**Assessing the bioaccumulation of ionic substances.**

Wiebke Drost1, Juliane Ackermann1, Ulrich Jöhncke1, Ele Treu1

1 Federal Environment Agency, Wörlitzer Platz 1, 06844 Dessau-Roßlau, wiebke.drost@uba.de

The methods used under REACH to assess and screen for potentially bioaccumulative substances were developed for neutral organic substances. While the sorption of neutral chemicals correlates well with the octanol-water portioning coefficient (KOW), the sorption of partly or totally ionized organic compounds is more complex and not well understood so far – despite the fact that 49% of the industrial chemicals under REACH (Franco, Ferranti, Davidsen, Trapp; Int J Life Cycle Assess, 2010, 15, 321–325) are charged substances. The decision whether a bioaccumulation test is necessary for the assessment of bioaccumulation in REACH is mainly based on the kow. A recent study concerning the compliance of registration dossiers (above 1000 t/a) in regard to data requirements within REACH screened 1932 dossiers. The project revealed that for about 18% of the registered substances, it was not conclusive whether the waiving of the bioaccumulation test was justified because the substances were ionisable at or hydrolytically unstable and screening approaches and criteria are lacking. Likewise the screening for potential PBT substances has so far been mainly restricted to neutral organic compounds.

As a case study the assessment of the bioaccumulation potential of the hydrolysis product of 4,4'-[(isopropylidene)bis(p-phenyleneoxy)]diphthalic dianhydride, a tetraprotic acid, shows the limitations of the actual used method. The substance is mainly dissociated under environmental relevant pH conditions and therefore more hydrophilic. Log D can be used to assess the portion of the neutral and ionic form of the substance and its partioning between water and octanol in dependence of the pH in the environment. It is however questionable if the further step to look at the neutral form and discard the ionic form in the bioaccumulation assessment is straightforward. A recent study has shown that ionic substances with a hydrophobic moiety can accumulate in membrane lipids and are therefore potentially bioaccumulative.( Bittermann, K., S. Spycher, S. Endo, L. Pohler, U. Huniar, K.-U. Goss, and A. Klamt, C. J. 2014. Phys. Chem. B: 14833-14842)

The considerations above are based on the assumption that neutral organic substances accumulate in fat tissues of organisms because of their hydrophobicity. Ionized organic molecules may, however, also be taken up into organisms and bound to proteins or phospholipids in membranes. There has recently been some work concerning sorption processes of ionized substances. Adequate methods for regulatory assessments are however missing.

The log Kow as the solitary screening criterion is not sufficient and not appropriate. The log-D approach for dissociating substances is questionable. Further screening criteria which take additional physical chemical properties and sorption processes especially in regard to hydrophic ions into account are needed. First thoughts on possible screening appraoches and criteria will be discussed.