2-N) and ammonium nitrogen (NH_4-N). Peaks in mineral phosphorus in 2011, 2016, and 2022 indicate episodic increases in phosphorus transport, which may be associated with surface runoff, drainage and irrigation return flows, or local sources of pollution.

The organic parameters were calculated based on a short series of observations from 2022 to 2025. Therefore, their background values should be considered preliminary. Because the background concentrations of BOD_5 and COD were estimated independently from their respective observation series, their ratio should not be interpreted as a conventional paired-sample BOD_5/COD indicator of organic-matter biodegradability. A reliable assessment of this relationship would require synchronous BOD_5 and COD measurements from the same samples.

Petroleum products, surfactants, and phenols were detected at low levels. However, their presence may indicate an anthropogenic influence on water quality. The potential sources discussed below should be regarded as plausible explanations based on previous studies and basin characteristics rather than as sources directly identified by the present study. In the Shu River basin, petroleum products may enter the river through road runoff, leakage, and wash-off from vehicles and agricultural machinery, runoff from fuel storage and maintenance areas, and local inputs from settlements within the catchment. Secondary transport with contaminated suspended solids may also contribute to their redistribution. Surfactants may be associated with domestic wastewater and local untreated or insufficiently treated effluents, while phenols may originate from both natural organic matter decomposition and anthropogenic inputs. The short duration of the data series requires further monitoring of these parameters.

For heavy metals, the most significant finding is that the *MPC* for copper is exceeded, even at the calculated background concentration level. This means that exceedances of the standard are recorded not only in specific years but also under calculated background conditions. This characteristic may be associated with the regional geochemical conditions of the watershed, the transport of copper in suspended form, secondary mobilization from bottom sediments, and diffuse anthropogenic impacts.

International studies show that concentrations of Cu, Pb, Zn, Cd, and Ni often have mixed origins and may reflect both natural and anthropogenic sources. Geochemical and statistical methods are used to distinguish between these sources, including normalization relative to background values, factor analysis, and spatial modeling [22,49,50]. Sediments are of particular importance, as they can act as reservoirs and secondary sources of heavy metals [36,37]. In regulated river systems, processes such as deposition, sorption onto suspended particles, and subsequent remobilization can significantly alter the migration and ecological availability of metals [38,51].

The differences in the trends of individual metals indicate that they do not form a single temporal trend. The decline in copper and zinc after the initial observation period

may reflect changes in input or migration conditions, whereas the increase in lead in recent years warrants further attention. A zero-background concentration value for cadmium should not be interpreted as its complete absence. It is more accurate to consider it as an indication of a concentration below the limit of quantification or as a result of the predominance of zero values in the original dataset.

A comparison of background concentrations with the reference *MPCs* shows that exceedances at the background-concentration level were observed for sulfates, nitrite nitrogen (NO_2-N), and copper. This is important for the interpretation of the results, because such exceedances cannot always be unambiguously explained by a contemporary local source of pollution [33,46,52]. They may reflect the combined effects of the regional geochemical background, arid climate, flow regulation, irrigation water use, and cumulative anthropogenic impacts. Suspended solids were considered separately because the applicable criterion is expressed relative to the background concentration rather than as a fixed *MPC*.

This interpretation is particularly important for the Shu-Talas basin. Given the significant water withdrawal for irrigation, the return flow of drainage and collector waters, and the regulation of runoff by reservoirs, the natural conditions for water dilution and self-purification are changing [23,24,30,48]. Recent reviews of river basins also emphasize that agricultural runoff, municipal wastewater, and industrial discharges remain the key sources of water quality degradation [31].

Calculations of the Comprehensive Water Pollution Index (*CWPI*) confirmed the conclusions drawn from the analysis of individual groups of substances. In most years, the index values corresponded to a moderate level of pollution. However, in 2002, 2003, 2006–2008, and 2016, water quality fell into the high pollution category. The use of integrated indices is a common approach for transitioning from the analysis of individual components to an overall assessment of a water body's condition [25–28]. The application of the CWPI in this study is methodologically justified by recommendations for the comprehensive assessment of surface water quality [40–43].

Further analyses of the mass transport of chemicals show that the environmental impact on downstream sections of the basin is determined not only by the concentration level of pollution but also by the annual water availability [29]. As water flow increases, the total transport of dissolved and suspended substances may rise even at moderate concentrations, whereas during low-flow periods, the concentration risk increases due to the reduced diluting capacity of the flow. Therefore, years with maximum concentrations do not always coincide with years of maximum mass transport of substances.

For the Shu River, this is reflected in the difference between concentration-based and mass-transport assessments. Nitrite nitrogen (NO_2-N) was the most problematic nutrient indicator in terms of the multiple by which the reference *MPC* value was exceeded, whereas nitrate nitrogen (NO_3-N) accounted for the largest share of nutrient mass transport. Among heavy metals, copper was the most significant in terms of concentration exceedance, whereas lead and zinc accounted for the largest shares of annual heavy-metal mass transport in recent years. This demonstrates the importance of considering both regulatory exceedances and the quantities of substances transported through the transboundary section [29,45].

The calculation of chemical mass transport has practical significance because it complements concentration-based assessment by quantifying the amount of substances transported through the transboundary section. This is particularly relevant for river basins with substantial interannual variability in discharge and intensive water use, where similar concentrations may correspond to different transported masses depending on waterflow volume.

The results obtained have several limitations. First, the background concentrations calculated for the entire 2002–2025 period represent integrated long-term estimates and may therefore incorporate gradual temporal changes in individual hydrochemical parameters. Interannual dynamics are presented separately in the corresponding figures and discussed for individual parameters. However, formal monotonic trend analysis was beyond the primary scope of the present study. Consequently, the calculated background concentrations should be interpreted as long-term regional reference levels for the observation period rather than as temporally invariant values. Second, background concentrations were calculated using annual averages, which increases the stability of the long-term assessment, but smooths out seasonal peaks and short-term pollution episodes. Third, some organic indicators were available only for 2022–2025; therefore, the corresponding background estimates should be considered preliminary. Fourth, the observation series for individual components differ in length and completeness, which limits the comparability among different groups of substances. Fifth, chemical mass-flux calculations for individual groups of substances were performed only for years with synchronous data on concentrations and water discharge.

The practical significance of this study lies in the fact that the calculated background concentrations and mass transport rates can be used to develop regionally adapted criteria for assessing water quality, interpreting monitoring results, and justifying water protection measures. This approach is consistent with the need to establish a robust research foundation for assessing conditions of river basins [39,52]. For the transboundary Shu-Talas basin, this is particularly important because the environmental assessment must account not only for local exceedances of standards, but also for the actual transport of pollutants across the border.

Thus, the water quality of the Shu River is shaped by a combination of natural and anthropogenically modified factors. Background-level exceedances of the reference *MPC* values for sulfates, nitrite nitrogen (NO_2-N), and copper indicate the importance of considering basin-specific hydrochemical characteristics in water-quality assessment. Suspended solids should be considered separately because the applicable criterion is expressed relative to the background concentration rather than as a fixed *MPC* value. At the same time, regulatory exceedances should remain an important component of water-quality assessment because they characterize the actual chemical condition of the river. Combining concentration-based assessment with chemical mass-transport analysis provides a more comprehensive characterization of the transboundary river and the transport of substances to downstream sections of the basin.

5. Conclusions

This study derived long-term background concentration estimates for the hydrochemical parameters of the Shu River at the Kaynar gauging station near the transboundary section in Kazakhstan, based on the available observation series. Calculations based on annual averages, with statistical extremes excluded according to the applied method, enabled comparisons among different groups of substances and characterization of long-term regional reference levels for the assessed hydrochemical parameters. For parameters represented by short observation series, particularly some organic indicators, the resulting background estimates should be regarded as preliminary.

The chemical composition of the Shu River water is shaped by a combination of natural and anthropogenically modified factors. Among the most significant are the arid conditions of the catchment, natural mineralization, soil erosion, transport of suspended solids, water abstraction for irrigation, irrigation return flows, and flow regulation. Therefore, the calculated background concentrations should not be interpreted as representing an

exclusively natural background; rather, they represent regionally determined reference levels reflecting the current condition of the water body.

Among the parameters assessed against fixed reference *MPCs*, sulfates, nitrite nitrogen (NO_2-N), and copper showed exceedances at the level of the calculated background concentrations, indicating persistently elevated levels during the observation period. Suspended solids were considered separately because the applicable criterion is expressed relative to the background concentration rather than as a fixed *MPC*. These results confirm the importance of considering basin-specific hydrochemical characteristics when interpreting *MPC* exceedances and developing water protection measures.

A comprehensive assessment based on the *CWPI* showed that the water quality of the Shu River corresponds to a moderate level of pollution in most years, whereas high pollution levels were recorded in 2002, 2003, 2006–2008, and 2016. These results indicate that the water-quality conditions of the river reflect the combined influence of mineralization, suspended solids, nutrient compounds, and certain heavy metals rather than a single component.

The calculation of chemical mass fluxes made it possible to assess not only concentrations in the river water but also the quantities of substances transported through the transboundary section. The calculated mass fluxes varied with river discharge, which is expected because water-flow volume is an explicit component of the mass-flux calculation. Therefore, the positive association between discharge and mass flux should not be interpreted as independent evidence of hydrological control. Between 2021 and 2023, the annual mass transport of ionic constituents increased from 555.2 to 899.6 thousand metric tons.

An analysis of nutrient mass transport showed that nitrate nitrogen (NO_3-N) accounted for the largest contribution to nutrient mass transport, whereas nitrite nitrogen (NO_2-N) was the most problematic parameter in terms of the multiple by which the *MPC* was exceeded. The total annual mass transport of nutrient compounds amounted to 3.14 thousand metric tons in 2021, 3.55 thousand metric tons in 2022, and 3.40 thousand metric tons in 2023. These results demonstrate the importance of considering both concentration exceedances and mass transport when assessing water quality.

For heavy metals, the pattern of mass transport was variable. During 2021–2023, lead and zinc made the largest contributions to heavy-metal mass transport, whereas copper remained the most significant element in terms of concentration exceedance. The total annual mass transport of the main heavy metals amounted to at least 19.23 metric tons in 2021, increased to 23.44 metric tons in 2022, and decreased to 12.87 metric tons in 2023. These results show that years with the highest concentration exceedances do not necessarily coincide with years of maximum mass transport.

The practical significance of this study lies in the fact that the background concentrations and mass transport rates can be used as regional benchmarks for the assessment of water quality, the interpretation of monitoring results, the analysis of *MPC* exceedances, and the justification of water protection measures in the Shu-Talas basin.

A limitation worth noting is that the calculations are based on annual averages. Consequently, seasonal peaks and short-term pollution episodes are smoothed out. Furthermore, for some organic parameters, the observation series are limited to 2022–2025, and mass transport for individual groups of substances was calculated only for years with a complete set of synchronous concentration and river-discharge data. Therefore, further research should focus on refining the seasonal patterns of pollution, analyzing concentration–discharge relationships, expanding the monitoring of organic pollutants and metals, and assessing the forms of substance migration in the suspended and dissolved phases.

Overall, the results demonstrate that reliable assessment of water quality in transboundary arid rivers requires the combined use of reference *MPC* values, region-specific

background concentrations, and chemical mass-transport estimates. From a scientific perspective, this integrated approach provides a more realistic basis for distinguishing persistent regional hydrochemical features from episodic pollution signals and for interpreting long-term monitoring data. From a management perspective, the identified priority parameters and mass-transport patterns can support the optimization of monitoring programs, the prioritization of water-protection measures, and more informed transboundary water-management decisions in the Shu-Talas basin. The proposed approach may also be applicable to other arid transboundary river systems where long-term hydrochemical and hydrological observations are available.

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Data Availability Statement: The hydrochemical monitoring data used in this study were obtained from the state monitoring materials of RSE "Kazhydromet" for the Shu River at the Kaynar monitoring section. The processed datasets generated during the study, including calculated annual mean values, background concentrations, water pollution indices, and chemical mass fluxes, are available from the corresponding author upon reasonable request. The raw monitoring data are not publicly archived by the authors because they originate from institutional monitoring records.

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Abbreviations

The following abbreviations are used in this manuscript:

BOD_5	Biochemical oxygen demand over five days
COD	Chemical oxygen demand
C_b	Calculated background concentration
K_b	Ratio of background concentration to maximum permissible concentration
MPC	Maximum permissible concentration
CWPI	Comprehensive Water Pollution Index
NH_4-N	Ammonium nitrogen
NO_2-N	Nitrite nitrogen
NO_3-N	Nitrate nitrogen
P_{min}	Mineral phosphorus
Q	River discharge
W	Water runoff volume
M	Mass flux of chemical substances
RSE	Republican State Enterprise
RD	Regulatory document

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