

Review of predictive risk assessment approaches for the transport of chemicals to groundwater

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BACKGROUND

The management of drinking water resources aims at providing water in sufficient quantity and quality and, as a consequence, this objective is reflected in European regulations. Chemicals can reach groundwater aquifers subsequent to accidental releases but may also reach drinking water resources as a result of their use in society. Acknowledging the different sources and release patterns of chemicals in the environment, regulations aiming at the proactive protection of humans and the environment from chemicals, such as the Plant Protection Product regulation (PPP) or the REACH regulation, include groundwater in their assessment frameworks. Several risk assessment tools have been developed to model and predict the leaching of chemicals to groundwater for the purpose of risk assessment in order to proactively protect drinking water. Information typically needed to support the assessment include the substance's properties, such as the physical-chemical and fate properties, the characterization of the environmental compartment(s) of release and the associated rates of emissions. Several risk assessment models were reviewed with a focus on routes of exposure, key metrics supporting the exposure assessment and their level of conservatism.

METHOD

Modelled route of exposure to drinking water

In regulatory risk assessment, several routes of exposure to drinking water are characterized in alignment with the purpose of the assessment.

- REACH Regulation: The exposure assessment informs the risk assessment of humans via the environment, via consumption of groundwater or surface water (figure 1, yellow arrows). The routes of exposure to drinking water direct (aerial deposition) and indirect (via sewage treatment plant (STP)) exposure of soil are modelled with EUSES (figure 2, yellow arrows).
- PPP Regulation: The route of exposure is direct application to land, modelled with the screening level model SciGrow or FOCUS GW, as a higher tier model.

Figure 1: Risk assessment of man via the environment in REACH guidance R.16 (ECHA, 2016)

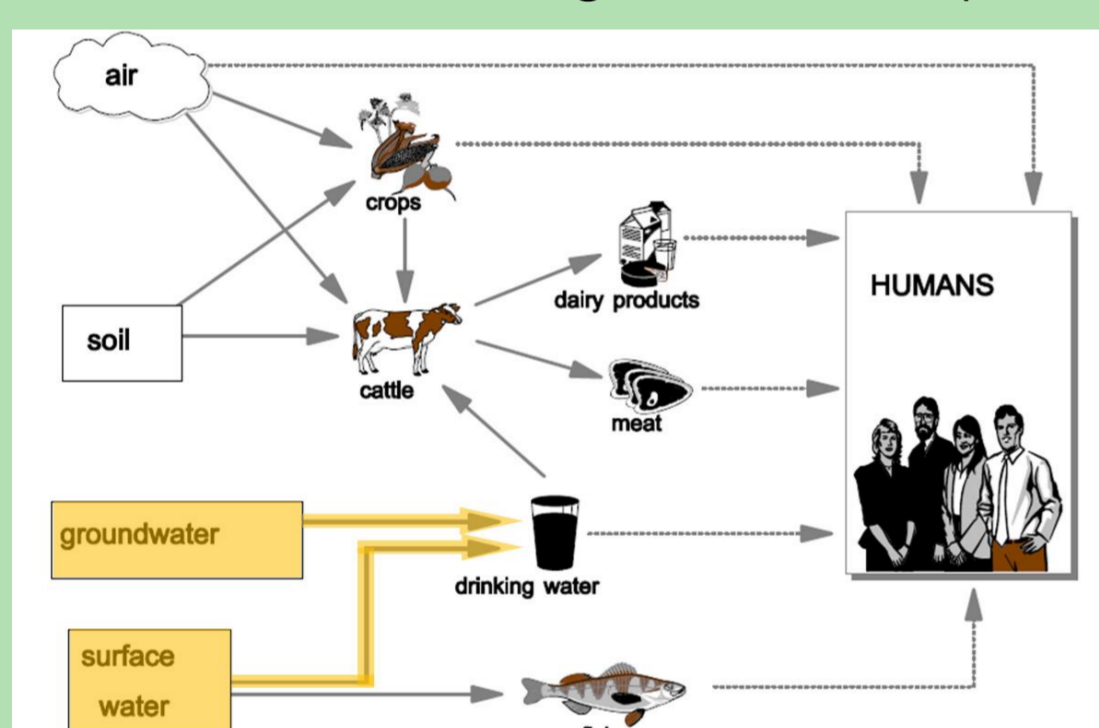
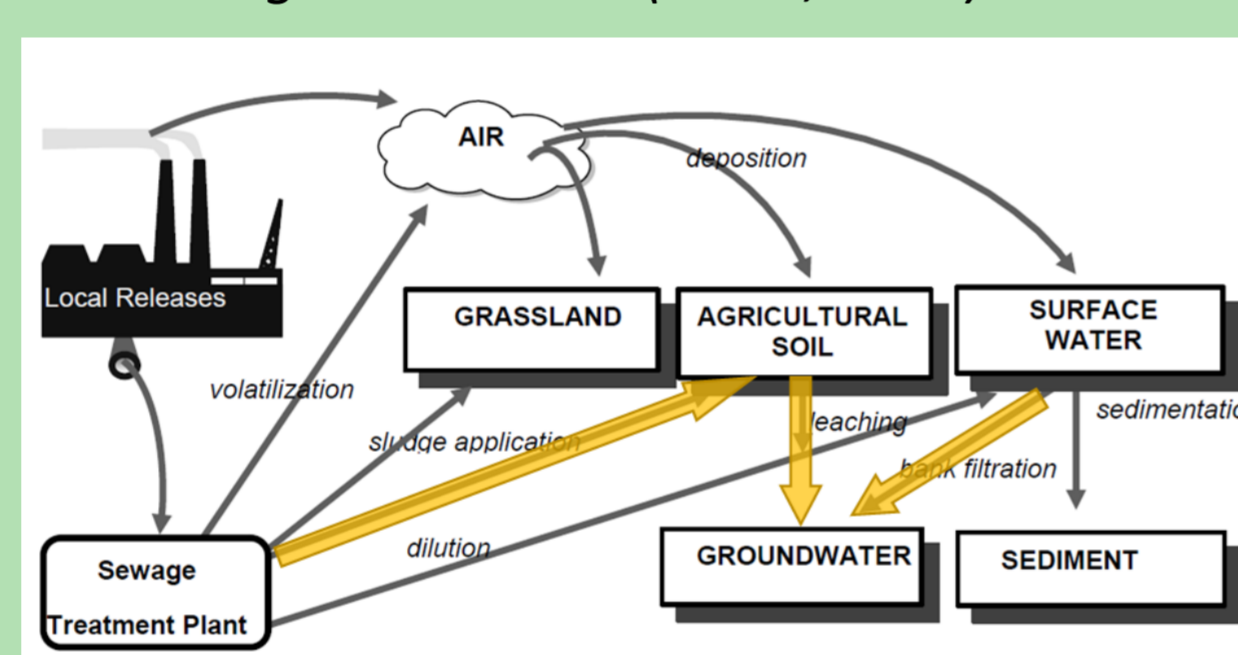


Figure 2: Direct and indirect exposure to groundwater in REACH guidance R.16 (ECHA, 2016)



Differences in model assumption & parametrization

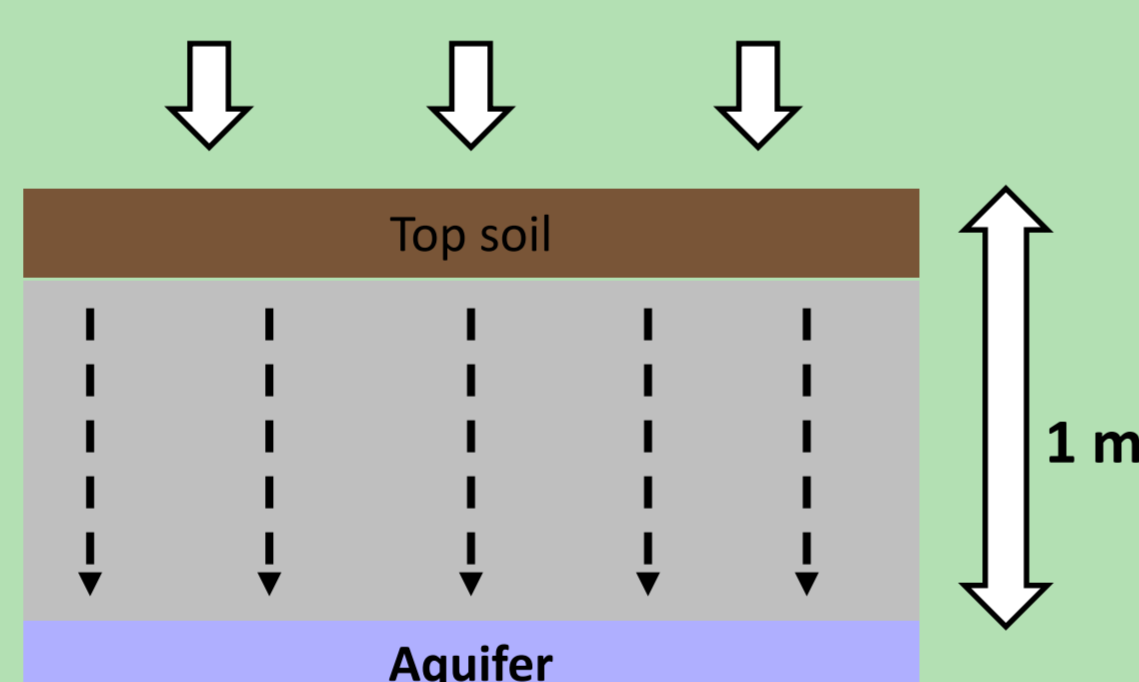
REACH: Potential direct and indirect exposure to land



Top soil = aquifer

- Dosing to land dependent on concentration in sewage sludge and aerial deposition
- Concentration in soil defined after 10 consecutive yearly applications on same field
- Predicted environmental concentration (PEC) in soil derived for 10 or 20 cm top soil
- Conservative derivation of groundwater concentration, as the PEC for groundwater equals PEC top soil pore water concentration

PPP: Direct application to land

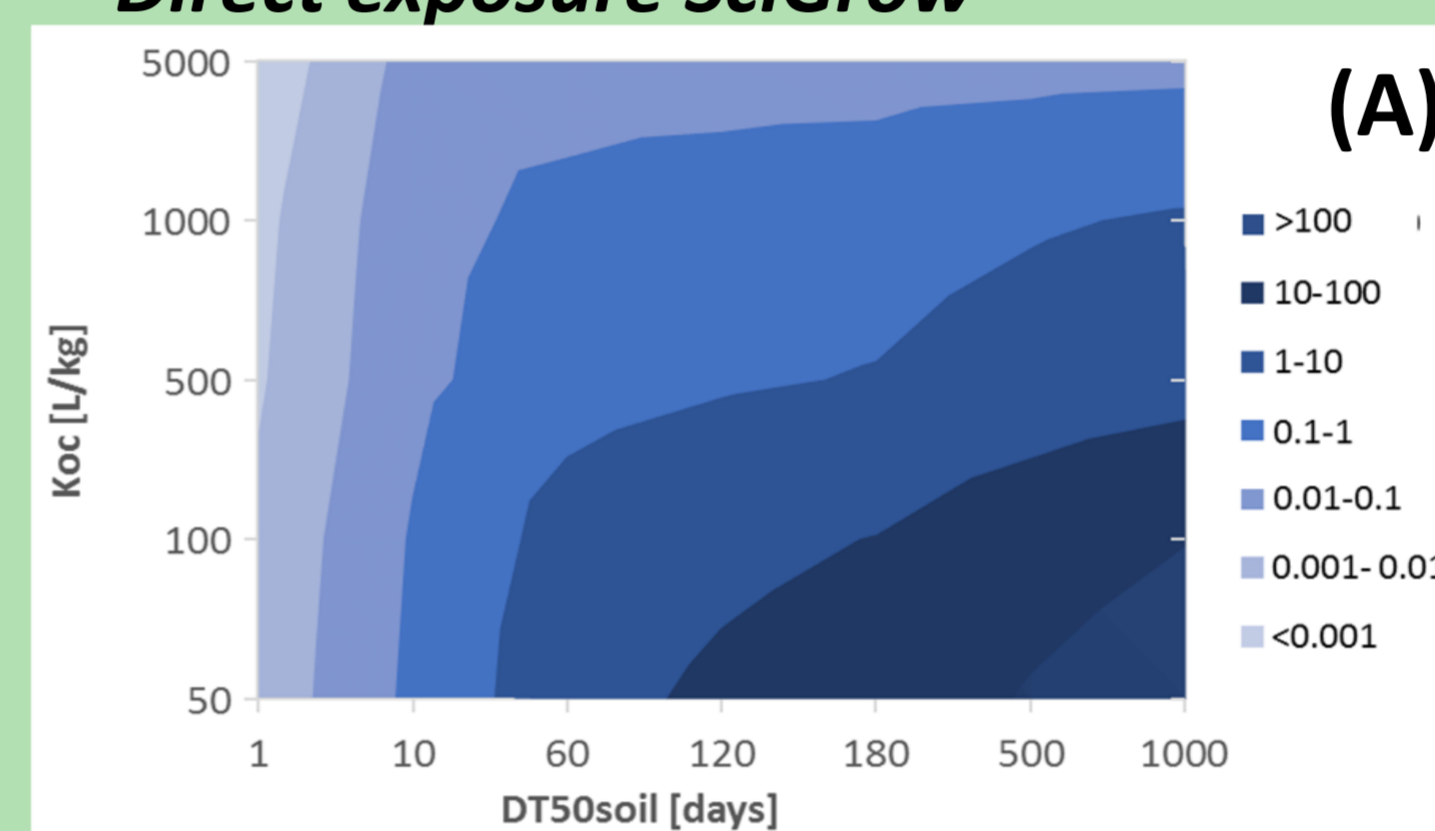


- Dosing to land as per use instructions
- Aquifer defined as 1 meter below ground
- PEC groundwater derived for aquifer after one dosing of active ingredient

RESULTS

Exposures in groundwater were estimated with the screening level models SciGrow and EUSES. Direct application to soil is considered for SciGrow, while emissions in EUSES were parametrized for the STP.

Direct exposure SciGrow



Indirect exposure EUSES

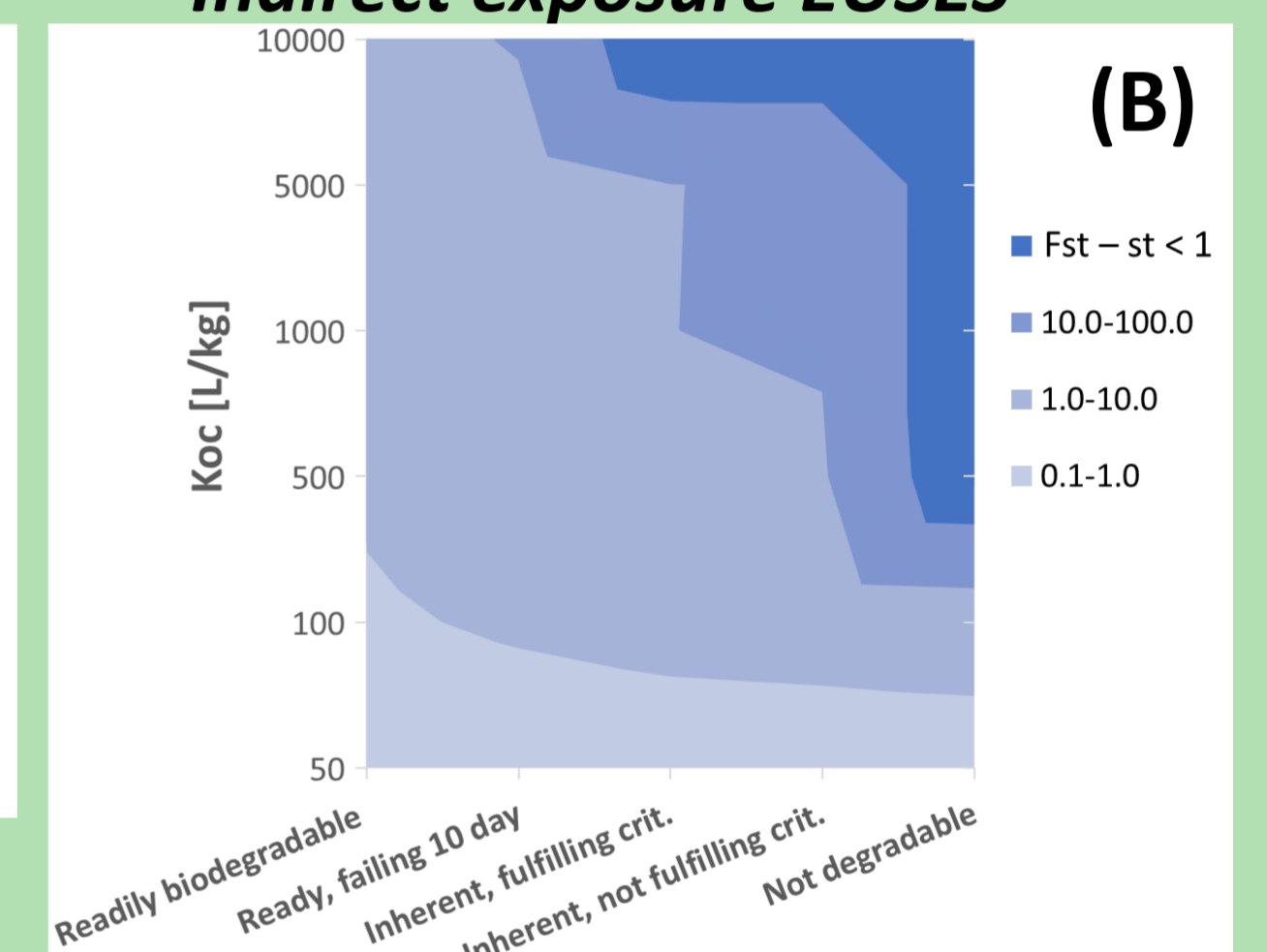


Figure 3: Influence of the route of exposure on groundwater exposure [$\mu\text{g/L}$] with selected soil degradation half-lives and K_{oc} values. Pattern of exposure reflecting direct application to soil 1000g/ha (A) and indirect exposure from release to the STP at 0.7 kg/d (B).

- For K_{oc} values > 5000L/kg, SciGrow model provides non-variable results
- Highest exposures are estimated for substances with long soil half-lives and low K_{oc} .
- Risk is determined by comparing the $PEC_{\text{groundwater}}$ to the World Health Organization guideline value for drinking water.
- The EUSES model deviates from steady-state assumption when the Fraction of steady state ($F_{st-st} < 1$).
- Substance with high K_{oc} have highest exposures, since adsorption of the substance to sewage sludge and the use of sludge as a fertilizer to land are prerequisite for exposure.

Predictions of concentration in groundwater can be refined with well established higher tier models from the agrochemical domain.

The REACH Regulation exposure modelling considers both surface water and groundwater PECs, taking the worst-case to derive the drinking water PEC. The $PEC_{\text{drinking water}}$ is in most cases derived from $PEC_{\text{surface water}}$ (see below matrix). No abatement or degradation during bank filtration would be considered for the majority of substances. Risk is determined by comparing the $PEC_{\text{drinking water}}$ to the $PNEC_{\text{oral}}$.

Biodegradation characteristics.	K_{oc} (L/kg)					
	1	10	100	500	1000	10000
Readily biodeg.						
Readily, failing 10-day window						
Inherent, fulfilling criteria						
Inherent, not fulfilling criteria						
Not degradable						

[Key: $PEC_{\text{drinking water}}$ derived from $PEC_{\text{groundwater}}$ (light green); $PEC_{\text{drinking water}}$ derived from $PEC_{\text{surface water}}$ (light blue); Respective source of $PEC_{\text{drinking water}}$ with deviation from steady-state (dark green/dark blue)]

CONCLUSIONS/NEXT STEPS

The potential for transport to groundwater is currently evaluated on the basis of information on the **compartment of release to the environment, the level of emissions, and the fate and partitioning characteristics of the substance.**

SciGrow and EUSES provide a screening-level estimate of groundwater concentration. Higher tier models from the agrochemical area are already well established, for example in the evaluation of biocides, and have a proven record for identifying potentially mobile compounds transported from the top soil to groundwater aquifer. A read-across will be proposed in the ECETOC Technical Report (ECETOC, 2020). Additionally, a cut-off for groundwater concentration needs to consider the allowable concentration, for example a health-based value in drinking water.

The route of exposure of surface water to drinking water via **bank filtration requires a refined characterisation of the exposure pathway.** Thus, it is suggested that future research develops quantitative approaches to characterise the fate and transport via bank filtration. The approach would gain realism in considering good practice in drinking protection schemes and the efficiencies of treatment methods routinely used for the preparation of drinking water.

References

ECHA (2016). Guidance on information requirements and Chemical Safety Assessment. Chapter R.16: Environmental exposure assessment. Version 3.0. February 2016
ECETOC (2020). ECETOC Technical Report 'Persistent chemicals and water resources protection' For Publication 2020.