
Summary

The release of a chemical in the environment may cause adverse effects. These effects result from the exposure to the chemical released, but also from the exposure to its transformation products. Accordingly, the *direct* impact is defined here as the sum of the effects caused by the chemical released, whereas the *overall* impact is the sum of the effects caused by the chemical released and its transformation products.

In the first part of this work, the status of transformation products in the current practice of chemical assessment is briefly reviewed, with the legislation of the European Union (Directives 67/548/EEC, 93/67/EEC, 91/414/EEC and Regulation 1488/98) taken as representative example. As it turns out, relevant transformation products of pesticides must be assessed at the same level as their precursors, but transformation products of non-pesticides are usually not assessed at all.

In the second part, it is shown that transformation products can be perfectly integrated in an assessment based on *spatial range*. The spatial range of a chemical is a proxy measure of the spatial extent of its impact. This concept was proposed by Scheringer, Berg and Müller-Herold (38). So far, only the spatial extent of the *direct* impact has been estimated (41; 40; 30), and the corresponding spatial range was called *characteristic spatial range*. The goal of this thesis is to estimate the spatial extent of the *overall* impact. The approach

chosen is based on the analytic method developed by Müller-Herold and Nickel for the calculation of characteristic spatial range (30). The model framework covers global long-range transport and first-order reactions. The result obtained is a closed formula for the *secondary spatial range* ϱ_{AB} , expressed as a function of the respective characteristic ranges ϱ_A and ϱ_B of a precursor A and its first-generation transformation product B. The exact form of secondary spatial range—given in Equation 6.30—is too complicated to provide an intuitive picture of the role of the different parameters involved. To this end, a simple, yet precise approximation is given:

$$\varrho_{AB} \cong \frac{\varrho_A + \varrho_B}{2} + \frac{\varrho_B}{2^{1+\varrho_A/\varrho_B}} + \frac{\varrho_A}{2^{1+\varrho_B/\varrho_A}}$$

Secondary spatial range ϱ_{AB} is interpreted as a proxy measure of the spatial extent of the overall impact, whereas the characteristic spatial range ϱ_A is a proxy measure of the direct impact of chemical A.

Quite surprisingly, the first-order rate constant k_{AB} of the reaction transforming A into B does not appear in the expression of secondary range. Moreover, it turns out that in a precursor/transformation product pair, the chemical with the larger characteristic range dominates the secondary range, regardless of being the precursor or the transformation product.

$$\max\{\varrho_A, \varrho_B\} \leq \varrho_{AB} \leq 1.4843 \cdot \max\{\varrho_A, \varrho_B\}$$

In particular, it was shown that the overall impact is significantly larger than the direct impact if the characteristic spatial range of the transformation product B is larger than the characteristic spatial range of its precursor A:

$$\varrho_B > \varrho_A \quad \implies \quad \varrho_{AB} > 1.5 \cdot \varrho_A$$