Modeling of water pollution in the basins of Arctic rivers

Aleksandra Bulavina*

Murmansk Marine Biological Institute RAS, Murmansk, 183010, Russia

Abstract. The goal hereof is mainly to model water pollution in the Arctic rivers on the basis of known natural and anthropogenic data on the drainage basins. The quality of water in rivers depends on the amount of pollutants entering the drainage basin and on the latter's ability to convert such substances. This paper investigates merging these two components into a single integral model by finding a balanced system of inputs. After reviewing the literature and theorizing on the concept, the model was tested on the river systems of the European part of the Russian Arctic. The experiments proved the integral river pollution model to be objective. The resulting integral indices show the extent of anthropogenic impacts on river waters. The use of integral indices in conjunction with hydrochemical ones gives insight into how far anthropogenic sources of chemicals affect the composition of river waters.

1 Introduction

The development of the Arctic resources is crucial to Russia's economy. The Arctic ecosystems are sensitive to anthropogenic impacts as their biogeochemical processes are slow. Russia adheres to the concept of sustainable development, and environmental protection of the Arctic is a national priority (Decree of the Russian President No. 440 dated April 1, 1996).

European North is one of the most developed regions of the Russian Arctic. Russia's areas in the region belong to the drainage basins of Barents and White Seas. Rivers of the European North are important for the economy and sustain extensive anthropogenic impact. River waters are a key source of freshwater for household and industrial use. Besides, the condition of land and coastal marine ecosystems largely depends on the quality of river waters.

Hydrochemical readings from observation stations are the key source of river water quality data. Hydrochemical indices of water pollution are an effective tool for assessing the status of rivers. However, some locations simply do not have enough observation stations. For instance, they are often absent in sparsely populated or hard-to-reach areas. Besides, sampling rates are not always sufficient for proper estimates.

This is why river water quality assessments based on indirect anthropogenic impact metrics are a relevant solution. They are based on modeling the functioning of river systems. Modeling is the primary source of water quality data where hydrochemical readings are not

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* Corresponding author: alexela@list.ru

available. Models of any natural systems have one important advantage: they can be reused as scenarios should inputs change. Modeling water pollution on indirect anthropogenic impact data is useful for quick water quality assessment and projection should the environment or the nature of water use change.

The goal hereof was to model the pollution of water in the river basins of the European part of the Russian Arctic.

Here are the requirements to such model:

1. The model should be simple yet sufficient to take into account the factors that determine the quality of river waters.
2. There should be enough data to make inputs.
3. The mathematical part of the model should include certainty testing.

2 Material and methods

2.1 Division of the area into basins

A drainage basin is a spatial unit that substances and energy move inside. This is why basin division is convenient for modeling river water pollution. Figure 1 shows the drainage basins analyzed herein.

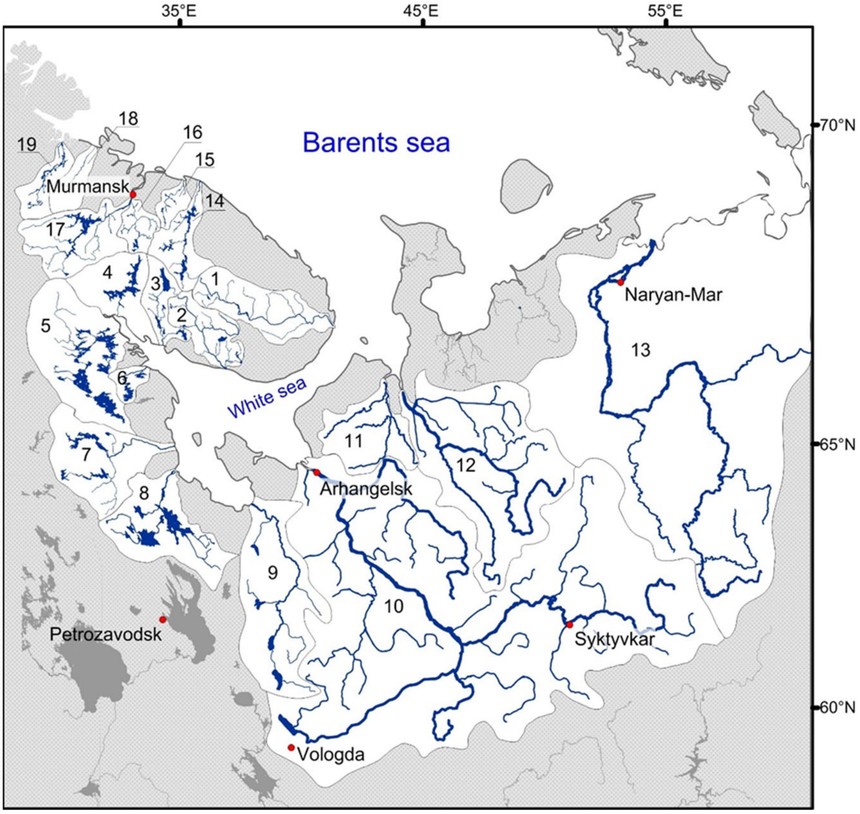

Fig. 1. Numbers denote catchments: 1 for Ponoy; 2 for Varzuga; 3 for Umba; 4 for Niva; 5 for Kovda; 6 for Keret; 7 for Kem; 8 for Vyg; 9 for Onega; 10 for Northern Dvina; 11 for Kuloy; 12 for Mezen; 13 for Pechora; 14 for Voronya; 15 for Teriberka; 16 for Kola; 17 for Tuloma; 18 for Pechenga; 19 for Paatsjoki.

2.2 Aggregated water pollution assessment: the algorithm

2.2.1 General description of the randomized aggregated indices method (RAIM)

The quality of river waters depends on many parameters of drainage basins and their internal processes. Further discussion will cover the most important parameters. Apparently, they are going to be diverse regardless of which parameters are actually picked. In order to combine several drainage basin properties that affect water pollution, and to make an aggregated quality assessment, the authors hereof chose the so-called aggregated indices method (AIM), first proposed by the Russian naval applied mathematician Aleksey Krylov and further presented in the papers of N.V. Hovanov [1; 2].

AIM essentially combines multiple assessments of a single object to make a single aggregated assessment by applying the synthesis function of choice. The following function was used in this study0:

$$Q = w_1 q_1 + w_2 q_2 + \cdots + w_m q_m \tag{1}$$

where Q is the aggregated index; $q_1, q_2, \ldots, q_m$ are the normalized initial values of indices (inputs) $x_1, x_2, \ldots, x_m$; $w_1, w_2, \ldots, w_m$ are the weights of the initial indices. The weights satisfy the following constraints:

$$\begin{cases} w_1 + w_2 + \cdots + w_m = 1, \\ \quad w_1 \geq 0 \ldots w_m \geq 0. \end{cases}$$

Inputs need to be dimensionless so that the aggregated index Q be independent from their units. The inputs are therefore subject to equalization by the normalization formulas of choice. The following formulas were used in this study:

$$q_m = \begin{cases} 1,\text{при } x_m > max(x_m) \\ \dfrac{x_m - min(x_m)}{max(x_m) - min(x_m)} \\ 0,\text{при } x_m < min(x_m) \end{cases}, \text{ at } min(x_m) \leq x_m \leq max(x_m) \tag{2}$$

$$q_m = \begin{cases} 0,\text{при } x_m > max(x_m) \\ \dfrac{max(x_m) - x_m}{max(x_m) - min(x_m)} \\ 1,\text{при } x_m < min(x_m) \end{cases}, \text{ at } min(x_m) \leq x_m \leq max(x_m) \tag{3}$$

where $min(x_m)$ and $max(x_m)$ are the minimum and maximum of a property in the tested sample.

If an increase in the input q_m implies an increase in summary index Q, use the Eq. (2). In case such an increase in q_m implies a decrease in summary index Q, use Eq. (3). These transforms bring the values of criteria within [0, 1]. Pareto set won't be changed by such transform, which is why it can be followed by linear convolution by the Eq. (1) [3].

The key challenge of applying aggregated indices is that precise weights are unknown. Information on weights is non-exact, non-numerical, and non-complete (NNN-information); it is essentially a system of inequalities that relate and constrain the weights. The required inequalities may hold true for multiple sets of weights. The choice of a particular set will affect the final result. For details on selecting the weight vector on the basis of NNN-information, see Hovanov et al. [1]. In order to adjust for the uncertainty of weights, they are randomized, i.e., certain weight vector $w = (w_1, w_2, \ldots, w_m)$ is replaced with the random vector $\widetilde{w} = (\widetilde{w}_1, \widetilde{w}_2, \ldots, \widetilde{w}_m)$. Therefore, the certain aggregated index also becomes randomized, and the convolution formula is written as

$$\tilde{Q} = \widetilde{w}_1 q_1 + \widetilde{w}_2 q_2 + \cdots + \widetilde{w}_m q_m \tag{4}$$

where $\tilde{Q}$ is the randomized aggregate index; $q_1, q_2, \ldots, q_m$ are the inputs; $\widetilde{w}_1, \widetilde{w}_2, \ldots, \widetilde{w}_m$ are random weights.

In order to simplify the calculations, count the weight vector coordinates discretely with at a step of $1/n$. Thus, instead of a continuous set, further analysis deals with a finite set of N elements:

$$N(m,n) = \frac{(n+m-1)!}{(m-1)!n!} \tag{5}$$

2.2.2 Configuring the model

The quality of river waters depends not only on the anthropogenic impact on the drainage basin, but also on the natural properties of the latter. To assess water pollution without hydrochemical readings, all the indirect anthropogenic impact metrics need to be adjusted for the multitude of natural properties of drainage basins. Such properties may facilitate either removal or accumulation of pollutants.

Thus, the quality of river waters depends on two components: self-cleaning potential (SP) and pollution potential (PP) of the drainage basin. Self-cleaning potential is the ability of a catchment to assimilate pollutants. Pollution potential is the rate at which chemicals are added to river waters. The ratio of these two values determines the relative water quality index (RWQI).

SP and PP are both affected by various natural and anthropogenic factors of catchment. PP factors are processes and conditions that contribute to greater inflow of suspended and dissolved substances to rivers. SP factors are processes and conditions that decrease such inflow or affect the rate of pollutant conversion. Which properties are exactly to be used in calculation depends on the physical and geographical features of the area, or on the availability of data. SP and PP calculations should use different parameters that neither directly affect each other nor are in a causative relationship.

The assumption is that SP is determined by the lake surface area as % of drainage area, % (L), forest cover as % of drainage area (W), and slope (F). A catchment rich in lakes and vegetation is capable of better retention and conversion of substances. Slope affects the current speeds and limits the time of the basin's exposure to self-cleaning factors. PP depends on the wastewater-to-runoff ratio (V), the catchment population density (P), and the sediment runoff (S). Wastewater volume and sediment runoff affect the concentration of various substances in water. Wastewater does not include storm water flowing from settlements. Population density is an implicit indicator of local development; it therefore indirectly measures the inflow of pollutants with storm water.

Inputs for pollution assessment in this study was collected from various sources. All the sources are publicly available, and it was a deliberate decision to use such. L, W, F, and annual average S were calculated from map and reference book data [4-6]. Catchment population density was calculated from the 2010 Census data [7]. In order to calculate the volume of discharged wastewater in the catchments, we used official data on water use [8] as well as the official water reports of major industrial facilities published under the Environmental Disclosure Standards (Federal Law No. 7-FZ On Environmental Protection). Table 1 presents the inputs for the river basins.

Table 1. Input data matrix.

River basin	1	2	3	4	5	6
Varzuga	3.00	30.00	0.80	14760.00	0.50	15.82
Voronya	4.00	30.00	0.99	18620.00	0.20	2764.23
Kem	9.30	50.00	0.53	55400.00	3.00	3049.89
Keret	11.20	50.00	1.10	7320.00	1.50	106.38

Kovda	14.00	50.00	0.50	52200.00	1.50	34.52
Kola	6.00	30.00	1.67	7315.00	4.00	3478.26
Kuloy	2.00	87.00	0.39	201210.00	0.50	7.54
Mezen	0.60	70.00	0.38	858000.00	0.50	4.29
Niva	12.00	50.00	3.77	25600.00	3.00	212.77
Nizhny Vyg	14.00	50.00	0.87	54200.00	3.00	3869.41
Onega	3.00	65.00	0.28	91040.00	3.00	562.14
Paatsjoki	7.00	60.00	0.81	34817.50	2.00	837.50
Pechenga	6.50	60.00	1.48	3458.00	0.50	2202.86
Pechora	1.20	35.00	0.35	8050000.00	0.50	38.78
Ponoy	2.10	30.00	0.69	21700.00	0.50	18.80
Northern Dvina	0.40	70.00	0.07	4284000.00	3.50	4539.99
Teriberka	7.20	30.00	2.09	4237.00	0.20	47.12
Tuloma	9.00	60.00	0.75	43320.00	4.00	667.59
Umba	13.10	30.00	1.20	2500.00	1.00	80.97

1 for L, %; **2** for W, %; **3** for F, m/km; **4** for S, ton/year; **5** for P, ppl/km^2; **6** for V, thous. m^3/km^3

2.2.3 Randomized aggregated indices for modeling water pollution in river basins

RWQI search used two-level convolution. Level 1: finding the aggregated indices SP and PP. Level 2: using SP and PP as inputs for RWQI search.

Each of the drainage basin properties in table 1 has a specific yet hard-to-determine significance with respect to water quality. Additional NNN-information was introduced to find the weights of the inputs. Each weight was assumed to be no less than 0.1, as using lower values would make no sense. Weights were also given non-numerical characteristics, see Table 2.

Table 2. Weight constraints.

SP	PP	RWQI
$w_L > w_W$	$w_V > w_P$	$w_{SP} = w_{PP}$
$w_F > w_L$	$w_P > w_S$	$w_{SP} + w_{PP} = 1$
$w_L \geq 0.1$; $w_W \geq 0.1$; $w_F \geq 0.1$	$w_V \geq 0.1$; $w_P \geq 0.1$; $w_S \geq 0.1$	
$w_L + w_W + w_F = 1$	$w_V + w_P + w_S = 1$	

Substances that end up in water due to human activity are diverse, often toxic, and sometimes have no natural counterpart. Apparently, manmade chemicals should have a greater weight than naturally occurring chemicals. The inflow of pollutants to the drainage basin and the self-cleaning capacity of the latter to self-clean is equally important for the quality of river waters. Thus, SP and PP are equally weighted.

Eq. (4) for calculating SP, PP, and RWQI is therefore written as follows:

$$\widetilde{SP} = \tilde{w}_L \times L + \tilde{w}_W \times W + \tilde{w}_F \times F$$
$$\widetilde{PP} = \tilde{w}_V \times V + \tilde{w}_P \times P + \tilde{w}_S \times S$$

$$\widetilde{RWQI} = w_{SP} \times \widetilde{SP} - w_{PP} \times \widetilde{PP}$$

Constraints in Table 2 only apply to a limited number of weight vectors. The weights w_{PS} and w_{PP} are not random, as for the given conditions, only one set of weights, w = (0.5, 0.5), is acceptable for calculating $\widetilde{RWQI}$. However, the aggregated index $\widetilde{RWQI}$ is still a random variable, as it calculation involves the random variables $\widetilde{SP}$ and $\widetilde{PP}$.

Final water pollution assessment algorithm is shown in Figure 2.

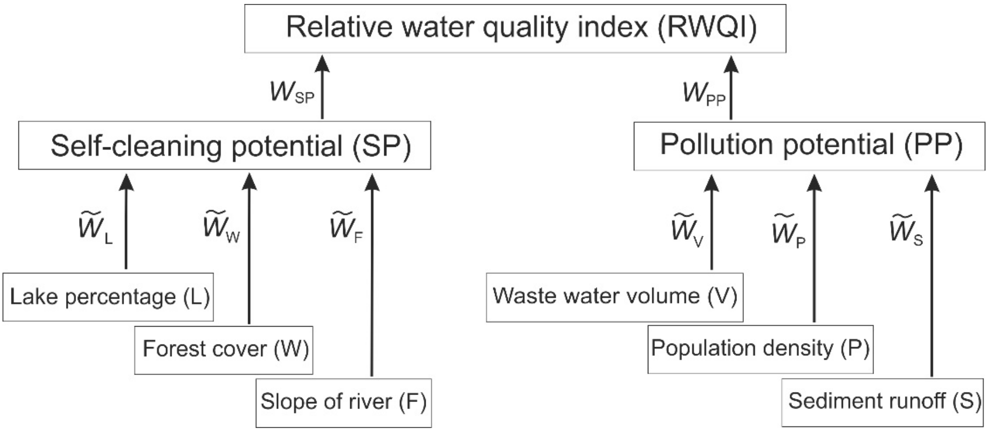

Fig. 2. Randomized final assessment of potential water pollution: the algorithm.

3 Results and discussion

The inputs were normalized by the Eq. (2) and Eq. (3). Coordinates of the weight vector were counted discretely with a step of 0.01. Calculating each of the aggregated indices SP and PP involved 5151 weight vectors, 408 met the requirements of the study. Mathematical expectations of random weights can be used as numerical estimates, whereas variance characterizes the accuracy of such estimates. Table 3 shows mathematical expectations of random weights and their variance.

Table 3. Values of weights.

Group	**SP**			**PP**			**RWQI**	
Index	L	W	F	V	P	S	SP	PP
Weight	$\tilde{w}_L$	$\tilde{w}_W$	$\tilde{w}_F$	$\tilde{w}_V$	$\tilde{w}_P$	$\tilde{w}_S$	w_{PS}	w_{PP}
E$\tilde{w}_i$	0.295	0.173	0.532	0.532	0.295	0.173	0.500	0.500
$\sigma^2\tilde{w}_i$	0.005	0.003	0.009	0.009	0.005	0.003	-	-
Number of valid vectors	408			408			1	

Randomized aggregated indices can also be characterized by the mathematical expectation E and variance σ^2, see Table 4.

Table 4. Characteristics of randomized aggregated indices $\widetilde{SP}$, $\widetilde{PP}$, $\widetilde{RWQI}$.

River	**E**$\widetilde{SP}$	$\sigma^2\widetilde{SP}$	**E**$\widetilde{PP}$	$\sigma^2\widetilde{PP}$	**E**$\widetilde{RWQI}$	$\sigma^2\widetilde{RWQI}$
Varzuga	0.483	0.005	0.032	0.000	0.225	0.001
Voronya	0.477	0.003	0.334	0.003	0.072	0.000
Kem	0.719	0.001	0.586	0.001	0.067	0.000

Keret	0.679	0.000	0.124	0.001	0.277	0.000
Kovda	0.826	0.001	0.116	0.001	0.355	0.000
Kola	0.423	0.001	0.713	0.002	-0.145	0.000
Kuloy	0.693	0.003	0.096	0.001	0.299	0.001
Mezen	0.613	0.005	0.098	0.001	0.257	0.002
Niva	0.313	0.005	0.253	0.002	0.030	0.000
Nizhny Vyg	0.773	0.001	0.682	0.002	0.046	0.000
Onega	0.664	0.004	0.291	0.002	0.186	0.003
Paatsjoki	0.660	0.001	0.248	0.000	0.206	0.001
Pechenga	0.553	0.000	0.291	0.002	0.131	0.000
Pechora	0.524	0.007	0.201	0.003	0.161	0.004
Ponoy	0.479	0.006	0.032	0.000	0.223	0.001
Northern Dvina	0.653	0.006	0.869	0.001	-0.108	0.001
Teriberka	0.389	0.001	0.016	0.000	0.187	0.000
Tuloma	0.712	0.001	0.384	0.004	0.164	0.002
Umba	0.645	0.002	0.071	0.000	0.287	0.000

Figure 3 shows a chart of RWQI estimates. Rivers are sorted by the RWQI value in descending order, i.e. the water quality worsens left-to-right.

Centers of segments correspond to the mathematical expectation of the random variable RWQI, ends show standard deviation. If the ends of segments for two rivers do not intersect, the quality of water in one of them is significantly (for any valid weight vector) higher than in the other one. Otherwise, the probability of dominance must be calculated to identify preference. Dominance probabilities were calculated for all the intersections. This effectively split rivers into four classes of quality:

1. Kovda, Kuloy, Umba, Mezen, Keret, Varzuga, Ponoy
2. Paatsjoki, Pechora, Teriberka, Onega, Tuloma, Pechenga
3. Voronya, Kem, Nizhny Vyg, Niva
4. Northern Dvina, Kola

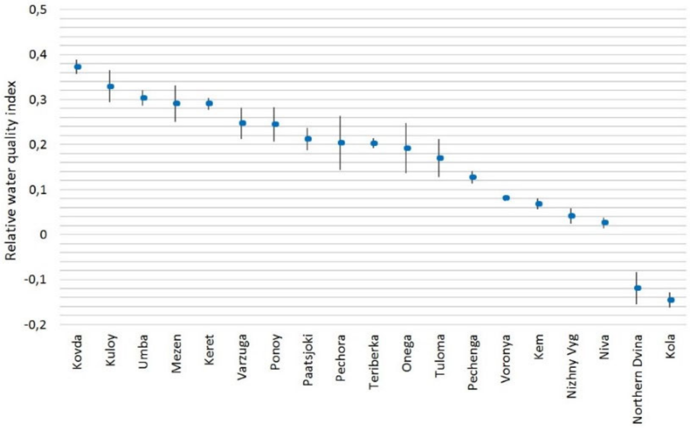

Fig. 3. Relative Water Quality Index estimates for the rivers in the European part of the Russian Arctic.

Higher class means a significantly higher quality of water. Let us designate the classes as follows: Class I for clean; Class II for mildly polluted; Class III for moderately polluted; Class IV for severely polluted.

The results of modeling can only be tested by comparing them against empirical data collected in field. The standard hydrochemical index used in Russia as a water quality indices is referred to as Specific Combined Water Pollution Index (SCWPI). Let us compare the quality assessments obtained herein against SCWPI values. For such a comparison, RWQI and SCWPI need to be clarified.

SCWPI value depends on how frequently the maximum permissible concentrations (MPC) of 15 chemicals on the list [9] are exceeded, and on the actual value to MPC ratio. If necessary, calculations of these metrics can involve substances specific to the body of water under analysis.

SCWPI calculations do not take into account the natural chemical of waters. Concentrations above MPC thresholds may occur in natural waters even without anthropogenic impact. Such waters are considered contaminated. However, if the drainage basin is highly resistant to pollution, the situation can be opposite. If the catchment is exposed to strong anthropogenic impact but can partially mitigate it so that the chemicals remain within their MPCs, river waters are considered clean.

Each particular study's theoretical background should be consulted to decide whether river waters should be considered contaminated where some chemicals exceed their respective MPCs for natural reasons. The theory behind assessing the status of natural systems is highlighted in V.V. Denisov's work [10]. The author defines the concept of normal natural status and the environmental quality norms as follows:

- Normal natural status is such condition of a natural system that is most likely to occur without anthropogenic impact due to its natural physical, chemical, and biological processes.
- Environmental quality norms are such values of physical, chemical, biological, or other indicators that are scientifically shown to enable sustainable functioning of natural ecological systems, natural and/or anthropogenic objects.

SCWPI shows how far the quality of water deviates from the quality norms regardless of why it happens. Background concentrations of chemicals in natural waters affect SCWPI; sometimes, these concentrations are decisive. RWQI shows how far the quality of river waters deviates from the normal natural status, i.e., the extent of anthropogenic impact.

This is why RWQI cannot be directly compared to SCWPI: they are different metrics. Comparison should involve data on the anthropogenic impact on catchments as well as MPC data for various substances.

Area under study is spread across three major geological structures: the Fennoscandian Shield, the Russian Plate, and the Timan-Pechora Plate. The Shield contains the drainage basins of Varzuga, Voronya, Kem, Keret, Kovda, Kola, Niva, Nizhny Vyg, Paatsjoki, Pechenga, Ponoy, Teriberka, Tuloma, Umba. The catchments of Kuloy, Mezen, Onega, Pechora, and Northern Dvina are confined to the plates.

Background concentrations of up to 5-6x MPC for copper, up to 10x MPC for iron, and up to 2x MPC for manganese are characteristic of the rivers whose drainage basins are in the Fennoscandian Shield. Above-MPC concentrations of copper, iron, and manganese are also typical of rivers with basins within the plates. However, the ratios there are an order of magnitude higher for manganese; besides, they have above-MPC concentrations of the ion SO_4^{2-} [11] due to the presence of soluble rock.

Let us compare the SCWPI estimates against anthropogenic impact assessment, see Table 5.

Table 5. Quality of water in the European rivers of the Russian Arctic and anthropogenic impact on their drainage basins.

Catchment	SCWPI quality class	RWQI quality class	Substances above MPC	Anthropogenic impact
Varzuga	III	I	Cu, Fe_{total}	low
Voronya	III	III	Fe_{total}, Mn, Cu, Zn, fluorides	moderate
Kem	III	III	Organic substances (COD), Cu, Fe_{total}	moderate
Keret	II	I	Cu, Fe_{total}	low
Kovda	II	I	Cu, Fe_{total}	moderate
Kola	III	IV	Cu, Fe_{total}, Mn, organic substances (COD), phenols, $NH4^+$, Al, Zn, Hg	high
Kuloy	IV	I	Mn, Cu, Fe_{total}, SO_4^{2-}	low
Mezen	IV	I	Mn, Cu, Fe_{total}	low
Niva	II	III	Cu, Zn, Mn, Ni, Mo, petroleum products	high
Nizhny Vyg	III	III	Cu, Fe_{total}, Organic substances (COD), petroleum products, NH_4^+	moderate
Onega	IV	II	Mn, Cu, $Fe_{total,}$ Al, Zn, petroleum products	moderate
Paatsjoki	II	II	Cu, Zn, Fe_{total}	low
Pechenga	III	II	Ni, Cu, Fe_{total}, Mn	moderate
Pechora	IV	II	Cu, Fe_{total}, Zn, Al, Mn, petroleum products	low
Ponoy	III	I	Cu, Fe_{total}	low
Northern Dvina	IV	IV	Fe_{total}, Cu, Mn, Al, Zn, organic substances (COD)	high
Teriberka	III	II	Cu, Fe_{total}, Mn, Zn	low
Tuloma	III	II	Cu, Fe_{total}, Mn	moderate
Umba	III	I	Cu, Fe_{total}	low

In most cases, RWQI showed an equal or higher quality of water than SCWPI due to the natural chemical of waters. However, the assessments were opposite of each other in some cases. Kuloy and Mezen are severely polluted per SCWPI. Yet, these rivers are barely affected by human activity. In particular, Mezen is one of Europe's most intact rivers [12]. In its natural state, the water of Kuloy may contain up to 100x MPC of manganese in annual average figures (240x MPC for Mezen) [11]. This inflates their SCWPI. RWQI, however, shows no deviation from the normal natural status and classifies these rivers as 'clean'.

Class I per RWQI (clean rivers) includes rivers that are exposed to virtually no anthropogenic impact; they only have above-MPC concentrations for substances typical of the natural waters in the region.

Class II (mildly polluted) includes rivers exposed to low or mild anthropogenic impact. They exceed MPCs for all the substances typical of the regions as well as for 1 to 3 substances that are not typical of the local natural waters.

Classes III and IV (moderate and severely polluted) include rivers whose drainage basins are exposed to moderate or high anthropogenic impact. They exceed MPCs for multiple substances including hazardous toxins.

RWQI metrics correlate well with the extent of anthropogenic transformation of river waters. RWQI shows the extent of anthropogenic pollution. However, it is not indicative of the quantity of impurities in water nor of its safety. Those should be analyzed by SCWPI or other hydrochemical indices.

Non-numerical data on the presence or absence of nearby sources of anthropogenic impact is often cited in addition to hydrochemical pollution indices to clarify the causes of low water quality. Such data is not sufficient to compare rivers in terms of how human activity affects their water quality.

V.A. Bryzgalo and I.M. Ivanova [13] calculated the extent and the proportion of anthropogenic pollution of river waters. Their estimates could be used to compare the anthropogenic pollution of river waters in space and time. Notably, they used MPC standards and ignored normal natural status. Thus, their method cannot fully separate the anthropogenic effects on river water chemistry from the natural causes.

RWQI has several advantages as a metric of anthropogenic water pollution: Namely, it:

1. uses normal natural status and thus shows only the anthropogenic effects
2. needs no hard-to-find data
3. allows for mathematical testing of certainty
4. can be used to make scenarios in order to project the effects of change in natural conditions or anthropogenic impact.

4 Conclusions

This paper presents a novel integral model of water pollution in river basins. The model has been tested on the rivers of the European part of the Russian Arctic and performed well. The chemistry of river waters depends on the natural and anthropogenic factors of drainage basins. The model takes that into account. RWQI assessments are consistent with the actual anthropogenic impact on drainage basins; they are sensitive to deviation from the normal natural status.

RWQI allows assessing the extent of anthropogenic transformation of river waters. Its potential applications are:

1. an independent model indicative of anthropogenic pollution of river waters.
2. A model to complement hydrochemical pollution indices, which could help clarify the contribution of anthropogenic impact to the chemistry of river waters as part of ecological studies of rivers or planning the development of drainage basin areas.

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