Supplementary material for

Evaluation of Surface Water Quality Using Various Indices for Heavy Metals in Sasolburg, South Africa

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Section S1. Pollution Indices

1.1 Modified heavy metal pollution index (m-HPI)

[1] specified a modified heavy metal pollution index (m-HPI) for improved evaluation of water quality for domestic use to improve the drawbacks of heavy metals pollution index and m-HPI is calculated as follows:

$$m - HPI = \sum_{i=1}^{n} m - HPI^{i} \quad (1)$$

where n is the number of metals that are evaluated and m-HPI^{i} is the modified heavy metal pollution index for the ith heavy metal, calculated as:

$$m - HPI^{i} = w_i Q_i \quad (2)$$

Where w_i is the relative weightage factor calculated as:

$$w_i = \frac{W_i}{\sum_{i=1}^{n} W_i} \quad (3)$$

Where W_i is the unit weighting factor calculated as:

$$W_i = \frac{1}{S_i} \tag{4}$$

S_i is the maximum standard value of the *i*th heavy metal. Sub index Q_i for the *i*th heavy metal is quantified as:

$$Q_i = \frac{M_i - S_i}{S_i} \tag{5}$$

M_i represents the analysed concentration of the *i*th heavy metal. Modified heavy metal index can be broken down into metals that meet the maximum allowable value or metals that do not meet the maximum allowable value. The previous m-HPI is referred to as the positive index (PI) and the latter as the negative index (NI) with U_L being the upper limit of PI. Therefore, water quality according to m-HPI may be grouped as shown in Table 1.

1.2 Heavy metal evaluation index (HEI)

HEI offers a description of water quality regarding heavy metal contamination. HEI is evaluated based on Maximum Allowable Concentration (MAC) using concentration of the metal of interest [1]:

$$HEI = \sum_{i=1}^{n} HEI^i \tag{6}$$

HEI^i is the contamination index related to the *i*th heavy metal calculated as:

$$HEI^i = \frac{M_i}{H^i_{MAC}} \tag{7}$$

The MAC of the *i*th heavy metal is H^i_{mac}. To distinguish the various levels of contamination, this method divides water quality into three groups as seen in Table 1:

1.3 Nemerow Index (NeI)

This approach is a multifactorial and integrated technique, where the index is determined using [1]:

$$NeI = \left[\frac{\{(M_i/S_i)^2_{average} + (M_i/S_i)^2_{max}\}}{n}\right]^{\frac{1}{2}} \quad (8)$$

Where $(M_i/S_i)_{average}$ is the mean value for all heavy metals of interest of a sample, $(M_i/S_i)_{max}$ is the maximum value for all metals of interest evaluated in the sample, and *n* is the number of heavy metals evaluated. For water quality purposes the technique has for categories for classification (Table 1):

1.4 Contamination factor (Cf)

The assessment of contamination in surface water may be evaluated using the contamination factor (C*f*). It is an essential technique for measuring contamination over time. C*f* is a ratio computed by dividing the average concentration of each element by the reference value and is calculated as follows [2]:

$$Cf = \frac{C_{heavy\ metal}}{C_{background}} \quad (9)$$

$C_{heavy\ metal}$ is the concentration of the target metal analysed and $C_{background}$ is the reference concentration of the permissible value. C*f* quality classifications are listed in Table 1.

1.5 Modified degree of contamination (m-Cd)

The purpose of m-C_d is to provide an assessment on the overall contamination in surface water at a given study area [3] and the equation is given as follows:

$$m - C_d = \frac{\left(\sum_{i=1}^{i=n} cf\right)}{n} \quad (10)$$

Where *n* is the number of elements evaluated for the *i*th heavy metal and C*f* is the sum of the contamination factor. For water quality statuses the m-C_d is divided into categories (Table 1).

1.6 Estimated daily intakes (EDI)

The estimated daily intake (EDI) for this study was investigated. Study was conducted for adult men, adult women, and children using the following equation (11) [4]:

$$EDI = C \times E_F \times E_D \times F_{TR}/W_{AB} \times T_A \quad (11)$$

Where C is the concentration of the analysed heavy metal (mg/L) in surface water, E_F is the frequency of exposure (365 days/year), E_D is the duration of exposure (60 years for men, 67 years for women, and 12 years for children), F_{IR} is the surface water ingestion rate (2.0 L/day for adult men and women, 1.0 L/day for children), W_{AB} is the Average body weight (65 kg for men, 60 kg for women, 20 kg for children), and T_A is the average exposure time ($E_F \times E_D$).

1.7 Non-carcinogenic risk of water consumption (HQ)

A hazard quotient (HQ) calculation was made in compliance with equation (12) to compute the potential non-cacinogenic risk values due to specific pollutants in the examined surface water [4]:

$$HQ = EDI/RfD_0 \quad (12)$$

Where HQ is the hazard quotient (unit-less), EDI is the estimated daily intake (mg/kg/bw/day), and RfD_0 is the oral reference dose value.

1.8 Carcinogenic risk of water consumption (R)

Potential carcinogenic risk values (R) of surface water was calculated using heavy metal concentrations analysed, and was determined using equation (13) [4]:

$$R = EDI \times SF \quad (13)$$

Where R is the carcinogenic risk value (unit-less), EDI is the estimated daily intake (mg/kg bw/day), and SF is the slope factor [(mg/kg bw/day)$^{-1}$]. SF were available for As = 1.5 [(mg/kg bw/day)$^{-1}$, Cr = 0.5 [(mg/kg bw/day)$^{-1}$, Pb = 0.0085 [(mg/kg.bw/day)$^{-1}$ [4].

1.9 Weighted arithmetic Water Quality Index (WQI)

Water quality for drinking purposes was determined with the weighted arithmetic method (WQI). The following formulae were used to calculate water quality rating [5]:

$$q_i = (C_i/S_i) \times 100 \quad (14)$$

Where q_i, C_i, and S_i represent the quality rating scale, concentration of *i* parameter, and standard value of *i* parameter, respectively.

Relative weight was calculated by

$$w_i = 1/S_i \quad (15)$$

Where the standard value of the *i* parameter is inversely proportional to the relative weight.

The overall WQI is calculated according to the following expression:

$$WQI = \Sigma q_i w_i / \Sigma w_i \quad (16)$$

WQI quality classifications are found in Table 1.

Table S1: Quality status for environmental and health parameters

Indices	Value	Quality status	References
m-HPI	$-1 \leq NI \leq 0$ and $PI = 0$	Excellent	[1]
	$-1 < NI < 0$ and $0 < PI \leq U_L/2$	Very good	
	$-1 \leq NI \leq 0$ and $U_L < PI \leq U_L$	Good	
	$NI \leq 0$ and $PI > U_L$	Unacceptable	
HEI	HEI < 10	Low	[1]
	HEI= 10 – 20	Medium	
	HEI > 20	High	
NeI	NeI < 1	Insignificant contaminated	[1]
	$1 \leq NeI < 2.5$	Slightly contaminated	
	$2.5 \leq NeI < 7$	Moderately contaminated	
	$NeI \geq 7$	Heavily contaminated	
C*f*	C*f* < 1	Low C*f*	[3]
	$1 \leq CF < 3$	Moderate C*f*	
	$3 \leq CF < 6$	Considerable C*f*	
	$CF \geq 6$	Very high C*f*	
m-C_d	m-C_d < 1.5	Nil to a very low degree of contamination	[3]
	$1,5 \leq$ m-C_d < 2	Low degree of contamination	
	$2 \leq$ m-C_d < 4	Moderate degree of contamination	
	$4 \leq$ m-C_d < 8	High degree of contamination	
	$8 \leq$ m-C_d < 16	Very high degree of contamination	
	$16 \leq$ m- C_d < 32	Extremely high degree of contamination	
	m-$C_d \geq 32$	Ultra-high degree of contamination	
WQI	< 50	Excellent	[5]
	50 - 100	Good water	
	101 - 200	Poor water	
	201 - 300	Very poor water	
	> 300	Unsuitable for drinking	

References

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