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The Role of Photochemistry in the Transformation of Propanil and 3,4-Dichloroaniline in Paddy Water

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Photochemical reactions play an important role in the transformation of water-dissolved pollutants in sunlit surface waters, such as lakes, rivers and paddy floodwater. However, other very important transformation pathways are those induced by microorganisms (biodegradation). Overall, the photochemical processes can be divided into direct photolysis and indirect photochemistry. Direct photolysis is triggered by the absorption of sunlight by the xenobiotic, which can induce its photodegradation. In contrast, indirect phototransformation occurs when a xenobiotic reacts with the so-called *Photochemically Produced Reactive Intermediates* (PPRIs), of which the most important are the hydroxyl radicals (HO), the carbonate radicals (CO_3^{-}), the excited triplet states of Chromophoric Dissolved Organic Matter ($^3CDOM^*$) and singlet oxygen ($^1O_2$). The PPRIs are formed upon sunlight absorption by naturally-occurring photosensitizers, such as CDOM, nitrate and nitrite [1]. By taking into account all these events and by using a suitable software to model photochemistry (APEX: *Aqueous Photochemistry of Environmentally occurring Xenobiotics* [2]), the photochemical fate of a water-dissolved pollutant can be foreseen.

This study assesses the photochemical fate of propanil [3], a post-emergence herbicide used in rice-crops, and that of its main metabolite 3,4-dichloaniline (34DCA). With the APEX software it was possible to model the relevant phototransformation pathways (both the direct and the indirect ones) and to evaluate their role in the overall (biotic + photochemical) transformation of the two compounds. Indeed, by comparing the literature-reported half-life times of the two molecules in the field [4,5] with those foreseen by our photochemical modelling, it was possible to compare the relative importance of photo- and biodegradation. Under water-chemistry conditions that are usually found in paddy floodwater, the biodegradation of propanil overcomes phototransformation and forms 34DCA as a compound of high environmental concern. Differently from propanil, 34DCA mainly undergoes photochemical transformation.

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