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Simulation of the fate of co-labeled $^{13}C_3$-^{15}N-glyphosate in a water-sediment system and formation of biogenic non-extractable residues

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The combination of dynamic simulation and stable isotope techniques allows tracking the assimilation of pesticides into biomass [1]. Here, we simulated the fate of co-labeled $^{13}C_3{}^{15}$N-glyphosate in an OECD 308 sediment-water degradation test [2]. The mathematical model used consisted of two compartments for sediment (slow and rapid ad-/desorption), one compartment for dissolved mass, and microbial growth and metabolism. The flow of both ^{15}N and ^{13}C were balanced. The model considers two biodegradation pathways for glyphosate, namely the sarcosine-pathway with complete mineralization, and the incomplete pathway with AMPA as a stable transformation product. Kinetic input parameters were partly estimated from the data, while others were calculated. The microbial growth yield was predicted from the MTB method, using thermodynamics and chemical structure [3]. The model can capture the dynamics of the system, including degradation of glyphosate, formation of AMPA and CO_2, formation of living and dead biomass (proteins) and chemical adsorption. At the end of the experiment (80 days), non-extractable residues accounted for 23% of the ^{13}C and 26% of the ^{15}N; 10% of the ^{13}C and 12% of the ^{15}N were recovered from the protein fraction (mostly non-living amino acids), which is equal to the biogenic non-extractable residues (NER). Biogenic NER consist of assimilated ^{13}C/^{15}N and are thus considered to be 'irreversibly bound' as proposed in the updated ECHA guideline for PBT/vPvB assessment [4]. This is the first study simulating the formation of biogenic NER using experiments with ^{15}N-labeled molecules.

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