Research article

Water Reuse: A Risk Assessment Model for Water Resources

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Abstract.
The increasing demands for water for multiple purposes combined with climate change challenges are leading to water scarcity and quality deterioration. Portugal is vulnerable to the impacts of climate change and therefore, the use of reclaimed waters has been identified as a suitable alternative water source for non-potable uses, such as irrigation, to overcome water shortages. In the last two years, new policies for water reuse have been approved at the Portuguese and European levels. The legal frameworks are supported in the international guidelines developed by the International Organization for Standardization, namely for irrigation, urban uses and health risk assessment. In this way, all reuse projects must follow a fit-for-purpose approach, i.e., the water quality needs to meet the requirements of its specific end-uses without compromising public health or the surrounding environment, and all reuse projects must conduct a risk assessment for health and the environment. Quantitative, qualitative or semi-quantitative models can be used. Although a quantitative assessment may be desirable, these models tend to be complex and present high uncertainty. Furthermore, these usually require extensive data which are often not available. Accordingly, this study intended to develop a conceptual model to deal with the risk assessment for water resources, namely surface and ground waters. A semi-quantitative approach was employed for the risk characterization, using empirical qualitative judgment to assess the relative importance of hazards, exposure routes, scenarios and barriers in place. The use of a strategic assessment allows the quality standards that meet the needs of each project to be validated. The developed model was applied to a case study to illustrate its applicability.

Keywords: water reuse, water resources, risk assessment, semi-quantitative model, compounds of emerging concern

1. Introduction

The increasing demands for water resources for multiple purposes such as public water supply, agriculture, industry, recreational uses and others are leading to water scarcity and quality deterioration. The intensification of severe weather conditions due to climate change, such as droughts, and urban development has put a significant strain on freshwater supplies [1]. Therefore, the search for new alternative water sources like reclaimed waters is rising in several countries, such as the United States of America,
Singapore, Australia, Spain, Malta, Cyprus, and even in Portugal [1-3]. However, the use of treated wastewaters may pose some risks, where microbial risks are usually the main focus to protect human health, but other aspects are also catching attention, in particular, disinfection by-products (DBP) and compounds of emerging concern (CoC) which can pose risk to water resources and aquatic ecosystems and through these to humans [2-4].

The current policies in the European Union for the use of reclaimed water for agriculture irrigation (Regulation EU 741/2020) and in Portugal for multiple uses (Decree-Law 119/2019, 21st August) emphases on the adoption of projects supported on a risk management framework and in quality standards defined according to a fit-for-purpose approach, based on ISO standards 16075. This approach is supported on the production of water quality that meets the needs of the intended end-users. Accordingly, the European and Portuguese policies establish that all projects shall follow a risk assessment for human health and to the environment, which includes water resources. This type of appraisal will allow to select the quality standards applicable to each reuse project and the risk management conditions that should be followed to ensure an associated minimum risk value [3]. For health risk assessment were already developed several qualitative, semi-quantitative and quantitative methods, but for water resources, the most popular methods are based on complex mathematical models to assess pollutants fate and transport on environmental compartments or to evaluate hydrological conditions [5]. In the quantitative methods, the risk characterization is usually based on the ratio between the predicted environmental concentrations (PEC) and the predicted no-effect concentration (PNEC) for water, sediment, and biota. However, this type of methodology presents several limitations, such as the use of standardized bioassays involving single species and unique substances, without taking into account the real routes of exposure and the effects of mixtures and large uncertainties in extrapolating data across doses, species, and life stages, namely due to the lack of data on dose-response relationships [6]. Hence, these type of approaches requires the existence of a significant number of monitoring data from reuse projects to establish the predicted concentrations associated with each exposure scenario, since in this practice no direct discharge to water occurs, which limits the applicability of these methodologies to water reuse projects. Consequently, the quality criteria applied to a certain project are usual flat legal requirements without taking into account local conditions, such as water bodies characteristics, status, and uses of surface and groundwaters.

However, the use of knowledge-based models already showed its feasibility and applicability with simple outputs that may provide support for environmental authorities
on the decision-making process [5, 7]. Taking into account these considerations, this study aims to propose the development of a semi-quantitative model to perform water reuse risk characterization for water resources, including surface and groundwater, and demonstrate its suitability to validate the quality standards for chemical parameters, like nutrients (N and P), DBP and CoC, to be applied to a water reuse project and to be noted in the water reuse permits issued by environmental authorities [5, 7-9]. The proposed model is a site-specific assessment, supported on the typical tier approach including hazard identification, exposure and pathway assessment, and risk characterization [6].

2. Methodology

The proposed model was supported on a previous conceptual model developed by Rebelo et al., named Risk Assessment Model for Water Resources (RAMWR) and the ISO 16075-2:2020 and all factors are measured according to an importance scale from 1 to 9 [3,7]. The model proposed the risk determination by the product between hazard, the vulnerability of water resources and damage.

The hazard identification, within the scope of the current study, is nutrients (nitrogen and phosphorous) and chemicals, such as DBP, CoC, and priority substances/priority hazardous substances or specific pollutants classified according to the Directive 2000/60/EC, usually known as Water Framework Directive (WFD). The classification of hazards, as can be seen in table 1, is made according to its characteristics, treatment level, and expected concentrations in reclaimed waters. For nutrients the used criteria are the treatment level, the legal classification of water bodies in terms of sensibility to eutrophication (Directive 91/27/EEC) and vulnerability due to nitrates pollution (91/676/EEC) and the ecological status of water bodies (when the concern parameters are N or P). For chemicals, the classification is made according to expected concentration, which can derive from monitoring data or from a proposal of a quality standard to write on a permit.

| Nutrients | Chemicals in water bodies | Hazard |
|-----------|---------------------------|--------|
| Treatment level | Units of concentration | Hazard level |
| Without N and P removal | N & P (mg L⁻¹) | >EQS² or >30 LoQ³⁴ | 9 |
| With partial removal of N or P | N ≤ 15 or P ≤ 3 | >10 LoQ⁴ | 7 |
| With partial removal of N or P | N ≤ 15 or P ≤ 3 | >LoQ | 5 |
| With partial removal of N and P | N ≤ 10 and P ≤ 3 | >LoD⁵ | 3 |
| With advance removal of N and P | N ≤ 5 and P ≤ 0,5 | <LoD | 1 |
1 In vulnerable areas to nitrate pollution or when water body status is less than "Good" due to parameter N, consider Hazard for N equal to 7 and for P equal to 5; In sensitive areas to eutrophication or when water body status is less than "Good" for parameter P, consider Hazard for N equal to 5 and for P equal to 7.

2 EQS – Environmental quality standard (legal value) applicable to water bodies according to its status or uses

3 LoQ – Limit of quantification of the applicable analytical method

4 Relationship established according to [10]

5 LoD – Limit of detection of the applicable analytical method

The pathway assessment considers runoff to surface waters and infiltration, leaching and percolation to groundwaters. The vulnerability of water resources ($V_{WR}$) is given by equation 1:

$$V_{WR} = V_{p\text{-GW}} \times f_{p\text{-GW}} + V_{p\text{-SW}} \times f_{p\text{-SW}}$$ (1)

Where $V_{p\text{-GW}}$ and $V_{p\text{-SW}}$ are partial vulnerabilities directly achieved by Figure 1 and $f_p$ are partial factors equal to $f_{p\text{-SW}} = V_{p\text{-SW}}/(V_{p\text{-SW}} + V_{p\text{-GW}})$ and $f_{p\text{-GW}} = V_{p\text{-GW}}/(V_{p\text{-SW}} + V_{p\text{-GW}})$, developed according to the same principles proposed by other authors [7].

From equation 1 is possible to obtain four different values which are prioritized through the importance scale according to table 2.

| Infiltration rate to groundwater | None | Low | Medium | High |
|----------------------------------|------|-----|--------|------|
| Groundwater Sensitivity          |      |     |        |      |
| Shallow aquifer with no protection | I    |     |        |      |
| Deep aquifer with clay protection | II   |     |        |      |
| Deep aquifer with significant clay protection | III  |     |        |      |
| No aquifer with hydrological continuity to the area | IV   |     |        |      |
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| Sensitivity to surface water     | IV   | III  | II    | I    |
| Surface runoff                   |      |      |       |      |

**Figure 1:** Matrix for surface and groundwater vulnerability assessment (adapted from ISO 16075-1:2020).

From the exposure evaluation of water resources is possible to determine through equation 2, the global vulnerability ($V_G$).
Table 2: Water resources vulnerably expressed in importance factors.

| Values for $V_{WR}$ given by equation 1 | N & P (mg L$^{-1}$) |
|----------------------------------------|---------------------|
| 5.2                                    | 9                   |
| 5.0                                    | 7                   |
| 4.0                                    | 5                   |
| 3.3                                    | 3                   |

$$V_G = V_{WR} \times \frac{\sum f_i \, \text{barrier}}{f_{\text{max}} \times n_{\text{Scen}}} \quad (2)$$

Where $f_{\text{barrier}}$ is the factor applicable to barriers according to table 3, where $f_{\text{max}} \times n_{\text{Scen}}$ is a normalization factor, to adjust the scale to a common range [11], where $n_{\text{Scen}}$ is the number of scenarios given by table 4 and $f_{\text{max}}$ is the maximum value of the used importance scale (9). The number of exposure scenarios depends on the barriers in place since a barrier is a mean that reduces or prevents the exposure of the receiving waters to the reclaimed waters [8,9]. In this study, the proposed barriers were adopted from Rebelo et al. and the number of exposure scenarios is displayed in table 4 [3,7].

Table 3: Applicable barriers for water resources protection

| Type of barrier                                           | Importance factor |
|-----------------------------------------------------------|-------------------|
| Absence of barriers                                      | 9                 |
| Leak detection system                                     | 7                 |
| Partial retention capacity/irrigation system according to water crop needs | 5                 |
| Total retention capacity                                  | 3                 |

Table 4: Number of exposure scenarios according to barriers in place.

| Type of barrier                                           | Number of exposure scenarios ($n_{\text{Scen}}$) |
|-----------------------------------------------------------|-----------------------------------------------|
| Absence of barriers                                      | 1                                             |
| Leak detection system                                     | 1                                             |
| Partial retention capacity/irrigation system according to water crop needs | 1                                             |
| Total retention capacity                                  | 1                                             |
| Leak detection system Partial retention capacity and irrigation system according to water crop needs | 2                                             |
| Leak detection system and total retention capacity        | 2                                             |

The final step to determine the risk is the definition of damage which can be attained by the severity of damage versus the likelihood of occurrence of failure in barriers (which also translates the likelihood of exposure occurrence). According to the ISO 20426:2018, a certain likelihood of exposure occurrence can be defined depending on data availability as can be seen in table 5.
Table 5: Likelihood of occurrence of water resources exposure to contamination (adapted from ISO 20426:2018).

| Likelihood of occurrence | Observations according to evidence (from other irrigation projects) and/or literature | Value |
|--------------------------|------------------------------------------------------------------------------------|-------|
| Unlikely                 | Has not happened in the past but may occur in exceptional circumstances in the reasonable period | 2     |
| Possible                 | May have happened in the past and/or may occur under regular circumstances in the reasonable period | 3     |
| Likely                   | Has been observed in the past and/or is likely to occur in the reasonable period | 4     |
| Almost certain           | Has often been observed in the past and/or will almost certainly occur in most circumstances in the reasonable period | 5     |

The reasonable period is defined according to the validity period of reuse permits as mentioned in the Portuguese legislation, i.e., 10 years (Decree-Law 119/2019, 21st August). The severity of damage depends on the characteristics of the receiving water resources, namely its classification according to existent legislation (e.g., sensitive areas according to the Directive 91/271/EEC), status of the water body according to the WFD and the respective existing uses (e.g., drinking waters). This correlation is presented in Table 6:

Table 6: The severity of damage for water resources from exposure to contamination.

| Severity of damage | Observations according to water resources evidence | Value |
|--------------------|--------------------------------------------------|-------|
| Severe             | Water body with status less than good            | 5     |
| Major              | Water body in good status, with defined use and classification (vulnerable to nitrate pollution or sensitive area) | 4     |
| Moderate           | Water body in good status, with defined use or classification (vulnerable to nitrate pollution or sensitive area) | 3     |
| Minor              | Water body in good status, without defined use or classification (vulnerable to nitrate pollution or sensitive area) | 2     |

The partial damage ($d_i$) associated with the exposure routes and exposure scenarios considered is given by the matrix presented in Figure 2, by combining the values obtained in Table 5 with the data from Table 6. The global damage ($D$) can be calculated by equation 3:

$$D = \sum_{i} d_i x n_{Scene} f_{max} x n_{Scene}$$

Where $n_{Scene}$ is the number of exposure scenarios from Table 4 and $f_{max} x n_{Scene}$ is a normalization factor similar to equation 2.

The risk for water resources ($R_{WR}$) is achieved by the product between the hazard ($Hz$), the global vulnerability ($V_G$), and associated damage ($D$), normalized to the maximum value of importance scale (9), i.e.:

$$R_{WR} = \frac{Hz x V_G x D}{f_{max}} = \frac{Hz x V_G x D}{9}$$
The $R_{WR}$ value varies from a minimum value above zero (0) to nine (9) depending on the number of scenarios, barriers and the characteristics of water bodies. The prioritisation is accomplished by conversion of the $R_{WR}$ results into a three-level qualitative scale as follows: Despicable Risk ($R_{WR} < 3$), Acceptable Risk ($3 \leq R_{WR} < 7$), and Unacceptable Risk ($R_{WR} \geq 7$), similar to descriptions used by other authors [3, 7]. When the risk presents an unacceptable, the process should be repeated considering additional minimization measures, such as additional barriers or increase of treatment level and as a result a lower level of hazard (Hz), which means a proposal for a quality standard more restricted. Nevertheless, a project may not be viable if it is not possible to below the $R_{WR}$ at least to an acceptable level. Similar to other risk management options, the proposed methodology follows a strategic appraisal where a reassessment will allow defining the best management options [3, 7, 12]. Whenever possible, the risk level should be despicable although some projects may be approved with an acceptable risk if supported on the evidence that further reduction would be highly disproportionate to the benefit gained.

### 3. Results and discussion

The model was applied to a casestudy, a golf course that intends to reuse water for irrigation. The course is located in an area classified as vulnerable to nitrate pollution. The hydrogeological conditions determine that is a local with a high infiltration rate for groundwater and there is an aquifer with some clay protection, in the area of the sports field. The aquifer is also classified as a strategic reserve for public water
supply. Both surface and groundwater present Good Status according to the River Basin Management in force. The effluents treatment level in place is a secondary plus disinfection (UV), and according the monitoring data, from the European Pollutant Release and Transfer Register, the treated wastewaters also present an annual average below the limit of quantification for Di(2-ethylhexyl)phthalate (DEHP). The methodology was used to define the quality standards to be applied to nitrogen and DEHP and the possible needs of additional treatment, taking into account that no barriers are in place.

From the above description is possible to define Hazard (Hz) level for DEHP, which is equal to three (3), and for nitrogen, since no nutrient removal is in place, the $H_z$ level is nine (9). The hydrogeological description allows to understand that partial vulnerabilities for surface and groundwaters ($V_{pSW}$ and $V_{pGW}$) are 2 and 6, respectively. By the application of equation 1 and table 2, is possible to obtain a value of seven (7) to the $V_{WR}$. The absence of barriers determines a $f_{barr}$ that matches the maximum level of importance (9) and a single scenario of exposure, leading to a global vulnerability value equal to seven (7). In the same way, the absence of barriers determines an “almost certain” likelihood of exposure occurrence, which translates to a value of five (5). The water body as mentioned presents a good status, has a defined use since is a reserve for drinking waters, and is also classified as vulnerable to nitrate pollution, which determines the severity of damage with a major level with a value of four (4). Therefore, the partial damage ($d_i$) reveals a value of nine (9) and the global damage will then be equal to one (1). All results are presented in table 7 where is possible to see that for the considered hazards (DEHP and N), the risk assessment reveals a despicable level for DEHP (2,3) and an unacceptable level for nitrogen (7,0). Consequently, in terms of DEHP the risk level defines that there is no need to establish a quality standard for this parameter. However, for nitrogen, an increase of treatment level could be desirable. A definition of a quality standard level equal to or below 5 mg L$^{-1}$ will result in a despicable risk while standard equal to or below 15 mg L$^{-1}$ will promote an acceptable risk. However, the final solution should be adopted based on a nitrogen balance study, since not all the nitrogen in the reclaimed waters is immediately available for consumption by the crop, namely the organic fraction will only be accessible after the mineralization process, which not only depends on the treatment level but also the retention time in the storage system. Hence, besides the previous risk assessment, the final quality standard to be defined should take into account the maximum amount of nitrogen from reclaimed waters that can be adsorbed by the crop (grass and other ornamental crops on the golf course) to minimize the use of synthetic fertilizers [13].
If a post-chlorination is proposed, the use of DBP formation models can also be used to predict possible risk levels for these types of pollutants [14]. For instance, using the model developed by other authors [14], the use of a typical chloride dose of 5 mg L\(^{-1}\) and a reaction time between 5 to 15 min will induce a formation of trichloromethane from 3.7 to 4.6 µg L\(^{-1}\), above the EQS of 2.5 µg L\(^{-1}\), previewed on the Directive 2008/105/EC and 2013/39/UE. These results reflect a Hz of maximum level and, thus, an unacceptable risk. However, it is quite common the use of a LoQ for this substance below 5 µg L\(^{-1}\), and real sampling results may result in a despicable risk. Thus, special attention should be paid to LoQ and EQS when results are displayed as below LoQ and further research could be useful to improve the model for this type of pollutants, namely, to apply to centralized systems for a more sustainable urban water management [15].

### 4. Conclusions

To promote and increase water reuse practices in Europe and Portugal, new policies, supported on the international guidelines, such as ISO standards, were adopted and one of its most critical features is the application of a flexible approach without jeopardizing the health and environmental safety. The main strength of the proposed model is its simplicity. The application of the methodology to a case study allowed to demonstrate its applicability and respective strengths, such as the use of a strategic assessment, that allows to evaluate the risks involved in each water reuse project for surface and groundwater and helps authorities, with simple outputs, on the validation process of the appropriate quality standards to be noted on water reuse permits and, subsequently, helps them on the decision-making process namely on the imposition of minimization measures. Although the model allows the determine the quality standards for reclaimed waters, these results should always be seen with other management options, namely for nutrients to minimize the use of synthetic fertilizers.
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