An update to this article is included at the end

Heliyon 9 (2023) e13007

Contents lists available at ScienceDirect

Heliyon

journal homepage: www.cell.com/heliyon

Research article

Development of a GIS-based knowledge hub for contaminants of emerging concern in South African water resources using open-source software: Lessons learnt

Tarryn Lee Botha [a,b,*], Emomotimi Bamuza-Pemu [c], Ashira Roopnarain [d], Zibusiso Ncube [d], Gert De Nysschen [d], Busiswa Ndaba [d], Ntebogeng Mokgalaka [e,f,k], Maryam Bello-Akinosho [g], Rasheed Adeleke [h], Akani Mushwana [d], Michael van der Laan [i,j], Phedisho Mphahlele [d,k], Fanelesibonge Vilakazi [d,h], Penny Jaca [l], Eunice Ubomba-Jaswa [l]

[a] *Institute for Nanotechnology and Water Sustainability, College of Science, Engineering and Technology, University of South Africa, Florida Science Campus, 1710, South Africa*
[b] *Water Research Group, Unit for Environmental Sciences and Management, North-West University, Private Bag X6001, Potchefstroom, 2520, South Africa*
[c] *OptimalEnviro; Postnet Suite 073, Private Bag X21, Queenswood, Pretoria, 0121, South Africa*
[d] *Microbiology and Environmental Biotechnology Research Group, Agricultural Research Council – Natural Resources and Engineering, Pretoria, South Africa*
[e] *University of Pretoria, Mamelodi Campus, Private Bag X20, Hatfield, Pretoria, 0028, South Africa*
[f] *Tshwane University of Technology, Faculty of Science, Department of Chemistry, Private Bag X680, Pretoria, 0001, South Africa*
[g] *Pathogenic Yeast Research Group, Department of Microbiology and Biochemistry, Faculty of Natural and Agricultural Sciences, University of the Free State, PO Box 339, Bloemfontein, 9300, South Africa*
[h] *Unit for Environmental Sciences and Management, North-West University, South Africa*
[i] *Agricultural Research Council (ARC) – Natural Resources and Engineering, Private Bag X79, Pretoria, 0001, South Africa*
[j] *Department of Plant and Soil Sciences, University of Pretoria, Private Bag X20 Hatfield, Pretoria, 0028, South Africa*
[k] *Department of Chemistry, Tshwane University of Technology, Private Bag X680, Pretoria, 0001, South Africa*
[l] *Water Research Commission, Lynnwood Bridge Office Park, Bloukrans Building, 4 Daventry Street, Lynnwood Manor, Pretoria, 0081, South Africa*

ARTICLE INFO

Keywords:
Interactive map
Biological contaminants
Freshwater
Collated data

ABSTRACT

With population growth and dwindling freshwater sources, protecting such sources has come to the forefront of water resource management. Historically, society's response to a problem is based on funding availability, current threat, and public outcry. Achieving this is largely dependent on the knowledge of the factors that are resulting in compromised water sources. These factors are constantly changing as novel contaminants are introduced into surface water sources. As we are in the information age, the interest in contaminants of emerging concern (CEC) is gaining ground. Whilst research is being conducted to identify contaminants in South African water sources, the research outputs and available information is not collated and presented to the science community and stakeholders in readily available formats and platforms. Current research outcomes need to be made known to regulators in order to develop environmental laws. By using fourth industrial revolution technology, we were able to collate available data in literature and display

* Corresponding author. Institute for Nanotechnology and Water Sustainability, College of Science, Engineering and Technology, University of South Africa, Florida Science Campus, 1710, South Africa.
E-mail address: bothatl@unisa.ac.za (T.L. Botha).

https://doi.org/10.1016/j.heliyon.2023.e13007
Received 17 November 2022; Received in revised form 12 January 2023; Accepted 12 January 2023
Available online 18 January 2023

these in a user-friendly online format to regulatory bodies as well as researchers. A standardized excel spreadsheet was developed and uploaded to a PostgreSQL, running a PostGIS extension and was then processed in the GeoServer to allow for visualization on an interactive map which can be continuously updated. The near real-time access to information will reduce the possibility of duplication of research efforts, enhance collaboration in the discipline, and act as a CEC early warning system.

1. Introduction

Rapid population growth, urbanisation and industrialisation have led to the production of myriads of compounds of varied classifications with new ones being introduced daily. Unfortunately, water bodies serve as an ultimate sink for most of these products and their degradates through various pathways. Several of these compounds are considered "emerging" pollutants or contaminants as they are not in the conventional list of monitored and regulated contaminants. These compounds have high potential of entering the environment and are widely distributed throughout environmental matrices [1,2]; with subsequent adverse ecological and/or human health effects [3,4]. Emerging contaminants are not limited to chemical pollutants as anthropogenic activities also result in contamination of water resources with particle contaminants (microplastics, nanomaterials) and biological microcontaminants (bacteria, viruses). Some of these biological CECs are potentially pathogenic causing waterborne diseases and remain a major cause of death worldwide [2] particularly in developing and underdeveloped countries where basic sanitation and potable water are lacking. This is compounded by the fact that conventional wastewater or drinking water treatment facilities are usually not (yet) equipped to remove these compounds because of their chemical structural stability and low concentrations detected [5]. Additionally, these compounds are often toxic to microbial species if used in the treatment processes [2].

South Africa is a semi-arid country with highly variable rainfall patterns and an average rainfall of 52% of the global average [6]. South Africa has very little surplus freshwater available, already placing a constrain on economic growth and development. Approximately 80–90% of water in South Africa is consumed by the agricultural industry and farmers will have to double their water use by 2050 if they are to meet growing food demands without significantly improving water productivity. Safeguarding South African water sources is key to realizing the vision of both the South African Department of Water and Sanitation (SDG 6) and the UN Millennium Development Target 10 of Goal 7. Both these goals require adequate and suitable quality water sources, and the quality of water ultimately determines its fitness for a particular end use.

Globally, different standards have been adopted by different countries for water quality. For instance, since 2014 the United States of America Environmental Protection Agency (US EPA) has 121 organic contaminants in its list of priority contaminants and the European Union (EU) has 45 organic compounds in its priority contaminants watch list [7]. Both lists are currently undergoing review with additional compounds under investigation for inclusion. The South African Water Quality Guidelines (SAWQ) on the other hand listed only atrazine, phenol and trihalomethanes [6] as organic contaminants of concern. Therefore, emerging contaminants regulation in our water resources is being neglected. This is further compounded by the poor state of wastewater treatment facilities in South Africa which receive intensive agricultural runoff. The National Water Resource Strategy sets out the vision and strategic actions for effective water management which include the security of water supply, environmental degradation, and pollution of resources.

A database of contaminants in South African water resources would act as a one stop information hub where all available research outputs that have been identified would be available at the click of a button; building towards digital specimen banking. The contaminants, and all available scientific data would be recorded together with their prevalence and potential toxicology. Currently, there is no integrated database of information on contaminants in water resources anywhere in Africa. Therefore, information on research that has been conducted on contaminants is not readily available, hence identifying, collating, and bridging knowledge gaps is currently a challenge. This leads to duplication of expensive research efforts and, delayed response to pollution events where and when they occur. The aim of this paper is therefore to i) review contaminants that are of major concern in South Africa, ii) to integrate data into a geospatial map using open-source software, and iii) to provide information on the methodologies related to setting up a similar platform to other researchers. It is envisaged that such a database be expanded to cover information not only for South Africa but for the African continent and the globe.

2. Contaminants of emerging concern

Contaminants of Emerging Concern are contaminants that have previously not been present or at levels below detection limits but are now being detected in our water bodies. These can include nanomaterials, flame retardants, microplastics, agricultural chemicals and waste, microbial contaminants, heavy metals, pharmaceuticals and personal care products. The effects of these contaminants on the environment are becoming increasingly important [1,2], and the continued unregulated use of these products will lead to further ecological risks.

Emerging contaminants are released into the environment due to several anthropogenic activities ranging from industrial effluent discharges, storm water runoff, product lifecycle, pharmaceuticals and personal care products (PPCPs), as well as mining and agricultural emissions. Some of these contaminants are or could be carcinogenic, mutagenic, or disruptive to reproductive systems, have endocrine disrupting properties, bioaccumulative and/or persistent in the environment. Because of this, there is no consensus or an all-inclusive classification of CECs and a number of them could fit broadly into several categories of any single classification type. Living systems have developed protective, defensive, or adaptive mechanisms for minimizing exposure and toxicity of many of the otherwise harmful, naturally occurring chemicals. For biological systems which have never been exposed to CECs, their defensive or avoidance mechanisms are sometimes inadequate [4,8] The quantities and complexity of emerging chemicals in the environment and the toxicities of individual chemicals span an extraordinarily broad range [2], posing major challenges for regulatory bodies [3].

3. Information and Communications Technology: application development

At the conclusion of the twentieth century, significant breakthroughs in the field of Information and Communications Technologies, as well as the introduction and widespread use of the Internet, resulted in the Fourth Industrial Revolution (4IR) [9]. The use of 4IR technology has changed the way we access information, and shifted working environments, educational capabilities and how we are able to use technology to draw information [10]. The application developed can be found at http://www.ceckh.agric.za/ [to be unlocked after the launch in March 2023 as firewalls are currently in place]. By collating and repackaging current peer reviewed data, together with 4IR technology, the collected information on freshwater CECs could be displayed in a user-friendly online format that can be made available to researchers, stakeholders, and regulators to assist in developing environmental laws with the most recent scientific data. This access to information would not only reduce the possibility of duplication of research efforts but will assist in identifying gaps in the knowledge and greatly enhance research efforts by allowing for research collaborations amongst researchers in the same discipline.

3.1. *World Wide Web Geographical Information Systems (Web-GIS)*

3.1.1. *Web based GIS development*

In designing, developing, and implementing a new web-based GIS/spatial visualization tool, open-source software packages and technologies were used. This tool provides the ability to view the data in an online map and visually explore the data in a web browser without the need for additional software. In developing an entirely new spatial viewer the following advantages were gained: The final product closely suits its intended purpose, it is user-friendly, and does not require GIS expertise to use.

3.1.2. *Basic system design and software selection*

A web GIS (spatial data viewer) system that consists of a geodatabase, a map server, and a web viewer was the basis of the entire design (see Figure S1, Supporting Information). The other considerations were that the whole system should be built using only open-source software. No propriety software or licences would be required making it cheaper to maintain. Other considerations were that the web viewer should be easy to develop by any party who has coding capabilities and user-friendly for anyone with basic computer skills.

For the Geodatabase PostgreSQL (in combination with PostGIS)(https://www.postgresql.org/; https://postgis.net/) was chosen as the Database Management System (DBMS). This has a very powerful spatial support system that is built into the DBMSs, and from a spatial capabilities perspective, the PostgreSQL PostGIS combination has the widest range amongst opensource alternatives. GeoServer (https://geoserver.org/) was the only software considered for the map server. A map server enables the access of, and display of the spatial content of the geodatabase. It allows users to query and analyze the displayed data. The data stored in a table in the database can be viewed as a layer in the map via a webservice. In our case the data was converted to GeoJSON (https://geojson.org/) and then converted in a Web Map Service (WMS)(https://www.ogc.org/standards/wms) which the front end could utilize to display the data. The main design criterion for the software web viewer was that no additional software would be used for either processing or inputting the data into the GeoServer and that the user in a standard web browser can view the spatial data. OpenLayers JavaScript library and Ext and GeoExt javascript libraries were used for their ease of development of a professional looking web interface. Leaflet was eventually used as the JavaScript library of choice (https://leafletjs.com/). In this instance leaflet had the ability to spiderfy sample points that were causing a challenge where the same coordinates were displaying on top of each other in the map viewer and hiding data points from the visual mapping system available to the user.

3.2. *Use case considerations*

The basic use case is that a researcher enters sample data that is then processed to be viewed in web pages or the web GIS viewer. It is a web-based system with different modules that researchers use to upload specific information regarding CECs (an example of the Excel spreadsheet format developed between researchers and ICT is provided in the Supplementary info). Regular users can view CEC information contained in the site as printable information sheets, and also view information on how to avoid CEC pollution to find a laboratory for specific CEC analyses. To ensure responsible science communication, registered users can enter data either manually or via spreadsheets in addition to what unregistered users can do. This data is then processed and uploaded to a PostgreSQL instance running PostGIS extension and sent to an internal inbox for further approval by researchers. Once approved internally, the data is then served to the public as a map after being processed in the GeoServer. As the data moves from the MySQL instance to the PostgreSQL instance the Python script that is used to replicate this data from one DBMS to another and also does secondary quality checks (formatting and referencing) on the data before it is loaded into Postgres (see Figure S2, Supporting Information).

3.3. Final system design

The final system is setup as shown in Fig. 1 for both the client and background server side. This elaborates on the different technologies that are linked together and shows the flow of data from the different views in the system.

3.4. Web map design

The web map (Fig. 2) is divided into the four functional parts: (1) Links to other pages on the website which are divided into basic information sheets and resources, (2) Shows the layers in the interactive map and these can be toggled on and off as required by the user, (3) Main map view area shows the contaminant layers as well as context layers displayed in different colours per contaminant group and, (4) Legend of functional/contaminant layers per CEC grouping. Additional page design and functions are available in Supplementary Information (see Figure S3 and S4, Supporting Information).

4. Contaminants currently featured in the CEC Knowledge Hub

The current version of the CEC Knowledge Hub (November 2022) has highlighted gaps in the knowledge which include specific provinces such as the Northern Cape where no CEC data has been reported. Organic contaminants have been detected in all provinces except for the Free State. While currently microbial CECs are only reported in Limpopo, Mpumalanga, and KwaZulu-Natal. Microplastic data is spread across South Africa and can be found in most provinces. The collated information at present is made up of 590 data inputs; with the highest number of inputs is 302 found in pharmaceuticals and personal care products, followed by microplastics

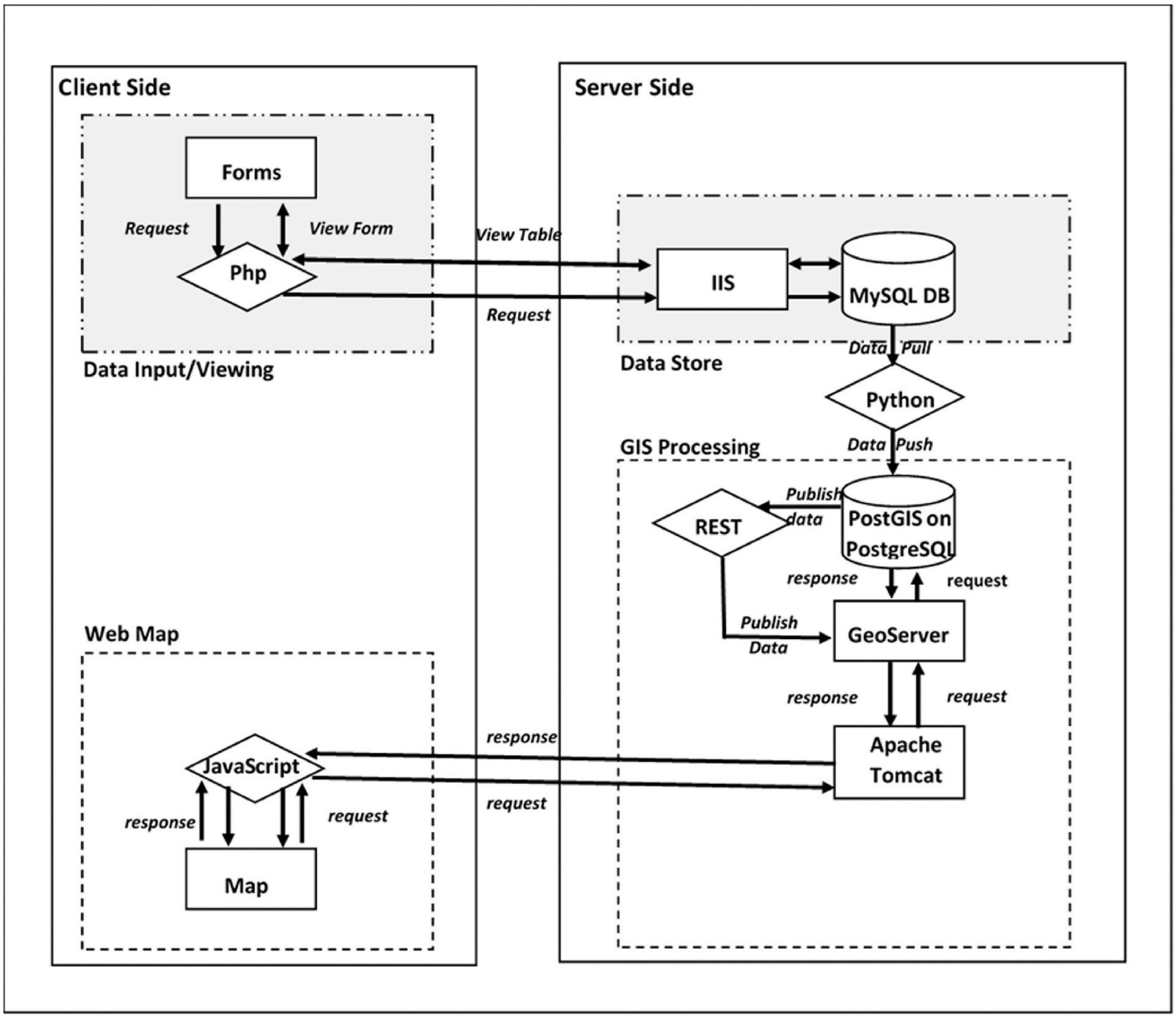

Fig. 1. The final system design flow and developed using open-source software for the contaminants of emerging concern Knowledge Hub.

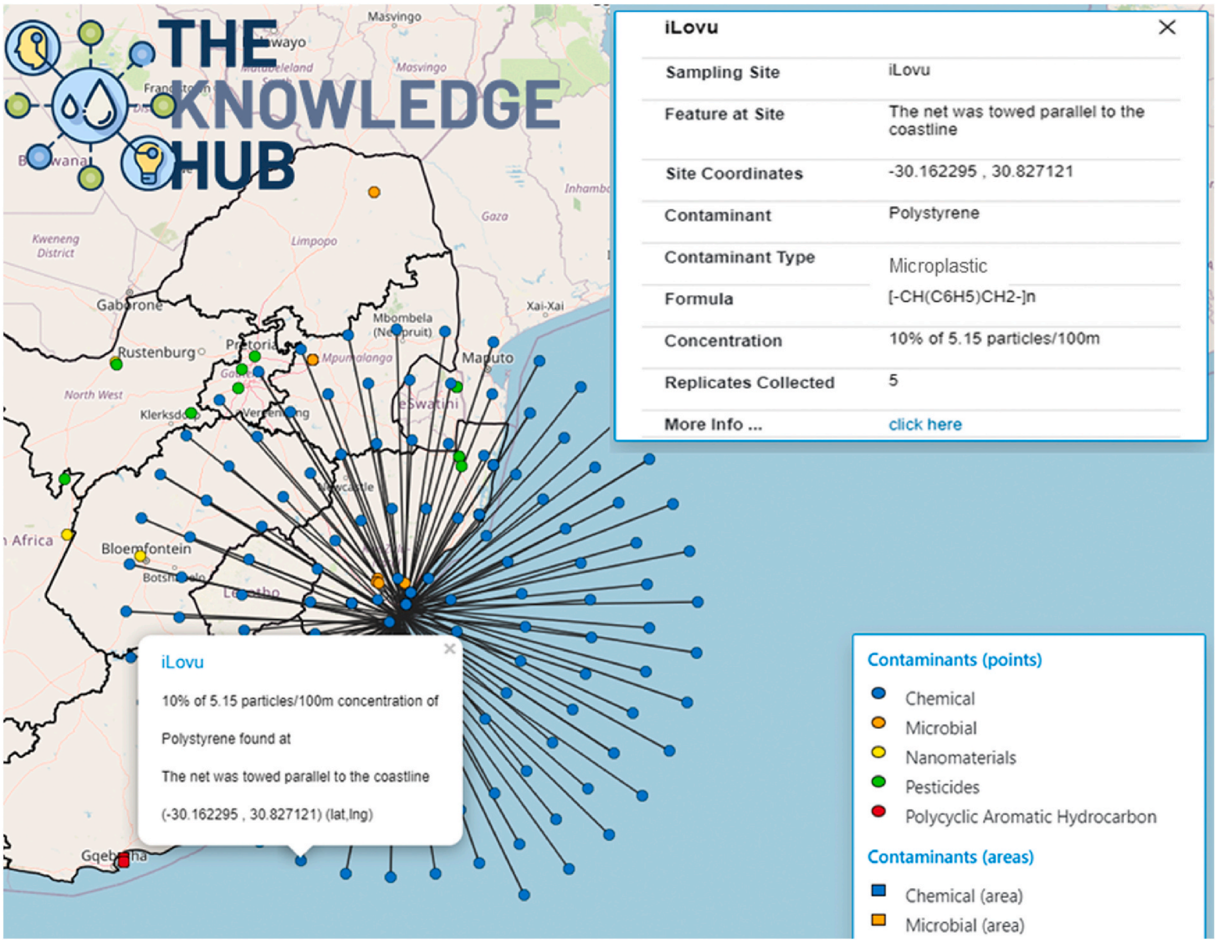

Fig. 2. Final map viewer of the CEC Knowledge Hub displaying the "spiderfied" sample points to avoid data overlap.

with 108 inputs while the remaining inputs of CECs range between 53 and 22 inputs, the least being nanomaterials with only four inputs. Specific information per contaminants class can be found in the following sections.

4.1. Organic contaminants

4.1.1. Alkylphenols and alkylphenol ethoxylates

Alkylphenols (APs) and their precursors, alkylphenol ethoxylates (APEs), are a group of synthetic chemicals used mainly as surfactants in detergents and cleaning products for domestic and industrial applications since the 1940s [11]. Other uses of APEs include additives to pesticide formulations as "inert ingredients" to enhance performance, in paper production, leather and textile processing, metalworking, as oil field chemicals and for dispersal of petroleum spills, and as ingredients in paints, adhesives, PCPs, and spermicidal lubricants. Globally, APEs are produced in excess of a million tons and thus classified as high production volume chemicals, the main toxicological concern is their potential to compete for the binding site of the natural estrogen receptor in vertebrates. These compounds are manufactured by reacting APs with ethylene oxide resulting in a molecule that consists of two parts: the AP and the ethoxylate (EO) moiety. This structure makes APEs soluble in water and helps disperse dirt and grease from soiled surfaces into water. The most commercially produced APEs are nonylphenol ethoxylates (NPEs), which account for 80–85% of all APEs produced in the USA (US EPA).

Based on literature, very few studies have been conducted in South Africa reporting the levels of APEs in surface waters; but concentrations assessed were all within the microgram per litre range. Farounbi and Ngqwala [12] reported NPs and OPs in the range of 0.031–2.55 μg/L and 0.0097–2.72 μg/L, respectively, in four major rivers of the Eastern Cape (Bloukrans, Buffalo, Swartkops and Tyume). The Vaal River and Jukskei River catchment areas, both in the Gauteng Province of South Africa, were well studied. The reported concentration range of the metabolites of APES in the Jukskei River Catchment Area were as follows: NP 0.38–9.35 μg/L [13]; NPEs 0.08–0.31 μg/L [11,12], nonylphenol monoethoxylate (NP-1EO) 0.044–0.73 μg/L [14], nonylphenol di-ethoxylates (NP-2EO) 0.13–0.94 μg/L [13], octylphenol penta ethoxylates (OPPEs) 0.31–6.01 μg/L [12,14] and octyl phenol ethoxylates ($OPnEO_3$) 60.1–92.7 μg/L [12]. The lack of published studies on the levels of APEs and their metabolites in freshwater in other provinces highlights an urgent need for more studies across South Africa.

4.1.2. Chlorinated paraffins

Chlorinated paraffins (CPs), also known as poly-chlorinated n-alkanes, are a class of industrial chemicals consisting of chlorinated straight-chain hydrocarbons, which have been widely produced since the 1930s. As a result of their thermal and chemical stability, CPs are frequently used as additives in cutting fluids, lubricants as well as flame retardants in sealants, leather and plastics [15,16]. As such, traces of CPs have been detected in several environmental compartments including freshwater and freshwater sediments, seawater, air, freshwater sediments, aquatic and terrestrial biota, marine mammals, human tissues and breast milk. Its ubiquity in nature is likely due to its array of uses as well as improper disposal methods of CP containing products [16]. Approximately 10 000 tonnes of CPs were produced per year in South Africa as reported in 2015 [17]. Whilst there is limited information on the biological effects, fate and levels of CPs in the environment, studies have indicated the possibility of carcinogenicity in humans and have identified target organs for toxicity to include kidneys, liver, the parathyroid and thyroid glands [18]. Coupled with mammalian toxicity, there have been suggestions that CPs are biomagnified and bioaccumulated in food webs [15]. In an aquatic environment, due to low water solubility and high carbon partition coefficients, CPs are adsorbed in sediment [19]. Therefore, most studies performed have focused on sediment, dust, and biological tissue as a source of these contaminants. This warrants further research into mechanisms of CP toxicity as well as monitoring and control in the environment. More focus on regulations to control CPs is also imperative due to the propensity of these chemicals to persist in the environment as well as their ability to undergo long-range environmental transport within aquatic ecosystems [18].

4.1.3. Current use pesticides

Pesticides are an extremely complex group of CECs due to their varied uses, distribution through different climate conditions, application methods and ability to enter the aquatic environment [20,21]. These contaminants are released into our water systems by runoff during rainstorms and air drift during spraying and once they are present, they can dissolve in soil but remain “relatively immobile” in water due to low solubility [22]. The risks associated with exposure include toxicity in fish, immobilization and possible death of untargeted insects and terrestrial animals [23]. Although there are pesticides that are being currently regulated in the country, there are many more that are not yet regulated nor monitored in freshwater. There is indeed a pronounced knowledge gap that still needs to be filled and prioritized for future research but there is also lack of regulatory standards for many of the pesticides. For example, in South Africa, DDT was banned for general use in 1974 but resumed in 2000 due to an increase in the incidence of malaria which is mainly transmitted along the upper border areas [24]. A study on the Luvuvhu River in Limpopo revealed concentration ranges below detection limit and also between 0.7 and 1.4 μg/L of p,p′-DDE and 1.1 and 7 μg/L ΣDDT [25]. However, since 2010 there are not many studies on DDT in freshwater due to low solubility and the high cost of analysis. Evidently, certain aspects of pesticides are receiving more attention and most studies focus on uptake in fish and sediment.

Twenty seven currently used pesticides which can be broken up into herbicides (namely Dimetachlor, Acetochlor, Metazachlor, S-Metolachlor, Alachlor, Diuron, Pyrazon, Chlorsulfuron, Simazine, Terbuthylazine, Atrazine, Metamitron, Metribuzin, Chlorotoluron and Isoproturon), Fungicides (namely Carbendazim, Prochloraz, Propiconazole and Tebuconazole) and Insecticides (namely Pirimicarb, Carbaryl, Azinfos-methyl, Dimethoate, Malathion, Chlorpyrifos, Fenitrothion and Terbufos) are listed in South Africa. A comprehensive report by Dabrowski [26] has categorized sixty-four pesticides of which 30% fell into a high risk and 23.4% fell into a medium risk category. The hazard potential (HP) can be ranked as follows: Ethylene-dibromide (HP- 92), Trichlorfon (HP- 100), Atrazine (HP- 68), Triadimenol (HP- 68), Tembotrione (HP- 64), Sulcotrione (HP- 64), Simazine (HP- 64), Cyproconazole (HP- 60), Carbofuran (HP- 60) and Imidacloprid (HP- 60).

Pyrethroid is commonly known as PYR or Pyrethrin and is produced from pyrethrums flowers (*Chrysanthemum cinerariaefolium* and *C. coccineum*) [27]. It is commonly used as a pesticide in agriculture and has been in use/production since 1977 for applications in the commercial agricultural market [28]. These compounds are known to cause ‘hyperexcitement’ in insects by attacking the voltage-gated calcium and voltage-gated chloride channels of their nervous systems [28]. Once they are present, they can partially dissolve and attach to soil sediments at shallow depth as they do not typically infiltrate into the groundwater table [29]. The risks associated with exposure include acute toxicity to aquatic inhabitants such as fish and other invertebrates [30]. Based on literature, a total of four studies have been performed of which five sites were selected in northern KwaZulu-Natal. The total PYR ranges detected in water were between 0.00006 and 132.88 μg/L [31] with the majority of the studies focusing only on water and its impact on human health and not so much on sediment accumulation and soil health. A recent study by Curchod et al. [20] detected 53 pesticide compounds in river water in the Western Cape, with 39% listed in farm spraying records while 23 discovered pesticides, mostly herbicides, were not previously listed. The study was performed during a drought period and found most of the two-week average pesticide concentrations to be less than 40 ng/L. The following insecticides at least once exceeded environmental quality standards (EQS): imidacloprid, thiacloprid, chlorpyrifos and acetamiprid their EQS 58-fold (EQS 13 ng/L), 12-fold (EQS 10 ng/L), 9-fold (EQS 0.46 ng/L) and 5-fold (EQS 24 ng/L) respectively and the herbicide terbuthylazine was 3-fold it’s EQS of 220 ng/L [20]. This further highlights the research need within pesticide usage as well as the urgent regulation updates.

4.1.4. Pharmaceuticals and Personal Care Products (PPCPs)

The production and use of consumer products are a major contributing factor to pharmaceuticals and personal care products (PPCPs) in our water bodies that are either not removed or chemically transformed throughout wastewater treatment processes [32]. Pharmaceuticals and personal care products are an intrinsic part of the human daily life and disposal of pharmaceuticals both by humans and in animal husbandry is on the increase. Pharmaceuticals are developed with the specific purpose of altering the physiology of the species (human or animal) [33], with the ultimate aim to improve health or growth. However, they could be very potent CECs in environmental matrices. Their presence and fate in the environment are not fully understood, although the last decade has witnessed a surge in research into the environmental impact of pharmaceuticals. This heightened research interest, coupled with improvements in available analytical technology and the capacity to detect these contaminants, even at very low levels, have revealed the extent of pollution of environmental matrices by PPCPs.

Research within South Africa on pollution of freshwater by PPCPs and their degradation products is limited considering the wide variety of possible contaminants in the group. Globally, South Africa is the country with the highest use of antiretroviral drugs per capita in the fight to control HIV/AIDS [34] and this is likely to result in increased release of these drugs through the sewage system. In the past decade, research has revealed a significant presence of pharmaceutical pollution in waterways. These include antiretroviral drugs in surface water sources across South Africa [34], nonsteroidal anti-inflammatory drugs (NSAIDs) along Umgeni and Msunduzi river sediments in KwaZulu Natal [35], antibiotics and analgesics river and sediment samples in Umgeni river/sediments and Hartbeespoort Dam [36]. Others include antipyretics and antibiotics in Msunduzi river in KZN [37,38]; analgesics/anti-inflammatory drugs in sludge of wastewater treatment plants (WWTPs) [39]. Archer et al. [40] detected 40 pharmaceuticals and PPCPs in a surface water source in Gauteng including antibiotics, NSAIDs, antihistamines, stimulants, anti-epileptics, anti-depressants, analgesics, medication for diabetics and hypertension, drug precursors, plasticizers, UV filters, parabens, x-ray contrast media and beta blockers. Targeted analysis in samples collected at rivers in the Eastern Cape (Buffalo, Bloukrans, Swartkops and Tyhume) revealed high levels of antibiotics (erythromycin −11.2 to 11 800 ng/L, clarithromycin −4.8 to 3280.4 ng/L, sulfamethoxazole −6.6 to 6968 ng/L), anti-epileptics (81.8–36 576.2 ng/L), and anti-inflammatory drug residues [41]. The presence of these compounds in South Africa surface waters is an indication of the fact that the WWTPs are not effective in removing these compounds during the sewage treatment process [39,42]. It is imperative to put in place regulations for the disposal of PPCPs to reduce/control the levels in the environment.

4.1.5. Polybrominated Diphenyl Ethers (PBDEs)

Polybrominated diphenyl ethers are a brominated flame retardant. Flame retardants are a functional class of a variety of chemical compounds that are added to certain manufactured products (such as furniture foam padding, wire insulation, draperies, upholstery rugs as well as plastic cabinets for televisions, personal computers and small appliances) in order to reduce the chances that the products will catch fire or slow the spread of fire. Flame-retardants are often categorized based on their chemical constituents such as whether they contain Chlorine, Bromine, Phosphorus, Nitrogen, metals or Boron. Brominated flame-retardants are most abundantly used and PBDE is a prominent brominated flame retardant. Polybrominated diphenyl ethers do not chemically bind with the products to which they are added; this enables their release from these products into air, water and soil during manufacture or throughout the product life and disposal. Fresh waterways are therefore vulnerable to receiving PBDEs when they are in proximity with heavily industrialised regions or when they are polluted with domestic and industrial wastes. Although information is limited about the production of PBDEs in African countries, many export products containing PBDEs [43].

Polybrominated diphenyl ethers have been in use since the 1970s when they came to replace the earliest flame retardants, polychlorinated biphenyls (PCBs), which were progressively banned in many countries due to their toxicity. The use of PBDEs is currently being scrutinized with countries such as the US and EU placing a complete or partial ban on their use and release into the environment [14]. In two sampling sites in the Eastern Cape, the concentration of $\sum$PBDEs detected in water samples from Sundays Estuary ranged from 2.5 to 39.1 ng/L and Swartkops estuary ranged from 2.5 to 168.8 ng/L [43]. Ohoro et al. [44] found a range of $\sum$PBDEs 30.1–785 ng/L in an estuary in East London, South Africa with different seasonal concentrations detected.

4.1.6. Polycyclic aromatic hydrocarbon (PAHs)

Polycyclic aromatic hydrocarbons are a class of ubiquitously distributed toxic organic compounds possessing two or more fused aromatic rings and they are persistent in the environment because of their hydrophobicity, low aqueous solubility, and stability of their aromatic ring structure. Depending on the number of aromatic ring, PAHs are classified as being low molecular weight (LMW), containing two or three rings or high molecular weight (HMW) containing four or more rings. The HMW PAHs being more persistent in the environment and more recalcitrant to being biodegraded [45,46]. Although naturally present in fossil fuels and produced during incomplete combustion of gasoline, diesel exhaust, asphalt, coal and coal tar, they are also generally produced from burning of organic compounds such as wood, refuse, smoked and barbecued foods while tobacco smoke contains a significant amount of PAHs [47,48]. They are usually introduced into freshwater systems by anthropogenic activities which include leakage (runoff) of mine wastewaters, industrial discharges and domestic wastes [45,48]. When PAHs react with oxidants such as NOx, O_3 and OH, they produce nitrated and oxygenated PAHs, which are attracted to atmospheric particulate matters and then find their way into aquatic environments as a fallout from rain [47].

Sixteen of the PAHs are prioritized and included in the European Union (EU) and United States Environmental Protection Agency (US EPA) priority list of contaminants. Currently reported are findings from three study sites in South Africa. The concentrations detected for each of the 16 priority PAHs ranged from no detection (bdl) to a high of 72.38 ± 9.58 μg/L [46,48,49]. Concentrations were found to be season-dependent with summer and autumn concentrations being consistently higher. Concentrations were also dependent on individual PAHs with many being below threshold values of regulatory bodies such as USEPA, SANS 241 and WHO but the sum total of the 16 priority PAHs was concerning [49].

4.1.7. Polyfluoroalkyl compounds (PFCs)

Polyfluoroalkyl compounds (PFCs) are man-made compounds with perfluorooctane sulfonate (PFOS) being the most studied among this class. These compounds are mostly used as surfactants and in oil and water repellents for fabric production applications as well is in chemical applications such as insecticides and firefighting foams. Hence, they are released to the environment via industrial applications and consequently become contaminants of emerging concern [50]. Their introduction into the market was validated in the 1940s, and eventually made their way to the environment infecting humans, domestic pets, and wildlife worldwide. Notwithstanding their fast-growing pace of environmental contamination, there is still limited knowledge on their extensiveness globally due to limited number of studies on PFOS, especially within Africa [51]. Therefore, extensive analyses need to be conducted for full understanding of the implications these compounds might have, since they are continuously released to the environment. Few studies have assessed perfluorooctanoic acid (PFOA) and PFOS levels in drinking water in South Africa but Mudumbi et al. [52] found PFOA (146–390 ng/L) levels to be higher than PFOS (23–182 ng/L) in river water in the Western Cape, and in some instances the levels were higher than that of the suggested levels in EPA drinking water guidelines [50]. While a South African-Belgium collaboration revealed that out of the fifteen PFCs assessed, thirteen PFASs were detected in water, sediment and biota samples in two estuaries in KwaZulu Natal, PFOA being detected in every sample. Perfluorooctanoic acid was found in high concentrations in all water samples with an average range between 171 and 258 ng/L in the Amatikulu and 711–788 ng/L in the Umvoti estuary [53]. While in the Vaal Dam a gradient decrease was seen in PFAS concentrations in water which ranged from <LOQ to 38.5 ng/L [54]. The main water source for the Kruger National Park, the Olifants River basin, however had PFASs levels all bdl (0.86 ng/L for PFOA, 0.73 ng/L for PFOS and 0.55 ng/L for PFNA) [55].

4.1.8. Triclosan

Triclosan known as TCS is commonly found in numerous households and agricultural antibacterial as well as antifungal products [56]. It has been in use/production since 1972 for applications in hospitals and other medical facilities but is now being applied in a wide range of consumer products such as soap, toothpaste, detergents, and pesticides [57]. These contaminants are released into our water systems by outflow from wastewater treatment plants, runoff, and domestic disposal [58] and once they are present, they can partially dissolve to form toxic compounds and metabolites. The risks associated with exposure include suspected possibility of being hormone disruptors and triggering antimicrobial resistance genes [59].

Based on literature a total of six studies have been performed, the ranges detected were between bdl and the highest at Bridle Drift Dam in the Eastern Cape (1264.2 ng/L) [60]. Other studies focused on wastewater treatment plants discharge in cities with only a few on rural settlements and hospitals with a focus on the release from PPCPs. There is currently a lack of studies on environmental and ecological impact of Triclosan in South Africa [61].

4.2. Inorganic contaminants

4.2.1. Heavy metals

Heavy metals (or trace elements) are metallic elements that usually have high density in comparison to water. Heavy metals such Cadmium (Cd), Chromium (Cr), Lead (Pb) and Mercury (Hg), are considered as potential hazardous elements and are considered CECs. These are mostly found in contaminated sites such as industrial effluents, water bodies and agro-ecosystems [62]. Some metals, in salt form, are highly soluble in aquatic environments and can be readily absorbed by aquatic organisms and transferred to humans through consumption. Heavy metal exposure can lead to adverse effects such as damage to the brain, kidneys as well as damage of developing foetuses, in some cases they may even be carcinogenic. However, there are safe limits of heavy metals allowable in water according to DWAF and WHO guidelines, and these levels are associated with low health risks in humans [63].

Some of these metals exceed the allowable levels in most of the investigated water research areas in South Africa but the rich geology and mining effects needs to be considered [64]. Hence, this calls for more concern for identification and quantification of such metals in South African water sources. According to Kinuthia et al. [63] toxicity levels of some selected metals for humans follows the sequence Co < Al < Cr < Pb < Ni < Zn < Cu < Cd < Hg. However, in the last decade, the heavy metals that have received increased attention are Cd, Hg and Pb. In a study on final effluent from WWTP in Cape Town, As and Cd levels in river water were within acceptable limits for human consumption but surpassed the requirements for aquatic life protection. In addition, Pb and Hg levels surpassed both human consumption and aquatic life sustainability standards [65]. In agriculture, while some of these heavy metals are essential plant nutrients at low concentrations, continued application with irrigation water can lead to accumulation to toxic levels for crops, or to animals consuming produce grown on these soils [66].

4.3. Particulate contaminants

4.3.1. Microplastics

Microplastics are plastic particles of <5 mm in diameter. Some of these particles are generated through degradation of larger plastic particles, some are introduced to the environment when plastic debris are carelessly disposed while others may arise as primary products (microbeads) [96]. Auta et al. [67] reported that microplastic contamination in the marine environment is caused by land activities. Non-functional waste management systems, poor infrastructure and ineffective regulations by legislative bodies have led to the introduction of microplastics in the aquatic environment through leaching from landfills, sewage leaks and effluents wastewater treatment plants [68]. The danger of microplastics is that they fit in the food range preferred by marine animals and thus, ingestion of microplastics by fish, mollusks, invertebrates and planktons is inevitable [69,70]. The large surface area of microplastics can cause higher toxicity as they can serve as adsorbents for other contaminants (e.g., pesticides, polyaromatic compounds and heavy metals) thus causing an organism to be exposed to a variety of contaminations in a single intake [71]. Mao et al. [69] reported that ingestion of microplastics by aquatic organisms leads to negative health implications because they cause inflammation and mineral deficiencies, disrupt reproductive abilities, and also reduce their food intake.

According to literature, at least twelve studies on microplastics were conducted in South African freshwater bodies. Five of which focused on the eastern coast sites, two in Orange and Vaal Rivers sites, two in Cape Town coast sites, two in Braamfonteinspruit site and the final one focused on all South African coast lines. Additionally, a scoping study by Bouwman et al. [72] sampled forty three freshwater sites across Gauteng and the North West Province and found microplastics in the range of 0.33–56 particles per litre, particle concentrations were extremely high in two sites, with 39 and 56 particles per litre, respectively. Fragments sizes were all <600 μm while fibres ranged between 20 μm and >1.5 mm. The main focus in the reviewed studies were classification of the microplastics and not identification of the polymer type due to technical difficulties. The microplastic pollution problem is still ongoing with no studies done on nanoplastics in South Africa to date.

4.3.2. Nanomaterials

Nanomaterials can be defined as materials possessing, at minimum, one external dimension measuring 1–100 nm. The definition given by the European Commission states that the particle size of at least half of the particles in the number size distribution must measure 100 nm or below (2011/696/EU). Nanomaterials can occur naturally, be created as the by-products of combustion reactions, or be produced for a specific application in industry as engineered nanomaterials (ENM). Nanomaterials usually have different physical and chemical properties compared to their bulk counterparts [73,74].

Nanomaterials can be produced as very thin surface coatings (one dimension), or as nanowires and nanotubes (two dimensions) or in three dimensions as nanoparticles [75]. By developing nanotechnology ENMs can be used to make long-lasting and better performing materials which exploit the unique properties present at the nanoscale. Medical uses of nanomaterials include diagnostic products, optical imagery enhancement and *in vivo* drug delivery vectors [74]. Due to their wide range of uses, nanomaterials have the potential to be released into the environment during any or all stages of the production process, from release during synthesis to the end of product life. Once these ENMs are released into the environment (determined by the product itself) they are able to interact with environmental media in which they aggregate, lightly bind to with suspended solids or sediment, or become ingested or accumulated by organisms and enter drinking water and food sources [76]. The fate of ENMs depends on their characteristics and the characteristics of the environmental partition they are released in to. Characteristics which can affect the fate of ENMs include size, surface charge, functional groups, and particle composition (metal or an organic). Therefore, by altering one part of the ENM they can react differently in the environment and have different toxicity. As the production of ENMs increases, human and environmental exposure to ENMs is also expected to increase [77].

Scientific authorities acknowledge that nanotechnology risk assessment is a considerable challenge, since monitoring diverse ENMs being produced, and their consequent impact is very difficult to track [78]. It was estimated that by 2020 the total amount of industrial nanomaterials was expected to increase from 1000 to 58,000 tons. This makes the release of nanomaterials during production a major concern [79]. A study by Maiga et al. [97] assessed ENM, titanium dioxide, in five rivers systems across five provinces and found a size range between 118.68 and 168.04 nm in size while the concentration range varied greatly (14.84–243.94 μg/L) with North West Province having the highest and Western Cape having the lowest concentration. In South Africa, a research platform was established by The Department of Science and Innovation in 2016 to investigate the environmental, safety and health related aspects of nanotechnology.

4.4. Biological contaminants

4.4.1. Microbiological CECs

Microbial contaminants of concern in environmental water bodies range from pathogenic viruses, bacteria and protozoa to cyanobacteria and helminths [80]. Microbial contaminants are introduced into waterways from several sources, including veterinary, domestic, agricultural as well as industrial sources [81] and once present have the potential to infect humans and animals, and may induce waterborne disease outbreaks. The ability of waterborne microbial contaminants to cause significant health risks warrants their careful monitoring and control [82].

Studies on microbial contaminants in South African waterways have predominantly centered on indicators of fecal contamination such as coliforms e.g., *Escherichia coli* [83–85]. Such indicator organisms have historically been utilized to assess fecal contamination of waterways. Unfortunately, this approach doesn't sufficiently address the challenge of CEC in the waterways. However, the need for continual testing of waterways for such organisms is imperative as an epidemiological link has been established between contact with fecal contaminated water and gastro-intestinal diseases. More so, the increased utilization of wastewater sources for irrigation purposes, due to the drive towards sustainable development, contributes to the risk of coliform contamination of food sources and downstream waterways.

Other enteric pathogens of bacterial, viral and parasitic origin can also be found in water [84]. Such emerging pathogens have often-times adapted strategies to evade antimicrobial agents and disinfectants that are utilized for conventional water treatment processes for the removal of coliforms. Hence, the presence of emerging pathogens, even when no coliforms are detected in a sample, is frequently being observed [86]. Emerging contaminants that are gaining rapid attention due to their ability to thrive within water distribution systems include opportunistic pathogens, antibiotic resistant bacteria, antibiotic resistance genes, metal resistance genes as well as free-living amoebae. These microbial CECs often-times have no link to fecal indicator bacteria-based standards [87,88].

Whilst limited reports have been published on such microbial CECs in South Africa, a few recent South African studies have reported on the use of advanced molecular methods such as Next Generation Sequencing (NGS) to reveal the plethora of potentially pathogenic microbes in several waterways without restricting results to cultivable microorganisms [89,90]. Such methods enable the detection of potential microbial contaminants of emerging concern such as pathogenic microbes belonging to the genera *Acinetobacter*, *Clostridium*, *Legionella*, *Pseudomonas, Tatlockia* and *Serratia* [89]. A significant research gap in SA still exists on the effect of aquatic contaminants on the shaping of microbial community structure, diversity and ecological function. For instance, several studies have highlighted the positive correlation between heavy metal pollution and the selection for antibiotic resistance genes [90,91,92]. Antimicrobial resistant organisms have been identified as a CEC in general since antimicrobial resistance in human pathogenic microorganisms forms a major public health concern [87,88] and these bacteria are thereafter able to persist under adverse conditions [93].

Technological advances including molecular tools such as qPCR enable the routine tracking of antibiotic resistant bacteria in environmental matrices [94]. Moreover, such tools are particularly valuable since they enable quantification of specific antibiotic resistance genes which in turn facilitates correlations between such genes and chemical CECs e.g., heavy metals and antibiotics. These correlations may aid in evaluating the influence of chemical CECs on shaping antimicrobial resistance which would direct mitigation strategies [95]. As such techniques evolve, they may become more cost effective for use in environmental monitoring [94].

4.4.2. Challenges and conclusions

The development of a South African based CEC Knowledge Hub has been critical in securing a digital specimen bank of acquired contaminant data. Although current data already gives an indication of where the most research has taken place and has raised areas of concern in South Africa, it's strength will improve as more information is added to the Hub. Challenges in the future would be to ensure that researchers upload data, and the ease of bulk imports will determine their willingness to do so. Responsible science communication is imperative and skilled researchers are required to evaluate and interpret information displayed due to seasonal variations in data and detection methods used which could be a limitation. Foreseen ICT challenges are that a virtual machine was used as servers were being upgraded therefore the Hub is currently running on AMD processors which are not ideal for graphic intensive processes that the Geoserver demands. In future developments switching to an Intel processor setup would be ideal as Intel server rated processors have built in graphical processing units (GPU) which share the load off the main CPU making the whole system faster and more powerful.

Author contribution statement

Tarryn Lee Botha: conceived and designed the experiments; performed the experiments; analyzed and interpreted the data; contributed reagents, materials, analysis tools or data; and wrote the paper.

Emomotimi Bamuza-Pemu; Ashira Roopnarain; Busiswa Ndaba; Ntebogeng Mokgalaka; Maryam Bello-Akinosho; Rasheed Adeleke; Michael van der Laan; Phedisho Mphahlele; Fanelesibonge Vilakazi; Penny Jaca; Eunice Ubomba-Jaswa: analyzed and interpreted the data; contributed reagents, materials, analysis tools or data; and wrote the paper.

Zibusiso Ncube; Gert De Nysschen; Akani Mushwana: contributed reagents, materials, analysis tools or data; wrote the paper.

Funding statement

Emomotimi Bamuza-Pemu was supported by Water Research Commission [2021/2022-00256].

Data availability statement

Data will be made available on request.

Declaration of interest's statement

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.

Acknowledgements

The authors wish to thank Hunted Wolf Design for assistance with logo design. We would further like to thank the Agricultural Research Council, Tshwane University of Technology, the University of South Africa and North-West University for all administrative assistance and student support.

Appendix A. Supplementary data

The Supplementary Information contains additional information in the development of the CEC Knowledge Hub. Supplementary data related to this article can be found at https://doi.org/10.1016/j.heliyon.2023.e13007.

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Update

Heliyon

Volume 9, Issue 3, March 2023, Page

DOI: https://doi.org/10.1016/j.heliyon.2023.e14083

Heliyon 9 (2023) e14083

Contents lists available at ScienceDirect

Heliyon

journal homepage: www.cell.com/heliyon

Corrigendum

Corrigendum to "Development of a GIS-based knowledge hub for contaminants of emerging concern in South African water resources using open-source software: Lessons learnt" [Heliyon 9 (1) (January 2023) Article e13007]

Tarryn Lee Botha [a,b,*], Emomotimi Bamuza-Pemu [c], Ashira Roopnarain [d], Zibusiso Ncube [d], Gert De Nysschen [d], Busiswa Ndaba [d], Ntebogeng Mokgalaka [e,f,k], Maryam Bello-Akinosho [g], Rasheed Adeleke [h], Akani Mushwana [d], Michael van der Laan [i,j], Phedisho Mphahlele [d,k], Fanelesibonge Vilakazi [d,h], Penny Jaca [l], Eunice Ubomba-Jaswa [l]

[a] *Institute for Nanotechnology and Water Sustainability, College of Science, Engineering and Technology, University of South Africa, Florida Science Campus, 1710, South Africa*
[b] *Water Research Group, Unit for Environmental Sciences and Management, North-West University, Private Bag X6001, Potchefstroom, 2520, South Africa*
[c] *OptimalEnviro, Postnet Suite 073, Private Bag X21, Queenswood, Pretoria, 0121, South Africa*
[d] *Microbiology and Environmental Biotechnology Research Group, Agricultural Research Council – Natural Resources and Engineering, Pretoria, South Africa*
[e] *University of Pretoria, Mamelodi Campus, Private Bag X20, Hatfield, Pretoria, 0028, South Africa*
[f] *Tshwane University of Technology, Faculty of Science, Department of Chemistry, Private Bag X680, Pretoria, 0001, South Africa*
[g] *Pathogenic Yeast Research Group, Department of Microbiology and Biochemistry, Faculty of Natural and Agricultural Sciences, University of the Free State, PO Box 339, Bloemfontein, 9300, South Africa*
[h] *Unit for Environmental Sciences and Management, North-West University, South Africa*
[i] *Agricultural Research Council (ARC) – Natural Resources and Engineering, Private Bag X79, Pretoria, 0001, South Africa*
[j] *Department of Plant and Soil Sciences, University of Pretoria, Private Bag X20 Hatfield, Pretoria, 0028, South Africa*
[k] *Department of Chemistry, Tshwane University of Technology, Private Bag X680, Pretoria, 0001, South Africa*
[l] *Water Research Commission, Lynnwood Bridge Office Park, Bloukrans Building, 4 Daventry Street, Lynnwood Manor, Pretoria, 0081, South Africa*

In the original published version of this article, the author contribution statement is inaccurate. **Here is the current statement:**

Tarryn Lee Botha: conceived and designed the experiments; performed the experiments; analyzed and interpreted the data; contributed reagents, materials, analysis tools or data; and wrote the paper.

Emomotimi Bamuza-Pemu; Ashira Roopnarain; Busiswa Ndaba; Ntebogeng Mokgalaka; Maryam Bello-Akinosho; Rasheed Adeleke; Michael van der Laan; Phedisho Mphahlele; Fanelesibonge Vilakazi; Penny Jaca; Eunice Ubomba-Jaswa: analyzed and interpreted the data; contributed reagents, materials, analysis tools or data; and wrote the paper.

DOI of original article: https://doi.org/10.1016/j.heliyon.2023.e13007.

* Corresponding author. Institute for Nanotechnology and Water Sustainability, College of Science, Engineering and Technology, University of South Africa, Florida Science Campus, 1710, South Africa.

E-mail addresses: 26964546@nwu.ac.za, tarrynb@uj.ac.za (T. Lee Botha).

https://doi.org/10.1016/j.heliyon.2023.e14083
Received 21 February 2023; Accepted 21 February 2023
Available online 5 March 2023
2405-8440/

Zibusiso Ncube; Gert De Nysschen; Akani Mushwana: contributed reagents, materials, analysis tools or data; wrote the paper.

Here is the correct author contribution statement:

Tarryn Lee Botha; Emomotimi Bamuza-Pemu: Conceived and designed the experiments; performed the experiments; analyzed and interpreted the data; contributed reagents, materials, analysis tools or data; wrote the paper.

Ashira Roopnarain; Busiswa Ndaba; Ntebogeng Mokgalaka; Maryam Bello-Akinosho; Rasheed Adeleke; Michael van der Laan; Phedisho Mphahlele; Fanelesibonge Vilakazi; Penny Jaca; Eunice Ubomba-Jaswa: performed the experiments; analyzed and interpreted the data; contributed reagents, materials, analysis tools or data; wrote the paper.

Zibusiso Ncube; Gert De Nysschen; Akani Mushwana: contributed reagents, materials, analysis tools or data; wrote the paper.

The authors apologize for the errors. Both the HTML and PDF versions of the article have been updated to correct the errors.

Declaration of interests statement

The authors declare no conflict of interest.