Journal of Environmental Management 348 (2023) 119383

Contents lists available at ScienceDirect

Journal of Environmental Management

journal homepage: www.elsevier.com/locate/jenvman

Research article

Development and testing of a new flexible, easily and widely applicable chemical water quality index (CWQI)

Lorenzo Chemeri [a,b,*], Jacopo Cabassi [c], Marco Taussi [a], Stefania Venturi [b,c]

[a] *Department of Pure and Applied Sciences, University of Urbino Carlo Bo, Via Ca' Le Suore 2/4, 61029, Urbino, Italy*
[b] *Department of Earth Sciences, University of Florence, Via G. La Pira 4, 50121, Florence, Italy*
[c] *Institute of Geosciences and Georesources (IGG), National Research Council of Italy (CNR), Via G. La Pira 4, 50121, Florence, Italy*

ARTICLE INFO

Handling editor: Jason Michael Evans

Keywords:
Water quality
Environmental geochemistry
Water management
Chemical pollution

ABSTRACT

Water quality indices (WQIs) are numeric parameters that summarize the overall quality status of freshwaters compared to quality standards by aggregating multiple physicochemical data into a single value. Among the available WQIs in the literature, several criticalities were recognized including: (a) mathematical complexity of the computation, (b) lack of inclusivity, (c) arbitrary weight assignment method, and (d) site-specificity of most of the indexes. The proposed index, the Chemical Water Quality Index (CWQI), aims to overcome these flaws and provides a computation based on simple mathematic equations that are easily manageable on spreadsheet software. The computation is divided into two steps: (i) parametrization of the variables and (ii) index determination. The parametrization consists of assigning a score (s) from ~1 to 10 to each chemical variable based on (i) measured concentrations and (ii) quality targets (e.g., the limits provided by the European legislation for drinking waters). In the second step, a weight (w), directly proportional to the score (s), is assigned to each parameter, allowing to overcome any bias related to subjective assignments from the user. The resulting CWQI ranges from ~1 (very good quality) to 10 (extremely poor quality). The reliability and accuracy of the CWQI were assessed by (i) applying the computation to 1,810 waters and (ii) comparing our results with another available WQI. The CWQI outputs showed an optimal response with the number of variables exceeding the quality target with high correlation coefficients ($r = 0.94$; $R^2 = 0.89$). Due to the simplicity of its computation, the absence of arbitrariness in the weightage of selected variables, and the independence of the proposed approach regarding the choice of the chemical parameters, CWQI can be easily and universally applied.

1. Introduction

Water shortage represents one of the major environmental and social issues that humanity must face in the upcoming years. The effects of climate change together with the increase of anthropogenic pressure, e.g., population growth, expansion of industrial activities, and increasing agricultural activities, are strongly endangering the water resource in terms of both quantity and quality. Consequently, the presence of toxic pollutants of different natures (organic, inorganic, or biological) makes surface water and groundwater unfit for drinking purposes in many places of the world (e.g., Ray, 2011; Yolcubal et al., 2016; Basheer, 2017; Gupta et al., 2021; Torres-Martínez et al., 2021; Taussi et al., 2022; Linhoff, 2022). Hence, correct management coupled with the quality assessment of the water resources is a paramount step to implement water protection and addressing its possible usage (e.g., drinking, irrigation, and/or industrial).

The most common tool used to evaluate the water quality status is the application of water quality indices (WQIs), i.e., numeric parameters that summarize the overall quality status of freshwaters compared to standard values (e.g., national, or international guidelines for drinking waters) by aggregating multiple physicochemical (or biological) data into a single value.

The first WQI was elaborated by Horton in 1965 (Horton, 1965) and since then several new and updated WQIs have been computed (e.g., Brown et al., 1970; Prati et al., 1971; Dinus, 1987; Saffran et al., 2001; Vasanthavigar et al., 2010; Centeno et al., 2023). A detailed and critical review of the available and most used WQIs in literature, from the Horton index to the most recent formulations, is presented by Kachroud et al. (2019) and Uddin et al. (2021).

The generic formulation of a WQI is divided into four steps

---

* Corresponding author.Department of Pure and Applied Sciences, University of Urbino Carlo Bo, Via Ca' Le Suore 2/4, 61029, Urbino, Italy.
E-mail address: l.chemeri@campus.uniurb.it (L. Chemeri).

https://doi.org/10.1016/j.jenvman.2023.119383
Received 17 August 2023; Received in revised form 26 September 2023; Accepted 15 October 2023

(Kachroud et al., 2019): (i) selection of the variables, (ii) their transformation into a common scale, (iii) weightage, and (iv) aggregation of the variables and computation of the index. Among the available WQIs, several criticalities can be recognized, including (a) the mathematical complexity of the computation; (b) the lack of inclusivity, since several water quality indexes are formulated for specific sets of variables (Uddin et al., 2021, and reference therein) preventing the inclusion of other parameters (Ma et al., 2020) such as emerging chemical pollutants (e.g., pesticides, pharmaceuticals, metalloids); (c) the weighting assignment, which is generally evaluated taking into account the relative importance of each parameter on water quality and it is frequently based on arbitrary criteria that strongly influence the final index values (e. g., Vasanthavigar et al., 2010); (d) the site specificity of most of the indexes, since WQIs are generally developed on single-case studies and therefore cannot be generalized or directly applied in different areas (Kachroud et al., 2019; Centeno et al., 2023).

The Chemical Water Quality Index (hereafter, CWQI) presented in this paper, aims to overcome the most common problems since it is based on simple mathematic equations easily manageable on common spreadsheet software (e.g., Excel) and it relies on a weight assignment procedure that allows to erase any arbitrariness. Moreover, its formulation is flexible and can include any possible chemical parameters, allowing an easy application to virtually any case study. To verify the reliability and accuracy of the proposed index, almost two thousand waters were tested with the CWQI, and the results were compared with another water quality index widely used in the literature (Vasanthavigar et al., 2010).

2. Limitations of available WQIs and advantages of the CWQI

The development of the CWQI aims to facilitate the water quality status computation and minimize or avoid the criticalities highlighted in other WQIs. As far as the selection of variables is concerned, most of the WQIs are based on a fixed number of (chemical, physical, and biological) variables, generally comprised between 8 and 11 (Uddin et al., 2021). Therefore, their formulation does not allow the inclusion of additional parameters that may be crucial in water quality evaluation (Ma et al., 2020). Trace elements (e.g., As, Mn, Cr), that can be potentially toxic and/or radioactive, are rarely considered in common WQIs (Uddin et al., 2021), thus representing a strong limitation since they can be extremely hazardous for both humans and ecosystems. Similar considerations can be extended to emerging contaminants (i.e., pesticides, pharmaceuticals, microplastics, and pathogens) which are related to domestic discharges, hospital effluents, industrial wastewaters, agricultural runoffs, livestock and aquaculture, and landfill leachates. Water contamination due to emerging pollutants is always more frequent in industrial and agricultural areas (Deblonde et al., 2011; Venturi et al., 2015; Basheer, 2018; Slejko et al., 2019; Morin-Crini et al., 2022; Kumar Mishra et al., 2023).

The weighting assignment represents the most influential step towards the final calculation of the index; hence a correct evaluation is fundamental since a wrong weightage (i.e., giving a parameter more importance than it merits or the opposite) can affect the entire calculation and produce unreliable results leading to an eclipsing problem (Ott, 1978), a major issue that was recognized in many WQIs models (Uddin et al., 2021). Generally, the weight is estimated on the relative importance of each parameter on water quality and assigned following different procedures. Most of the WQIs assign unequal weights to the different variables, e.g., the Horton (1965) and *Bascaron* (Pesce and Wunderlin, 2000) *Indexes*. Other indexes assign an equal weight to each parameter (e.g., *Oregon Index*; Dunette, 1979; Cude, 2001) or some models do not involve the weighting step, e.g., the *Canadian Council of Minster of the Environment* (Saffran et al., 2001) and the Smith (1990) *Indexes*. The weight computation can be carried out either by applying different mathematical equations involving the use and the aggregation of different sub-indexes or following the evaluation from a panel of experts and/or directly by the user (Uddin et al., 2021 and references therein).

A further problem is represented by the specificity of the indices. Indeed, they strongly depend on the water body they were computed for, and WQIs that were tested for rivers and streams may not be suitable to evaluate lakes or groundwaters (Uddin et al., 2021). Additionally, since most of the indexes were only tested on a restricted number of case studies (Centeno et al., 2023) their application in different contexts worldwide is not always feasible.

Indeed, the CWQI proposed in the present study was designed to (a) include any chemical parameters based on data availability or at the user's discretion, (b) rely on a weightage method exclusively related to the concentrations of each parameter in the water, considering the correspondent quality target value, allowing to overcome any bias related to the subjective assignments from the user, and finally (c) provide accurate outcomes. The fulfillment of the last requirement was tested using 1,810 waters of different types (e.g., bottled waters, tap waters, springs, rivers, groundwaters, and thermal waters).

3. Materials and methods

3.1. Variables parametrization

The first step in the development of CWQI consists in the selection of the variables to be included in the index computation and, since they may be reported in different scales, a transformation (or parametrization) phase is required. The choice of the variables is at the user's discretion. We suggest considering, at least, the two main physico-chemical parameters, i.e., pH and electrical conductivity (EC, when not available can be computed from total dissolved solids (TDS) according to eq. (1), Walton, 1989), and major anions and cations, i.e., fluorine (F^-), chlorine (Cl^-), nitrate (NO_3^-), sulfate (SO_4^{2-}), sodium (Na^+) and water hardness (h expressed in °F, French degrees following eq. (2)), since these are the main water parameters/components and are always regulated due to their toxicity when they exceed the quality target (WHO, 2017).

$$computed\ EC = \frac{TDS\ (total\ dissolved\ solids)}{0.7} \tag{1}$$

$$h = \frac{(2.39 * Ca) + (4.118 * Mg)}{10};\quad Ca\ and\ Mg\ in\ mg \Big/ L \tag{2}$$

To have a better and multi-comprehensive characterization of the water quality status, the inclusion of trace elements (e.g., As, B, Cr, Cu, Mn) is highly recommended since some of them are extremely toxic and hazardous to humans, vegetation and aquatic life even when present in low concentrations (Costa and Klein, 2008; Bakirdere et al., 2010; O'Neal and Zheng, 2015; Kolarova and Napiórkowski, 2021; Prakash and Verma, 2021).

The parametrization consists in assigning a score (s) from 1 to 10 to each variable based on measured value/concentration and quality targets, the latter represented by the European quality standards for drinking waters (EU Directive 2020/2184/EC, 2020). For the score assignments, two functions were developed. The first one (eq. (3)) is applicable to all variables for which the quality target is a specific concentration value not to be exceeded (hereafter, A-variables type), and the second (eq. (4)) for pH, for which the quality target is represented by a range of values (i.e., 6.5 to 8.5).

$$s = \frac{10}{1 + 6.714e^{2.234(0.148-a)}};\quad a = \frac{measured\ value}{reference\ value}\quad \left(R^2 = 0.94\right) \tag{3}$$

$$s_{pH} = \frac{10}{1 + 1.953e^{6.381(0.985-b)}};\quad b = \left|7.5 - pH_{measured}\right|\quad \left(R^2 = 0.93\right) \tag{4}$$

Eqs. (3) and (4) were derived by fitting the values shown in Supplementary Materials (SM1) according to the following sigmoid equation (eq. (5)):

$$y(x) = \beta + \frac{\alpha - \beta}{1 + qe^{m(c-x)}} \tag{5}$$

were β is the lower asymptote (in this case, set equal to zero), α is the upper asymptote (in this case, set equal to 10) and x value corresponds to the ratio between the measured concentration of each variable and the corresponding quality target in the case of A-type variables (i.e., a in eq. (3)), and the absolute value of the difference between the central value (arithmetic mean) of the quality target range and the measured value for pH (i.e., b in eq. (4)). The other three unknown parameters in eq. (5) (q, m and c) were determined through a least squares iterative procedure for finding the best-fitting curve to the given set of points. The fitting curve was forced to pass through (1,5) and for every value of the variable x higher than 3, $y(x)$ will always equal 10.

3.2. Weight assignments and index computation

As previously mentioned, the weightage is one of the main problems affecting the WQIs final computation since an incorrect weight assignment can lead to an overestimation or underestimation of the index. According to the proposed CWQI, the weight (w) assigned to each parameter is directly proportional to the score (s), obtained in the previous step, following eq. (6):

$$w_x = \frac{S_x}{\sum_{i=1}^{n} S_i} \tag{6}$$

where w_x indicates the weight of the parameter x, S_x is the score computed for the parameter x and the denominator is the sum of the scores of all the n parameters considered. This formulation gives to the parameter a relative importance that only depends on the parameter concentration (or value) measured in the sample and the corresponding quality target, avoiding any arbitrary assignment made by the single user or further complex mathematical computations (Kachroud et al., 2019; Uddin et al., 2021).

The final step is the index computation in which all the single scores and weights are aggregated together producing a single number that will summarize the overall water quality status. The CWQI uses a weighted geometric average, since a multiplicative aggregation was found to be more suitable because it allows to reduce the eclipsing problem and to produce more reliable results with respect to an additive aggregation (Brown et al., 1973; Bhargava, 1983; Kachroud et al., 2019). The CWQI index is computed as it follows, eq. (7):

$$CWQI = \prod_{i=1}^{n} S_i^{W_i} \tag{7}$$

Hence, according to the proposed approach, in the worst-case scenario where $S_i = 10\ \forall i \in [1; +\infty]$ (eq. (8)), the limit of the function will always tend asymptotically to 10.

$$\lim_{n \to +\infty} \prod_{i=1}^{n} S_i^{W_i} = \lim_{n \to +\infty} CWQI = 10 \tag{8}$$

On the other hand, the calculated CWQI will be ~1 for high quality waters. This mean that the CWQI will be comprised between ~1 (very good chemical quality) and 10 (extremely poor chemical quality) regardless of the number of the variables involved.

3.3. CWQI testing towards universal application

Site-sensitivity and water body dependence represent two further limits found in the already published WQIs that prevent their application in other areas. The calibration phase is an innovative and necessary step that allows the application of the CWQI computation worldwide and to any water body.

For this purpose, a calibration test was performed to evaluate the response of the CWQI to various types of waters both in terms of type (e.g., bottled waters, tap waters, springs, rivers, groundwaters, and thermal waters) and elemental abundances. In the calibration test, 1,810 waters (Table 1), from different datasets available in the literature and belonging to different regional and hydrogeological contexts (i.e., 1050 from Italy and 760 from other European countries), were evaluated with respect to the quality targets provided by the European Union legislation for drinking waters (EU Directive 2020/2184/EC, 2020). The following parameters were included in the computation: pH, EC, F^-, Cl^-, NO_3^-, SO_4^{2-}, Na^+, and hardness (for each water sample), while trace elements were selected upon their availability in the considered datasets (Table 1), since it was proven that this approach is independent on the choice of the variables (eq. (8)).

To verify the reliability of the proposed index, the results obtained with the CWQI application were then compared with those resulting from the WQI formulated by Vasanthavigar et al. (2010), hereafter VQI, which is widely used in literature (e.g., Gaagai et al., 2023; Manu et al., 2023). The VQI was chosen since it is also characterized by a simple computation and allows the inclusion of the desired variables (eq. (9.1)-(4)), although it uses an additive aggregation formula, more influenceable by the eclipsing problem, and the weights are assigned at user's discretion so that its determination can be biased. The VQI grows from 0 to beyond 300 and the water quality classes are defined as follows: excellent (<50), good (50–100), poor (100.1–200), very poor (200.1–300) and water unsuitable for drinking purposes (>300).

$$VQI = \sum_{i=1}^{n} SI_i \tag{9.1}$$

$$SI_i = W_i * q_i \tag{9.2}$$

where SI_i is the sub-index of the ith parameter, q_i is the rating based on the concentration of the ith parameter, W_i is the relative weight of the ith

Table 1
Summary of the datasets used in the testing phase. Number of waters analyzed (N_{waters}), study area, literature reference and available trace elements are reported.

N_{waters}	Area	Reference	Trace elements
255	Vicano-Cimino Volcanic District	Cinti et al. (2014)	Al, B, Fe and Mn
215	Eastern Sabatini Volcanic District	Cinti et al. (2017)	Al, B, Fe and Mn
114	Gioia Tauro coastal Plain	Vespasiano et al. (2023)	Al, B, Fe and Mn
34	Porretta Terme hydrothermal system	Tassi et al. (2022)	As, Fe and Mn
30	Metauro River coastal Plain	Nisi et al. (2022)	As, B, Cr, Cu and Mn
17	Montecatini thermal system	Capecchiacci et al. (2015)	As, Cr, Cu and Mn
37	Argo Avezzano and Caiazzo plains	Rufino et al. (2022)	B, Cu, Mn, Ni and U
18	Lessini's Mountain thermal area	Lelli et al. (2022)	B, Fe and Mn
34	Po Plain's shallow aquifers	Sciarra et al. (2013)	B, Fe, Mn and U
35	Campidano Plain	Frau et al. (2020)	As, B, Mn and Pb
104	Umbria and South Tuscany aquifers	Frondini (2008)	Fe and Mn
36	Arno river and tributaries	Nisi et al. (2008)	As, Cr, Cu and Mn
52	Bottled and tap waters from Calabria	Apollaro et al. (2019)	As, Cr, Cu and Mn
21	Mt. Amiata former mining area	Lazzaroni et al. (2022)	As, Hg and Sb
808	European stream and surface waters	Salminen et al. (2005)	As, B, Cr, Cu e Mn

parameter and *n* is the number of parameters.

W_i and q_i are computed as follows:

$$W_i = \frac{w_i}{\sum_{i=1}^{n} w_i} \tag{9.3}$$

$$q_i = \frac{C_i}{S_i} * 100 \tag{9.4}$$

where w_i is the weight assigned to each parameter, C_i is the concentration of each chemical parameter in the water sample (in mg/L) and S_i is the drinking water standard for each parameter (in mg/L) according to the considered legislation or guidelines.

Moreover, to prove the influence of the subjective weightage method on the VQI computation, the comparison was performed under three different conditions: C_1 (*geochemical weightage*, each weight assigned to the parameter based on their relative importance in affecting water quality and that will be used to test the CWQI reliability and efficiency), C_2 (*overestimation* of trace elements) and C_3 (*underestimation* of trace elements), according to Table 2.

Finally, for those elements with contents below detection limit (DL), the value corresponding to DL/2 was used in the computation (Helsel and Gilliom, 1986).

4. Results and discussion

According to the results obtained in the testing phase (Fig. 1), the CWQI outcomes are classified as follows (Table 3). Waters are defined as *good* when the CWQI is below or equal to 2, these waters generally do not show any parameters above the quality target and therefore they may be considered for drinking purposes, obviously upon microbiological analyses. Since the number of variables considered in the CWQI computation was limited (10–13 parameters) concerning the possible number of parameters that can be determined in a water sample, although higher than the variables generally included in other WQIs (Uddin et al., 2021), as a precautionary measure the classification term *excellent* was not included. It is also worth noticing that some water showed CWQI ≤ 2 despite having one parameter higher than the corresponding quality target (Fig. 1). However, in most of these cases the variables exceeding the target are represented either by pH, since the range considered as optimal in our computation was narrow (6.5–8.5), or by hardness. Therefore, this may not represent a limit in their possible use as drinking waters, since bottled waters on the worldwide markets are usually characterized by a pH lower than 6.5 or higher than 8.5, as well as hardness values above 31 °F (Birke et al., 2010; Frengstad et al., 2010; Dinelli et al., 2010; Raco et al., 2013; Daniele et al., 2019).

The chemical quality status of waters showing a CWQI comprised between 2.01 and 4.00 is classified as *fair*, indicating a medium to low quality. Thus, these waters may be used for irrigation or industrial purposes, and in some cases, they may be evaluated for drinking usage after specific treatment steps (e.g., dilution or potabilization). For $4.01 \leq \text{CWQI} \leq 6.00$, the water is defined as *poor*. In this case, water is not suitable for drinking purposes since one or more parameters exceed the quality target. Other uses (e.g., industrial) may be evaluated depending on elemental abundances.

Table 2
Summary of the weights assigned to each parameter for the VQI computation under three different conditions: C_1 (geochemical weightage), C_2 (overestimation of trace elements) and C_3 (underestimation of trace elements).

Variable	C_1_geochemical weightage	C_2_traces overestimation	C_3_traces underestimation
EC	4	2	4
F	5	4	3
Cl	4	2	4
NO_3	5	4	3
SO_4	3	1	3
Na	3	1	3
Hardness	2	1	3
Trace elements	5	5	1

For values of the CWQI included between 6.01 and 8.00, the water is classified as *very poor*, whilst for values of the index higher than 8.01, the water is defined as *extremely poor*. Both these classification terms indicate that the water quality is extremely and irreversibly compromised and therefore its use is not recommended since it may be harmful to humans, vegetation, and aquatic life. As can be observed in Fig. 1, the CWQI increases in agreement with the number of parameters that do not meet the quality target for each tested sample, indeed the correlation coefficients (Pearson *r*, R^2) showed a very strong linear association between the two terms (Table 4).

The reliability and the efficiency of the CWQI were evaluated by comparing the outcomes with the VQI (Vasanthavigar et al., 2010) under C_1 conditions (Table 2). The results are reported in Fig. 2 and the full datasets are available in Supplementary Material (SM2).

In most of the tested waters, the results obtained with the CWQI computation tend to agree with the outcomes obtained by applying the VQI, although the aggregation function and the weightage method used in the VQI calculation caused an underestimation and/or an overestimation of the index in several cases. Additionally, the first limit that can be highlighted for the VQI computation is the impossibility of including the pH in the quality evaluation.

For example, all the waters with no parameters above the quality target are classified as *excellent* according to the VQI, whereas some of these waters showed a CWQI above 2 and sometimes approaching the value of 4 (Fig. 1), meaning that despite no variable exceeds the quality target, a few parameters may be close to the limit. The overestimation of the water quality following the VQI is due to the use of an additive aggregation function which is more likely to suffer the eclipsing problem than a multiplicate aggregation function (Kachroud et al., 2019). As a matter of fact, throughout almost the entire dataset, the VQI produces lower values compared to the CWQI thus overestimating the overall quality status; hence, the CWQI overperforms the VQI by offering a more balanced and reliable outcome.

The major disagreements between the two indexes were determined by the different weightage methods. Since in the VQI computation, the weight of each parameter is assigned by the user, major components, such as sodium, sulfate, and chlorine, are generally weighted less compared to trace elements. Consequently, when the chemical quality status of water is exclusively endangered by those elements (with low concentrations of trace elements), the VQI produces a strong overestimation of the quality. Indeed, waters with three parameters above quality standard are classified as *excellent,* and waters up to six parameters exceeding the limit are defined as *good* (Fig. 3). In these cases, the VQI computed under conditions C_3 (i.e., underestimation of trace elements) agrees slightly better with the CWQI.

On the contrary, the weightage method used for the CWQI computation gives the parameter a relative importance only depending on the concentration of that parameter in the water with respect to its quality target. Hence, for the CWQI the weights are not established *a priori* but are recalculated for each parameter every time a new water is tested. Thus, the CWQI outcomes grow together with the number of variables above the quality standard, showing an optimal response. The same trend is not always granted by the VQI, which shows lower correlation coefficients (Table 4). This may represent a fault of the VQI calculation that should be considered when dealing with water management. Consequently, for those cases where the chemical quality of the water depends on parameters to which lower weights are assigned, the VQI has more chances to provide an incorrect result with respect to the CWQI. These results clearly show that the CWQI overcomes those inconsistencies and/or uncertain results of the VQI in most of the cases tested.

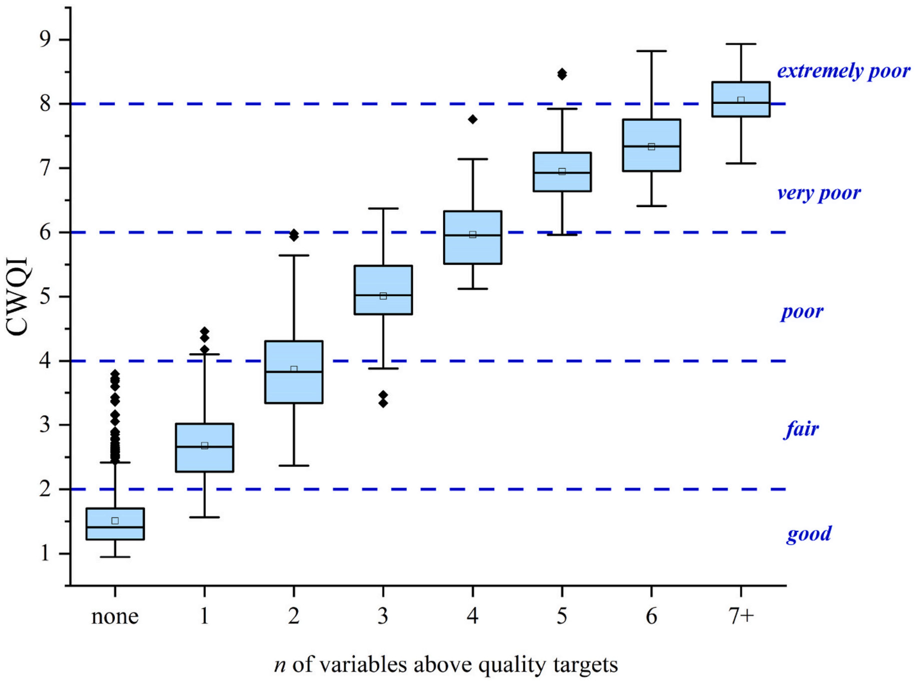

Fig. 1. Box-plot describing the variation of the Chemical Water Quality Index with respect to the number of variables above quality targets. Horizontal dashed blue lines indicate the chemical quality classes proposed for the CWQI.

Table 3
The proposed chemical quality ranking classes based on the CWQI outcomes are presented. Possible use for water resource and correspondent classification according to VQI computation are also reported.

CWQI value	Classification	Possible use	VQI correspondent
≤2.00	good	water may be considered for drinking purposes, upon microbiological analyses	excellent
2.01–4.00	fair	water may be considered for irrigation or industrial usage, water may be evaluated for drinking purposes, upon microbiological analyses and treatment is necessary (e.g., dilution, purification)	good poor
4.01–6.00	poor	water not suitable for drinking purposes, other uses may be evaluated depending on elements concentrations	poor very poor
6.01–8.00	very poor	water quality is extremely damaged, the use is not recommended.	very poor unsuitable
8.01–10	extremely poor	water quality is irreversively damaged, the use is not recommended.	unsuitable

The testing phase also highlighted a limitation for the CWQI which is represented by those waters characterized by a limited number of variables that strongly exceed the quality target. In those specific cases, the result produced by the CWQI computation was underestimated since the maximum score assigned to a parameter is 10 when that parameter overcomes the quality target at least 3 times. This flaw was detected for 19 water samples out of the 1,810 tested (1.05% of the total cases) that were classified as fair, while they were defined according to VQI as poor, very poor, or unsuitable. It is worth mentioning that those waters were characterized by the presence of some elements exceeding the reference value at least 20 times and therefore their indexing may not be necessary since their chemical status is clearly damaged, and as Horton already pointed out during his first index formulation “water containing such substances, therefore, is considered not eligible for index rating” (Horton, 1965; Kachroud et al., 2019).

Table 4
Summary of correlation coefficient (Pearson r, R^2) used to evaluate the CWQI and VQI indexes’ response to the increase of variables that do not meet the quality standards. Correlation coefficients were applied to (i) the entire dataset and (ii) to the median values of the indexes computed for waters characterized by the same number of variables above quality standards.

	CWQI	VQI
N of variables above quality target		
Pearson (r) (entire dataset)	0.94	0.36
R squared (R^2) (entire dataset)	0.89	0.13
Pearson (r) (median values)	0.98	0.86
R squared (R^2) (median values)	0.96	0.73

5. Conclusions

In this paper, we presented a new simple, fast, and flexible method to compute an index able to summarize the water chemical quality status: the chemical water quality index (CWQI).

The CWQI presented strong advantages compared to the other indexes available in the literature: (i) the inclusivity of the variables, as shown in eq. (8) any parameter can be considered in the computation overcoming the lack of inclusivity found in most WQIs; (ii) the simple and unbiased weightage method; (iii) the universal applicability without limitations due to site-specificity and water body dependence. The high reliability, replicability, and efficiency of the CWQI were proven and

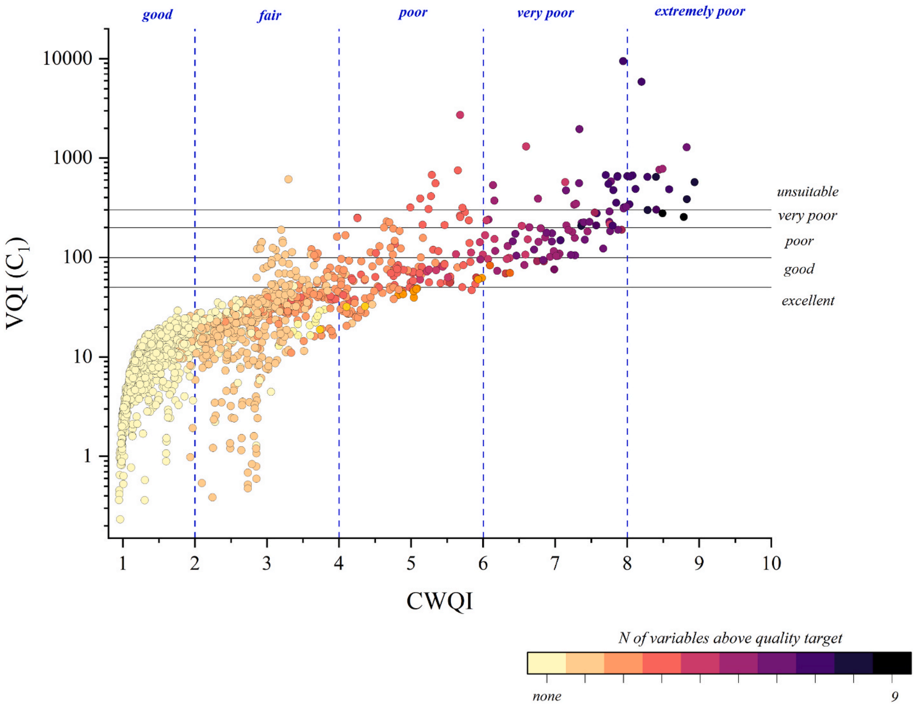

Fig. 2. Binary plot of the VQI (C_1) v. CWQI reporting he results obtained in the testing phase. VQI values are reported in log10 scale. The color intensity increases with number of parameters that does not meet the quality target. Vertical dashed blue lines indicate the chemical quality classes proposed for the CWQI, while horizontal black lines indicate the quality classes for the VQI (Vasanthavigar et al., 2010).

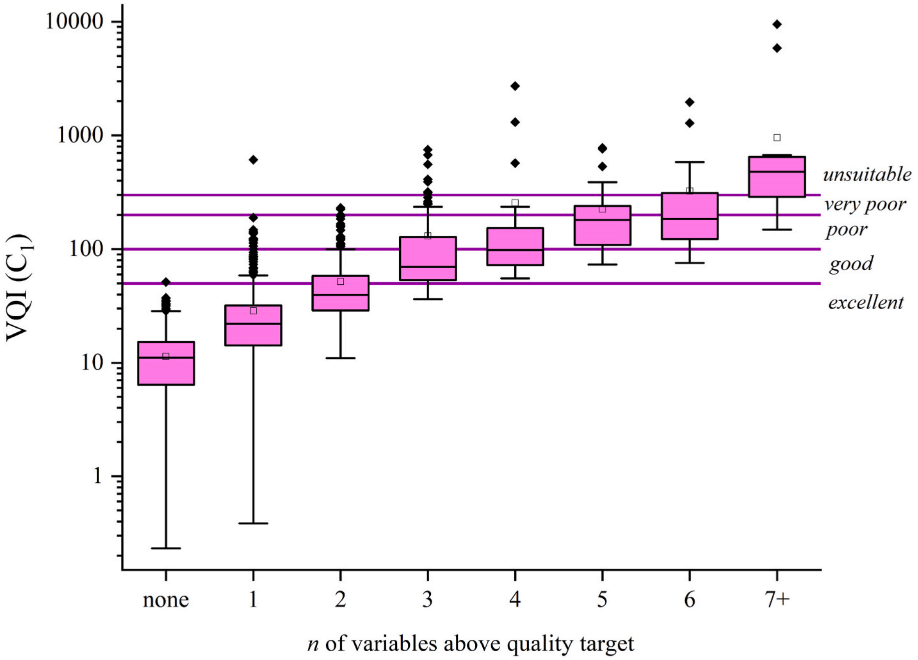

Fig. 3. Box-plot describing the variation of the VQI (under C_1) with respect to the number of variables above quality targets. VQI values (Vasanthavigar et al., 2010) are reported in log10 scale and horizontal red lines indicate the quality classes.

tested by evaluating the quality status of 1,810 waters of different types belonging to various geological and hydrological contexts. The results showed an optimal correlation between the CWQI outcomes and the number of parameters exceeding the quality target (r = 0.94), allowing the definition of clear and univocal quality classes (i.e., good, fair, poor, very poor and extremely poor). The results obtained confirmed that the CWQI may represent a powerful tool to assess the chemical quality status of any kind of water in any environment, supplying an important instrument in the water management field.

Although in our test the waters were evaluated concerning the European guidelines, the resulting CWQI is strongly related to the number of parameters above the reference values, therefore its computation can be applied using different national or international guidelines as reference values and always maintaining unchanged the quality classes used for the classification.

Although the index is defined as a chemical one, the method and the formulation used for the CWQI do not prevent the inclusion of variables of different nature (e.g., physical, biological, and/or microbiological), i. e., any variable that can be parametrized following eq. (3) and eq. (4) may be included in the computation. Lastly, the CWQI formulation is extremely flexible, and it may not be limited to water, indeed, the applicability of the proposed method to different matrices is currently under evaluation and testing.

Credit author statement

All authors contributed to the study and manuscript. LC: conceptualization, methodology, investigation, validation, formal analysis, visualization, writing – original draft, writing – review & editing. JC and MT: conceptualization, investigation, writing – review & editing. SV: conceptualization, methodology, investigation, validation, writing – review & editing. All authors have approved the final article.

Funding

LC is financially supported by a ReMeST PhD Grant (XXXVII cycle) financed by the University of Urbino. MT is financially supported by a research contract co-financed by the European Union “ESF-REACT-EU, PON Research and Innovation 2014–2020 DM1062/2021 (grant n. 63-G-19603-1)”.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

The CWQI computation spreadsheet will be provided by corrisponding author on request.

Acknowledgments

The authors wish to thank the two anonymous reviewers for their useful and constructive reviews which helped to improve the quality of the manuscript. J. M. Evans and C. Lin are also thanked for editorial handling. The authors also thank Dr. A. Venturi for her help in the development of the mathematical approach of the CWQI and to Dr. R. Biagi for her hints provided during the beginning of the index development.

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.jenvman.2023.119383.

References

Apollaro, C., Buccianti, A., Vespasiano, G., Varde, M., Fuoco, I., Barca, D., Bloise, A., Miriello, D., Cofone, F., Servidio, A., De Rosa, R., 2019. Comparative geochemical study between the tap waters and the bottled mineral waters in Calabria (Southern Italy) by compositional data analysis (CoDA) developments. Appl. Geochem. 107, 19–33. https://doi.org/10.1016/j.apgeochem.2019.05.011.

Barikdere, S., Örenay, S., Korkmaz, M., 2010. Effect of boron on human health. Open Miner. Process. J. 3, 54–59.

Basheer, A.A., 2017. Chemical chiral pollution: impact on society and science and need of the regulations in the 21th century. Chirality 30, 402–406. https://doi.org/10.1002/chir.22808.

Basheer, A.A., 2018. New generation nano-adsorbents for the removal of emerging contaminants in water. J. Mol. Liq. 261, 583–593. https://doi.org/10.1016/j.molliq.2018.04.021.

Bhargava, D., 1983. Most rapid BOD assimilation in Ganga and Yumana rivers. J. Environ. Eng. 109, 174–178.

Birke, M., Rauch, U., Harazim, B., Lorenz, H., Glatte, W., 2010. Major and trace elements in German bottled waters, their regional distribution, and accordance with nationals and internationals standards. J. Geoch. Explor. 107, 245–271. https://doi.org/10.1016/j.gexplo.2010.06.002.

Brown, R.M., McClelland, N.I., Deininger, R.A., Landwehr, J.M., 1973. Validating the WQI. The Paper Presented at the National Meeting of American Society of Civil Engineers on Water Resource Engineering. American Society of Civil Engineers, Washington, DC.

Brown, R.M., McClelland, N.I., Deininger, R.A., Tozer, R.G., 1970. A water quality index: do we dare? Water Sew. Work 117, 339–343.

Capecchiacci, F., Tassi, F., Vaselli, O., Bicocchi, G., Cabassi, J., Giannini, L., Nisi, B., Chiocciora, G., 2015. A combined geochemical and isotopic study of the fluids discharged from the Montecatini thermal system (NW Tuscany, Italy). Appl. Geochem. 59, 33–46. https://doi.org/10.1016/j.apgeochem.2015.03.010.

Centeno, L.N., Cecconello, S.T., Vieira, R.R., Soares Guedes, H.A., Reichardt, K., Timm, L. C., 2023. Methodological proposal for the establishment of a water quality index using multivariate analysis based on Brazilian legislation. Environ. Earth Sci. 82, 196. https://doi.org/10.1007/s12665-023-10847-w.

Cinti, D., Tassi, F., Procesi, M., Bonini, M., Capecchiacci, F., Voltattorni, N., Vaselli, O., Quattrocchi, F., 2014. Fluid geochemistry and geothermometry in the unexploited geothermal field of the Vicano-Cimino Volcanic District (Central Italy). Chem. Geol. 371, 96–114.

Cinti, D., Tassi, F., Procesi, M., Brusca, L., Cabassi, J., Capecchiacci, F., Delgado Huertas, A., Galli, G., Grassa, F., Vaselli, O., Voltattorni, N., 2017. Geochemistry of hydrothermal fluids from the eastern sector of the Sabatini Volcanic District (central Italy). Appl. Geochem. 84, 187–201.

Costa, M., Klein, C.B., 2008. Toxicity and carcinogenicity of chromium compounds in humans. Crit. Rev. Toxicol. 36, 155–163.

Cude, C.G., 2001. Oregon water quality index: a tool for evaluating water quality management effectiveness. J. Am. Water Resour. Assoc. https://doi.org/10.1111/j.1752-1688.2001.tb05480.x.

Daniele, L., Cannatelli, C., Buscher, J.T., Bonatici, G., 2019. Chemical composition of Chilean bottled waters: anomalous values and possible effects on human health. Sci. Total Environ. 689, 526–533. https://doi.org/10.1016/j.scitotenv.2019.06.165.

Deblonde, T., Cossu-Leguille, C., Hartemann, P., 2011. Emerging pollutants in wastewater: a review of the literature. Int. J. Hyg Environ. Health 216 (6), 442–448. https://doi.org/10.1016/j.ijheh.2011.08.002.

Dinelli, E., Lima, A., De Vivo, B., Albanese, S., Cicchella, D., Valera, P., 2010. Hydrogeochemical analysis on Italian bottled mineral waters: effects of geology. J. Geoch. Explor. 107, 317–335. https://doi.org/10.1016/j.gexplo.2010.06.004.

Dinus, S.H., 1987. Design of an index of water quality. J. Am. Water Resour. Assoc. 23, 833–843.

Dunette, D.A., 1979. A geographically variable water quality index used in Oregon. J. Wat. Pollut. Control Fed. 51 (1), 53–61.

EU Directive 2020/2184/EC, 2020. Council Directive of 16 December 2020 on the quality of water intended for human consumption. Off. J. Euro. Union L 435, 23.12.2020.

Frau, F., Cidu, R., Ghiglieri, G., Caddeo, G.A., 2020. Characterization of low-enthalpy geothermal resources and evaluation of potential contaminants. Rendiconti Lincei. Sci. Fis. Nat. 31, 1055–1070.

Frengstad, S.B., Lax, K., Tarvainen, T., Jaeger, O., Wigum, B.J., 2010. The chemistry of bottled mineral and spring waters from Norway, Sweden, Finland and Iceland. J. Geoch. Explor. 107, 350–361. https://doi.org/10.1016/j.gexplo.2010.07.001.

Frondini, F., 2008. Geochemistry of regional aquifers systems hosted by carbonate-evaporite formations in Umbria and Southern Tuscany (central Italy). Appl. Geochem. 23, 2091–2104.

Gaagai, A., Aouissi, H.A., Bencedira, S., Hinge, G., Athamena, A., Heddam, S., Gad, M., Elsherbiny, O., Elsayed, S., Eid, M.H., Ibrahim, H., 2023. Application of water quality indices, machine learning approaches, and GIS to identify groundwater quality for irrigation purposes: a case of study of Sahara aquifer, Doucen plain, Algeria. Water 15 (2), 289. https://doi.org/10.3390/w15020289.

Gupta, P., Singh, J., Verma, S., Chandel, A.S., Bhatla, R., 2021. Chapter 1 – impact of climate change and water quality degradation on food security and agriculture. In: Water Conservation in the Era of Global Climate Change, p. 22.

Helsel, D.R., Gilliom, R.J., 1986. Estimation of distributional parameters for censored trace level water quality data: 2. Verification and applications. Water Resour. Res. 22 (2), 147–155.

Horton, R., 1965. An index number system for rating water quality. J. Wat. Pollut. Control Fed 37, 300–306.

Kachroud, M., Trolard, F., Kefi, M., Jebari, S., Bourrié, G., 2019. Water quality indices: challenges and application limits in the literature. Water 11 (2), 361. https://doi.org/10.3390/w11020361.

Kolarova, N., Napiórkowski, P., 2021. Trace elements in aquatic environment. Origin, distribution, assessment and toxicity effects for the aquatic biota. Ecohydrol. Hydrobiol. 21 (4), 655–668. https://doi.org/10.1016/j.ecohyd.2021.02.002.

Kumar Mishra, R., Samyukthalakshmi Mentha, S., Misra, Y., Dwivedi, N., 2023. Emerging pollutants of severe environmental concern in water and wastewater: a comprehensive review on current developments and future research. Water-Energy Nexus 6, 74–95. https://doi.org/10.1016/j.wen.2023.08.002.

Lazzaroni, M., Vetuschi Zuccolini, M., Nisi, B., Cabassi, J., Caliro, S., Rappuoli, D., Vaselli, O., 2022. Mercury and arsenic discharge from circumneutral waters associated with the former mining area of Abbadia San Salvatore (Tuscany. Central Italy). Int. J. Environ. Res. Publ. Health 19, 5131. https://doi.org/10.3390/ijerph19095131.

Lelli, M., Agostini, L., Monegato, G., Cavazzini, G., Fasson, A., Giaretta, A., Galgaro, A., Doveri, M., 2022. Fluid geochemistry of Lessini's Mountain thermal area: new data from Caldiero, S. Ambrogio-Cola di Lazise and Sirmione hydrothermal districts (Verona-Brescia Provinces, Italy). Geothermics 101, 102377.

Linhoff, B., 2022. Deciphering natural and anthropogenic nitrate and recharge sources in arid region groundwater. Sci. Total Environ. 848, 157345 https://doi.org/10.1016/j.scitotenv.2022.157345.

Ma, Z., Li, H., Ye, Z., Wen, J., Hu, Y., Liu, Y., 2020. Application of modified water quality index (WQI) in the assessment of coastal water quality in main aquaculture areas of Dalian, China. Mar. Pollut. Bull. 157, 111285 https://doi.org/10.1016/j.marpolbul.2020.111285.

Manu, E., De Lucia, M., Kuhn, M., 2023. Hydrogeochemical characterization of surface water and groundwater in the crystalline basement aquifer system in the Pra Basin (Ghana). Water 15 (7), 1325. https://doi.org/10.3390/w15071325.

Morin-Crini, N., Lichtfouse, E., Liu, G., Balaram, V., Lado Ribeiro, A.R., Lu, Z., Stock, F., Carmona, E., Teixeira, M.R., Picos-Corrales, L.A., Moreno-Pirajàn, J.C., Giraldo, L., Li, C., Pandey, A., Hocquet, D., Torri, G., Crini, G., 2022. Worldwide cases of water pollution by emerging contaminants: a review. Environ. Chem. Lett. 20, 2311–2388.

Nisi, B., Buccianti, A., Vaselli, O., Perini, G., Tassi, F., Minissale, A., Montegrossi, G., 2008. Hydrogeochemistry and strontium isotopes in the Arno River Basin (Tuscany, Italy): constraints on natural controls by statistical models. J. Hydrol. 360, 166–183.

Nisi, B., Vaselli, O., Taussi, M., Doveri, M., Menichini, M., Cabassi, J., Raco, B., Botteghi, S., Mussi, M., Masetti, G., 2022. Hydrogeochemical surveys of shallow coastal aquifers: a conceptual model to set-up a monitoring network and increase the resilience of a strategic groundwater system to climate change and anthropogenic pressure. Appl. Geochem. 142, 105350.

O'Neal, S.L., Zheng, W., 2015. Manganese toxicity upon overexposure: a decade in review. Curr. Environ. Health Report 2, 315–328.

Ott, W.R., 1978. Environmental Índices: Theory and Practice. Arbor Science Publications, AnnAnn Arbor, Michigan, p. 317.

Pesce, S.F., Wunderlin, D.A., 2000. Use of water quality indices to verify the impact of Cordoba City (Argentina) on Suquia River. Water Res. 34 (11), 2915–2926.

Prakash, S., Verma, A., 2021. Arsenic: it's toxicity and impact on human health. Int. J. Biol. Innov. 3 (1), 38–47.

Prati, L., Pavanello, R., Pesarin, F., 1971. Assessment of surface water quality by a single index of pollution. Water Res. 5, 741–751.

Raco, B., Dotsika, E., Cerrina Feroni, A., Battaglini, R., Poutoukis, P., 2013. Stable isotope composition of Italian bottled waters. J. Geoch. Explor. 124, 203–211.

Ray, S., 2011. Impact of population growth on environmental degradation: case of India. J. Econ. Sustain. Dev. 2 (8), 72–77.

Rufino, F., Busico, G., Cuoco, E., Muscariello, L., Calabrese, S., Tedesco, D., 2022. Geochemical characterization and health risk assessment in two diversified environmental settings (Southern Italy). Environ. Geochem. Health 44, 2083–2099. https://doi.org/10.1007/s10653-021-00930-1.

Saffran, K., Environment, A., Cash, K., Canada, E., 2001. Canada Water Quality Guidelines for the Protection of Aquatic Life CCME Water Quality Index 1.0 Users' Manual. Quality 1-5.

Salminen, R., Batista, M.J., Bidovec, M., Demetriades, A., De Vivo, B., De Vos, W., Duris, M., Gilucis, A., Gregorauskiene, V., Halamic, J., Heitzmann, P., Lima, A., Jordan, G., Klaver, G., Klein, P., Lis, J., Locutura, J., Marsina, K., Mazreku, A., O'Connor, P.J., Olsson, S.Å., Ottesen, R.-T., Petersell, V., Plant, J.A., Reeder, S., Salpeteur, I., Sandström, H., Siewers, U., Steenfelt, A., Tarvainen, T., 2005. Geochemical atlas of europe. Part 1: background information, methodology and maps. Espoo. Geol. Surv. Finland 526, 36, 362 maps, •F020.

Sciarra, A., Cinti, D., Pizzino, L., Procesi, M., Voltattorni, N., Mecozzi, S., Quattrocchi, F., 2013. Geochemistry of shallow aquifers and soil gases surveys in a feasibility study at the Rivara natural gas storage site (Po Plain, Northern Italy). Appl. Geochem. 14, 3–22.

Slejko, F.F., Petrini, R., Lutman, A., Forte, C., Ghezzi, L., 2019. Chromium isotopes tracking the resurgence of hexavalent chromium contamination in a past-contaminated area in the Friuli Venezia Giulia Region, northern Italy. Isot. Environ. Health Stud. 55 (1), 56–69. https://doi.org/10.1080/10256016.2018.1560278.

Smith, D.G., 1990. A better water quality indexing system for rivers and streams. Water Res. 24 (10), 1237–1244. https://doi.org/10.1016/0043-1354(90)90047-A.

Tassi, F., Garofalo, P.S., Turchetti, F., De Santis, D., Capecchiacci, F., Vaselli, O., Cabassi, J., Venturi, S., Vannini, S., 2022. Insights into the Porretta Terme (northern Apennines, Italy) hydrothermal system revealed by geochemical data on presently discharging thermal waters and paleofluids. Environ. Geochem. Health 44, 1925–1948. https://doi.org/10.1007/s10653-020-00762-5.

Taussi, M., Gozzi, C., Vaselli, O., Cabassi, J., Menichini, M., Doveri, M., Romei, M., Ferretti, A., Gambioli, A., Nisi, B., 2022. Contamination assessment and temporal evolution of nitrates in the shallow aquifer of the metauro river plain (adriatic sea, Italy) after remediation actions. Int. J. Environ. Res. Publ. Health 19, 12231. https://doi.org/10.3390/ijerph191912231.

Torres-Martínez, J.A., Mora, A., Mahlknecht, J., Daesslé, L.W., Cervantes-Avilés, P.A., Ledesma-Ruiz, R., 2021. Estimation of nitrate pollution sources and transformations in groundwater of an intensive livestock-agricultural area (Comarca Lagunera), combining major ions, stable isotopes and MixSIAR model. Environ. Pollut. 269, 115445.

Uddin, M.G., Nash, S., Olbert, A.G., 2021. A review of water quality index models and their use for assessing surface water quality. Ecol. Indicat. 122, 107218.

Vasanthavigar, M., Srinivasamoorthy, K., Vijayaragavan, K., Rajiv Ganthi, R., Chidambaram, S., Anandhan, P., Manivannan, R., Vasudevan, S., 2010. Application of water quality index for groundwater quality assessment: thirumanimuttar sub-basin, Tamilnadu, India. Environ. Monit. Assess. 171, 595–609.

Venturi, S., Vaselli, O., Tassi, F., Nisi, B., Pennisi, M., Cabassi, J., Bicocchi, G., Rossato, L., 2015. Geochemical and isotopic evidences for a severe anthropogenic boron contamination: a case study from Castelluccio (Arezzo, central Italy). Appl. Geochem. 63, 146–157. https://doi.org/10.1016/j.apgeochem.2015.08.008.

Vespasiano, G., Cianflone, G., Marini, L., De Rosa, R., Polemio, D., Walraevens, K., Vaselli, O., Pizzino, L., Cinti, D., Capecchiacci, F., Barca, D., Dominici, R., Apollaro, C., 2023. Hydrogeochemical and isotopic characterization of the Gioia Tauro coastal plain (Calabria – southern Italy): a multidisciplinary approach for a focused management of vulnerable strategic systems. Sci. Total Environ. 862, 160694 https://doi.org/10.1016/j.scitotenv.2022.160694.

Walton, N.R.G., 1989. Electrical conductivity and total dissolved solids – what is their precise relationship? Desalinization 72 (3), 275–292. https://doi.org/10.1016/0011-9164(89)80012-8.

World Health Organitazion (WHO), 2017. Guidelines for drinking-waters quality. In: Fourth Edition Incorporating First Addendum. WHO Press, p. 564.

Yolcubal, I., Gündüz, Ö.C., Sönmez, F., 2016. Assessment of impact of environmental pollution on groundwater and surface water qualities in a heavily industrialized district of Kocaeli (Dilovası), Turkey. Environ. Earth Sci. 75, 170. https://doi.org/10.1007/s12665-015-4986-2.