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Modelling releases from tailings in life cycle assessments of the mining sector: from generic models to reactive transport modelling

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Highlights:

- Impacts associated with tailings releases are poorly quantified in LCA
- Comparison of different approaches to account for releases from tailings
- Generic inventory datasets may overestimate tailings releases to environment
- Interdisciplinarity is key to develop more complete models to be applied in LCA

Abstract

Extracting mineral ores to produce mineral concentrates and finally metals that enter the value chains of different sectors is a waste intensive activity. In particular, mineral processing activities generate yearly and globally several billion tons of wastes called tailings. Tailings storage is associated with significant environmental risks due to different sources such as releases to groundwater. Yet, these environmental impacts are poorly taken into account in the environmental life cycle assessment of a concentrate or metal production, in particular due to a lack of representative data in the inventory.

This paper aims at coupling geochemical modelling geochemical modelling with life cycle assessment to quantify releases from tailings and the associated environmental impacts. In the present work, reactive transport modelling was implemented to quantify more accurately short-term (100-year timeframe) and long-term (10,000 year-timeframe) tailings releases. Reactive transport modelling allows modelling and estimating the distributions in space and in time of chemical reactions occurring in a specific environment. The resulting tailings releases are compared with those calculated through the approach, based on a first order law of kinetics, used in the ecoinvent database. The results from the ecoinvent approach are calculated both with generic and site-specific parameters. These different approaches are applied on the case-study of a polymetallic sulphidic ore from a mine in Northern Europe.

The tailings releases obtained through the different approaches differ. Overall, the reactive transport model leads to quantities released at both short-term and long-term timeframes being smaller than those calculated with the ecoinvent approach. As a result, the impacts on ecotoxicological and toxicological categories show differences between two to eight orders of magnitude. Each approach used to model the tailings releases differ in the nature and amount of data needed as well as in the sophistication of the model used. While the approach based on reactive transport modelling is exhaustive and presumably provides a more accurate prediction

41 for the releases from tailings, it also requires massive computational resources and much larger
42 volumes of data, some of which being difficult to obtain on-site. Consequently, a consensus has
43 to be found between the complexity of the model used, the data availability and the expected
44 reliability of the results.

45 **Keywords:** life cycle inventory, tailings, reactive transport, groundwater releases

46

1. Introduction

1.1. The problematic of tailings in the mining sector

The dependence of our modern societies to metals has no longer to be proven. From the agricultural sector to the numerical sector, all industrial activities rely on metals, and by extension on the mining and metallurgical sector. Extracting mineral ores to produce mineral concentrates that are, *in fine*, refined into metals is a weak sustainable activity where the natural capital, the ores, is irreversibly transformed to the human capital, e.g. infrastructures (Tost et al., 2018). Moreover, mining activities are linked to environmental costs such as land disturbances, pollution legacies or solid waste generation (Azapagic, 2004; Moran et al., 2014; Mudd, 2007; Worrall et al., 2009). Mining waste in particular have the potential to increase the environmental liabilities associated with a mine site (Mudd, 2007). On a mine site, three main sources of waste can be cited, each associated with the unit processes transforming an extracted ore to a metal: mining that extracts the ore from the ground, mineral processing that separates the valuable minerals from the gangue, and metallurgical processing that refines the valuable minerals into metals. Thus, leading to different types of waste: waste rocks (associated with mining); tailings (mineral processing) and slag (metallurgical processing) (Lèbre et al., 2017; Lèbre and Corder, 2015).

This paper focuses more particularly on tailings, fine particles in suspension in water that remain after the treatment of minerals by separation processes (Bellenfant et al., 2013; Cuesta-Lopez et al., 2016; Lèbre and Corder, 2015). In the 2010s, yearly tailings production ranged between five and seven billion tons worldwide (Edraki et al., 2014; Xie et al., 2013). Given the trends in the mining sector, where production increases to meet the demand and ore grades decrease, tailings generation may also increase over the next decades (Mudd, 2007). Different methods of mine tailings disposal, usually occurring on site, exist; see Edraki et al. for a review (2014). In the European Union, the directive 2006/21/EC on the management of wastes from extractive industries regulates mining companies to manage tailings in a way that limits their effect on human health and the environment. In particular, the directive mentions the need for the operator to have a major-accident prevention policy and to establish monitoring procedures not only during the operation phase but also after closure of the site and its associated tailings facilities (European Commission, 2006).

The storage of tailings poses environmental risks for the surrounding ecosystems and residential areas, specifically due to contaminant releases through wind borne disposal, leakages into groundwater or tailings dam failures (Bes et al., 2014; Broadhurst and Petrie, 2010; Edraki et al., 2014; Xie et al., 2013). These risks might happen on a short to a long-term time frame (after mine closure) (Kossoff et al., 2014). If tailings dam failures are catastrophic events with harmful consequences for human lives and fauna in the local ecosystem (see for example the case of the Córrego do Feijão mine in Brazil in January 2019¹ or the review of dam failures made by Kossoff et al. (2014) and Rico et al. (2008)); the generation of leakages to groundwater can also have long term harmful consequences. Since these environmental risks are directly linked to the tailings properties, which are themselves related to the ore characteristics and the technologies implemented in the mineral separation process (Broadhurst and Petrie, 2010), they are by essence, site-specific. In particular, if the tailings contain sulfidic minerals, these latter can oxidize in the unsaturated zone that is in direct contact with the atmosphere (Brookfield et al., 2006; Elberling et al., 1994). The produced sulfuric acid is dragged downward through the tailings by precipitation (rainwater or snowmelt) leading itself to further leaching of metal

¹ CNN. February 1 2019. "Death toll rises in Brazil dam collapse as mining company faces criticism" <https://edition.cnn.com/2019/01/27/americas/brazil-dam-collapse/index.html>

92 elements from the tailings to the surrounding environment, especially in water (Bellenfant et al.,
93 2013; Broadhurst and Petrie, 2010; Edraki et al., 2014; Mudd, 2007).

94 1.2. Consideration of tailings releases in life cycle assessment

95 Life cycle assessment (LCA) is a decision-making tool that assesses the potential environmental
96 impacts a system (product, service or organization) has during its whole life cycle: from the
97 extraction of resources to its end of life management. LCA is an ISO standardized tool (ISO/TC
98 207/ SC 5, 2006) widely used in various sectors, including in the mining and metal sector (see
99 for example Durucan et al., 2006; Ferreira and Leite, 2015; Mearns et al., 2012; Norgate and
100 Haque, 2010; Nuss and Eckelman, 2014; Santero and Hendry, 2016). Despite this wide use, only
101 few LCA studies currently include tailings management and their associated environmental
102 impacts within the boundaries of the mine site under study. (Beylot and Villeneuve, 2017; Edraki
103 et al., 2014). Edraki et al., underline that data availability regarding tailings management and the
104 associated emissions is a reason of this non-inclusion (2014). An assessment of the Web of
105 science bibliography database made in June 2020 shows that about 400 scientific publications
106 address the specific topics of “LCA” and “mining” while ten times less publications address “LCA”
107 and “tailings”. Yet, when taken into account, tailings disposal generally contributes to the
108 environmental impacts of mining operations assessed in a life cycle perspective. For example, a
109 LCA of a lead-zinc ore mining and concentration system showed that tailings disposal is the
110 highest contributor for 4 environmental impact categories out of 18 using the ReCiPe life cycle
111 impact assessment (LCIA) method (Tao et al., 2019). A similar conclusions can be drawn when
112 assessing the mining datasets of the ecoinvent 3.6 database, a life cycle inventory (LCI) database
113 widely used in the LCA community (Wernet et al., 2016). As an example, for the dataset ‘copper
114 concentrate, sulphide ore, copper mine’, tailings management contributes the most to 7 impact
115 categories out of 18 using ReCiPe as well.

116 Such important contributions to the environmental impacts emphasize the need to accurately
117 accounting for the releases induced by tailings when carrying out the LCA of mining operations.
118 However, the lack of consideration for tailings releases may, in part, pertain to the difficulty for
119 mining companies to obtain precise on-site measurements of direct leakages from tailings to
120 groundwater. Only two studies were found to rely on on-site measurements from mining
121 companies for quantifying these releases to water. Firstly, Beylot and Villeneuve (2017)
122 considered the volume of infiltrations to groundwater and measurements of pollutants
123 concentrations performed by KGHM (Polish mining company) in their study looking at the
124 storage of sulfidic tailings resulting from copper production. Secondly, Tao et al. (2019)
125 considered direct releases data (encompassing water discharge and metal ions migration)
126 monitored by a Chinese mining company in their study about lead-zinc ore mining and
127 beneficiation in China. Other studies rather rely on estimations, either based on experimental
128 data or on public literature information for quantifying tailings releases to water: Song et al.
129 (2017) estimated values of metals leaching from tailings to water based on experimental data
130 (electrodialytic extraction) obtained from samples of the mine tailings; Reid et al. (2009)
131 estimated them based on both data drawn from literature and data obtained from experiments
132 on samples of the mine tailings at a laboratory scale, further complemented by numerical
133 modelling for longer-term horizons; Broadhurst et al. (2015) primarily derived their
134 groundwater releases from literature information, their own knowledge and calculations. The
135 ecoinvent database, also relies on literature data and calculations to account for releases to
136 groundwater from tailings, considering worldwide averages in terms of tailings composition or
137 substances leakages to water. One may identify different limits with respect to these different
138 quantification approaches:

- 139 • Considering worldwide averages for the tailings composition may show significant
140 uncertainties and a certain lack of representativeness, given that ores and tailings

141 compositions are significantly different from one deposit to another, which accordingly
142 may not reflect the characteristics relative to a specific mine site (Doka, 2008; Rader et
143 al., 2019; Turner et al., 2019).

- 144 • Toxicity-related impacts are highly sensitive to long-term temporal horizons (with
145 releases from tailings up to 60,000 years as currently considered in LCA; (Beylot and
146 Villeneuve, 2017; Doka, 2008), however, obtaining reliable data regarding such releases
147 appears relatively complicated (Reid et al., 2009).
- 148 • The releases to water as considered in these different approaches may fail to capture the
149 behavior of these releases when flowing from the tailings pond to groundwater e.g. in
150 terms of temporal behavior (Broadhurst et al., 2015) or physical and chemical
151 interactions with the surrounding environment.

152 This literature review accordingly reveals that, the modelling of releases from mine tailings
153 overall suffers from a certain lack of representativeness. These limits are moreover present in a
154 context where the legislation around the use of LCA is developing, e.g. through the
155 implementation of the Product Environmental Footprint (PEF). Accurately accounting for the
156 environmental impacts relative to tailings therefore appears crucial, especially for the mining
157 industry, as such impacts may significantly stand out in the LCA of metals-containing products
158 and accordingly affect decisions relative to these products (Rader et al., 2019).

159 In this paper we propose to couple the use of reactive transport modelling (RTM) with LCA to
160 quantify more accurately short-term and long-term releases associated with tailings. In
161 particular, this coupling enables the generation of new data associated with the management of
162 mine tailings (and by extension mining operations), towards more comprehensive and
163 representative LCIs for the mining sector. In fact, the goal of reactive transport modelling is to ,
164 to better understand and represent the distribution in space and time of the chemical reactions
165 occurring in a specific environment (Muniruzzaman et al., 2020). In this study, reactive
166 transport modelling is applied on releases associated with tailings generated in an European
167 copper mine. The results are then compared with the approach used in the ecoinvent database,
168 using both generic and site-specific data. The different compared approaches as well as the
169 considered case study are described in the next chapter. Chapter 3 describes and discusses the
170 results of the comparison between the approaches used to quantify tailings releases to the
171 environment. Chapter 4 concludes on the assessment and provides some perspectives on the
172 coupling between RTM and LCA.

173 2. Materials and methods

174 2.1. Models to consider releases from tailings to groundwater

175 Releases to groundwater resulting from tailing ponds after mine closure can be modelled
176 through different methods. This section presents the three approaches applied in this study to
177 obtain these releases for each substance. These three approaches consider transfer coefficients
178 expressing the fraction of the element presents in the tailings that can be released during a
179 specific time period. From these transfer coefficients the releases are derived using Eq.1 where
180 the initial mass of the substance in the tailings is obtained from on-site data collection (see
181 section 2.2). In this study, the tailings releases are considered over two time frames representing
182 respectively short-term and long-term behaviors (see section 2.3).

183 **Eq.1** $m_i(t) = TK_i(t) * m_{initial,i}$

184 Where $m_i(t)$: mass of substance i released to groundwater over a time period t

185 $TK_i(t)$: transfer coefficient of substance i that can be released during a time period t

186 $m_{initial,i}$: initial mass of substance i in the tailings

187 2.1.1. Generic and semi-specific approach: Use of Doka’s model as applied in the
 188 ecoinvent database

189 The primary ecoinvent dataset “treatment of sulfidic tailings” (Althaus and Doka, 2018) was
 190 developed by Gabor Doka (2017, 2009, 2008), originally to consider releases resulting from
 191 landfills and then adapted for tailings ponds. For each chemical element present in the tailings,
 192 the model defines a $TK_i(t)$ that expresses the cumulative mass fraction released at time t . Generic
 193 TKs were determined for each element based on average tailings composition, leaching
 194 concentration and climatic conditions derived from literature data. In the ecoinvent mining
 195 datasets, these TKs are applied to quantify releases to groundwater following Eq.1 regardless of
 196 the composition of the sulfidic ore mined and the geographic context, thus leading to significant
 197 uncertainty factors associated with these TKs. Indeed, uncertainty values on parameters used to
 198 derive TKs and expressed as GSD vary from 147% to 11500% (Doka, 2017, 2009, 2008). This
 199 dataset “treatment of sulfidic tailings”, is commonly used to model tailings management in
 200 diverse sulfidic ores mining datasets in the ecoinvent database regardless the type of ore mined
 201 or the mine’s geographic location.

202 If generic TKs were used until the release of ecoinvent 3.5, the model developed by Doka could
 203 also be applied to obtain more specific TK associated with a given mine site with a given tailings
 204 composition. This was done for ecoinvent 3.6 in which specific literature data on tailings
 205 composition and climatic conditions of various mine sites were gathered allowing defining TKs
 206 for these specific cases turning the number of datasets concerning the treatment of tailings from
 207 2 in ecoinvent 3.5 to almost 40 (Turner et al., 2019). The model developed by Doka is accessible
 208 through a specific Excel file “Tailings Impoundment 2020” that can be retrieved from doka.ch
 209 website (Doka, 2020). This Excel file allows determining specific TKs over different timeframes.
 210 Depending on the leaking substance, either an exponential model (Eq.2) or a linear model (Eq.3)
 211 is applied. In particular, the linear model is applied to substances that are not easily leached out.
 212 Differences between both models are imperceptible for short time frames but grow larger for
 213 longer period. For a complete description of the models developed, see Doka (2008).

214 **Eq. 2:** $TK_i(t) = TK_{\infty,i}(1 - e^{-(V_{eff} \cdot C_{o,i} / m_{initial,i} \cdot TK_{\infty,i}) \cdot t})$

215 **Eq. 3:** $TK_i(t) = \frac{V_{eff} \cdot C_{o,i}}{m_{initial,i}} \cdot t$

216 Eq.2. represents a first order law of kinetics equation taking into account the initial composition
 217 of the tailings at the end of the active phase (i.e. at mine closure) and the volume of water that
 218 flows through the tailings depending on the site climatic conditions such as rainfall and
 219 evapotranspiration. All the parameters included in Eq.2 and Eq.3 are more specifically described
 220 in Table 1 and can be quantified from on-site data collection (see section 2.2) or using generic
 221 values.

222 Table 1 : Definition of parameters included in Equation 2 and Equation 3, as described in Doka
 223 (2017, 2009)

Parameter	Description	Unit
$TK_{\infty,i}$	Fraction of the observed element i that can be mobilized at the end of the initial active phase, i.e. at the moment of mine closure	kg/kg _{tailings}
V_{eff}	Effective leachate volume, i.e. the water that interacts with the tailings $V_{eff} = \frac{1 - w\%}{\frac{h\delta}{I} - \frac{Tp \cdot w\%}{v\%}}$	liter/kg.year
$w\%$	Share of preferential water flow in the leachate output	%

h	Tailings dam height	m
δ	Tailings density	kg/m ³
I	Rain infiltration rate $I = (MAP - ETa/2) * (1 - e^{-ft(MAT+15)})$	mm/m ² year
MAP	Mean annual precipitation	mm/m ² year
Et_a	Actual evapotranspiration rate	mm/m ² year
ft	Factor for temperature dependence	
MAT	Mean annual temperature	°C
T_p	Residence time of the preferential water flow	year
$v\%$	Water content in the tailings	%
$c_{0,i}$	Mean concentration of the observed element i in the leachate during the first year after the active phase, i.e. after mine closure	kg/l _{leachate}
$m_{initial,i}$	Total amount of the observed element i in the tailings at the end of the active phase, i.e. after mine closure	kg/kg _{tailings}

224

225 In this study, Doka's model will be applied to derive **semi-specific** TKs (referred to as *semi-*
226 *specific scenario*) taking into account the specific composition and climatic conditions of the
227 studied mine site (see section 2.2). These calculated semi-specific TKs and the associated
228 releases will be compared to the ones from the **generic** dataset "treatment of sulfidic tailing, off-
229 site - GLO" (referred to as *generic scenario*) and from the most representative dataset, regarding
230 both the main exploited metal and the climatic conditions, of the mine site under study
231 "treatment of sulfidic tailings, from copper mine operation, tailings impoundment - RU"
232 (**generic, Cu** dataset and referred as *generic, Cu scenario*) both as modeled in ecoinvent 3.6

233 2.1.2. Specific approach: reactive transport models

234 Reactive transport models are used in the mining industry to predict and describe the fate and
235 transport of metals, in particular for tailings ponds, during mine operations or after mine closure
236 in order to assess the associated environmental impacts (Butler et al., 2008; Nordstrom and
237 Nicholson, 2018; Strömberg and Banwart, 1994; Zhu et al., 2001). More specifically, multi-
238 component transport modelling aims at understanding the distribution in space and time of
239 chemical reactions occurring in a specific environment and in particular at the interfaces
240 between the gas, aqueous and solid phases. Steefel and Maher described in details the rationale
241 and the physical and biochemical processes driving transport modelling, which depends on mass
242 transport, heat transport and geochemical reactions (2009). To facilitate the solving of the
243 thermodynamics and kinetics equations that drive the transport phenomena, specific databases
244 on properties of the chemical elements and specific software were developed (Jacques et al.,
245 2008; Lichtner, 2007; Mayer et al., 2002; Steefel, 2009; Thiéry, 2015).

246 In this study, a representative cross-section of the tailings dam under assessment is considered
247 in a 2D model (see Figure 1). In this cross-section, several hydrogeochemical units are
248 considered, each with their specific properties: porosity, permeability, dispersivity,
249 mineralogical composition and pore water chemical composition. The numerical model applied
250 is the coupled reactive transport simulator MARTHE-PHREEQC (Thiéry, 2015) that couples a
251 geochemical code, PHREEQC (Parkhurst and Appelo, 2013; Parkhurst and Wissmeier, 2015), to a
252 flow and mass transport code MARTHE (Thiéry, 2013; Thiéry and Picot-Colbeaux, 2020). This
253 coupling, described in details as applied in this study in Lassin et al. (2021a), allow the
254 simulation of chemical elements' fate in the modelled system and in particular their fate at the
255 boundary between the system, the tailings ponds, and the environment. At the outlet of the
256 system (Figure 1), releases into the groundwater are quantified. The groundwater is
257 consequently considered as the final receiving compartment. More specifically, this coupling

258 allows simulating the aqueous concentration of the studied chemical elements at the inlet and
 259 outlet of the system at each simulated time step, permitting to determine the concentration at
 260 the outlet and the cumulated mass outflow at a certain timeframe. However, the concentration at
 261 the outlet results both from the presence of the tailing pond and its leakages and the initial
 262 concentration of the studied substances in the environment. In order to quantify the
 263 concentration variation induced by the presence of the tailings ponds only, the difference
 264 between the outlet and the inlet cumulated concentrations as reported in Lassin et al. (2021a) is
 265 calculated and used to derive the specific TKs following Eq.4. and Eq.5. for which the specific
 266 data are available in the Supplementary Information.

267 Applying Eq.1 to these TKs will lead to **site-specific releases** (referred to as *site-specific*
 268 *scenario*) resulting from the tailings.

269

270 **Eq. 4:**
$$m_i(t) = \frac{(c_{outlet,i}(t)*M_i - c_{inlet,i}(t)*M_i)*1000}{m_{total}}$$

271 **Eq. 5:**
$$TK_i(t) = \frac{m_i(t)}{m_{initial,i}}$$

272 With: - $c_{outlet,i}$ and $c_{inlet,i}$ the cumulated outflows at the year t of the observed substance i
 273 respectively at the outlet and at the inlet of the system (expressed in mol);

- 274 - M_i : the molar mass of the observed substance i (expressed in g/mol);
- 275 - m_{total} : The total mass of tailings (expressed in kg);
- 276 - $m_i(t)$: the mass at the year t of the observed substance i that is effectively leached out;
- 277 - $m_{initial,i}$: Total amount of the observed element i in the tailings at the end of the active
 278 phase, i.e. after mine closure (in kg/kg_{tailings})

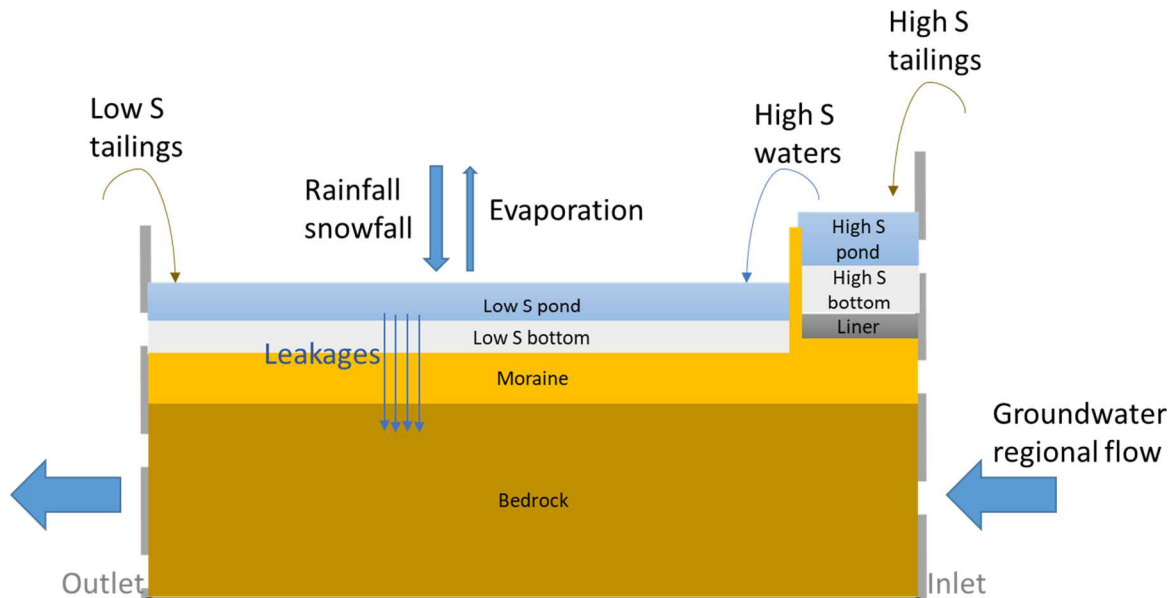


Figure 1 : Simplified vertical cross-section of the system under study showing the different flows considered, adapted from Lassin et al. (2021a). The different layers are representative of the site's morphology

279 **2.2. Case study and data**

280 This study aims at analyzing specific methodological issues, the coupling between RTM and LCA.
 281 In line with the ILCD Handbook recommendations, this study therefore does not specifically
 282 meet the ISO 14040/14044 requirements. (ILCD, 2010). More particularly, only the post-closure

283 tailings releases to the groundwater are considered in the scope of the study. As the specific
 284 modeling of air emissions as dust due to climatic conditions are outside the scope of the paper
 285 they are not considered here. Similarly, tailings management systems that can be put in place
 286 after closure are also not considered: in a conservative approach where no actions are supposed
 287 to be taken to limit tailings releases, they are considered out of the scope of this study.

288 The quantified releases are related to a mine site located in Northern Europe, which currently
 289 exploits a polymetallic sulphidic ore. The operators of this site provided access to the required
 290 data, in the frame of multi-partners R&D project funded under the European H2020
 291 program. The exploited ore leads to copper and nickel as a primary concentrates and some other
 292 metallic concentrates as co-products. The tailings generated during the mineral processing steps
 293 are mainly wastes from flotation operations, where flotation uses chemical reagents and water
 294 to separate and concentrate the minerals of interest using the hydrophobic and hydrophilic
 295 properties of materials. Here, post-closure tailings releases are modelled using the three
 296 approaches considering a short term and a long term timeframe (see section 2.3). The releases
 297 are related to the specific functional unit “The post-mining storage of 1 kg sulfidic tailings
 298 resulting from the exploitation of a polymetallic ore. In the absence of information as to potential
 299 future post-mining operations, it is decided in this study to not consider any tailings
 300 management operations that could potentially limit releases to groundwater from tailings in the
 301 long-term. Different datasets are needed to apply Eq.1 in the different approaches. Table 3
 302 provides a summary of the data and their sources needed to perform the TKs calculation for
 303 each scenario. The first dataset is the initial tailings composition (i.e. $m_{initial,i}$) given in Table 2.
 304 This composition is quantified based on the assessment of the tailings mineralogical
 305 composition using QXRD (quantitative X-Ray Diffraction) on a specific tailing sample and is used
 306 for the *semi-specific* and the *site-specific scenarios*. When available for the mine site, data needed
 307 to derive Eq.2 for the *semi-specific scenario* were used. The specific term $c_{o,i}$ is obtained from the
 308 simulation conducted by Lassin et al. (2021a). If data are not available from the mine site nor
 309 from the simulation conducted by Lassin et al. (2021a), by default values used in Doka’s model
 310 are considered, cf. Table 1 and Table 3 (Doka, 2020, 2008). The quantification of Eq.2
 311 parameters as well as the data sources are available in the Supporting Information. All data used
 312 to simulate the TKs using the reactive transport model are also available in the Supporting
 313 Information as well as in Lassin et al. (2021a).

314

315 Table 2 : Composition of the tailings assessed in this study, this composition was obtained using
 316 analytical techniques on site samples (QXRD)

Element	Symbol	$m_{initial,i}$ (kg / kg _{tailings})
Sulfur	S	5.63E-3
Copper	Cu	5.19E-3
Silicon	Si	2.12E-01
Iron	Fe	1.70E-01
Calcium	Ca	9.71E-2
Aluminium	Al	1.26E-2

Potassium	K	4.61E-3
Magnesium	Mg	9.25E-2
Nickel	Ni	7.08E-4
Sodium	Na	6.16E-4

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Table 3 : Summary of the data and their sources needed to perform the assessment for each approach

	Generic	Generic, Cu	Semi-specific	Site-specific
Initial composition $m_{initial,i}$	Data from Turner et al., (2019)	Data from Turner et al., (2019)	Data coming from on-site sampling, see Table 2	Data coming from on-site sampling, see Table 2
Parameters to estimate $TK_i(t)$	Data from Turner et al., (2019)	Data from Turner et al., (2019)	TK_{∞} , $w\%$, T_p , $v\%$, ft : Generic data available in (Doka, 2017) $c_{0,i}$: Simulated data Lassin et al. (2021a) h , δ , MAP , Eta , MAT : Values obtained from the mine site	Reactive transport modelling as described in Lassin et al. (2021a)
Model used to estimate $TK_i(t)$	First order law of kinetics: Equation 2 resolved using (Doka, 2020)	First order law of kinetics: Equation 2 resolved using (Doka, 2020)	First order law of kinetics: Equation 2 resolved using (Doka, 2020)	Reactive transport modelling: Equation 5 resolved using model from Lassin et al. (2021a)

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In the context of LCA, specific limits exist in the quantification of the impacts associated with metals emissions, especially on impacts related to ecotoxicity. First, not all LCIA characterization models provide characterization factors for the same metals, and not all metals are characterized. Then, metal speciation is often not considered (Aziz et al., 2018; Plouffe et al., 2016). In order to investigate these aspects in the present study, the releases determined from the three approaches will be characterized using in a first place the EF LCIA method that is the method used in the European environmental footprint initiative and recommended by the European Commission (Fazio et al., 2018). The EF method based the calculation of toxicity and ecotoxicity impacts on the USEtox 2.1 model. To assess the effects of the choice of the LCIA method on the comparison results, two other methods will be used to characterize the releases: the EDIP LCIA model with its specific characterization model (Hauschild and Potting, 2005) and the ReCiPe LCIA method that is based on the USES-LCA characterization model for the toxicity and ecotoxicity impacts (Huijbregts et al., 2017). The applied characterization factors are available in the Supplementary Information. Furthermore, considering the EF characterization

335 method, recommendations from the European Commission to discard long-term releases
336 (beyond 100 years) in the impacts calculations for the three assessed impact categories (“Non
337 cancer human health effects”, “Cancer human health effects” and “Ecotoxicity”) are followed
338 (Fazio et al., 2018). That should be kept in mind when interpreting the results, if long-term
339 releases are quantified, they are not characterized using the EF method, only short-term releases
340 are. In other terms, for both the short-term and the long-term perspectives (see section 2.3),
341 only the cumulated emitted masses in the short-term time frame are characterized with the EF
342 method. For other methods, long-term releases are characterized.

343 2.3. Considered timeframes

344 In the approach applied in ecoinvent, transfer coefficients are calculated for two different time
345 horizons: 100 and 60,000 years. The 60,000 year-timeframe was chosen as it represents an
346 “ecological planning horizon” at which landscape and ecospheres would be redefined (for
347 example Swiss landscapes might be recovered with glaciers). The damages implied by diffuse
348 pollution as we know it will also be redefined (Doka, 2008). Doka also underlined that a 60,000
349 year-timeframe represents a conservative approach in the quantification of long-term releases
350 associated with a tailings dam (2008). In this study, the 100 year-timeframe is kept to consider
351 the short term perspective. However, for the long term perspective, a 10,000 year perspective is
352 preferred. This choice is justified by two considerations. Firstly, if for the generic and the semi-
353 specific TKs determination, the chosen time frame has no incidence, this is not the case for the
354 site specific TKs obtained by simulation. In fact, complex computer simulations
355 require significant computational resources, from 6 to 24 hours of computer calculations
356 depending on the initial considerations. Here the 10,000 year-timeframe is chosen as a
357 compromise between simulation time and representation of a long-term perspective. Secondly,
358 results in Lassin et al. (2021a) show that, for each followed parameter (water inflow and
359 outflow rates, pH, and substances’ concentration) a steady state value seems to have been
360 reached out after around a 1,000 year-timeframe. Finally, to simplify the modelling, it is
361 assumed that no rehabilitation actions are done during these timeframes.

362 3. Results and discussion

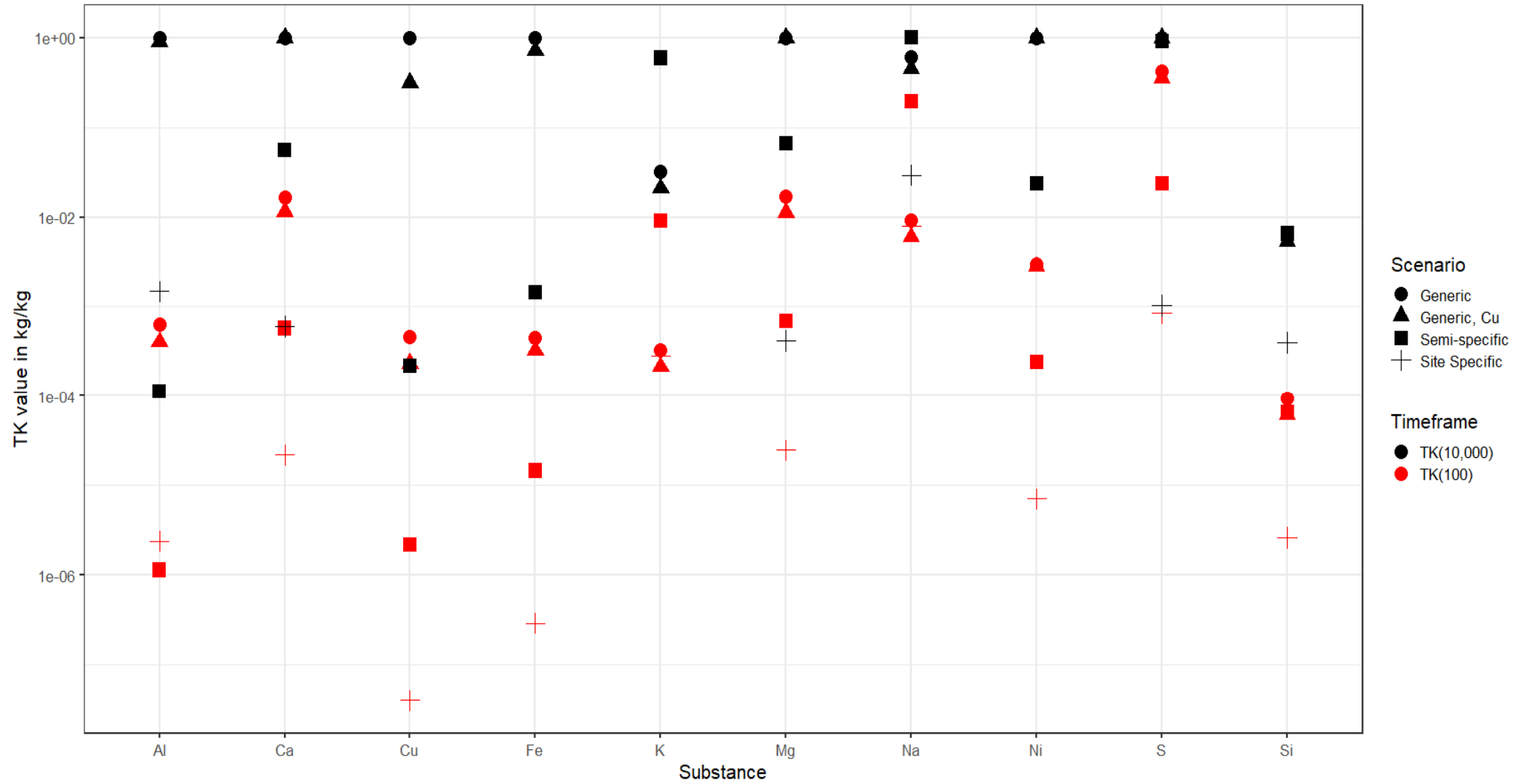
363 3.1. Resulting TKs and impacts

364 Figure 2 presents the TKs obtained for the four scenarios and for the short-term and the long-
365 term timeframes. The graphically represented TKs are the ones that correspond to the substance
366 initially present in the studied tailings (cf. Table 2). When looking at the scenario ‘Generic’
367 (linked to the ecoinvent dataset “treatment of sulfidic tailing, off-site – GLO”) or ‘Generic, Cu’
368 (linked to the ecoinvent dataset “treatment of sulfidic tailings, from copper mine operation,
369 tailings impoundment – RU”) for which the model as applied in ecoinvent 3.6 are used, TKs are
370 available for a larger amount of substances. In fact, they are available for substances present in
371 the average tailings composition considered in the Doka model (Turner et al., 2019). These
372 generic TKs values are reported in the Supplementary Information.

373 The long-term TKs for four substances, calculated for the ‘site specific’ scenario are not
374 represented in Figure 2: copper, potassium, nickel and iron. These TKs, which are based on
375 reactive transport modelling, are obtained through the difference of masses between the outlet
376 and the inlet of the system (cf. Figure 1). In this case study, these four cumulated substances
377 flows at the inlet are larger than at the outlet (see Supplementary Information) showing that,
378 over the long term, the regional groundwater will be naturally more charged than the water
379 coming out of the tailings. Indeed, the surrounding groundwater are representative of the local
380 geochemical background which, in this case, is characterized by high contents in copper and
381 nickel. That means, that in a long timeframe, the presence of the tailings would not influence the

382 concentration of these four substances in the groundwater Conversely, at a shorter timeframe,
383 the TKs for these four substances are positive, leading to their short-term release, as illustrated
384 in Figure 2 and in the Supplementary information.

385



386

387

Figure 2: Resulting short-term and long-term TKs for the four studied approaches, log-scale

388 The TKs obtained through Doka's formula using site specificities ('semi-specific') or through
389 transport modelling ('site specific') are often much smaller than the ones obtained using generic
390 values except for sodium and potassium, for which values from the semi-specific scenario are
391 larger than the generic values in both short-term and long-term. This might be due to the
392 parameter $c_{0,i}$ (average leachate concentration, see Table 1) that differs from two to three orders
393 of magnitude between the values used in ecoinvent that were obtained from a literature survey
394 and the ones used in the semi-specific approach that were obtained through reactive transport
395 simulations (see Table 3 and Supplementary Information). The differences between generic and
396 site specific TKs vary from zero (e.g. sodium, potassium) to four orders of magnitude (e.g.
397 copper) in a short-term timeframe. The differences between 'site specific' and 'semi-specific' TKs
398 result from the model employed to derive these values: a first order law of kinetics in the case of
399 the 'semi-specific' TKs and reactive transport modelling in the case of the 'site specific' TKs.
400 These differences in the TKs values translates into differences in the cumulative masses of
401 substances released, and therefore also in the calculated impacts. Regarding the mass released
402 (results in Supporting Information), the reactive transport modelling leads to quantities
403 released in both short-term and long term time perspectives smaller than masses calculated by
404 Doka's model, except for aluminum and potassium at short term. For these two substances, the
405 difference does not exceed an order of magnitude. As a result, the impacts of the site-specific
406 scenario are smaller than the impacts calculated for the three other scenarios for every
407 characterization methods and impact categories. These impacts are presented in Table 4.
408 Besides being driven by differences in the models themselves, the orders of magnitude of
409 differences between the impacts of the Generic/Generic, Cu scenarios and the Semi-specific/Site
410 specific scenarios are also driven by the number of substances considered as released in both
411 groups of scenarios. In fact and as stated above, in Doka's model for the "Generic" and the
412 "Generic, Cu" scenario it is assumed that a larger amount of substances are initially present in
413 the tailings. In other terms, the initial tailings composition in the "Generic" and the "Generic, Cu"
414 scenarios, is assumed different from the on-site *real* composition.
415 Nickel and copper are the only contributive substances to the impacts when looking at the
416 "semi-specific" and the "site-specific" scenarios and at the EF method. This is due to the fact that
417 they are the only substances present initially in the assessed tailings pond that are characterized
418 in the EF method. Looking at these two scenarios, this is the same for ReCiPe, while in EDIP, iron
419 and aluminum complete this list of contributive substances because both present in the tailings
420 and characterized. If for the EF method only short term emissions are considered in the
421 characterization results (see Section 2.2), this is different for EDIP and ReCiPe where
422 characterized results differ for the short-term and the long-term perspectives (see Table 4). For
423 all scenarios and all impact categories, as expected, long-term impacts are greater than in a
424 short-term perspective by up to 4 orders of magnitude; except for ReCiPe and the "Site-specific"
425 scenario. This is due to the fact, as said earlier, that only copper and nickel are characterized in
426 ReCiPe and that in the long-term the presence of the tailings does not influence the
427 concentration of these substances in the environment.
428 However, when assessing the results obtained by the EF characterization methods for the
429 "Generic" scenario, respectively 99.9%, 96.6% and 70.5% of the impacts for the categories "Non-
430 cancer human health effects", "Cancer human health effects" and "Ecotoxicity" are driven by
431 other substances, mainly zinc, arsenic and chromium VI. These substances that are not initially
432 present in the tailings under study but assumed to be present in the average tailings
433 composition are used to derive TKs for the "Generic" scenario. Figure 3 shows the specific
434 contribution of such substances not present in the tailings generated by the mine under study
435 for the "Generic" and "Generic, Cu" scenarios.
436

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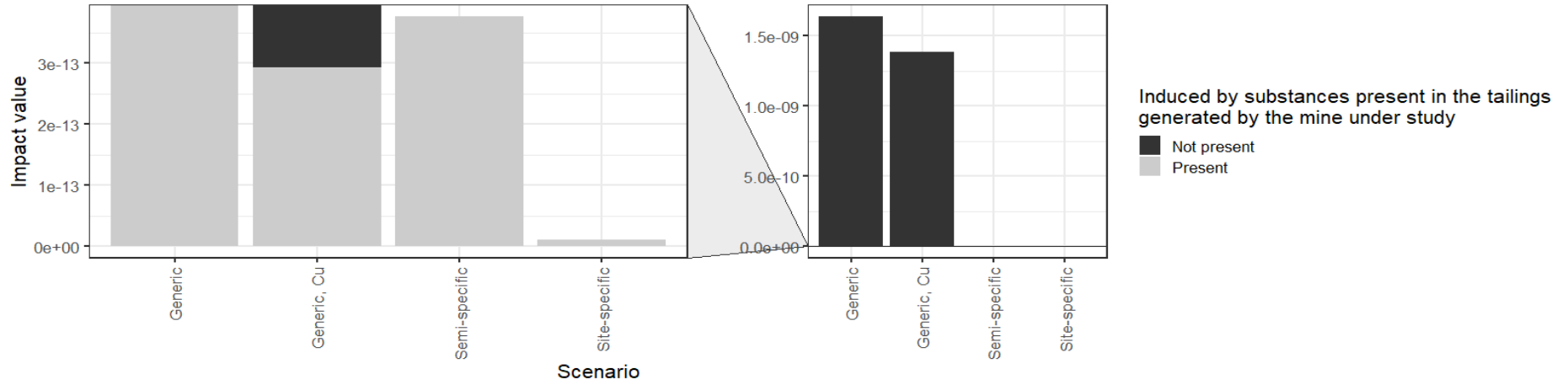
Table 4 Resulting characterized toxicity and ecotoxicity impacts per kg of tailings for the four studied scenarios for both the short term (ST) and the long term (LT) perspectives

Method	Impact	Units	Scenario			
			Generic	Generic, Cu	Semi-specific	Site-specific
EF (both ST and LT)	Non-cancer human health effects	CTUh	1.64E-09	1.39E-09	3.77E-13	1.10E-14
	Cancer human health effects	CTUh	9.19E-11	5.99E-11	6.53E-12	1.92E-13
	Ecotoxicity freshwater	CTUe	6.01E-02	4.52E-02	3.17E-03	8.69E-05
EDIP (ST)	Human toxicity water	m ³	1.32E-01	8.41E-02	3.12E-04	6.22E-06
	Ecotoxicity water chronic	m ³	8.32E00	5.50E00	4.59E-01	1.40E-02
	Ecotoxicity water acute	m ³	1.64E+02	1.38E+02	4.66E-02	2.83E-03
EDIP (LT)	Human toxicity water	m ³	2.86E+02	7.80E+01	3.12E-02	3.66E-05
	Ecotoxicity water chronic	m ³	1.12E+04	5.27E+03	4.58E+01	2.51E+00
	Ecotoxicity water acute	m ³	1.83E+03	1.21E+03	4.65E+00	1.14E+00
ReCiPe (ST)	Terrestrial ecotoxicity	kg 1.4-DCB	1.61E-20	1.28E-20	6.11E-22	1.68E-23
	Freshwater ecotoxicity	kg 1.4-DCB	2.62E-04	2.08E-04	9.68E-06	2.66E-07
	Marine ecotoxicity	kg 1.4-DCB	3.59E-04	2.89E-04	1.19E-05	3.29E-07
	Human carcinogenic toxicity	kg 1.4-DCB	6.53E-05	4.26E-05	3.89E-06	1.14E-07
	Human non-carcinogenic toxicity	kg 1.4-DCB	9.24E-03	7.91E-03	7.83E-07	2.27E-08
ReCiPe (LT)	Terrestrial ecotoxicity	kg 1.4-DCB	9.83E-18	5.21E-18	6.05E-20	0.00E+00
	Freshwater ecotoxicity	kg 1.4-DCB	1.59E-01	8.46E-02	9.59E-04	0.00E+00
	Marine ecotoxicity	kg 1.4-DCB	2.01E-01	1.12E-01	1.18E-03	0.00E+00
	Human carcinogenic toxicity	kg 1.4-DCB	4.45E-03	4.15E-03	3.84E-04	0.00E+00
	Human non-carcinogenic toxicity	kg 1.4-DCB	2.08E+00	2.03E+00	7.74E-05	0.00E+00

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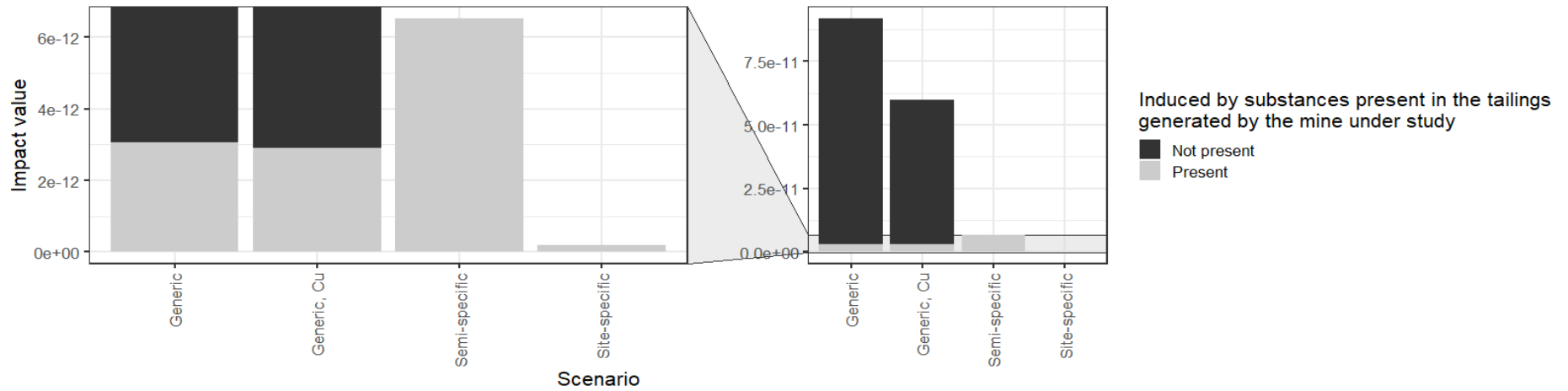
Non cancer human health effects

CTUh



Cancer human health effects

CTUh



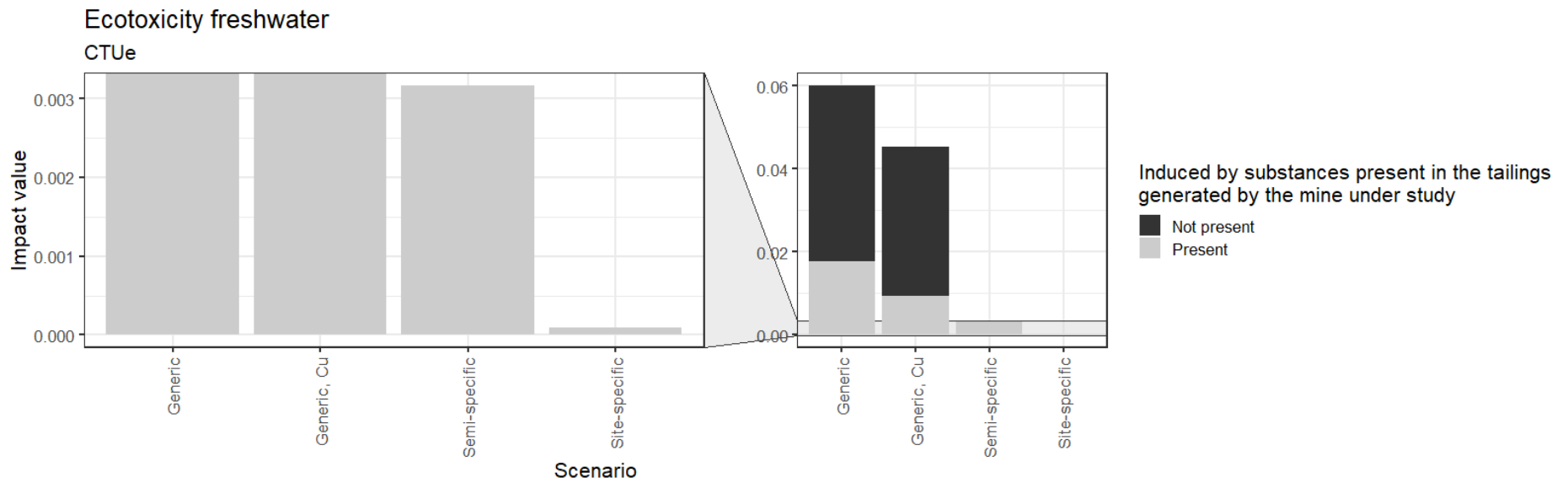


Figure 3 : Representation of the resulting toxicity and ecotoxicity impacts per kg of tailings using the EF method and for a 100 year-time frame. The left graphic is a zoom in of the representation of the right graphic window.

440 Results presented in both Table 4 and Figure 3 show large differences between the different
 441 scenarios, with a maximizing trend when looking at the 'Generic' and the 'Generic, Cu' scenarios
 442 based on a first order law of kinetics equations and a minimizing trend when looking at the 'Site-
 443 specific' scenario based on reactive transport modelling. More specifically and as summarized in
 444 Table 4, comparing results from the 'Site specific' scenario and the 'Semi-specific' scenario
 445 underlines the differences implied by the model used to quantify the releases associated with
 446 the tailings from the same initial composition dataset. When using a model based on the first
 447 order law of kinetics ('Semi-specific' scenario), resulting impacts are overestimated from 0 to 4
 448 orders of magnitude compared with the ones obtained through reactive transport modelling.
 449 Comparing results from the 'Generic' scenario and the 'Semi-specific' scenario underlines the
 450 differences implied by the use of different initial data conditions used in a same model
 451 framework. In this case, the differences vary from 1 to 5 orders of magnitude. Mainly, differences
 452 between 'site-specific' and 'semi-specific' scenarios are less or as significant as between 'generic'
 453 and 'semi-specific' scenarios showing here the importance to consider the proper tailings
 454 mineralogical composition when assessing its environmental impacts. However, this conclusion
 455 should be considered with caution as only one case study is assessed here.

456 3.2. Representativeness of tailings releases modelling approaches

457 Table 5 : Data and approaches used to quantify the long-term releases associated with tailings

		GENERIC and GENERIC, Cu SCENARIO	SEMI-SPECIFIC SCENARIO	SITE-SPECIFIC SCENARIO
<i>Tailings characteristics</i>	<i>Initial composition</i>	Average data representing worldwide mining sites (representing Russian copper mining sites in case of the scenario 'Generic, Cu')	Site specific data	Site specific data including mineralogical composition
	<i>Initial leachate</i>			Site specific data
	<i>Dimensions</i>			
	<i>Density</i>			
<i>Environmental parameters</i>	<i>Climatic conditions</i>	Not considered	Not considered	Site specific data
	<i>Underground layers composition</i>			
	<i>Regional groundwater flow</i>			
<i>System hydrodynamics</i>		Modeled using a first order law of kinetics considering only climatic waters		Modeled using MARTHE considering all waters inputs and outputs
<i>Geochemical interactions including mass and heat transport</i>		Not considered	Not considered	Modeled using PHREEQC associated to the THERMODDEM database as well as MARTHE

458

459 Table 5 summarizes the different elements that are effectively considered in each scenario.
 460 Every scenario differs in terms of data needed to run the model and in terms of sophistication of

461 the considered model. If for the 'Generic' and the 'Generic, Cu' scenarios, resulting releases are
462 directly available in the ecoinvent database, for the 'semi-specific' scenario, a data collection
463 considering the site tailings characteristics and climatic conditions is necessary to perform the
464 calculation manually or using Doka's dedicated Excel's file (2020). More initial data as well as
465 competencies in modelling hydrogeochemical systems are needed in the case of the reactive
466 transport model ('Site-specific' scenario). Using a more sophisticated model helps reduce the
467 uncertainty associated with the model in the obtained results. It also allows a better
468 understanding and therefore interpretation of the resulting tailings releases. For example,
469 applying the reactive transport modelling to the studied tailings, Lassin et al. concluded that the
470 level of releases is quite small as there is a progressive dilution of tailings waters (with the
471 inputs of climatic waters and the regional groundwater flow) (2021a). Moreover, Lassin et al.
472 also explain the individual substances emission behavior based on the model results, for
473 example here aluminum is released in concordance with a pH rise in the system, induced by the
474 dissolution of carbonate minerals that leads to the dissolution of aluminate and aluminosilicate
475 minerals (2021a).

476 If model uncertainty can be reduced using more sophisticated models, another source of
477 uncertainty is parameter uncertainty. In the 'Generic' scenario based on the ecoinvent generic
478 dataset, the uncertainty, expressed in terms of a geometric standard deviation (GSD), associated
479 with the resulting long-term releases varies between 100 % and 3,158 %. This parameter
480 uncertainty takes into account uncertainty associated with the considered waste composition
481 and the TKs calculations (Doka, 2020). Expressing uncertainty in terms of GSD implies
482 expressing the uncertainty as following: there is a 95% chance that the studied value belongs to
483 the interval $[\mu_g/GSD; \mu_g * GSD]$ where μ_g expresses the geometric mean. Thus, a GSD value of
484 3,158% implies quite a large interval where maximal values might not even be physically
485 reached (for explanation on uncertainty as defined and expressed in the ecoinvent database see
486 Muller et al. (2016). Parameter uncertainty can be reduced using on-site data, as it has been
487 done here in the 'Semi-specific' scenario. However, if the parameter uncertainty is expressed for
488 the datasets available in the ecoinvent database ('Generic' and 'Generic, Cu' scenarios), it was not
489 quantified for on-site parameters leading to no quantification of the uncertainty reduction
490 potential associated with the use of more reliable data. Even if parameter uncertainty remains in
491 on-site data (due to the data acquisition method for example, see next paragraph), one may
492 consider such data as less uncertain compared to data coming from average mining sites drawn
493 from literature.

494 Despite reactive transport modelling provides sound bases for understanding coupled processes
495 and thus improve predictions (Glassley et al., 2003; Steefel and Maher, 2009; Steefel et al., 2015,
496 2005), uncertainties must also be reported for more mechanistic and site specific models for the
497 following reasons. *i)* The whole set of site-specific data required for a fully comprehensive
498 reactive transport model may never be available at the scale of the mining site and over
499 sufficient time frames to calibrate unequivocally the model. However, one can expect that the
500 site-specific information about the mineralogical data will be more systematically acquired, and
501 thus made available for numerical simulations, thanks to the development of on-site
502 characterization tools aimed at optimizing the exploitation of the mines (Dold, 2017). *ii)*
503 Measured data are inherently error-prone. In particular, chemical data are measured at the lab,
504 on samples taken on site. More specifically, aqueous solutions properties may have evolved in
505 the meantime because of their extraction from the field. *iii)* Simplifying assumptions are made in
506 order to help the numerical convergence, speed-up the calculations, or because not all of the
507 numerous ongoing processes are fully understood or identified. *iv)* Property values reported in
508 thermodynamic and kinetic databases are also characterized by uncertainty or could be missing.
509 For all these reasons, even if reactive transport modelling improves the estimation of the release

510 of chemical elements from tailings ponds compared to more generic approaches, its results must
511 also be considered with caution.

512 The timeframe considered for estimating long term releases, namely 10,000 years, is also a
513 matter of discussion since there is no such model capable of predicting the evolution of climate
514 and its consequences on surficial facilities over such long time durations. Such a timeframe can
515 possibly be considered for contexts where only geological times apply, as in the case of nuclear
516 waste storage in deep geological sedimentary layers that are known to not have evolved for
517 million years. For shallow or surficial facilities, as here, a shorter timeframe should lead to more
518 reliable results. Limits of current impact characterization methods with respect to tailings
519 releases

520 In the context of LCA, specific limits are identified when quantifying impacts of metals releases,
521 especially on ecotoxicity and toxicity. A first limit is the consideration of metals fate in
522 characterization mechanisms. Ecotoxicity characterization models, and especially terrestrial
523 ecotoxicity models, do not take into consideration metal speciation and the soil and water
524 properties that can affect this speciation, and so the potential toxicity of the metals (Aziz et al.,
525 2018; Plouffe et al., 2016). A second limit is the completeness of characterization methods
526 regarding metals. Not all metals are characterized in each method. In the ecotoxicity and toxicity
527 impacts considered here, in average almost 60% of the released substances (of the total
528 considered for the 'Generic' and the 'Generic, Cu' scenarios) are not characterized. This is the
529 case for substances such as aluminum and iron for the EF characterization model for example;
530 despite their TKs value, characterization factors for these substances are not available in EF.
531 This percentage varies both per characterization method and impact category. Given these
532 limits, in USEtox, the characterization method recommended by the Product Environmental
533 Footprint program of the European Commission for the ecotoxicity and toxicity impacts,
534 characterization factors applied to metals are considered as interim ones. Moreover, the
535 European Commission recommends to discard long-term releases for the three impact
536 categories assessed using USEtox characterization model: 'Human toxicity, cancer effect',
537 'Human toxicity, non-cancer effect' and 'Ecotoxicity' (Fazio et al., 2018). This recommendation
538 has been followed in this work meaning that long-term releases (i.e. beyond 100 years) are not
539 characterized in the EF method in Table 4 and Figure 3. This fact has to be kept in mind when
540 interpreting results using this method.

541 4. Conclusions and perspectives

542 This work presents different approaches to quantify releases resulting from tailings in the
543 mining sector. Using these approaches allow assessing the effect of using more representative
544 data and model sophistication when quantifying the tailings releases and their associated
545 impacts. In this specific case study, large differences in the results are observed when comparing
546 a simplified model coupled with generic data and a more complex model coupled with site-
547 specific data. The latter being associated with much smaller calculated impacts. More
548 specifically, the more complex model considers on-site information to define the tailings
549 characteristics and the environmental parameters in combination with both the system
550 hydrodynamics and the geochemical interactions occurring in the system (see Table 5). Results
551 differ by two to eight orders of magnitude depending on the considered characterization model
552 and impacts categories. Each of the approaches have pros and cons. While more reliable results
553 may be brought by reactive transport models, their accuracy depend on the access to specific
554 data from the mine site and on the required time and competencies to run the model. While
555 generic data and models used in LCI database are less representative of a certain reality, they
556 give nonetheless an idea of potential impacts induced by mining. In fact, no matter the value
557 chain assessed in a LCA study, there is a good chance that production of metals and so the

558 mining and the beneficiation of the associated ores are part of this value chain somewhere in the
559 background system. In this case, the practitioner or the study sponsor have no access to the
560 specific mine site and to the specific value chain of the metals present in the system. In this
561 absence of specific knowledge of the background, using generic data allows quantifying these
562 impacts rather than ignoring the potential significant impacts in the life cycle of the system
563 under study. Finally, this coupling allows to generate more robust and reliable data regarding
564 releases from tailings and thus to generate more reliable and complete mining LCI datasets.

565 One common assumption to the different approaches is the time duration used for the long-term
566 perspective. In each approach, the model was applied in a 10,000 year time perspective without
567 considering changes such as climatic variations that can possibly occur in this time frame.
568 Results expressed in this long term time perspective must therefore be seen as a tendency rather
569 than a reliable quantification of long-term releases associated with tailings.

570 Thus, the use of the ‘appropriate’ model and/or the ‘appropriate’ data is a consensus to find
571 between the quality of the study to reach and as defined in the goal and scope, the data
572 availability and the availability of the ‘right’ competency to mobilize. The availability of the
573 ‘right’ competency also underlines the necessity of an interdisciplinary approach when
574 modelling complex systems in LCA and especially for dealing with data gaps. For example,
575 hydrogeologists can help the practitioner having a better model to consider specific emissions to
576 the environment, while process simulations can help closing data gaps regarding specific
577 exchanges at the level of the unit operations (Segura-Salazar et al., 2019).

578 The conclusion of this study was drawn on a single case-study in a specific climatic context.
579 Therefore the considerations on the reliability associated with the use of a simplified model and
580 generic data cannot directly be generalized. In order to draw some generalizations, the same
581 study should be conducted on various mine sites having differences in the treated ores and in
582 the operating climatic conditions, especially regarding precipitations and evapotranspiration).

583 A more precise evaluation of tailings releases over time is crucial, not only to assess their
584 potential environmental impacts but also to have a better estimate of what remains in the
585 tailings. Knowing the characteristics of tailings in terms of mineral composition can bring
586 arguments against or in favor of tailings reprocessing. In fact, during the exploitation, some
587 elements are not recovered because of the absence of economic viability of their exploitation
588 (processing costs might be too important compared to the market prices). Because of metals
589 market prices fluctuations and processes costs reduction through process amelioration for
590 example, these substances present in the tailings could be seen as secondary raw materials
591 resources in a short to long timeframe depending on their concentration in the tailings dam.

592 These considerations on metals releases to the environment versus the fact that they potentially
593 remain in the technosphere in a tailings dam are in line with discussions occurring today in LCA
594 around the area of protection “Resources” and in particular regarding resources dissipation. The
595 quantification of resources dissipation, in other words resources losses, is still subject to
596 methodological discussions today in LCA. Being able to quantify long-term metals behavior in
597 tailings, as done here, is a result that can be used in the quantification of resources dissipation in
598 the mining stage of a metal life cycle.

599

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