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2  
3 **Development of a qualitative approach to assessing risks associated with the use of**  
4 **treated wastewater in agricultural irrigation**

5  
6 **Abstract**

7 The European Commission's draft regulation for minimum water requirements for water reuse  
8 in agriculture addresses microbial and basic water quality parameters but does not consider  
9 the potential impacts of chemicals of emerging concern (CECs) on human and environmental  
10 health. Because insufficient data prevents the quantitative characterisation of risks posed by  
11 CECs in treated wastewater (TWW), this paper presents a framework which combines data  
12 and expert judgement to assess likelihood of occurrence and magnitude of impact. An  
13 increasing relative scale is applied where numeric values are pre-defined to represent  
14 comparative levels of importance. Subsequently, an overall assessment of the level of risk  
15 associated is characterised by multiplying together allocated scores, to obtain a single discrete  
16 overall score per CEC. Guidelines to support implementation of the framework as far as soil  
17 (the initial receiving compartment and pathway to further protected targets) are developed and  
18 applied. The approach is demonstrated through its application to clarithromycin, where results  
19 indicate that – under the considered scenario - there is limited possibility of its occurrence in  
20 soil in a bioavailable form. The role of a qualitative risk assessment approach is considered  
21 and the opportunity for its outputs to inform future research agendas described.

22  
23 **Keywords** Qualitative risk assessment; treated wastewater reuse; chemicals of emerging  
24 concern; agricultural irrigation; minimum water quality requirements

25  
26 **1. Introduction**

27 Facilitating the reuse of treated wastewater (TWW) is a priority objective towards the  
28 achievement of sustainable water resources both internationally (UN SDG 6, 2015) and within  
29 several European Union strategies (EU 2012 and 2015). As an alternative source of irrigation  
30 water, TWW offers a range of potential benefits including a predictable water quantity, a  
31 reduced need for chemical fertilisers and improved soil conditioning leading to increased crop  
32 yield (Navarro et al., 2015). However, despite these practical and economic benefits, TWW is  
33 an under-exploited water resource. In Europe it is estimated that only 2.4% of TWW is reused,  
34 rising to 5-12% in the more water-scarce Mediterranean countries (Saliba et al., 2018). While  
35 the needs for additional infrastructure to transfer and/or store TWW are identified as barriers  
36 to uptake, a key issue limiting its use is public concern over potential impacts on human and  
37 environmental health (Maryam and Buyukgungor, 2017; Garcia and Pargament, 2016). A  
38 range of guidelines have been developed to support the safe use of TWW in agriculture (e.g.  
39 WHO, 2006; FAO, 1992, ISO 2015) and the European Commission recently published draft  
40 regulations on minimum quality requirements for reuse (EC, 2018). However, the focus of  
41 these guidelines is the protection of human health through a reduction of pathogenic risks and  
42 little, if any, attention has been paid to the risks (perceived or actual) associated with chemicals  
43 present in TWW (Gardner et al., 2013).

44  
45 Selected guidelines (e.g. US EPA, 2012) identify limit values for a range of metals however,  
46 TWW may contain a myriad of further organic and inorganic substances, as a combined  
47 function of catchment-specific land use activities and wastewater treatment plant design. The  
48 risks associated with many of these chemical substances have yet to be robustly assessed,  
49 particularly chemicals of emerging concern (CECs; defined here as substances which are not  
50 regulated under existing EU water quality regulations but which have been identified as having  
51 the potential to impact negatively on human health and/or environmental endpoints). CECs  
52 represent a diverse group of substances and include various pharmaceuticals, perfluoroalkyl  
53 substances, biocides, plasticisers, plastics components, pesticides and oestrogenic  
54 compounds (NEREUS D20, 2018; EC, 2017).

56 With the increasing drive from both policy and practice to facilitate TWW reuse in agricultural  
57 irrigation, there is an urgent need to identify and characterise the risks associated with the  
58 occurrence of CECs in TWW. However, despite considerable activities undertaken to comply  
59 with, for example, the EU REACH requirements, the human and environmental health impacts  
60 of only a fraction of the 95,872 substances registered to-date have been fully evaluated  
61 (ECHA, 2019, EC, 2017). There is a lack of knowledge on CECs compositions in different  
62 products, relevant hazard data and /or details on levels of exposure (EC, 2017). In the absence  
63 of these data sets, it is not possible to undertake a quantitative risk assessment of the  
64 problems posed to human and environmental health by the occurrence of CECs in TWW.  
65 However, with the drive to reuse TWW accelerating, this paper presents a novel framework  
66 which combines data and (where this is not available) expert judgement to support a  
67 qualitative assessment of risks associated with the occurrence of CECs in TWW used in  
68 agricultural irrigation. Guidelines to support the application of the framework are identified up  
69 to the receiving soil environment, which represents the primary receiving compartment leading  
70 to a host of protection targets (including humans, plants and animals). Hence the specific risk  
71 evaluated is the occurrence of a CEC in soil in a bioavailable form. The developed approach  
72 is applied to clarithromycin (an advanced generation macrolide antibiotic which is included on  
73 both the WHO Model list of Essential Medicines (WHO, 2013) and the 2<sup>nd</sup> Watch List of  
74 Substances under the EU WFD; JRC, 2018) to illustrate the use of the methodology and the  
75 opportunities for its use within emerging research and policy agendas.

## 77 **2. Methodological approach to framework development**

78 A conventional risk assessment (RA) approach involves identification of the hazards within an  
79 exposure scenario, followed by analysis of available data on its likelihood of occurrence (LO)  
80 and magnitude of impact (MI) to inform both risk characterisation and management decisions  
81 (US NRC, 1983). While the OECD (2018) has published a range of exposure scenarios as  
82 part of its approach to chemical risk assessment, a standardised exposure scenario pertaining  
83 to the reuse of TWW irrigation has yet to be developed. The key variables with the potential  
84 to influence the fate of CECs present in TWW reused within agricultural irrigation have been  
85 identified (NEREUS D20, 2018), and are presented as a source-pathway-receptor (SPR)  
86 model (Figure 1) to inform development of the risk scenario utilised within the worked example  
87 (which considers pathways as far as the soil only; see Section 4).

### 89 **Add Figure 1 here**

91 Within the context of the use of TWW in agricultural irrigation, LO refers to frequency of  
92 occurrence of specific CECs in TWW and MI is considered in terms of whether a direct effect  
93 can be detected within the environment (e.g. change in soil microbial composition) and  
94 whether detected changes are considered to be permanent or reversible following cessation  
95 of TWW irrigation. Standard approaches to quantifying LO and MI typically draw on the use of  
96 dose response models (in human health RA) or 'no observable effect levels' data  
97 (environmental RA). However, data on the behaviour and fate of many CECs is limited, with  
98 models to predict CECs exposure to either humans or environmental receptors still in the early  
99 stages of development. Where data are not yet available to support a quantitative RA, a  
100 qualitative approach can be adopted (DEFRA, 2004; Standards Australia 2004, USDA, 2003).  
101 Both LO and MI may be assessed using an increasing relative scale where numeric values  
102 are pre-defined to represent the comparative seriousness of the problem as indicated in Table  
103 1 for the discharge of a specific CEC within a TWW flow which comes into contact with a  
104 protected target.

### 106 **Add Table 1 here**

108 The values presented in Table 1 are ordinal in nature and therefore represent only, for  
109 example, the order of LO of specific CECs in TWW at point of use relative to other CECs and  
110 do not have an exact quantitative meaning. For both LO and MI, scores are allocated across

111 a range of 1 – 4, where a score of 1 indicates least likelihood/impact to up to a maximum of 4  
112 (highest likelihood/impact). respectively. An overall assessment of the level of risk associated  
113 with a specific CEC in TWW used in agricultural irrigation can then be deduced by multiplying  
114 together the ranked scores allocated to LO and MI, developing a single discrete overall score  
115 per CEC.

116

### 117 **3. Results and discussions**

118 The scoring approach set out in Table 1 has been applied to the SPR model presented in  
119 Figure 1. Due to the lack of field data, dose response models and understanding of cumulative  
120 exposures, it is currently only possible to apply the approach as far as soil as the target  
121 receptor.

122

#### 123 3.1 Benchmarking the likelihood of CECs reaching the soil environment

124 The likelihood of a CEC reaching the soil environment is identified as a function of the  
125 untreated WW characteristics, the type of treatment applied, whether the TWW is subjected  
126 to transportation/storage prior to use and the type of irrigation used. The following sections  
127 discuss each of these influencing factors and draw on a combination of literature data and  
128 expert judgement (provided by the NEREUS network; a global network of 380 researchers  
129 working in the field of TWW in a variety of disciplines) to inform the application of the approach  
130 set out in Table 1 within an agricultural irrigation context.

131

##### 132 3.1.1 Dependence on sources of wastewater

133 CECs may be discharged into the WW treatment system from a range of urban and non-urban  
134 sources. The latter will be mainly rural residential areas from which WW will potentially contain  
135 CECs from a diversity of everyday activities, including the washing of textiles, the disposal of  
136 unused items and, in the case of pharmaceuticals, due to excretion in an unchanged state. In  
137 addition to housing, urban areas will additionally include hospitals and commerce/industry  
138 which, in the absence of on-site treatment facilities, are potentially major sources of CECs  
139 (Vidal-Dorsch et al., 2012; Fairbairn et al., 2016). The greater the variety of sources, the  
140 greater the likelihood that CECs will be present in the WW directed to the wastewater  
141 treatment plant (WWTP). However, a proposed rank scoring needs to take into account the  
142 different combinations of sources which may contribute CECs to WW and the relative  
143 importance of their contribution as shown in Table 2 (column 1). In the case of  
144 pharmaceuticals, the LO is greatest when the WWTP influent contains effluent from  
145 pharmaceutical industries followed by hospitals, residential areas and other industry (Brown  
146 et al., 2006; Santos et al., 2013).

147

##### 148 3.1.2 Level of wastewater treatment

149 Although it has been recommended that secondary TWW should not be used for agricultural  
150 irrigation in the EU (JRC, 2017), the highest rank score (4) is allocated to this category of  
151 TWW as there may still be circumstances under which it could be used (Table 2; column 2).  
152 Conventional treatment systems (e.g. activated sludge) are typically not designed to treat  
153 CECs with the result that a high proportion of the parent compounds and their metabolites can  
154 be discharged. This is particularly true of surfactants, pharmaceuticals and personal care  
155 products (PPCPs) and polar pesticides (Petrovic et al., 2003). The increased efficiency  
156 achieved in microbiological WW treatment through the use of membrane bioreactors (MBR)  
157 is indicated by allocating a rank score of 3 to this treatment (Table 2). Gonzalez et al. (2016)  
158 report that MBR systems enhance the removal of many CECs compared to activated sludge  
159 systems, particularly in the case of hydrophobic compounds which have lengthy residence  
160 times. Although high levels of elimination (>90%) have been observed for many compounds  
161 there are some PPCPs, for example amitriptyline, diazepam and sulfamethoxazole, for which  
162 removal is less efficient (24-68%) (Trinh et al., 2012).

163

164 Tertiary and advanced wastewater treatments include adsorption, ozonation and advanced  
165 oxidation processes. Light-driven oxidation (with or without H<sub>2</sub>O<sub>2</sub>) and ozonation processes

166 may involve the formation of unwanted toxic by-products, which is recognised by allocating a  
167 lower rank score (1) where there is the possibility of producing toxic by-products compared to  
168 a treatment scenario where this is known not to be the case (rank score 2) (Table 2; column  
169 2). Potentially toxic by-products associated with the ozonation of WW include nitrosamine and  
170 N-Nitrosodimethylamine (Hollender et al., 2009).

171

### 172 **Insert Table 2 here**

173

174 The treatment of secondary effluents with high doses of ozone has demonstrated increased  
175 toxicity due to the formation of toxic by-products (Petala et al., 2008). Similar problems are  
176 associated with advanced oxidation processes (AOPs) such as UV/H<sub>2</sub>O<sub>2</sub>, photo-Fenton,  
177 heterogeneous photocatalysis, and O<sub>3</sub>/H<sub>2</sub>O<sub>2</sub>. Although ozonation generally provides efficient  
178 removal of CECs (Nakada et al., 2007) there are some compounds which are resistant to this  
179 process including mecoprop, benzotriazole and sucralose (Margot et al., 2013; Reungoat et al.,  
180 2012). Adsorption techniques using activated carbon are widely practised treatment  
181 processes with removal efficiency depending on contact time and the physico-chemical  
182 properties of the adsorbate and the adsorbent. Removal efficiency increases as a substance's  
183 octanol-water partitioning coefficient (pK<sub>ow</sub>) increases with pK<sub>ow</sub> values >4 indicating a high  
184 potential for sorption to activated carbon (AC) (Margot et al., 2013). Granulated AC is reported  
185 to be capable of removing a range of different PPCPs and flame retardants to levels below  
186 detection limits (Kim et al., 2007). Together with sand filtration, AC filtration is recommended  
187 for the removal of oxidation by-products (Rizzo et al., 2019; Krzeminski et al., 2019).

188

#### 189 3.1.3 Effect of storage and transportation prior to use

190 If TWW is stored before irrigation, CECs may be degraded to daughter products which are  
191 either less toxic, or more toxic, than the original substance. A critical factor will be the time  
192 between the TWW discharge from the WWTP and its use for irrigation, including both transfer  
193 within a distribution system and storage within either an open or closed system. CEC  
194 properties will also determine its susceptibility to physical (e.g. adsorption to suspended  
195 solids), chemical (e.g. hydrolysis) and biological (e.g. biodegradation) processes. The  
196 efficiency of biotic/abiotic degradation processes varies widely between CECs. Ryan et al.  
197 (2011) found that allowing photolysis in WW stabilisation ponds led to enhanced PPCP  
198 removal, although direct UV radiation is reported as ineffective for the removal of antibiotics  
199 (Adams et al., 2002). There is also disagreement regarding the role of hydrolysis reactions  
200 with data showing only limited evidence of ciprofloxacin, sulfamethoxazole and trimethoprim  
201 removal (Alexy et al., 2004). Where degradation does occur, the occurrence of increased  
202 toxicity of daughter products needs to be considered. The worst TWW storage scenarios  
203 would be where there is either no degradation of the original CEC or degradation results in  
204 the formation of a toxic daughter product. These scenarios are both allocated a rank score of  
205 2 compared to a rank score of 1 where the degradation of the original CEC results in the  
206 formation of a non-toxic daughter product (Table 2; column 3), with scores of 2 and 1 reflective  
207 of the current limited understanding of the behaviour of CECs in stored/distributed TWW.

208

#### 209 3.1.4 Technique used for soil irrigation

210 The efficiency with which TWW, and hence the CECs, reach the receiving soil is dependent  
211 on the irrigation method. Four categories of irrigation (surface, spray/sprinkler, drip irrigation  
212 and sub-surface) system were identified (Doneen and Westcot, 1988), all of which have the  
213 potential to contaminate the soils. However, drip irrigation and sub-surface irrigation represent  
214 a targeted process of TWW delivery in which the supply of TWW to the soil is regulated to  
215 crop requirements. This limits TWW percolation to groundwater and/or CEC build-up in the  
216 soil. Therefore, both these irrigation procedures have been given a rank score of 1 (Table 2;  
217 column 4). The same level of control is not possible with surface irrigation where gravity  
218 systems are employed to effectively flood the irrigated area. The increased potential for soil  
219 contamination merits a rank score of 2. In spray/sprinkler irrigation, which is correctly adjusted  
220 to avoid surface ponding, the level soil contamination will be less severe but the potential for

221 direct contamination of the plant surfaces also merits a rank score of 2 (Table 2). The allocation  
222 of scores of 1 and 2 (as opposed to for example, 3 and 4) within this binary approach is  
223 reflective of the relatively limited data sets pertaining to CECs in TWW used in agricultural  
224 irrigation.

225

### 226 **3.2 Benchmarking the magnitude of the impact of CECs in the soil environment**

227 The MI of a CEC reaching the soil environment is considered to be a combined function of  
228 CEC load in TWW, the environmental behaviour of a specific CEC within the receiving soil  
229 environment and the type of soil management practices applied. The following sections  
230 discuss each of these factors to inform the application of the scoring scheme set out in Table  
231 1.

232

#### 233 **3.2.1 Dependence on CEC load in TWW**

234 The potential impact to the receiving soil will be influenced by the quantity of CEC delivered  
235 during the irrigation process. On the basis that constant irrigation flow rates will be used it is  
236 possible to use CEC concentrations as a surrogate for pollutant loads. The influent and effluent  
237 concentrations for a range of pharmaceuticals associated with a traditional activated sludge  
238 municipal treatment plant receiving a mean daily load of ~25 million gallons per day have been  
239 reported by Du et al. (2014). Influent concentrations ranged from 104 ng/l (diclofenac) to  
240 47,500 ng/l (sucralose). The variabilities in treatment efficiencies and therefore effluent  
241 concentrations (16.1 to 39,425 ng/L) require that this breadth of values is considered when  
242 assigning scores for the assessment of the impact of contaminants to the receiving soil (Table  
243 3; column 1).

244

#### 245 **3.2.2 Dependence on the CEC bioavailability/bioaccessibility in the soil**

246 CEC bioavailability in soil pore-water is dependent on sorption/desorption and transformation  
247 processes which, in turn, are influenced by the soil properties and the chemical form of the  
248 CEC. The physical nature of a soil as well as the existence of voids/channels affect the ease  
249 of movement of solutes and contaminants. The heterogeneous nature of agricultural soils in  
250 terms of both organic content (e.g. soil organic matter; SOM) and mineral fractions control the  
251 availability of CECs as a result of partitioning between pore-water and soil solids according to  
252 the distribution coefficient ( $K_d$ ). This parameter together with the octanol-water partition  
253 coefficient ( $K_{ow}$ ; reflecting the degree of hydrophobicity of a contaminant), are critical  
254 parameters for assessment of soil-contaminant behaviour. Colloids can play an important role  
255 in sorption processes and CECs strongly associated with colloidal particles have limited  
256 bioaccessibility/bioavailability.

257

#### 258 **Insert Table 3 here**

259

260 Hydrophobicity-independent mechanisms which contribute to reduced CEC availability include  
261 cation exchange/bridging, surface complexation and hydrogen bonding (Yamamoto et al.,  
262 2009). CECs may vary from being highly hydrophilic ( $\log K_{ow} < 1$ ; e.g. sucralose) to  
263 hydrophobic in nature ( $\log K_{ow} > 4$ ; e.g. ciprofloxacin) affecting their affinity for the soil-water  
264 phase. They can also occur as neutral or ionic forms depending on the value of the acid  
265 dissociation constant ( $pK_a$ ) relative to the soil pH.

266

267 The binding of CECs to soils can result in the formation of non-extractable residues (NER).  
268 This is often a controlling factor in relation to the fate and persistence of pesticides and may  
269 also apply to pharmaceuticals. Acetaminophen has been shown to be rapidly converted to  
270 bound residue (73.4-93.3%), compared to carbamazepine (retained at <4.2% in the same soil)  
271 (Li et al., 2013). Sulfadiazine and triclosan have also exhibited irreversible formation of NER.  
272 In contrast, it is the reversibly sorbed fractions together with dissolved species which are  
273 readily available for migration. The bioavailability of CECs introduced into soils can be reduced  
274 by biodegradation, volatilisation and photodegradation. Microorganisms have been shown to  
275 biodegrade diclofenac (Xu et al., 2009) whereas less than 1.2% of carbamazepine was

276 mineralised (Dodgen et al., 2016). The volatility of CECs from topsoil is limited (Undeman et  
277 al., 2009). Photodegradation of soluble pharmaceuticals can be a significant removal pathway  
278 (e.g. Fatta-Kassinos et al., 2011) but is confined to the soil surface.

279

280 The overall bioavailability of CECs is hence determined by their ease of movement through  
281 the soil, the established sorption/desorption equilibria and the existence of transformation  
282 processes. The latter are either of minimal importance or, as in the case of biodegradation,  
283 occur relatively slowly. Therefore, a scoring scheme (Table 3; column 2) has been developed  
284 based on the balance between the ease of movement of the CEC within the soil and its  
285 bioavailability based on soil properties and the chemical characteristics of the CEC.

286

### 287 **3.2.3 Biosolid/fertiliser addition to soils and ploughing**

288 The addition of biosolids/animal manures and the action of ploughing can influence the  
289 bioavailability of CECs in soils. Cultivation improves drainage and aeration, typically by  
290 breaking up undisturbed soil and reducing the size of soil aggregates. Ploughing can facilitate  
291 the transport of contaminants within soils (Dominguez et al., 2014). Application of biosolids or  
292 animal manures leads to an increase in SOM (enhancing adsorption and reducing CEC  
293 mobility) as well as elevated cation exchange capacity (facilitating CEC complexation).  
294 Biosolids are also sources of CECs with Kinney et al. (2006) detecting 30-45 contaminants  
295 per biosolid sample at sum total concentrations ranging from 64 to 1811 mg/kg. Animal  
296 manures have also been shown to contribute CECs to soil and therefore the possible  
297 introduction of an additional CEC load to soil has to be balanced against the advantages  
298 conferred by increased SOM as a result of non-composted biosolids or animal manure  
299 application.

300

301 Soil organic carbon content can inhibit PPCP biodegradation by reducing contaminant  
302 bioavailability and hence inhibiting contaminant availability to microbial populations (Stumpe  
303 and Marschner, 2010). Therefore, biosolid amendment of soils reduces biodegradation (Li et  
304 al., 2014) and prolongs PPCP persistence in soil due to increased sorption. In addition,  
305 biosolids may serve as a more readily available nutrient or carbon source for microorganisms  
306 compared to PPCP, further contributing to a reduced biodegradation. However, the major  
307 impact of biosolids is on CEC availability in the soil environment. The soil structural changes  
308 brought about by ploughing to some degree counteract the effects of biosolids/manure  
309 amendment by assisting CECs movement within the soil but at a considerably reduced level.  
310 Therefore, in developing a scoring system relating to the combined effect of biosolid/animal  
311 manure application and ploughing on CEC availability in soils the following order is proposed:  
312 no biosolids/manure + ploughing > manure (only) + ploughing or no ploughing > biosolids +  
313 ploughing > biosolids + no ploughing. The composting of animal manures, which has been  
314 demonstrated to degrade veterinary pharmaceuticals (Song and Guo, 2014), reduces CECs  
315 load associated with manure application and hence lowers the assigned score. The rank  
316 scores are allocated as shown in Table 3 (column 3).

317

### 318 **3.3 Calculation of discrete scores for LO and MI**

319 The different factors which influence the likelihood of CECs reaching the soil environment after  
320 irrigation with TWW (see Section 3.1) can be combined by multiplication of the individual  
321 ranking scores to give a single score indicating LO per CEC. These can be ranked to give a  
322 prioritised list varying from most likely (highest combined score) to least likely (lowest  
323 combined score). Likewise, in relation to MI, multiplying together each of the scores allocated  
324 to the factors that influence the impact of CEC bioavailability within soil generates a discrete  
325 combined score which can be used to indicate the relative MI of a CEC. The range of scores  
326 generated when calculating single combined values for either LO or MI range from 1 to 64 in  
327 both cases. These scores are grouped into four ranges and descriptors allocated to indicate  
328 an increasing overall likelihood of a CEC occurring in soil following irrigation with TWW or an  
329 escalating overall MI in terms of bioavailability within the soil environment. Ranges of scores  
330 and supporting LO and MI descriptors are as follows:

- 331 • scores 1-6: rare (LO: a lack of evidence but possible; MI: impact not detectable;  
332 integrated score = 1)
- 333 • scores 7-16: unlikely (LO: uncommon but know to occur; MI: uncommon but impact  
334 may occur; integrated score = 2)
- 335 • scores 17-36: possible (LO: may occur sometimes; MI: may create an impact  
336 sometimes; integrated score = 3)
- 337 • scores 37-64: LO: likely to occur; MI likely to exert an impact; integrated score = 4  
338

### 3.4 Calculation of an overall risk score

340 Multiplying the LO and MI scores (described in Tables 2 and 3) together supports development  
341 of a ranked list of CECs with regard to their potential to occur in soil in a bioavailable form. As  
342 an ordinal dataset, it does not provide information on what, for example, a ‘high probability’  
343 means, nor can it be used to determine how important the difference is between CECs ranked  
344 first as opposed to second. However, the ranked risk scores can be used to short-list CECs  
345 which are relatively of most concern and should be prioritised for further research. Whilst the  
346 score itself has no quantitative meaning, such risk scores are often interpreted using a ‘traffic-  
347 light’ style matrix. Despite their widespread use, there are no clear guidelines on how scores  
348 should be segregated into discrete ranges or how these sets of values should be interpreted.  
349 In the absence of specific guidelines, the approach below is proposed, together with an  
350 example of how score ranges can be interpreted:

- 351 • A risk score of 12-16 indicates a high probability of the occurrence and bioavailability of a  
352 CEC in soil resulting in uptake by a receptor;
- 353 • A risk score of 9-11 indicates the possibility of the occurrence and bioavailability of a CECs  
354 in soil resulting in uptake by a receptor;
- 355 • A risk score of 5-8 indicates the unlikely (or limited possibility of) the occurrence and  
356 bioavailability of a CEC in soil resulting in uptake by a receptor;
- 357 • A risk score of 1-4 indicates that only on very rare occasions would the occurrence and  
358 bioavailability of a CEC in soil result in uptake by a receptor;

### 4. Example of the application of the developed qualitative RA framework

361 The scenario considered focusses on clarithromycin and involves WW from a residential area  
362 (no major industrial or hospital contributions) undergoing secondary treatment with MBR. The  
363 TWW is piped directly to a closed tank, and is used for spray irrigation within 24 hours to a  
364 neutral, sandy soil. The soil is not amended with biosolids/animal manure but has been  
365 subjected to ploughing. By following the SPR model outlined in Figure 1 and considering the  
366 scoring systems described in Tables 2 and 3, the following assessments can be deduced.

#### 4.1 The likelihood of CECs reaching the soil environment

367 This will be dependent on:

- 368 • source of WW: WW derived from a residential area without industrial or hospital sources  
369 is allocated a score of 2.
- 370 • level of wastewater treatment: enhanced secondary treatment with MBR receives a score  
371 of 3.
- 372 • effect of storage prior to use: TWW is transferred to the irrigation site in a closed system  
373 and used within 24 hours allowing limited time for breakdown of the clarithromycin by  
374 hydrolysis or biodegradation. Lack of exposure to light eliminates opportunity for  
375 photolysis hence a score of 2 is allocated.
- 376 • soil irrigation technique: spray irrigation is considered to pose an increased CEC risk due  
377 to increased opportunity for soil contamination and is allocated a score of 2.

380 Therefore, the overall score relating to the likelihood of CECs reaching the soil environment is  
381  $2 \times 3 \times 2 \times 2 = 24$ . This falls within the ‘16-36’ range indicating an integrated LO score of 3  
382 which is indicative of the possibility of clarithromycin being found in the soil.  
383

384

## 4.2 The MI of CEC bioavailability within the receiving soils

This will be dependent on:

- CEC load in TWW: Following conventional activated sludge treatment, effluent clarithromycin concentrations in the range 57-598 ng/L have been reported (Tuckwell, 2014). After primary and secondary clarifiers followed by sand filtration, McArdell et al. (2003) found clarithromycin concentrations of 57-135ng/L in TWW from a WWTP receiving WW from an urban catchment without industrial or hospital inputs. The level of treatment and the catchment type are considered similar to the described scenario, leading to the allocation of a score between 2 and 1.
- CEC bioavailability in soil: the bio-physico-chemical factors which need to be balanced against one another to provide an overall assessment of the bioavailability of a given CEC in a particular soil are outlined in Table 4. Clarithromycin movement in a sandy soil will be limited due to electrostatic attraction to negatively-charged soil minerals although clarithromycin is likely to exhibit only moderate interaction with SOM. Therefore, the category in Table 3 which best fits this behaviour is 'ready movement of CECs within soil'.
- biosolid/animal manure addition and ploughing: ploughing is practised but there is no application of biosolids/animal manure hence a score of 4 is allocated.

### Insert Table 4 here

Therefore, the overall MI score relating to the impact of CEC bioavailability within the receiving soil is  $2/1 \times 2 \times 4 = 16/8$ . This falls within the '7-16' range indicating an integrated MI score of 2 which is indicative of clarithromycin being unlikely to exert an impact in the soil environment.

## 4.3 Overall risk assessment score

Combination of the LO and MI scores yields an overall risk score of 6 (3x2) which fits into the '5-8' band (see Section 3.4) and corresponds to a scenario in which there is limited possibility of the occurrence and bioavailability of clarithromycin in the soil.

## 5. Conclusions

Recognising that the development of complete data sets on the occurrence, behaviour and fate of CECs in TWW reused in agriculture is a long-term goal, this paper sets out a novel approach to qualitatively characterising the risk that a CEC will occur in soil in a bioavailable form. The utility of the approach is demonstrated through its application to clarithromycin and the scope for this approach to be applied to further CECs is clear. However, the identity of substances to be evaluated to inform a robust assessment of risks to human and environmental health from TWW reuse in this application is less so. The development of a short-list of priority CECs is a dynamic target influenced by both the development of new products (e.g. levels of CECs) and the perspective of the list-maker (e.g. a focus on potential to be bioaccumulated as opposed to those most resistant to treatment etc.). An initiative which could make a significant contribution to identifying a short(-er) list of CECs is the European Chemical Agency's chemical screening programme, involving the evaluation of data on hazardous properties to identify all 'substances of very high concern' (SVHCs) by 2020. Whilst the ECHA SVHCs short-list itself would not be fully fit for purpose (see Deviller et al., (under review) for a comprehensive evaluation of existing chemical legislation in relation to sources of CECs potentially present in TWW), it will provide a useful starting-point to which further CECs of concern can be added on a systematic basis. The results of the application of the developed approach to a prioritised list of CECs will enable future research and policy initiatives to focus on CECs in TWW reused in agricultural irrigation from the perspective of potential to occur in a bioavailable form. This represents a significant step forwarding in understanding, and one which can underpin efforts to address a further critical research question: do CECs identified as having a high probability of being present in soils in a bioavailable form have the potential to accumulate within an identified receptor and – if so – to what level?

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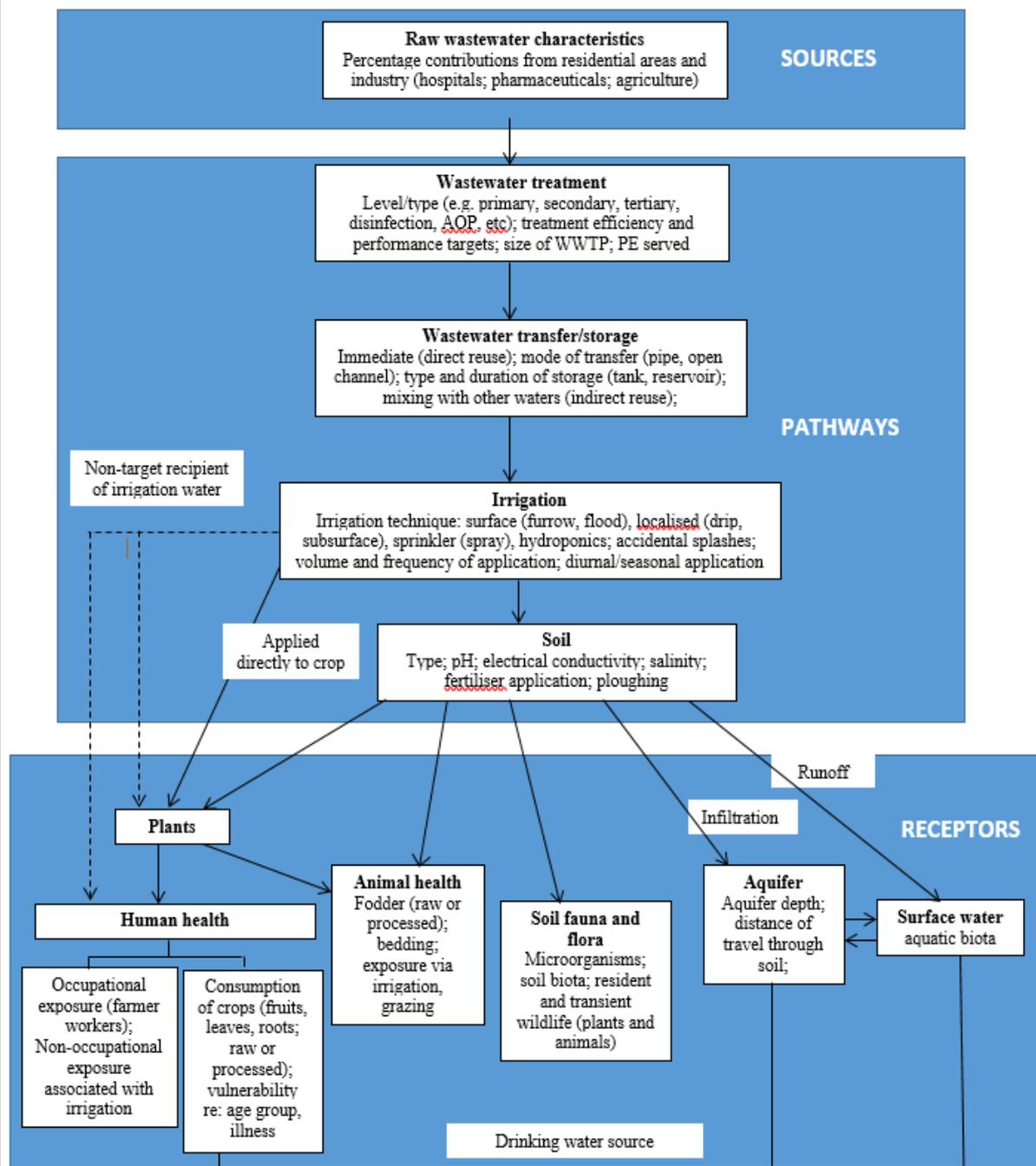
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667 **Table 1. Descriptors and scores to benchmark the likelihood of a specific CEC**  
668 **occurring in TWW and the magnitude of the impact occurring when a specific CEC is**  
669 **discharged in TWW**

<b>Factor</b>	<b>Possible descriptors for relative grading</b>	<b>Ordinal value associated with identified factor</b>
Likelihood of occurrence	Likely (expected to occur)	4
	Possible (may occur sometimes)	3
	Unlikely (uncommon but known to occur)	2
	Rare (lack of evidence but not impossible)	1
Magnitude of impact	High (; available for uptake)	4
	Medium (; may be available for uptake)	3
	Low (; unlikely to be available for uptake)	2
	Very low (not available for uptake)	1

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675 Key: AOP = advanced oxidation processes' PE = person equivalent

676 **Figure 1 Source-pathway-receptor model related to the use of TWW in agricultural**  
 677 **irrigation**

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684 **Table 2 Example of an approach for developing a single combined score which represents the likelihood of CECs occurring in soil**  
685 **following irrigation with TWW.**

Sources of wastewater				Characteristics of WW treatment				Storage prior to use		Soil irrigation										
Rural WW	Urban/Municipal WW			Secondary treatment (employing filter beds/ activated sludge aeration)	Enhanced secondary treatment (e.g. membrane bioreactors)	Tertiary/ advanced treatment; where oxidation processes can lead to toxic by-products	Tertiary/ advanced treatment; where there is NO possibility of toxic by-products	During the storage/ distribution process there is no breakdown of the original CECs or breakdown results in a toxic daughter product	During the storage/ distribution process breakdown of the original CECs results in a non-toxic daughter product	Surface irrigation	Spray/ sprinkler irrigation	Drip irrigation	Sub-surface irrigation							
	Residential sources	Industrial/ hospital sources with on-site treatment	Industrial/ hospital sources with NO on-site treatment																	
	4													4			2	1	2	1
	3													3			2	1	2	1
	2													2			2	1	2	1
1				1			2	1	2	1										

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693 **Table 3 Example of an approach for developing a single score which represents the impact of CECs bioavailability within the soil**694 **environment**

CECs load (concentration) in treated wastewater				CECs bioavailability/bioaccessibility in the soil				CECs availability in the soil due to biosolids/fertiliser application and ploughing			
CECs concentration in TWW exceeds 10,000 ng/L	CECs concentration range in TWW is 1,000 to 10,000 ng/L	CECs concentration range in TWW is 100 to 1,000 ng/L	CECs concentration in TWW is less than 100 ng/L	Ready movement of CECs within soil and ready availability for uptake	Limited movement of CECs within soil and ready availability for uptake	Ready movement of CECs within soil and limited availability for uptake	Limited movement of CECs within soil and limited availability for uptake	No biosolids/ animal manure application + ploughing	Animal manure (fresh or slurry) only application + ploughing or no ploughing	Biosolids/ composted animal manure application + ploughing	Biosolids/ composted animal manure application + no ploughing
4				4				4			
	3				3				3		
		2				2				2	
			1				1				1

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**Table 4 Factors influencing the bioavailability of clarithromycin in soil in the example**

Influencing factor	Situation for hypothetical scenario	Impact for soil bioavailability/bioaccessibility
Soil structure	Sandy soil	No inhibition of movement
log $K_{ow}$ for clarithromycin	3.16; indicative of moderate hydrophobicity	Some tendency for clarithromycin to associate with solid as opposed to aqueous phase
log $K_{oc}$ for clarithromycin	2.17; 1.37 (calculated values from EPI suite); indicative of fairly weak sorption to organic soil particles	Limited tendency for clarithromycin to sorb to organic matter associated with soil particles
p $K_a$ for clarithromycin	8.99; compared to soil pH of 7 indicates a tendency for clarithromycin to exist in cationic form	Cationic form of clarithromycin will promote sorption to predominantly negatively charged soil particles.
Biodegradation / volatilisation / photo-degradation	Not expected to readily occur in the soil environment.	Introduced clarithromycin levels in soil expected to be maintained.

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