Do the substances banned by REACh actually have a significant toxicological impact?

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Abstract: *REACH is a European Union regulation concerning the Registration, Evaluation, Authorisation and restriction of Chemicals. REACH has established limits for physicochemical properties of substances, which are related with their fate in the environment (persistence and bioaccumulation) and their effect (toxicity) in Human Health and Ecosystems. The evaluation of the fate and effect of substances is carried out independently for each physicochemical property, and if at least one of the limits is exceeded, the production and use of a substance shall be limited or banned. Therefore, REACH regulation will restrict or ban some chemical materials that are used for manufacturing gun propellants for military ammunitions and alternatives need to be procured. However, this evaluation neglects some properties of the substances and the combinatorial effect of different properties in the potential toxicity impacts.*

Keywords*: numerical models, concrete structures, impact and penetration, RHT model.*

The goal of this paper is to show how to improve the toxicological assessment of substances based on the limits defined by REACH regulation. The limits defined by REACH that are used to calculate the toxicity characterization factors are applied in this research to create "virtual substances". A virtual substance is characterized by having one of its physicochemical properties on the limit defined by REACH to be considered persistent, bioaccumulative or toxic (PBT), or very persistence or very bioaccumulative (vPvB). The physicochemical properties of the "virtual substance" are inputted in the USEtox method to calculate the respective toxicity characterization factors. The USEtox is a Life-Cycle Impact Assessment method which, based on the physicochemical properties of substances and environmental characteristics, calculates the fraction of chemical substance that is exchanged between the different compartments (air, water and soil); the real fraction taken by the organisms; and the effect on humans and

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different trophic organisms (e.g. plants, microorganisms, algae, fish, etc). Therefore, the USEtox method converts the physicochemical properties into potential impacts for ecosystems and human health. The characterization factors calculated for a "virtual substance" can act as thresholds for the toxicological assessment, since they reflect the behaviour of substances that overcome the limits imposed by REACH. The thresholds calculated can be used to i) assist in the toxicological assessment in order to provide a reference for understanding the significance of the impacts and ii) to comprehend the possible effects of combining different physicochemical properties into potential impacts.

Fourteen virtual substances were defined based on the physicochemical property limits considered in the toxicity assessment (seven for the PBT limits and seven for the vPvB limits). The properties considered were: persistence in air (t1/2 air), water (t1/2 water), soil (t1/2 soil) and sediment (t1/2 sediment); octanol-water partition coefficient (kow); water solubility at 25ºC (Sol25) and Effect Dose for human toxicity (ED50). The calculation was carried out for six different compartments: continental air, urban air, freshwater, sea water, natural soil and agricultural soil. Overall, eighty four threshold values were calculated considering the combination of the fourteen virtual substances and the six different emission compartments.

The results show that the thresholds are higher for the properties LD50, kow and t1/2 water, principally for the vPvB limits, while the thresholds calculated for the other five parameters presents similar impacts. The only exception is the parameter t1/2 soil which presents higher values for emissions into the soil, which is expected since this parameter represents the persistence of substance into the soil. The interpretation of the characterisation factors shows that the calculation are influenced by the emission compartments, in which direct emissions to freshwater have higher values for all the eight properties considered. The characterization factors are also influenced by the parameters Henry´s law constant (kH) and vapour pressure (Pvap) with variations between one to six orders of magnitude. For high values of kH (which implies also high values of Pvap) the characterisation factors thresholds decreases due to the high volatility of the substances which leads to low bioavailable concentrations.

The calculated threshold impacts can be used to assist in the toxicological assessment of substances. The threshold for the virtual substances mimics the limits defined by REACH (and other regulations), so that all the substances with impacts above the calculated thresholds can be considered hazardous for Human Health. The conclusions sum-up how this approach can improve the toxicological assessment, based on limits imposed by reach regulation.