Developing Ecological Life Cycle Impact Assessment Characterization Factors for CdTe

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***Abstract* — A variety of regulated metals are currently being used in three generations of photovoltaic technologies. Understanding the potential life cycle environmental impacts from use of these materials requires data on their physico-chemical and (eco)toxicological properties. For the thin film semiconductor CdTe, the documentation of physical, chemical, and toxicological properties in conjunction with the consensus toxicity model USEtox can be used to evaluate the potential impact of CdTe emissions on ecosystems. The freshwater ecotoxicity characterization factors (CF) are in a low range compared to metal ions in the USEtox database, due primarily to lower ecotoxicity effects on freshwater ecosystems measured for three trophic levels (algae, crustaceans, fish). Potential ecotoxic impacts of CdTe are approximately 3 orders of magnitude lower than Cd. Given the uncertainty of a factor 10-100 for freshwater ecotoxicity characterization factors, this difference is superior to the uncertainty range.**

***Index Terms* —ecosystems, environmental factors, photovoltaic cells, thin films.**

I. Introduction

While commercial photovoltaic modules based on wafer crystalline silicon (c-Si) account for more than 90% of global PV manufacturing capacity [1], there is increasing parity in record cell efficiency among first, second, and third generation PV technologies. For example, record cell efficiencies for multi-c-Si (22.3%), CIGS (22.6%), CdTe (22.1%), and perovskite (22.7%) differ by less than 1% [2]. Continued technology development and evolution in aspects such as cost, efficiency, lifetime, and capital intensity are needed to achieve terawatt levels of global PV deployment [3][4].

As evidenced in the above examples, PV technologies rely on a variety of regulated metals such as compounds of lead, cadmium, selenium, indium, silver, copper, tin, and nickel [5]. Understanding the potential life cycle environmental impacts from use of these materials and potential emissions in the environment occurring at manufacturing, use, or end-of-life requires data on their physico-chemical and (eco)toxicological properties.

When thin film cadmium telluride photovoltaic (CdTe PV) technology began to be commercialized about two decades ago, CdTe was hypothesized to have lower toxicity than cadmium (Cd) due to its stability (bond strength >5 eV) [6] and low solubility [7]. In recent years, a CdTe dossier of physical, chemical, and toxicological properties has been registered with the European Chemicals Agency [8], providing a more complete profile of the substance and enabling comparisons with other inorganic substances.

In parallel, methodologies for characterizing the potential human health and ecosystem impact of chemicals emissions in air, water or soil have evolved in the form of the USEtox scientific consensus model endorsed by the UNEP/SETAC Life Cycle Initiative [9]. The purpose of this evaluation is to demonstrate how freshwater ecotoxicity characterization factors (CF) for CdTe can be derived using data from the CdTe dossier and the USEtox model (Fig. 1), enabling comparisons to Cd and other inorganic substances.

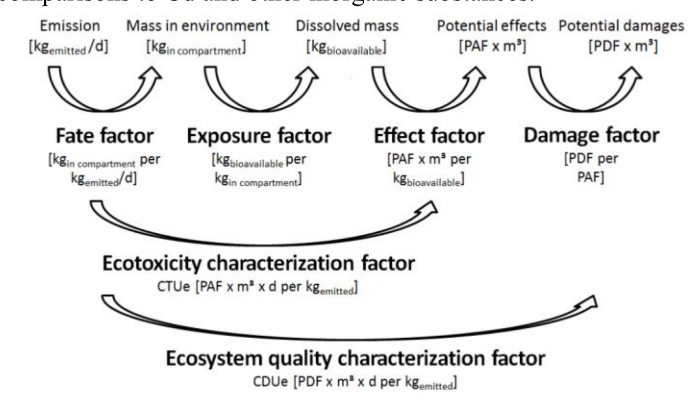

Fig. 1. USEtox framework for ecotoxicity impacts [10].

II. Methods

The derivation of USEtox ecotoxicity characterization factors involves two main steps: establishing physico-chemical data for the fate and exposure factor calculation (Table I), and compiling toxicological properties for use in dose response slope factor for the effect factor calculation (Table II). Physico-chemical data is available in the CdTe dossier or estimated using the U.S. EPA's EPI Suite physico-chemical property and environmental fate estimation program [11].

Partitioning coefficients (K_{DOC}, Kp_{SS}, Kp_{SD}, Kp_{SL}) for CdTe in Table I are derived from the USEtox partitioning coefficient for Cd^{2+} adjusted for 2.4-5.9% long-term transformation/dissolution of CdTe [8]. Transformation and dissolution testing is designed to determine the rate and extent to which sparingly soluble metal compounds can produce soluble ionic species in aqueous media under a set of standard laboratory conditions representative of those generally occurring in the environment (28 days at 1 mg/L loading in a pH 6 aqueous medium with shaking at 100 rpm) [12].

TABLE I. CdTe physico-chemical data used as inputs for the fate and exposure factor calculation in USEtox

Parameter	Value
Molecular weight (g/mol)	240.01
Water solubility at 25 ˚C (mg/L)	1.1×10^{-12} (based on solubility product K_{sp} of 9.5×10^{-35} [13])
Vapor pressure at 25°C (Pa)	1.13×10^{-33} [11] based on boiling point of 1050 ˚C
Partitioning coefficient between octanol and water (log K_{OW}) unitless	-0.07 [11]
Partitioning coefficient between dissolved organic carbon and water (K_{DOC}) in L/kg*	2.24×10^{6}
Partitioning coefficient between suspended solids and water (Kp_{SS}) in L/kg*	7.42×10^{4}
Partitioning coefficient between sediment particles and water (Kp_{SD}) in L/kg*	4.82×10^{4}
Partitioning coefficient between soil particles and water (Kp_{SL}) in L/kg*	3.61×10^{3}

*USEtox partitioning coefficient for Cd^{2+} adjusted for 2.4-5.9% long-term transformation/dissolution of CdTe [8].

Acute and chronic ecotoxicity testing has been conducted on CdTe, yielding median effects concentrations (EC50) for three trophic levels (algae, crustaceans, and fish) (Table II). Effects measured are growth rate for algae (acute testing); mobility for crustaceans (acute testing); mortality and reproductive impairment for crustaceans (chronic testing); and weight, mortality, and body length for fish (acute testing). For the latter, no acute effects were observed for the test species (Brachydanio rerio) in saturated solution (1 g CdTe/L).

Where only acute data is available, acute-to-chronic adjustment factors have been applied (15, 10, and 20 for algae, crustaceans, and fish, respectively) [14]. The adjusted ecotoxicity data results in an average chronic log EC50 (avlogEC50) value of 0.13 log(mg/L), which is an input to the USEtox model along with the physico-chemical data in Table I. While all three trophic levels are represented in the chronic avlogEC50 value, there is some uncertainty due to the extrapolation from acute data for algae and fish.

III. Results and Discussion

Based on the above data inputs, the USEtox model provides estimates of impacts on freshwater ecosystems for an emission of CdTe to air, water, and soil. These results are compared to values for Cd^{2+} and other metal ions covered in the USEtox 2.01 database in Figures 2-4. The unit of the characterization factor for ecotoxicity (PDF.m^3.d/kg) is the potentially disappeared fraction of species (PDF; *i.e.*, loss of biodiversity) integrated over the compartment volume (m^3) and the duration of 1 day (d) per kg emission. The other metal ions shown in Figures 2-4 are Ag(I), Al(III), As(III), As(V), Ba(II), Be(II), Co(II), Cr(III), Cr(VI), Cs(I), Cu(II), Fe(II), Fe(III), Hg(II), Mn(II), Mo(VI), Ni(II), Pb(II), Sb(III), Sb(V), Se(IV), Sn(II), Sr(II), Tl(I), V(V), and Zn(II).

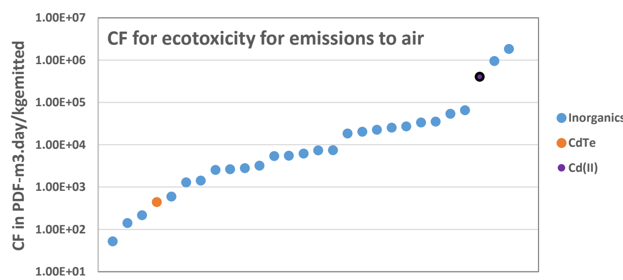

Fig. 2. USEtox ecotoxicity characterization factors (CF) for emissions to continental rural air for CdTe, Cd^{2+}, and metal ions.

TABLE II

USEtox ecotoxicity data inputs for CdTe [8]

Trophic level	Species	EC50 acute (µg/L)	EC50 chronic (µg/L)	EC50 chronic equivalent (mg/L)	EC50 chronic equivalent per species (mg/L)	Log EC50 chronic (log mg/L)
Algae	Pseudokirchnella subcapitata	3100	Not available	0.21	0.21	-0.68
Crustaceans	Daphnia magna	>2200		0.22	0.23	-0.63
	Daphnia magna		200-290	0.25		
Fish	Brachydanio rerio	>1000000	Not available	50	50	1.7
Average (avlogEC50)						0.13

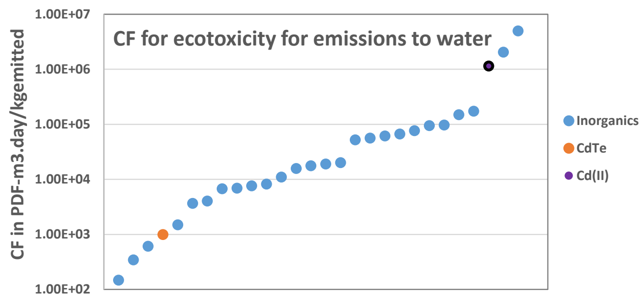

Fig. 3. USEtox ecotoxicity characterization factors (CF) for emissions to continental freshwater for CdTe, Cd^{2+}, and metal ions.

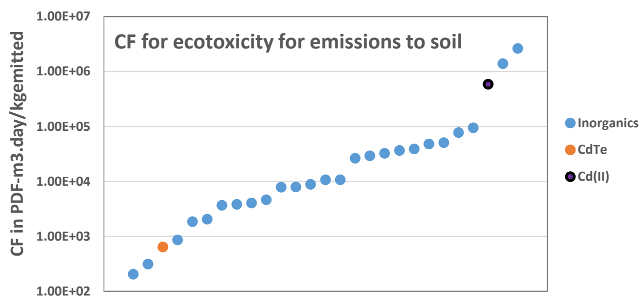

Fig. 4. USEtox ecotoxicity characterization factors (CF) for emissions to continental natural soil for CdTe, Cd^{2+}, and metal ions.

Compared to metal ions documented in USEtox 2.01, CdTe is below the first quartile for ecotoxicity impact, for an emission into air, water, and soil. Its ecotoxicity impact is thus in a low range compared to metal ions. The CdTe ecotoxicity characterization factor is around 3 orders of magnitude lower than Cd. This is mainly due to a lower effect factor of CdTe on freshwater aquatic ecosystems (3.74×10^2 $PAF.m^3.kg^{-1}$) than Cd (3.30×10^4 $PAF.m^3.kg^{-1}$), where PAF is the potentially affected fraction of species. The effect factor (see Fig. 1) represents the chronic toxicity of a substance to a freshwater ecosystem and is based on the avlogEC50 value derived in Table II covering three trophic levels. PAF is related to PDF by a damage factor for freshwater ecotoxicity (PDF/PAF) (Fig. 1).

When comparing ecotoxicity characterization factors for inorganic substances, uncertainties have to be taken into consideration related to the modeling of metals in USEtox. These uncertainties are due to factors such as insufficient ecotoxicity effect data for some inorganic substances, complexity of variables (e.g., pH, redox potential) affecting solid-liquid partitioning, and variability in chemical sequestration effects on bioavailability [14]. Taking these uncertainties into consideration results in an uncertainty factor of 10-100 for inorganic freshwater ecotoxicity characterization factors derived in USEtox.

IV. Conclusion

Because the documentation of ecotoxicity data for CdTe covers three trophic levels, fair data quality is available for following the USEtox methodology, including a CdTe-specific avlogEC50 value of 0.13 log(mg/L). Despite the high uncertainty of metals in USEtox, the freshwater ecotoxic impact of CdTe is estimated as lower than Cd, given that the 3 orders of magnitude between the CF results exceeds the 1-2 orders of magnitude uncertainty. These results are consistent with earlier hypotheses regarding CdTe stability. Based on the USEtox results, potential life cycle ecological impacts for CdTe are in a low range compared to metal ions in the USEtox database, due primarily to lower ecotoxicity effects on freshwater ecosystems than other metal ions such as Cd.

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