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Microbial growth yield as a new parameter in environmental chemistry and risk assessment

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Chemicals traded on the European market subject to a chemical safety assessment are assessed for their persistency, bioaccumulation and toxicity (PVB/vPvB) [1]. If the degradation half-life in soil is more than 120 days the chemical is labelled persistent. In soil incubation experiments non-extractable residues (NER) are often formed. NER are defined as residues that are not extractable using extraction methods that do not alter the matrix [2]. Kästner *et al.* [3] differentiated between three types of NER: sequestered NER (type I); covalently bound NER (type II); and biogenic NER (type III). Only type I and II can be considered NER according to the IUPAC definition [2]. A considerable fraction of NER can be of biogenic origin (e.g. [4]). Despite this, ECETOC [5] recommends that NER is considered as a 'separate component' in risk assessment; however, analytical methods are needed to differentiate biogenic NER from other types of NER and currently not part of standard procedures. In REACH [6] incorporation of labelled carbon into biomass should be considered as a potential removal pathway. Consequently, a method to distinguish biogenic NER from type I and II NER is needed. Biogenic NER is the sum of microbial biomass X formed by degradation and its decay products (soil organic matter SOM). The biogenic NER is thus related to the microbial growth yield which is defined as the mass of microorganisms formed per mass of substrate consumed [7,8]:

$$\left[X_{biogenic\ NER}\right] = \frac{Y}{1-Y}\left[CO_2\right] \quad (1)$$

$$\left[SOM_{biogenic\ NER}\right] = \frac{f\times Y}{(1-Y)+(1-f)\times Y}\left[CO_2\right] \quad (2)$$

Eqs. 1 and 2 quantify the upper ($X_{biogenic\ NER}$) and lower ($SOM_{biogenic\ NER}$) boundaries of biogenic NER formed due to microbial growth, decay and incorporation into SOM. Since the CO_2 released during degradation is measured, estimation of the yield enables us to elucidate the nature of NER. Recently, we developed a yield estimation method based on the molecule's nutritional value. The method is based on the Gibbs free energy released from mineralisation, the Nernst equation, and structural information [7]. The advantage is that it can be used to all kind of molecules, including xenobiotics and pesticides, without knowledge about microbial metabolic pathways. Using this method, typical carbon yields of xenobiotics range from 0 (chlorobenzenes) to 0.57 g cell carbon (g substrate carbon)$^{-1}$ (synthetic plant hormones) under aerobic conditions. Under nitrate-reducing conditions, yields are somewhat lower, while under sulfate-reducing conditions the range is from 0 to 0.24 g cell carbon (g substrate carbon)$^{-1}$. Bacterial growth, and thus high yield, is a prerequisite for the rapid degradation unless other growth substrates can be used [8], which is often the case in co-metabolic degradation processes. Using Eq. (1) and (2) we found that for many pesticides a considerable part of the NER formed in degradation experiment is likely biogenic [9]. The approach outlined provides a method to quantify the biogenic NER fraction of NER observed in soil degradation studies. Beyond NER estimation, the method enables identification of compounds which are non-stable, and allows closing the carbon cycle in turnover models.

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