Prediction of the formation of biogenic non-extractable residues during degradation of environmental chemicals from biomass yields

Degradation tests with radio or stable isotope labeled compounds enable the detection of the formation of non-extractable residues (NER). In PBT and vPvB assessment, remobilisable NER are considered as a potential risk while biogenic NER from incorporation of labeled carbon into microbial biomass are treated as degradation products. Relationships between yield, released CO2 (as indicator of microbial activity and mineralization) and microbial growth can be used to estimate the formation of biogenic NER. We provide a new approach for calculation of potential substrate transformation to microbial biomass (theoretical yield) based on Gibbs free energy and microbially available electrons. We compare estimated theoretical yields of biotechnological substrates and of chemicals of environmental concern with experimentally determined yields for validation of the presented approach. A five-compartment dynamic model is applied to simulate experiments of 13C-labeled 2,4-D and ibuprofen turnover. The results show that bioNER increase with time, and that most bioNER originate from microbial proteins. Simulations with pre-calculated input data demonstrate that pre-calculation of yields reduces the number of fit parameters considerably, increases confidence in fitted kinetic data and reduces the uncertainty of the simulation results.