Life cycle inventory data for critical mineral mining: Recommendations and new U.S. data compendium

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1. Estimating ecotoxicity, human health-cancer, and human health-noncancer values for select compounds

Some chemical or metal species that mines emit as reported in the Toxic Releases Inventory (TRI) and National Emissions Inventory (NEI) are not included within the Tool for Reduction and Assessment of Chemicals and Other Environmental Impacts (TRACI) based on chemical abstract service (CAS) number. These species therefore do not have a unique toxicity characterization factor (CF). This was especially true of more complex molecules, like volatile organic compounds and compounds that contain metal ions. We implemented one of three strategies for filling these data gaps for each IC:

1) *We omitted these compounds from the analysis.* Releases of metal-containing compounds or other general classes of chemical compounds that didn't specify the chemical identity of the compound were excluded. An example is "manganese compounds." An example of non-metal containing compounds is polycyclic aromatic compounds. This type of chemical and metal-containing compound reporting in the TRI did not allow us to match the emissions with a characterization factor. We therefore assumed a CF of zero.

2) *We used a best-case proxy value.* For metal-containing compounds, we used the lowest CF of that metal among the oxidation states reported in TRACI. For organic compounds, the lowest CF of a compound with the same element as the generic compound (e.g., arsenic compounds) within the generalized group was used (e.g., arsenic (III) for arsenic compounds for ecotoxicity CF to freshwater from air emissions or ethylene glycol for VOCs for human health cancer CF for emissions to freshwater).

3) *We used a worst-case proxy value.* The highest respective TRACI value of a compound with the same element as the generalized group or of a compound within the generalized group was used (e.g., arsenic (IV) for arsenic compounds for ecotoxicity to freshwater from air emissions or 1,3-butadiene for VOCs for human health cancer CF for emissions to freshwater).

Corresponding compounds that were considered for scenarios 2 and 3 are listed in Table S1. We note that the compound that fit the criterion for scenario 2 sometimes was, but not always, the same compound that fit the criterion for scenario 3. Also, some generalized compound groups did not have any corresponding substances in TRACI, namely, manganese compounds and cyanide compounds. The CFs for these groups were assigned as zeroes. For many of the organic compounds, the list below is not comprehensive of all chemicals. However, we limited our list to those that had data entries within TRACI and are common pollutants from mining and/or diesel combustion.[1–6]

These scenarios allowed us to determine a range of total impact on ecotoxicity (ECO), human health-cancer (HHC), and human health-noncancer (HHNC) across the critical mineral mines.

Table S1. Corresponding TRACI Compounds by Generalized Compound Group

Type	Generalized Compound Group	Corresponding TRACI Compounds
Metal	Antimony Compounds	Antimony (III), Antimony (V)
	Arsenic Compounds	Arsenic (III), Arsenic (IV)
	Beryllium Compounds	Beryllium (II)
	Cadmium Compounds	Cadmium (II)
	Chromium Compounds	Chromium (III), Chromium (VI)
	Cobalt Compounds	Cobalt (II)
	Lead Compounds	Lead (II)
	Manganese Compounds	No manganese compounds in TRACI
	Mercury Compounds	Mercury (II)
	Nickel Compounds	Nickel (II)
	Selenium Compounds	Selenium (IV)
Organic	Cresol/Cresylic Acid (Mixed Isomers)[6]	4,6-dichloro-o-cresol, 4,6-dinitro-o-cresol, Cresol(s), Cresyl diphenyl phosphate, m-Cresol, o-Cresol, p-Cresidine, p-Cresol, Tri-m-cresyl phosphate, Tri-o-cresyl phosphate, Tricresyl phosphate
	Cyanide Compounds	No cyanide compounds in TRACI
	Polycyclic Organic Matter[1,2]	1-methylnapthalene, 1,3-dimethylnapthalene, 2,3-dimethylnapthalene, Benzo[A]pyrene, Pyrene, 2-acetylaminofluorene, 9H-fluorene-9-carboxylic acid 2-chloro-9-hydroxy fluorene, n-hydroxy-n-acetyl-2-aminofluorene
	Volatile Organic Compounds (VOC)[3–5]	1,3-Butadiene, Benzene, Ethylene glycol, Formaldehyde, Tetrachloroethanes, Toluene
	Xylenes (Mixed Isomers)	m-Xylene, o-Xylene, p-Xylene, Xylenes

2. Statistical correlations

We investigated correlations between emissions, production, and impacts. We probed linear correlations as we hypothesized that an increase in production would result in an increase in emissions. However, there are no correlations between emissions, production, and impacts. We tried fitting other regressions (polynomial and logarithmic), but these efforts did not improve the correlation. We also calculated outliers using interquartile range and determined correlations for non-outlier values. The correlations were weakly positive excluding outliers. We investigated a specific emission to test if there would be a correlation, but the same trend occurred. Table S2 provides the relationship and respective R^2 value.

Table S2. Relationship correlations and R^2 values.

Relationship	**R^2 values (including outliers)**	**R^2 values (excluding outliers)**
Production (mineral equivalents per year) & Total emissions (kg per year)	0.0066	0
Production (mineral equivalents per year) & Lead compound emissions to land (kg per year)	0.0039	0.0507
Production (mineral equivalents per year) & Ecotoxicity impacts (CTUeco per year)	0.0084	0.0828
Production (mineral equivalents per year) & Noncancer/Cancer impacts (CTUnoncancer or CTUcancer per year)	0.0137	0.0433

3. Sample Calculations for Life Cycle Impact Assessment

As an example, an imaginary mine emits 3 metric tons of *toluene* into the air and 20 metric tons of *lead compounds* onto soil and land resources in a given year. What are the total ecotoxicity, human health cancer, and human health non-cancer impacts from these emissions?

We first start by looking up the impact characterization factors of toluene and lead compounds (by Table S1, only lead (II)) in the Tool for Reduction and Assessment of Chemicals and Other Environmental Impacts (TRACI) dataset. We must account for the medium in which these chemicals are emitted (air, water, or land). Table S3 contains these characterization factors and their units.

Table S3. TRACI values for select chemical pollutants

Chemical Pollutant	**Emissions Medium**	**Ecotoxicity (CTUeco/kg)**	**Human health cancer (CTUcancer/kg)**	**Human health non-cancer (CTUnoncancer/kg)**
Toluene	Air	0.0131	3.17E-12	9.62E-08
Lead (II)	Land	221	2.02E-07	7.08E-05

Despite being released into two different media, the characterization factors within TRACI translate the emissions into common units (comparative toxicity units). The general equation for calculating the total of an impact is in Equation S1. This equation is individually applied to each impact (namely, ecotoxicity, human health cancer, and human health non-cancer).

Equation S1.

$$\sum_i (mass\ of\ emissions\ of\ i) * (characterization\ factor\ of\ i)$$

Applying Equation S1 to the emissions from the imaginary mine for each impact category:

Ecotoxicity

$$(3\ tons\ toluene) * \left(\frac{1000\ kg}{1\ ton}\right) * \left(\frac{0.0131\ CTUeco}{kg\ toluene}\right) +$$

$$(20\ tons\ lead\ compounds) * \left(\frac{1000\ kg}{1\ ton}\right) * \left(\frac{221\ CTUeco}{kg\ lead\ compounds}\right) = 4.42 * 10^{6}\ CTUeco$$

Human Health Cancer

$$(3\ tons\ toluene) * \left(\frac{1000\ kg}{1\ ton}\right) * \left(\frac{3.17 * 10^{-12}\ CTUcancer}{kg\ toluene}\right) +$$

$$(20\ tons\ lead\ compounds) * \left(\frac{1000\ kg}{1\ ton}\right) * \left(\frac{2.02 * 10^{-7}\ CTUcancer}{kg\ lead\ compounds}\right) = 4.04 * 10^{-3}\ CTUcancer$$

Human Health Non-Cancer

$$(3\ tons\ toluene) * \left(\frac{1000\ kg}{1\ ton}\right) * \left(\frac{9.62 * 10^{-8}\ CTUnoncancer}{kg\ toluene}\right) +$$

$$(20\ tons\ lead\ compounds) * \left(\frac{1000\ kg}{1\ ton}\right) * \left(\frac{2.02 * 10^{-7}\ CTUnoncancer}{kg\ lead\ compounds}\right) = 1.42\ CTUnoncancer$$

4. References

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