

MCA – Water Quality Risk Assessment Tool

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Abstract

Industrial, mining and agricultural industries in South Africa are legally obligated by the Constitution of South Africa and Environmental Legislation to identity, quantify, monitor, and manage their pollution sources and the potential environmental impact of these sources. A risk assessment, based on the Monte Carlo analysis (MCA) of random sampling, was developed to characterize, quantitatively, the uncertainty and variability in assessing possible environmental impacts and risk. The program is a screening tool applied to historical time-series monitoring data for a monitoring site to determine the risk of probability of environment impact on water quality parameters for the groundwater regime.

Keywords: Risk assessment, Monte Carlo analysis, monitoring programmes

Introduction

Handling, processing, and storage of different type of wastes and end-products of all industrial, agricultural, and mining facilities can release contaminants into the natural water environment. It is for this reason that these industries are legally obligated by the Constitution of South Africa and Environmental Legislation to identify, quantify, monitor, and manage these pollution sources and potential environmental impact of these sources on the natural environment.

Apart from the initial capital cost for the installation of a monitoring network, the cost for analyzing the water quality for different industries can outweigh the cost for sampling, data processing, storage, and reporting. The cost for analyzing the water quality can be reduced if it is possible to identify water quality parameters that have a high risk of impacting the groundwater regime and modify the water quality parameters to be monitored, and the frequency of monitoring according to the risk of probable impact. The aim of this research was to develop a quantitative risk assessment tool to assist geohydrologists in the optimization of groundwater monitoring programmes.

Approach to the Quantitative Risk Assessment

The Monte Carlo analysis of random data sampling was used in this research to characterize, quantitatively, the uncertainty and variability in assessing possible impacts and risk. The U.S. Environmental Protection Agency (1997) defines the Monte Carlo analysis as a random data sampling techniques in obtaining a probabilistic approximation to the solution of a mathematical equation/ model. The random sampling Monte Carlo Algorithm applied in the Microsoft Excel Program for this research study is given below (equation 1, see more Microsoft (2022) and EXCELTV (2022) for a detailed explanation).

{NORM.INV[RAND(), A, Sdev.]} -{NORM.INV[RAND(), A, Sdev.]}

Equation 1

Where NORM.INV = the Normal Inversion Function, RAND () = function that elicit a random number (probability) based on the other criteria within the distribution, A =arithmetic mean of the selected/input water quality parameter, Sdev. = the standard deviation of the selected/input water quality parameter.



Figure 1 Illustration explaining the concept of the Monte Carlo random sampling analysis.

Table 1 Results of the Monte Carlo algorithm versus a selected standard.

Value/Answer	Frequency	Probability of Impact							
>0	8524	85.24%							
Value/Answer	Frequency	Probability of Impact exceeding first limit of standard							
>250	6631	66.31%							
Value/Answer	Frequency	Probability of Impact exceeding second limit of standard							
>500	4082	40.82%							

The concept of the algorithm in Equation 1 is illustrated in Fig. 1. The algorithm takes a random sample from the distribution of the downstream/monitoring site quality data and a random sample from the distribution of the upstream/background quality data. The random sampling points is then subtracted from each other. This process is repeated 10 000 times for each water quality parameter. A value equal or less than zero is regarded as no impact, and a value greater than zero is regarded as an impact (Fig. 1)

The algorithm is applicable to data that is normally distributed (Gaussian or Bell-Shaped Curved distribution). According to Reimann, Filzmoser and Garrett (2005), geochemical data distributions are generally symmetrical (normally distributed) or can be logarithmic transformed to be symmetrical. The distribution of each water quality parameter in terms of non-normality (skewness) was evaluated by calculating the coefficient of variation (COV). If the COV is smaller than 100% a normal distribution is assumed and when greater than 100%, a logarithmic scale was prepared (Reimann, Filzmoser and Garrett, 2005) and the Normal Inversion Function in Equation 1 was replaced by the Log-Normal Inverse Function (LOGNORM. INV)(EXCELTV, 2022).

The frequency percentage of the values above zero equals the percentage of probability of impact (see Tab. 1). The values are then evaluated in terms of the limits of a selected standard. The frequency percentage of the values above the limit of the standard equals the percentage of probability of impact exceeding the limit of the selected standard (Tab. 1).

The probability percentages are then converted to a value between one and five based on the percentage intervals shown in Tab. 2. Based on these ratings, the basic concept of a risk equals the probability multiplied by the severity of consequence (Duijm, 2015) are then used to compute a risk rating for each water quality parameter. The probability of impact is regarded as the probability, where the probability of the exceedance of the limits of the selected standard is regarded as the severity of consequence. In the case where a water quality parameter has two limits, the sum of the ratings assigned to each of these two categories are then multiplied by the probability. The computed risk ratings are then classified according to the intervals shown in Fig. 2.

Monitoring data from two different Industrial Facilities within South Africa, with varies types of waste management facili-

0 71	71	0											
Probability Per	centage	0-20	20-40	40-60	60-80	80-100							
Rating		1	2	3	4	5							
	Risk Rating												
$(Probability \times Severity)$													
Very Low	Low	Ν	ledium	High	V	/ery High							
1-2	3-9		10-15 16-20										

Table 2 Rating of probability percentage.

Figure 2 Risk rating categories.

ties was used to test the approach of the quantitative risk assessment. The number of monitoring points of the two different sites ranges between 200 and 350, with a data coverage period ranging between 15 and 20 years. This research is part of an unpublished PhD thesis completed at the University of the Free State, South Africa.

MCA – Water Quality Risk Assessment Tool Interface

The MCA-Water Quality Risk Assessment Tool is a Microsoft Excel-based program. The tool consists of the nine sheets that will be discussed in the paragraphs below.

Title Sheet (MCA_WQRAT) – When the MCA-Water Quality Risk Assessment Tool

is opened, it will show a Title sheet (Fig. 3). The sheet also indicates the information and data input sequence to be followed. The user should read through the sequence, and once familiar they can continue by clinking on the "START" button. The user will then be navigated to the General Info sheet.

Menu Sheet – the MENU sheet (Fig. 4) enables the user to navigate between the different worksheets. These worksheets include the General Inf, BH-ID, CHEM, and RESULTS sheets.

General Info Sheet – The user is navigated to the General Info sheet (Fig. 5) by clicking on the "START" button in the Title sheet. This is where the user defines the general information for the monitoring



Figure 3 Title sheet of the MCA-Water Quality Risk Assessment Tool.

	Α	В	С	D	E	F	G	н	1	J	К	L	М	N	0	Р	Q
1																	
2																	
3																	
4																	
5	General Info				BHID				CHEM				RESULTS				
6																	
7																	
8																	
9																	
10																	
11																	
12																	
13																	
14																	

Figure 4 MENU sheet of the MCA-Water Quality Risk Assessment Tool.

	A	B	C	D	E	F	G	н	1	J	К	L	м	N	0	P
1	Project A	rea Delineatio														
2	Project A	rea Denneatio									Chemi	cal Parameter	's			
3 4	Number of Areas	5			1) Area Info	M	enu	Physical Parameters	Macro Chem	ical Parameters						
5	AREA		AREA ID		No. of AQUIFERS			77.00	T 0	E HOMM		-	T CHITCHIN	_		
6	AREA 1		В		3			W EC	i≊ G	MO2(N)	A	≥ Ca	M CN(IDtal)	✓ Mn	i∞ se	
7	AREA 2		с		2						SI Ar	2 Co		Z Mo	el si	
8	AREA 3		D		1			100	. n	1105(11)	~~		entitee)	mo		
9	AREA 4		E		2			M pH	Mg Mg		⊠ B	Cr(Total)	CN(WAD)	🖂 Ni	⊡ Sr	
10	AREA 5		F		3											
11 12									🗹 Na	🗹 NH4(N)	🗹 Ba	🗹 Cr(+6)	✓ Fe(Total)	🗹 Pb	⊠ U	
13									T (0)		-10-	71.0		-	-	
14									IV 504	l∾ 2n	i∾ Be	v cu	i≊ ng	50	No. V	
15									⊡ F	TALK						
17									1							
18						i i			CI 🛛		4) Ch	emical Parameter	3			
19					2) Create Aquifer Info											
20	AREA ID	AQUIFER 1	AQUIFER 2	AQUIFER 3	Sheet											
21	В	Unconfined	Confined	Uncertain		1		Sta	indard Sele	ction						
22	С	Confined	Sandstone					CANE 313 2001		-	Ī					
23	D	Shallow						34145 2412005		· ·	1					
24	E	Unconfined	Deep													
25	F	Shallow	Sandstone	Gravel												
26																
2/															PROJECT RESET	
28																
30																
31					3) Create BH											
32					information Sheet											
	MCA_WQRA	T MENU	General_Info	BHJD EC	K CI NO3(N) Fe(To	otal) Mn	CHEM RESL	ILTS RISK	Controls Star	idards 🕀						1

Figure 5 General Info sheet of the MCA-Water Quality Risk Assessment Tool.

	А	В	С	D	E	F	G	н	I.	J	
1	Back to G	eneral Info									
2				С							
3	1: Unc	onfined	2: Co	nfined	3: Uno	ertain	1: Co	nfined	2: Sandstone		
4	Borehole	Туре	Borehole	Туре	Borehole	Туре	Borehole	Туре	Borehole	Туре	
5	BH1	Background	BH10	Background	BH20	Background	BH30	Background	BH40	Background	
6	BH2	Monitoring	BH11	Monitoring	BH21	Monitoring	BH31	Monitoring	BH41	Monitoring	
7	BH3	Background	BH12	Background	BH22	Background	BH32	Background	BH42	Background	
8	BH4	Monitoring	BH13	Monitoring	BH23	Monitoring	BH33	Monitoring	BH43	Monitoring	
9	BH5	Monitoring	BH14	Monitoring	BH24	Monitoring	BH34	Monitoring	BH44	Monitoring	
10											
11											
12											
13											

Figure 6 BH_ID sheet of the MCA-Water Quality Risk Assessment Tool.

site. Information includes area information, aquifer classification, and chemical parameter and standard selection.

Borehole-ID Sheet (BH_ID) – This is where the user lists the borehole names per area and per aquifer as defined in the General Info sheet. The user should also select or indicate if the borehole is a reference (background) or monitoring borehole by using the dropdown menu (Fig. 6). CHEM Sheet – The CHEM sheet (Fig. 7) is where the user calculates the parameters statistics and probability of impact per chemical parameter. This can only be completed if the chemical parameter sheets (generated when the chemical parameters were selected in the General Info sheet) have been populated. First the user should click on the "Calculate Parameter Statistics" button. The average, standard deviation and



4	A	B	C	D	E	F	G	H	1.1	J	К	L	M	N	
	Area ID	Aquifer ID	Parameter	standard	Range	Bin	Frequency	Relative Frequency	Cumulative %	Probability: Impact %	Probability: Exceed Aesthetic %	Probability: Exceed Limit %			1
В		1: Unconfined	EC	SANS 241:2005	<=0	0	3622	36.22	36.22%				Cali	culate Risk	
В		1: Unconfined	EC	SANS 241:2005	0-150	150	5705	57.05	93%	63 7956	6 72%	0.00%			1
В		1: Unconfined	EC	SANS 241:2005	150-370	370	673	6.73	100%	03.7676	0.73%	0.00%			Ξ.
В		1: Unconfined	EC	SANS 241:2005	>370	More	0	0	100%						
В		1: Unconfined	EC	Own Standard	<=0	0	3622	36.22	36.22%			63.78%		Monu	
В		1: Unconfined	EC	Own Standard	0-0	0	0	0	36%	63 708/	63 78%			menu	
В		1: Unconfined	EC	Own Standard	0-0	0	0	0	36%	03.78%	03.7878				
В		1: Unconfined	EC	Own Standard	>0	More	6378	63.78	100%						
В		2: Confined	EC	SANS 241:2005	<=0	0	5349	53.49	53.49%						
В		2: Confined	EC	SANS 241:2005	0-150	150	3108	31.08	85%	46 5184	15 430	0.000			
В		2: Confined	EC	SANS 241:2005	150-370	370	1457	14.57	99%	40.31%	13.43%	0.80%			
В		2: Confined	EC	SANS 241:2005	>370	More	86	0.86	100%						
В		2: Confined	EC	Own Standard	<=0	0	5349	53.49	53.49%		46.51%				
В		2: Confined	EC	Own Standard	0-0	0	0	0	53%	6 46.51% 6		45 5494			
В		2: Confined	EC	Own Standard	0-0	0	0	0	53%			40.51%			
в		2: Confined	EC	Own Standard	>0	More	4651	46.51	100%						
В		3: Uncertain	EC	SANS 241:2005	<=0	0	5053	50.53	50.53%		10.22%	0%			
В		3: Uncertain	EC	SANS 241:2005	0-150	150	3925	39.25	90%	10.171					
В		3: Uncertain	EC	SANS 241:2005	150-370	370	1016	10.16	100%	49.47%					
В		3: Uncertain	EC	SANS 241:2005	>370	More	6	0.06	100%						
В		3: Uncertain	EC	Own Standard	<=0	0	5053	50.53	50.53%						
В		3: Uncertain	EC	Own Standard	0-0	0	0	0	51%	40.47%	40.47%	101/			
В		3: Uncertain	EC	Own Standard	0-0	0	0	0	51%	49.47%	49.47%	49%			
В		3: Uncertain	EC	Own Standard	>0	More	4947	49.47	100%						
C		1: Confined	EC	SANS 241:2005	<=0	0	4805	48.05	48.05%						
c		1: Confined	EC	SANS 241:2005	0-150	150	3897	38.97	87%	54.05W	43.000				
C		1: Confined	EC	SANS 241:2005	150-370	370	1274	12.74	100%	51.95%	12.98%	0%			
С		1: Confined	EC	SANS 241:2005	>370	More	24	0.24	100%						
с		1: Confined	EC	Own Standard	<=0	0	4805	48.05	48.05%						
C		1: Confined	EC	Own Standard	0-0	0	0	0	48%	54.0524	54.0594	500			
С		1: Confined	EC	Own Standard	0-0	0	0	0	48%	51.95%	51.95%	52%			
с		1: Confined	EC	Own Standard	>0	More	5195	51.95	100%						

Figure 7 CHEM sheet of the MCA-Water Quality Risk Assessment Tool.

1	A	В	с	D	E	F	G	н	1	J	К	L	м	N	0
1	Area ID	Aquifer ID	Parameter	Standard	Range	Bin	Frequency	Relative Frequency	Cumulative %	Probability: Impact %	Probability: Exceed Aesthetic %	Probability: Exceed Limit %			1
2 B		1: Unconfined	EC	SANS 241:2005	<=0	0	3622	36.22	36.22%				Calci	alate Risk	
3 B		1: Unconfined	EC	SANS 241:2005	0-150	150	5705	57.05	93%	C3 700/	6 720	0.000			
4 B		1: Unconfined	EC	SANS 241:2005	150-370	370	673	6.73	100%	03.76%	0.73%	0.00%			_
5 B		1: Unconfined	EC	SANS 241:2005	>370	More	0	0	100%						
6 B		1: Unconfined	EC	Own Standard	<=0	0	3622	36.22	36.22%					Monu	
7 B		1: Unconfined	EC	Own Standard	0-0	0	0	0	36%	63 700/	C3 700/	62 702/		menu	
8 B		1: Unconfined	EC	Own Standard	0-0	0	0	0	36%	03.78%	03.76%	03.76%			
9 B		1: Unconfined	EC	Own Standard	>0	More	6378	63.78	100%						
10 B		2: Confined	EC	SANS 241:2005	<=0	0	5349	53.49	53.49%						
11 B		2: Confined	EC	SANS 241:2005	0-150	150	3108	31.08	85%	46 619/	15 439/	0.969/			
12 B		2: Confined	EC	SANS 241:2005	150-370	370	1457	14.57	99%	40.31%	13.4374	0.80%			
13 B		2: Confined	EC	SANS 241:2005	>370	More	86	0.86	100%						
14 B		2: Confined	EC	Own Standard	<=0	0	5349	53.49	53.49%			46 514			
15 B		2: Confined	EC	Own Standard	0-0	0	0	0	53%	46 510	46 519				
16 B		2: Confined	EC	Own Standard	0-0	0	0	0	53%	+0.31%	40.51%	40.51%			
17 B		2: Confined	EC	Own Standard	>0	More	4651	46.51	100%						
18 B		3: Uncertain	EC	SANS 241:2005	<=0	0	5053	50.53	50.53%		10.22%				
19 B		3: Uncertain	EC	SANS 241:2005	0-150	150	3925	39.25	90%	40.470/		0%			
20 B		3: Uncertain	EC	SANS 241:2005	150-370	370	1016	10.16	100%	43.47%					
21 B		3: Uncertain	EC	SANS 241:2005	>370	More	6	0.06	100%						
22 B		3: Uncertain	EC	Own Standard	<=0	0	5053	50.53	50.53%						
23 B		3: Uncertain	EC	Own Standard	0-0	0	0	0	51%	40.470/	40.470/	1021			
24 B		3: Uncertain	EC	Own Standard	0-0	0	0	0	51%	49.47%	49,47%	49%			
25 B		3: Uncertain	EC	Own Standard	>0	More	4947	49.47	100%						
26 C		1: Confined	EC	SANS 241:2005	<=0	0	4805	48.05	48.05%						
27 C		1: Confined	EC	SANS 241:2005	0-150	150	3897	38.97	87%	F4 0F0/	42.000/				
28 C		1: Confined	EC	SANS 241:2005	150-370	370	1274	12.74	100%	51.95%	12.98%	0%			
29 C		1: Confined	EC	SANS 241:2005	>370	More	24	0.24	100%						
30 C		1: Confined	EC	Own Standard	<=0	0	4805	48.05	48.05%						
31 C		1: Confined	EC	Own Standard	0-0	0	0	0	48%	F4 0F0/	54 0501	5044			
32 C		1: Confined	EC	Own Standard	0-0	0	0	0	48%	51.95%	51.95%	52%			
33 C		1: Confined	EC	Own Standard	>0	More	5195	51.95	100%						
	MCA_WQRAT ME	NU General_Info E	с к сі	BHJD NO3(M	4) Fe(To	tal) M	vin CHEM	RESULTS RISK	Standards 0	ontrols 🕘 🛞					

Figure 8 RESULTS Sheet of the MCA-Water Quality Risk Assessment Tool.



Figure 9 RISK Sheet of the MCA-Water Quality Risk Assessment Tool.

coefficient of variance is calculated for each chemical parameter for the monitoring boreholes and reference boreholes and the sheet is automatically populated. If the coefficient of variance is greater than 100% the log-transformed statistics is selected by default for the probability calculation (Monte Carlo analysis). Then the user should click on the "Calculate Probability" button. The user is then navigated to the RESULTS sheet (Fig. 8).

RESULTS Sheet – this is where the probability percentages calculated is presented and where the user can calculate the risk. The user should click on the "Calculate Risk" button. The risk is then calculated based on the probability percentages and the user is navigated to the RISK sheet (Fig. 9).

RISK Sheet – This sheet represents the final product of the risk assessment process, which is the calculated risk matrix per monitoring area, indicating the probable risk of impact per chemical parameter.

Application for Groundwater Monitoring Programme Optimization

Based on the risk rating calculated by the MCA-Water Quality Assessment Tool, a monitoring programme can be optimized by applying the following rules:

- Water quality parameters with a risk rating of high to very high should be monitored at minimum on a quarterly basis.
- Water quality parameters with a risk rating of medium should be monitored at a minimum on a biannual basis (wet and dry season).
- The water quality parameters with a risk rating of very low to low should be monitored on an annual basis if the concentration of these parameters exceed the limits of the selected standard at one of the monitoring localities, then the frequency of monitoring for that parameter at that specific locality should be increased to determine if it was a once off occurrence or if the concentration is increasing over time.

Conclusions

The MCA-Water Quality Risk Assessment Tool should be regarded as a screening tool applied to historical time-series monitoring data for a specific monitoring site to determine the risk of probability of impact for the inorganic water quality parameters. The Tool can be applied to varies industries that have the potential to impact or have impacted the groundwater regime if historical timeseries monitoring data is available. Other applications include:

- Determination of which potential pollution source at an industrial and/or mining facility is impacting the water resources (surface-and groundwater) the most or which one have the highest risk of possible impact.
- Industrial and/or mining post-closure screening tool to estimate which water quality parameters have the highest risk of impacting the water resources of the area.
- Incorporation into monitoring reports to assist management in identifying problem areas and the management thereof.

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