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Input of plant protection products into groundwater via bank filtration

Literature research and recommendations for action

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On behalf of the German Environment Agency

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Abstract: Input of plant protection products into groundwater via bank filtration - Literature research and recommendations for action

Plant protection products (PPPs) can be transported from the target area to other environmental compartments after application. To minimize potential negative impacts on the environment and human health, their environmental fate is assessed as part of the authorization process. Bank filtration describes the process where surface water infiltrates into groundwater systems, transporting dissolved or particulate compounds through the subsurface. The study aims to review the state of the art on the processes and influencing factors of bank filtration, to assess bank filtration rates for pesticides, and to evaluate the suitability of the model Exposit 3.02 to represent the removal of PPPs via bank filtration. Based on this analysis, recommendations for integrating the bank filtration pathway into the EU approval process are suggested.

During bank filtration, the concentration of compounds in the infiltrating water is reduced by processes such as physical filtration, sorption, microbial degradation, and dilution. These processes are influenced by factors such as site characteristics, subsurface properties, hydrometeorological conditions, and the properties of the compounds themselves. The hyporheic zone plays a crucial role as it can enhance pollutant retention due to its characteristics. Other important factors include hydrodynamic dispersion, subsurface porosity, as well as hydrophobicity and polarity of the compounds. Bank filtration is significant given that groundwater is generally a particularly protected resource and that raw water for drinking water production is obtained from bank filtrate in 16% of cases in Germany. Since compounds cannot be completely retained during this passage, there is potential for groundwater contamination. Studies show considerable heterogeneity in bank filtration rates for individual compounds, due to high variability in study design and research focus as well as the influence of various parameters. Therefore, mostly qualitative statements can be made, with quantitative statements being limited mainly to laboratory studies. Statistical analysis of the data was found unsuitable.

The model Exposit 3.02 used in Germany's authorization process of PPP estimates groundwater risk from bank filtration. Based on the sorption potential, half-life in soil under aerobic conditions, and water solubility of the compound, groundwater risk groups for active ingredients of PPPs are defined, to which certain bank filtration rates (75%, 90%, and 100%) are assigned. For 13 selected PPPs, individual bank filtration rates were defined based on literature data. These bank filtration rates are then used to estimate the concentrations of the PPPs after subsurface passage. However, comparing these rates with data from the literature shows significant differences. Additionally, subsurface properties and distance from the water body are not considered. To improve the Exposit model, alternative models were analyzed to see how compound retention is considered, including subsurface properties. A simplified approach based on the advection-dispersion equation was proposed, and a realistic worst-case scenario was defined.

The study recommends developing a standardized approach for determining bank filtration rates supported by a comprehensive database of field studies. Additionally, classifying the groundwater hazard potential of compounds using databases like the Pesticides Properties Data Base (PPDB) is suggested. This could help to verify the applicability of risk potential classes and improve the accuracy of assessments.

The results of this study highlight the complex processes during bank filtration and identify research gaps. At the same time, they provide valuable insights for improving the Exposit 3.02 model in the authorization process and outline the requirements necessary for the potential implementation of the bank filtration pathway at European level.

Kurzbeschreibung: Eintrag von Pflanzenschutzmitteln über den Pfad Uferfiltration in das Grundwasser – Literaturrecherche und Handlungsempfehlungen

Pflanzenschutzmittel können nach der Anwendung von der Zielfläche in andere Umweltkompartimente transportiert werden. Um mögliche negative Auswirkungen auf die Umwelt und die menschliche Gesundheit zu minimieren, wird ihr Verhalten in der Umwelt im Rahmen des Zulassungsverfahrens bewertet. Uferfiltration beschreibt den Prozess, bei dem Oberflächenwasser in Grundwassersysteme eindringt und dabei gelöste oder partikuläre Stoffe durch den Untergrund transportiert. Die vorliegende Studie zielt darauf ab, den Stand der Forschung zu den Prozessen und Einflussfaktoren der Uferfiltration zu untersuchen, Uferfiltrationsraten für Pflanzenschutzmittelwirkstoffe zu erfassen und das Modell Exposit 3.02 auf seine Eignung hin zu prüfen, den Rückhalt von Pflanzenschutzmittelwirkstoffen bei der Uferfiltration abzubilden. Auf Basis dieser Analyse werden Empfehlungen für die Integration des Uferfiltrationspfades in das Verfahren der EU-Wirkstoffgenehmigung vorgeschlagen.

Während der Passage der Uferfiltration wird die Konzentration von Stoffen im infiltrierenden Wasser durch Prozesse wie physikalische Filtration, Sorption, mikrobiellen Abbau und Verdünnung verringert. Diese Prozesse werden durch Faktoren wie Standortcharakteristika, Untergrundeigenschaften, hydrometeorologische Bedingungen sowie die Eigenschaften der Wirkstoffe beeinflusst. Die hyporheische Zone spielt dabei eine entscheidende Rolle, da sie durch ihre Eigenschaften die Schadstoffretention erhöhen kann. Weitere wichtige Einflussgrößen sind die hydrodynamische Dispersion, die Porosität des Untergrunds sowie auch die Hydrophobie und Polarität der Wirkstoffe. Der Uferfiltration kann vor dem Hintergrund, dass Grundwasser generell eine besonders schützenswerte Ressource ist und dass in Deutschland Rohwasser für die Trinkwasserwasseraufbereitung zu 16 % aus Uferfiltrat gewonnen wird, eine besondere Bedeutung beigemessen werden. Da Stoffe sich auf dieser Untergrundpassage nicht generell vollständig zurückhalten lassen, besteht die Möglichkeit einer Gefährdung des Grundwassers. Die Studien zeigen aufgrund der hohen Variabilität im Studiendesign und beim Forschungsfokus eine große Heterogenität in Bezug auf die Uferfiltrationsraten für die einzelnen Wirkstoffe, aber auch in Bezug auf den Einfluss der verschiedenen Parameter auf die Uferfiltrationsrate. Daher können vorwiegend qualitative Aussagen getroffen werden. Quantitative Aussagen waren vorwiegend auf Laborstudien begrenzt. Eine statistische Auswertung der Daten erwies sich als ungeeignet.

Das in Deutschland im Zulassungsverfahren für Pflanzenschutzmittel verwendete Modell Exposit 3.02 schätzt die Grundwassergefährdung durch Uferfiltration ab. Anhand des Sorptionspotentials, der Halbwertszeit im Boden unter aeroben Bedingungen und der Wasserlöslichkeit des Wirkstoffs, werden Grundwassergefährdungsgruppen für Pflanzenschutzmittelwirkstoffe definiert, denen bestimmte Uferfiltrationsraten (75 %, 90 % und 100 %) zugeordnet sind. Für 13 ausgewählte Wirkstoffe wurden auf Basis von Literaturdaten individuelle Uferfiltrationsraten definiert. Diese Uferfiltrationsraten fließen dann in die Abschätzung der Wirkstoffkonzentrationen nach der Untergrundpassage ein. Der Vergleich dieser Raten mit Daten aus der Literaturrecherche zeigt jedoch zum Teil große Unterschiede. Ferner werden die Untergrundeigenschaften und die Distanz zum Gewässer nicht berücksichtigt. Zur Verbesserung des Exposit-Modells wurde betrachtet, wie der Stoffrückhalt unter Einbeziehung der Untergrundeigenschaften in alternativen Modellen berücksichtigt wird. Ein vereinfachter Ansatz, der auf der Advektions-Dispersions-Gleichung basiert, wurde vorgeschlagen und ein realistisches Worst-Case-Szenario definiert.

Die vorliegende Studie empfiehlt die Entwicklung eines standardisierten Ansatzes zur Bestimmung von Uferfiltrationsraten, unterstützt durch eine umfassende Datenbank mit Feldstudien. Zusätzlich wird die Klassifizierung des Gefährdungspotenzials von Substanzen anhand von Datenbanken wie der Pesticides Properties Data Base (PPDB) vorgeschlagen. Dies

könnte helfen, die Anwendbarkeit der Gefährdungspotenzialklassen zu überprüfen und die Genauigkeit der Bewertungen zu erhöhen.

Die Ergebnisse heben die komplexen Prozesse bei der Uferfiltration hervor und zeigen Forschungslücken auf. Gleichzeitig liefern sie wertvolle Hinweise zur Verbesserung des Modells Exposit 3.02 im Zulassungsverfahren und zeigen auf, welche Vorraussetzungen für eine mögliche Implementierung des Uferfiltrationspfads in das Verfahren der EU-Wirkstoffgenehmigung notwendig sind.

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Abbreviation	Explanation
2,4 D	2,4-dichlorophenoxyacetic acid
2,4 DP	dichlorprop
AMPA	aminomethylphosphonic acid
AR	artificial recharge
BfR	Federal Institute for Risk Management (Bundesinstitut für Risikobewertung)
2,4 D	2,4-dichlorophenoxyacetic acid
BFR	bank filtration rate
BVL	Federal Office of Consumer Protection and Food Safety (Bundesamt für Verbraucherschutz und Lebensmittelsicherheit)
c	concentration
C_{org}	organic carbon
Δ	delta, difference between to values
DIN	Deutsches Institut für Normung
DOC	dissolved organic carbon
DT_{50}	degradation time (half-life)
exp	exponential function with the base e

Abbreviation	Explanation
JKI	Julius Kühn Institute
K_d	sorption coefficient to soil
K_{oc}	sorption coefficient to soil organic carbon matter
L_{H2O}	water solubility
logD	octanol-water partition coefficient dependent on pH values
$logK_{ow}/P_{ow}$	octanol-water partition coefficient
MAR	manual aquifer recharge
MCPA	2-methyl-4-chlorophenoxyacetic acid
MCPP	methylchlorophenoxypropionic acid
OECD	Organisation for Economic Co-operation and Development
OMP	organic micropollutant
PEC_{ini}	initial predicted environmental concentration
PflSchG	Plant Protection Act (Pflanzenschutzgesetz)
pH	power of hydrogen (negative logarithm of the hydrogen ion concentration)
pK_a	dissociation constant
PPDB	Pesticides Properties Database
PPP	plant protection product
R_d	retardation
TOC	total organic carbon
UBA	German Environment Agency (Umweltbundesamt)
v_p	flow velocity
λ	degradation time
ρ_b	bulk density
θ	porosity
°C	degree celsius
cm	centimeter
d	day
g	gram
h	hour
kg	kilogram
L	liter
m	meter

Abbreviation	Explanation
m^3	cubic meter
mg	milligram
min	minute
mL	milliliter
ng	nanogram
s	second
µg	microgram
µL	microliter
INR	Institute of Natural Resource Conservation

Summary

Introduction and objectives of the study

Plant protection products (PPPs) can be transported from the target area after application. Therefore, the environmental behavior of PPP is assessed as part of the authorization process to minimize negative impacts on human health and the environment. Germany, unlike other EU member states, considers the entry of PPPs via the bank filtration pathway to evaluate the potential risk to groundwater. Bank filtration refers to the process where surface water infiltrates into groundwater systems and transports dissolved or particulate compounds through the riverbed and subsurface. In the German authorization process of PPPs, the bank filtration rate (BFR) of a PPP is determined with the model Exposit 3.02 (UBA 2018) based on groundwater risk groups. Individual bank filtration rates from literature are provided for 13 PPPs. The BFR is then used to estimate the expected environmental concentration of a PPP in groundwater through bank filtration. Based on a literature review, the study aims

- to review the current research on the processes and influencing factors of the bank filtration pathway,
- to assess bank filtration rates for pesticides in relation to compound characteristics, subsurface properties, and environmental conditions at the study site,
- to evaluate the suitability of the Exposit 3.02 model for accurately representing bank filtration and to identify potential suggestions for improvement,
- to elaborate recommendations for incorporating the bank filtration pathway into the EU approval process for active ingredients of PPPs.

A total of 174 suitable sources were extracted from various literature databases, including literature reviews, field and laboratory studies, and modeling. Using this database, the research questions were addressed. The results of the studies were systematically categorized by influencing factors and study types, as different effects may dominate depending on the study context/type. Bank filtration rates were compiled, and research gaps and data deficiencies based on the study results were identified. The study shows that there is little data on the natural bank filtration of PPPs. Only one field study specifically addressed this aspect, while all other field studies were conducted under technically initiated conditions. Laboratory studies did not differentiate between these conditions. Furthermore, only 91 PPPs were examined, so pharmaceuticals were also included in the literature review, with 124 compounds identified. To evaluate and optimize the model Exposit 3.02, further literature research was conducted to identify how other models represent bank filtration and especially the retention of PPPs along this pathway. Recommendations for integrating the bank filtration pathway of PPPs into the approval process at EU level are also provided.

Current state of the art on the bank filtration pathway

Bank filtration involves several interrelated processes that reduce the concentration of compounds as surface water infiltrates into the subsurface. These processes include physical filtration, sorption, microbial degradation, and dilution by surrounding groundwater. Water infiltrates due to hydraulic gradients from surface waters into the subsurface, penetrating through fine-grained sediments in the hyporheic zone and flowing through coarser subsurface matrix. The infiltration process is influenced by the hydraulic potential gradient, which can be natural or artificially created by damming or groundwater extraction. Seasonal fluctuations, particularly dry periods in spring and summer or flooding, can affect the hydraulic gradient and thus the infiltration rate.

The clogging of pores in the hyporheic zone by fine sediments can reduce infiltration and improve pollutant retention due to increased residence time.

The transport of water and dissolved compounds is influenced by hydrodynamic dispersion, which depends on molecular diffusion and mechanical dispersion. The porosity and hydraulic conductivity of the aquifer, the spatial distance of the measurement point from the surface water, and the residence time of the compound affect the transport and retention of compounds. Organic and inorganic components (e.g., clay) in the subsurface can remove compounds from the aqueous phase through various sorption mechanisms, thereby retaining them. The hyporheic zone, with its high organic content, exhibits the highest sorption potential. Sorption efficiency depends on the properties of the compound and the subsurface material such as organic carbon content, clays oxides. Microbial communities in the subsurface play a critical role in the degradation of compounds. The efficiency of microbial degradation depends on environmental factors such as temperature, redox conditions, and the availability of electron donors and acceptors. The redox potential influences whether aerobic or anaerobic microbial processes take place. Depending on the compound, redox conditions can either enhance or reduce its degradation.

Bank filtration rates and influencing factors

The bank filtration rates identified in various studies and the factors influencing them vary considerably. Bank filtration rates are highly dependent on subsurface properties, environmental conditions, and substance characteristics. Subsurface properties such as the content of organic material and hydraulic conductivity, influence bank filtration rates. High clay and organic material content increase sorption and degradation rates, whereas sandy subsurfaces with low organic content can allow for greater substance mobility. Longer residence times and greater distances between the surface water and the measurement point generally lead to higher bank filtration rates due to increased microbial degradation processes and sorption. Wells located further from surface water benefit from better mixing of infiltrating water with surrounding groundwater, which can reduce compound concentrations. Seasonal fluctuations and extreme weather events such as floods and droughts can influence bank filtration rates by varying water levels, flow rates, and redox conditions. Initial concentrations of compounds also affect their retention. Higher compound concentrations in infiltrating water lead to faster adaptation of microorganisms and increased degradation rates. Higher temperatures promote microbial growth and activity, leading to increased degradation rates. However, elevated temperatures can also create anoxic conditions due to higher oxygen consumption during intensified microbial activity. Redox conditions generally affect microbial degradation processes: oxic conditions generally promote the degradation of most compounds, while anoxic conditions may favor the degradation of specific compounds like certain sulfonamides. Suitable environmental conditions such as temperature, oxygen content, and the amount of degradable organic material contribute to effective microbial degradation. Compound properties such as hydrophobicity, polarity, and molecular structure were analyzed to determine how they influence the mobility and persistence of a compound and contribute to its environmental behavior. Hydrophobic compounds tend to be more readily sorbed, while polar and water-soluble compounds may be more persistent and mobile.

Similar to the groundwater risk groups in Exposit 3.02, a classification for PPPs is proposed to provide an initial assessment of their risk potential without direct measurement data. Since the study findings were not sufficiently conclusive, a classification of risk potential was developed using the Pesticide Property Data Base (PPDB). The classification is based on mobility (using the adsorption coefficient) and persistence (using the half-life in the water-sediment system) of a PPP from the PPDB. Combining different value ranges of these properties results in eight classes for the risk potential of a PPP, with Class 1 representing "low risk potential" and Class 8 representing "high risk potential." This classification requires validation with suitable data, ideally from standardized studies.

The studies generally show significant differences in study design, subsurface properties, site conditions, and the compounds studied. Furthermore, the completeness of reporting on examined factors in the studies varies considerably. Generally, the studies provide mostly qualitative information, with quantitative data found only in laboratory studies. The variability in study design and execution results in wide ranges of bank filtration rates, making it difficult to determine statistically significant correlations between influencing factors and bank filtration rates. The data basis from the studies is neither homogeneous nor specifically distributed, making the reliability of statistical analyses uncertain. A standardized approach to design and conduct studies on bank filtration rates and their influencing factors at both field and laboratory scales is necessary to draw reliable conclusions and potentially adjust the authorization process.

There are concerns about groundwater risk from bank filtration. Groundwater is a valuable resource and is subject to special protection. This protection is anchored in legal limits in the Plant Protection Regulation (Regulation (EC) No 1107/2009 2009) and groundwater quality standards in the Groundwater Directive (Directive 2006/118/EC 2006). Furthermore, bank filtrate is relatively common as raw water for drinking water production in Europe, especially in Germany, the Netherlands, Austria, and France (Sprenger et al. 2017). Many studies examining compound retention along the bank filtration pathway show that compounds are retained to varying extents through bank filtration. This points to a potential risk for groundwater or possible exceedances of legal limits/standards. The extent of the risk cannot be conclusively assessed based on the available data. A quantification of the water volume transported through bank filtration would be helpful, which can be calculated using the water budget equation of the respective water body, including spatial and temporal variabilities.

Approaches to optimize the Exposit 3.02 model

The Exposit 3.02 model currently used in Germany for the authorization process of plant protection products to estimate the expected environmental concentration in groundwater through bank filtration has been evaluated for its methodology and limitations. Recommendations for possible optimization were provided. In the current version, the substance properties of sorption potential, microbial degradability in soil under aerobic conditions, and water solubility are indirectly considered, as they are included in so-called groundwater risk groups. Based on the groundwater risk group, bank filtration rates of 75% to 100% are assigned to plant protection products. Additionally, individual bank filtration rates for 13 selected plant protection products were defined based on literature data (Schmidt 2006; Sturm et al. 2006). A comparison of the 13 individual bank filtration rates with data from the compiled studies shows that the comparability of the data is challenging due to the wide range of bank filtration rates for individual substances. Eleven PPPs have a higher BFR in Exposit 3.02 compared to the minimum BFR from literature and two PPPs have the same minimum BFR comparing the values in Exposit 3.02 and the minimum BFR from literature.

The literature review highlights the significant impact of subsurface properties and the distance to the water body, which are not considered in the current Exposit Model 3.02. To define optimization potentials for the Exposit model, literature was specifically analyzed for models that represent the bank filtration pathway, including the compound retention along this entry pathway. Only a few models such as MODFLOW/MT3D, FEFLOW, or MIKE SHE were deemed suitable for simulating bank filtration processes. A simplified advection-dispersion equation under generalized hydrogeological conditions (Parker and Van Genuchten 1984; Toride et al. 1995; Bjerg et al. 1996) was considered. A 5-step calculation integrates subsurface and substance properties of mobility (through the sorption coefficient K_{oc}) and persistence (through $DT_{50,}$ water-sediment) into the determination of bank filtration rates. By calculating retardation, residence time, and degradation of the compound, its concentration in groundwater after bank filtration and the BFR can be determined.

A realistic worst-case scenario was defined to calculate bank filtration rates under these conditions. Since the studies did not provide sufficient information on unfavorable subsurface conditions, data from literature not sourced from the literature review were used. Unfavorable conditions that favor high transport of PPPs from surface water to groundwater include a sandy subsurface with low organic content and low bulk density, as well as high porosity and hydraulic conductivity. The suggestions for the Exposit model aim to optimize the assessment of the potential groundwater hazard of a substance through bank filtration.

Recommendations for implementing a model-based approach at the EU Level

The literature review on bank filtration processes and relevant factors affecting bank filtration rates reveals that a standardized method for determining bank filtration rates in field and laboratory studies is lacking. Therefore, a coordinated concept should be developed and applied in all studies in the future to improve the accuracy of depicting bank filtration rates. On one hand, a comprehensive database of bank filtration rates generated from field studies is needed to validate the 5-step calculation for the realistic worst-case scenario and other scenarios. On the other hand, another database is required to assess the applicability of the proposed groundwater hazard potential classification for PPPs. To capture the impact of compound properties in studies, these should be conducted under defined and controlled laboratory conditions, where only the tested substances vary. Using this data, the applicability of the concept with the eight groundwater hazard potential classes could be validated. Furthermore, research is needed to understand how individual influencing factors interact and affect the bank filtration rate, and to determine the contribution of bank filtration in the hydrological context.

The report emphasizes the variability and complexity of bank filtration processes and their significance in groundwater contamination by PPPs. The results contribute to a better understanding of bank filtration but also reveal knowledge gaps. They provide a basis for developing suggestions to improve the Exposit 3.02 model and identify the requirements necessary for the potential implementation of the bank filtration pathway into the European approval process.

Zusammenfassung

Einleitung und Ziele der Studie

Pflanzenschutzmittel können nach Applikation aus der Zielfläche transportiert werden. Daher wird im Rahmen des Zulassungsverfahrens für Pflanzenschutzmittel deren Umweltverhalten bewertet, um negative Auswirkungen auf die menschliche Gesundheit und die Umwelt zu minimieren. Deutschland berücksichtigt hierbei im Gegensatz zu anderen EU-Mitgliedstaaten den Eintrag von Pflanzenschutzmittelwirkstoffen über den Pfad der Uferfiltration, um das Potenzial einer Grundwassergefährdung zu bewerten. Uferfiltration bezeichnet den Prozess, bei dem Oberflächenwasser in Grundwassersysteme eindringt und dabei gelöste oder partikuläre Stoffe durch die Gewässersohle und den Untergrund transportiert. Im deutschen Zulassungsverfahren für Pflanzenschutzmittel wird die Uferfiltrationsrate eines Pflanzenschutzmittelwirkstoffs mit dem Modell Exposit 3.02 (UBA 2018) auf Basis von Grundwassergefährdungsgruppen ermittelt. Für 13 PPPs sind individuelle Uferfiltrationsraten aus der Literatur hinterlegt. Die Uferfiltrationsrate fließt in die Abschätzung der voraussichtlichen Umweltkonzentration eines Pflanzenschutzmittelwirkstoffs im Grundwasser durch Uferfiltration ein. Im Rahmen der Studie sollen anhand einer Literaturrecherche

- der Stand der Forschung zu Prozessen und Einflussfaktoren beim Transportpfad Uferfiltration recherchiert werden,
- Uferfiltrationsraten für Pflanzenschutzmittelwirkstoffe sowie der Einfluss von Stoff-, Untergrundeigenschaften und weiteren Umweltbedingungen des Untersuchungsstandorts auf die Uferfiltrationsrate erfasst werden,
- das im Zulassungsverfahren verwendete Model Exposit 3.02 auf seine Eignung, die Uferfiltration geeignet abzubilden, bewertet und mögliche Verbesserungsvorschläge aufgezeigt werden,
- Handlungsempfehlungen für eine Berücksichtigung des Pflanzenschutzmitteleintrags über den Pfad Uferfiltration in das Grundwasser im Rahmen der EU-Wirkstoffgenehmigung erarbeitet werden.

Aus verschiedenen Literaturdatenbanken wurden 174 geeignete Quellen extrahiert, die sich in Literaturrecherchen, Feld- und Laborstudien sowie Modellierungen unterteilen lassen. Mithilfe dieser Datenbasis wurden die Aspekte bearbeitet. Die Ergebnisse der Studien wurden systematisch nach Einflussfaktoren und Studientypen kategorisiert, da unterschiedliche Effekte je nach Studienkontext/-art dominieren können. Uferfiltrationsraten wurden zusammengetragen sowie Forschungsdefizite und Datenlücken basierend auf den Ergebnissen der Studien aufgezeigt. Die vorliegende Studie zeigt auf, dass es kaum Daten zur natürlichen Uferfiltration von Pflanzenschutzmittelwirkstoffen gibt. Zum einen wurde lediglich eine Feldstudie gefunden, die sich mit genau diesem Aspekt beschäftigte, alle anderen Feldstudien wurden unter technisch initiierten Bedingungen durchgeführt. Bei den Laborstudien konnte dazwischen nicht unterschieden werden. Weiterhin ergab sich, dass die Anzahl der untersuchten Pflanzenschutzmittelwirkstoffe nur bei 91 lag, so dass auch Pharmazeutika in die Literaturrecherche einbezogen wurden, deren Anzahl bei 124 Wirkstoffen lag. Zur Bewertung und Optimierung des Models Exposit 3.02 wurde eine weitere Literaturrecherche durchgeführt, um bei anderen Modellen die Abbildung der Uferfiltration und insbesondere des Rückhalts von Stoffen entlang dieses Pfades zu identifizieren. Schließlich wurden Empfehlungen zur Integration des Uferfiltrationspfads in das Genehmigungsverfahren auf EU-Ebene formuliert.

Aktueller Stand der Forschung zum Uferfiltrationspfad

Die Uferfiltration umfasst mehrere, sich gegenseitig beeinflussende Prozesse, die die Stoffkonzentration reduzieren, während Oberflächenwasser in den Untergrund infiltriert. Zu diesen Prozessen zählen die physikalische Filtration, die Sorption, der mikrobielle Abbau und die Verdünnung durch umgebendes Grundwasser. Wasser infiltriert aufgrund hydraulischer Gradienten aus Oberflächengewässern in den Untergrund, indem es durch feinkörnige Sedimente in der hyporheischen Zone eindringt und durch grobkörnigere Matrix des Untergrunds strömt. Der Infiltrationsprozess wird durch das hydraulische Potentialgefälle beeinflusst, das natürlich sein kann oder künstlich durch Aufstauung oder Grundwasserentnahme erzeugt wird. Saisonale Schwankungen, insbesondere trockene Phasen im Frühling und Sommer oder Überschwemmungen können das hydraulische Gefälle und damit die Infiltrationsrate beeinflussen.

Die Verschlämmung von Poren der hyporheischen Zone durch feine Sedimente kann die Infiltration verringern und die Schadstoffretention aufgrund der erhöhten Aufenthaltszeit verbessern.

Der Transport von Wasser und gelösten Stoffen wird durch hydrodynamische Dispersion beeinflusst, die von molekularer Diffusion und mechanischer Dispersion abhängt. Die Porosität und hydraulische Leitfähigkeit des Aquifers, die räumliche Entfernung der Messstelle vom Oberflächenwasser und die Verweilzeit der Substanz beeinflussen den Transport und den Rückhalt von Stoffen. Organische und anorganische Anteile (z.B. Ton) im Untergrund können Substanzen durch verschiedene Sorptionsmechanismen aus der wässrigen Phase entfernen und damit zurückhalten. Die hyporheische Zone mit ihrem hohen organischen Gehalt zeigt das höchste Sorptionspotenzial. Die Sorptionseffizienz hängt von den Eigenschaften der Substanz und des Untergrundmaterials ab, wie z. B. dem Gehalt an organischem Kohlenstoff, Tonen und Oxiden. Mikrobielle Gemeinschaften im Untergrund spielen eine entscheidende Rolle beim Abbau von Substanzen. Die Effizienz des mikrobiellen Abbaus hängt von Umweltfaktoren wie Temperatur, Redoxbedingungen und der Verfügbarkeit von Elektronendonatoren und -akzeptoren ab. Das Redoxpotential beeinflusst, ob aerobe oder anaerobe mikrobiellen Prozesse ablaufen. Je nach Substanz können die Redoxbedingungen deren Abbau verbessern oder verringern.

Uferfiltrationsraten und sie beeinflussende Faktoren

Die in verschiedenen Studien identifizierten Uferfiltrationsraten und die sie beeinflussenden Faktoren variieren erheblich. Uferfiltrationsraten hängen stark von den Eigenschaften des Untergrunds, den Umweltbedingungen und den Substanzeigenschaften ab. Untergrundeigenschaften wie der Gehalt an organischem Material und die hydraulische Leitfähigkeit beeinflussen die Uferfiltrationsraten. Hoher Ton- und organischer Materialgehalt erhöhen die Sorptions- und Abbauraten, während sandige Untergründe mit niedrigem organischem Gehalt eine größere Mobilität der Substanzen ermöglichen können. Längere Verweilzeiten und größere Entfernungen zwischen dem Oberflächenwasser und der Messstelle führen in der Regel aufgrund erhöhter mikrobieller Abbauprozesse und Sorption zu höheren Uferfiltrationsraten. Brunnen, die weiter vom Oberflächengewässer entfernt sind, profitieren von einer besseren Durchmischung des infiltrierenden Wassers mit dem umgebenden Grundwasser, wodurch die Stoffkonzentrationen reduziert werden können. Saisonale Schwankungen und extreme Wetterereignisse wie Überschwemmungen und Dürreperioden können die Uferfiltrationsraten beeinflussen, indem sie Wasserstände, Flussraten und Redoxbedingungen variieren. Die Anfangskonzentrationen der Substanzen beeinflussen ebenfalls ihren Rückhalt. Höhere Stoffkonzentrationen im infiltrierenden Wasser führen zu einer schnelleren Anpassung der Mikroorganismen und erhöhen dadurch die Abbauraten. Höhere Temperaturen fördern das mikrobielle Wachstum und dessen Aktivität, was ebenfalls zu erhöhten Abbauraten führt. Erhöhte

Temperaturen können jedoch auch anoxische Bedingungen schaffen, die durch einen höheren Sauerstoffverbrauch bei verstärkter mikrobieller Aktivität entstehen. Redoxbedingungen beeinflussen generell die mikrobiellen Abbauprozesse: oxische Bedingungen fördern im Allgemeinen den Abbau der meisten Substanzen, während anoxische Bedingungen den Abbau spezifischer Verbindungen wie bestimmter Sulfonamide begünstigen können. Weiterhin tragen geeignete Umweltbedingungen wie Temperatur, Sauerstoffgehalt und der Gehalt an abbaubarem organischem Material zum effektiven mikrobiellen Abbau bei. Stoffeigenschaften wie Hydrophobie, Polarität und molekulare Struktur wurden daraufhin analysiert, inwieweit sie die Mobilität und Persistenz eines Stoffes beeinflussen und damit zu seinem Umweltverhalten beitragen. Es zeigt sich, dass hydrophobe Verbindungen leichter sorbiert werden, während polare und wasserlösliche Verbindungen möglicherweise persistenter und mobiler sind.

Ähnlich der Grundwassergefährdungsgruppen in Exposit 3.02 wird eine Klassifikation für Pflanzenschutzmittelwirkstoffe vorgeschlagen, um eine erste Bewertung ihres Gefährdungspotenzials ohne direkte Messdaten vorzunehmen. Da die Ergebnise aus den Studien dazu nicht aussagekräftig genug waren, wurde eine Klassifizierung des Gefährdungspotentials mithilfe der Pesticide Property Data Base (PPDB) erarbeitet. Dazu wurden die Klasseneinteilungen der Mobilität anhand des Adsorptionskoeffizienten und der Persistenz mithilfe der Halbwertszeit im Wasser-Sediment-System eines Stoffes aus der PPDB übernommen. Aus der Kombination verschiedener Wertebereiche der beiden Stoffeigenschaften ergeben sich acht Klassen für das Gefährdungspotenzial eines Wirkstoffs mit Klasse 1 „geringes Gefährdungspotential“ und Klasse 8 „hohes Gefährdungspotential“. Diese Klassifizierung bedarf allerdings einer Validierung durch geeignete Daten, die möglichst aus standardisierten Studien stammen.

Generell zeigen die vorliegenden Studien erhebliche Unterschiede in Studiendesign, Untergrundeigenschaften, Standortbedingungen und den untersuchten Substanzen. Darüber hinaus variiert der Grad der Vollständigkeit bei der Angabe der untersuchten Faktoren in den Studien erheblich. Generell finden sich in den Studien vorwiegend qualitative Angaben, quantitative Angaben sind vereinzelt in den Laborstudien zu finden. Die Variabilität im Design und der Durchführung der Studien führt zu großen Spannbreiten der Uferfiltrationsraten, wodurch die Bestimmung statistisch signifikanter Korrelationen zwischen Einflussfaktoren und Uferfiltrationsraten erschwert wird. Die aus den Studien entstandene Datenbasis ist weder homogen noch spezifisch verteilt, wodurch die Aussagekraft von statistischen Analysen unsicher ist. Ein standardisierter Ansatz zur Konzeption und Durchführung von Studien zu Uferfiltrationsraten und deren Einflussfaktoren im Feld- und Labormaßstab ist notwendig, um verlässliche Schlussfolgerungen zu ziehen und gegebenenfalls die Bewertung im Zulassungsverfahren anzupassen.

Es gibt Bedenken hinsichtlich einer Grundwassergefährdung über den Pfad der Uferfiltration. Grundwasser ist eine wertvolle Ressource und unterliegt einem besonderen Schutz. Dieser ist in Form von Grenzwerten in der Pflanzenschutzverordnung (Regulation (EC) No 1107/2009 2009) und als Grundwasserqualitätsnormen in der Grundwasserrichtlinie (Directive 2006/118/EC 2006) verankert. Weiterhin ist die Verwendung von Uferfiltrat als Rohwasser für die Trinkwasserproduktion in Europa verbreitet, insbesondere in Deutschland, den Niederlanden, Österreich und Frankreich (Sprenger et al. 2017). Zudem zeigen viele Studien, die den Rückhalt von Stoffen entlang des Uferfiltrationspfads untersuchen, dass Wirkstoffe meist nur zum Teil zurückgehalten werden. Dies weist auf ein potenzielles Risiko für das Grundwasser bzw. auf mögliche Überschreitungen der gesetzlichen Grenzwerte/Normen hin. Wie hoch das Maß der Gefährdung ist, kann anhand der vorliegenden Daten nicht abschließend beurteilt werden. Hier wäre eine Quantifzierung des über Uferfiltration transportierten Wasservolumens hilfreich, das über die Wasserhausthaltsgleichung des jeweiligen Wasserkörpers inklusive räumlicher und zeitlicher Variabilitäten berechnet werden kann.

Ansätze zur Optimierung des Modells Exposit 3.02

Das in Deutschland im Zulassungsverfahren für Pflanzenschutzmittel derzeit verwendete Modell Exposit 3.02 zur Abschätzung der voraussichtlichen Umweltkonzentration im Grundwasser durch Uferfiltration wurde auf seine Methodik und Einschränkungen hin bewertet. Darüber hinaus werden Empfehlungen zu einer möglichen Optimierung gegeben. In der aktuellen Version werden die Stoffeigenschaften Sorptionspotenzial, mikrobielle Abbaubarkeit im Boden unter aeroben Bedingungen und die Wasserlöslichkeit indirekt berücksichtigt, da sie in sogenannte Grundwassergefährdungsgruppen einfließen. Basierend auf der Grundwassergefährdungsgruppe werden den Pflanzenschutzmitteln Uferfiltrationsraten von 75 %, 90 % und 100 % zugewiesen. Außerdem sind für 13 ausgewählte Pflanzenschutzmittel individuelle Uferfiltrationsraten basierend auf Literaturdaten (Schmidt 2006; Sturm et al. 2006) definiert. Ein Vergleich der 13 individuellen Uferfiltrationsraten mit Daten aus den zusammengetragenen Studien zeigt, dass die Vergleichbarkeit der Daten aufgrund der großen Spannbreiten der Uferfiltrationsraten für die einzelnen Wirkstoffe schwierig ist. Elf Wirkstoffe zeigen in Exposit 3.02 eine höhere Uferfiltrationsrate im Vergleich zu den niedrigsten Uferfiltrationsraten, die im Rahmen der Literaturrecherche gefunden wurden. Zwei Wirkstoffe weisen dieselbe Uferfiltrationsrate auf wie die Minimum-Uferfiltrationsraten aus der Recherche.

Die Literaturübersicht verdeutlicht den erheblichen Einfluss der Untergrundeigenschaften und der Distanz zum Gewässer, die im aktuellen Exposit-Modell 3.02 nicht berücksichtigt werden. Um Optimierungspotentiale für das Exposit-Modell definieren zu können, wurde die Literatur gezielt auf Modelle analysiert, die den Uferfiltrationspfad einschließlich des Stoffrückhalts entlang dieses Eintragspfades darstellen. Nur wenige Modelle, wie MODFLOW/MT3D, FEFLOW oder MIKE SHE, wurden als geeignet für die Simulation der Uferfiltrationsprozesse bewertet. Eine vereinfachte Advektions-Dispersions-Gleichung unter verallgemeinerten hydrogeologischen Bedingungen (Parker und Van Genuchten 1984; Toride et al. 1995; Bjerg et al. 1996) wurde in Betracht gezogen. Eine 5-Schritte-Berechnung integriert die Untergrund- und Stoffeigenschaften Mobilität (durch den Sorptionskoeffizienten K_{oc}) und Persistenz (durch $DT_{50,\text{Wasser-Sediment}}$) in die Ermittlung der Uferfiltrationsraten. Über die Berechnung der Retardation, die Verweilzeit und den Abbau des Wirkstoffs lässt sich dessen Konzentration im Grundwasser nach Uferfiltration und die Uferfiltrationsrate berechnen.

Es wurde ein realistisches Worst-Case-Szenario definiert, um Uferfiltrationsraten unter diesen Bedingungen zu berechnen. Da die Studien keine ausreichenden Informationen zu ungünstigen Untergrundeigenschaften boten, wurden Daten aus Literatur verwendet, die nicht aus der Literaturrecherche stammen. Ungünstige Bedingungen, die einen hohen Transport von Pflanzenschutzmitteln aus dem Oberflächengewässer ins Grundwasser begünstigen, umfassen einen sandigen Untergrund mit geringem Gehalt an organischem Material und geringer Lagerungsdichte sowie hoher Porosität und hydraulischer Leitfähigkeit. Die Vorschläge zum Exposit-Modell zielen darauf ab, die Bewertung der potenziellen Grundwassergefährdung einer Substanz durch Uferfiltration zu optimieren.

Empfehlungen zur Implementierung eines modellbasierten Ansatzes auf EU-Ebene

Durch die Literaturrecherche zu Uferfiltrationsprozessen und relevanten Faktoren, die Uferfiltrationsraten beeinflussen, wird deutlich, dass eine standardisierte Methode zur Bestimmung von Uferfiltrationsraten in Feld- und Laborstudien fehlt. Daher sollte ein abgestimmtes Konzept entwickelt und in allen Studien zukünftig angewendet werden, um die Genauigkeit bei der Abbildung von Uferfiltrationsraten zu verbessern. Zum einen wird eine umfassende Datenbank von Uferfiltrationsraten benötigt, die aus Feldstudien generiert wurden, um die 5-Schritte-Berechnung für das realistic worst-case Szenario und andere Szenarien zu validieren. Zum anderen ist eine weitere Datenbank erforderlich, um die Anwendungsmöglichkeiten der vorgeschlagenen Gefährdungspotenzialklassifikation für Substanzen abzuschätzen. Um den Einfluss von Stoffeigenschaften in Studien zu erfassen, sollten diese unter definierten und kontrollierten Laborbedingungen durchgeführt werden, bei denen nur die getesteten Verbindungen variieren. Mit Hilfe dieser Daten könnte die Anwendbarkeit des Konzepts mit den acht Gefährdungspotenzialklassen überprüft werden. Ferner besteht Forschungsbedarf, wie die einzelnen Einflussfaktoren sich gegenseitig beeinflussen und auf die Uferfiltrationsrate wirken und wie hoch der Beitrag der Uferfiltration im hydrologischen Kontext ist.

Der Bericht unterstreicht die Variabilität und Komplexität der Uferfiltrationsprozesse und ihre Bedeutung bei der Grundwassergefährdung durch Pflanzenschutzmittelwirkstoffe. Die Ergebnisse tragen zum besseren Verständnis der Uferfiltration, zeigen aber auch Wissenslücken auf. Sie ermöglichen, Vorschläge zur Verbessserung des Modells Exposit 3.02 zu erarbeiten und Voraussetungen aufzuzeigen, die für eine mögliche Implementierung des Transportpfads Uferfiltration in das europäische Verfahren der Wirkstoffgenehmigung notwendig sind.

1 Introduction

All types of water bodies are threatened by a large variety of pollutants such as plant protection products (PPP). Therefore, PPP usage is only permitted after an authorization procedure. Active ingredients of a PPP are regulated based on Regulation (EC) No 1107/2009 (2009) by the European Food Safety Authority (EFSA). At the national level in Germany, the Federal Office of Consumer Protection and Food Safety (BVL), the German Environment Agency (UBA), the Julius Kühn Institute (JKI), and the Federal Institute for Risk Assessment (BfR) are involved in the regulation of PPPs according to the Plant Protection Act (PflSchG 2012). The role of the UBA is to assess the impact of PPP on ecosystems and groundwater (Umweltbundesamt 2015). Drinking water, mainly received from groundwater, is the most valuable resource for humans, warranting special protection. This is reflected in various national and international laws and programmes such as the European Drinking Water Directive (Directive (EU) 2020/2184 2020), the national Drinking Water Ordinance (TrinkwV 2023), and the Sustainable Development Goals (including SDG 6) (WHO 2012). In context of the authorization process for PPPs, the transport of an active compound into groundwater is given particular attention. In Germany, approx. 16% of drinking water is obtained via bank filtration (BDEW 2022). The interaction between shallow groundwater (hereafter referred to simply as groundwater) and surface water, especially in regions with low hydraulic gradients such as lowlands and during water extraction through near surface water, represents a potential exchange pathway for PPPs. Depending on the hydrological conditions, the surface water feeds the groundwater leading to the transport of PPPs from surface water into groundwater (Puckett and Hughes 2005; Hintze et al. 2020; Willkommen et al. 2022). Conversely, during weather periods with high groundwater levels, PPPs may be transferred from groundwater into surface water (Puckett and Hughes 2005; Hintze et al. 2020; Willkommen et al. 2022). To protect groundwater, which can serve as drinking water resource for humans, and ecosystems, the bank filtration pathway is recognized in Germany during the authorization process of PPPs (Regulation (EC) No 1107/2009 2009; PflSchG 2012). Bank filtration refers to the transport of water, along with dissolved or particulate matter, from a surface water body through the riverbed and subsurface passage into the groundwater, excluding percolating (DIN 4049-3: 1994). Therefore, it is important to thoroughly understand and control the environmental behavior of PPPs along the bank filtration pathway.

The aim of the project is to document the current state of research on the bank filtration pathway for PPPs in agricultural landscapes and its relevance in terms of groundwater contamination in Germany and Europe. Bank filtration rates (BFR) for PPPs are compiled and the factors influencing this transport pathway are identified and described. Furthermore, the concept of the Exposit model 3.02 (UBA 2018), which so far is solely applied in the authorization procedure in Germany (PflSchG 2012; Regulation (EC) No 1107/2009 2009), will be examined for its suitability to estimate BFR. Recommendations will be developed to optimize the Exposit model with regard to the results of the bank filtration pathway. Based on the findings, actionable recommendations for the potential implementation of this pathway in the EU approval procedure will be provided.

1.1 Term clarification

To ensure clarity, the following terms are defined and clarified. Hereafter, the term

- “compound” refers to both the active ingredients of PPPs and pharmaceuticals. When specifically referring to one of these groups, the terms 'PPP' and 'pharmaceutical' are used to denote the respective active ingredients,

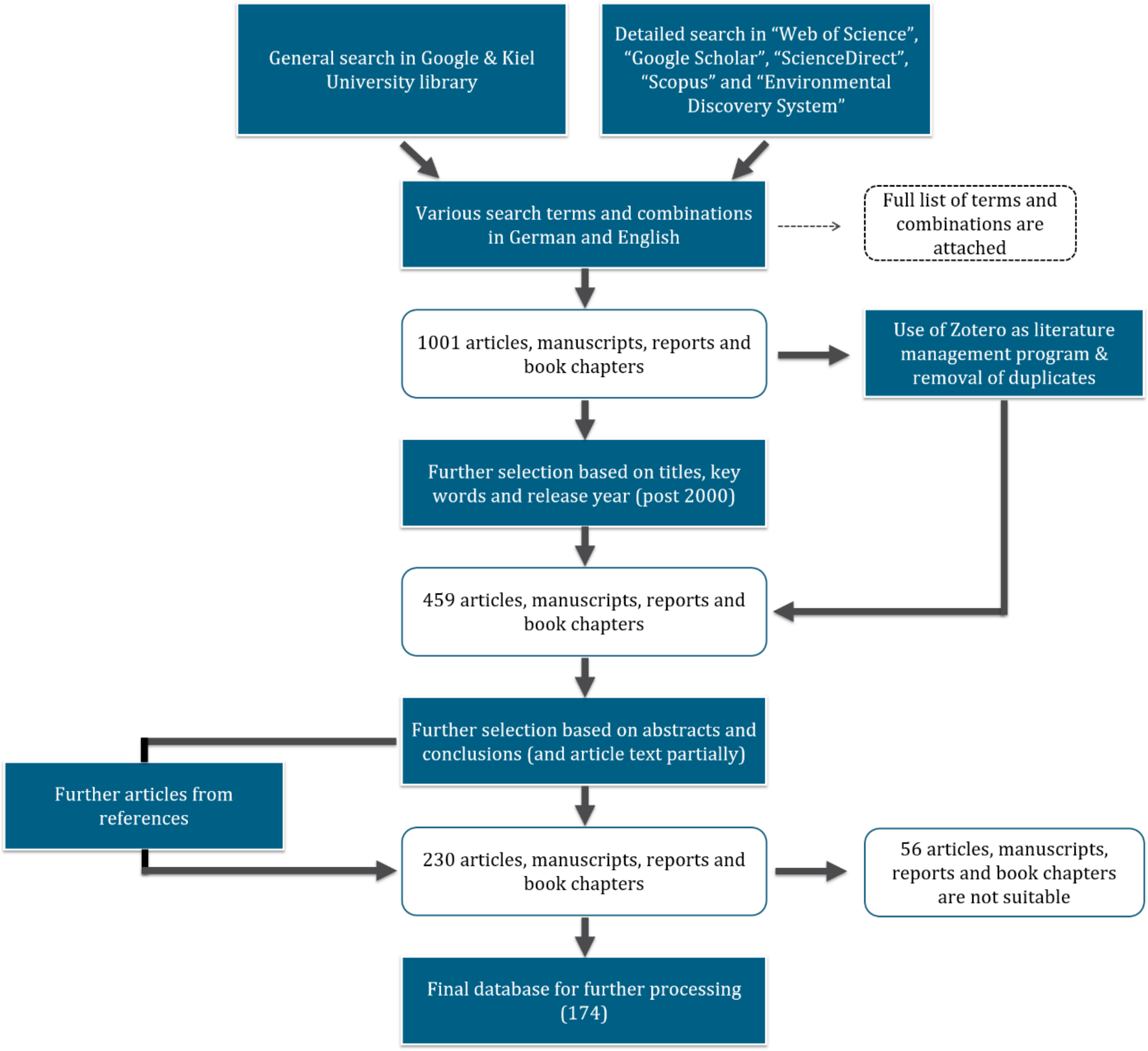
- half-life of a compound "degradation time DT_{50}" is reported this way, when the matrix in which the degradation takes place is not specified. When specified, the matrix is indicated as a subscript such as $DT_{50,\ soil}$ or $DT_{50,\ water\text{-}sediment}$,
- "site characteristics" refer to the redox potential, temperature and microbial activity at a study site,
- "subsurface properties" include soil type, hydraulic conductivity, porosity, organic carbon content (C_{org}), dissolved organic carbon (DOC), total organic carbon (TOC), and clay minerals at at study site,
- "hydrometeorological factors" considers the discharge regime and the water level in surface water at a study site,
- "environmental conditions" combines site characteristics, subsurface properties, and hydrometeorological properties,
- "compound properties" refers to functional groups, charge, adsorption coefficient (K_{oc}), and persistence (DT_{50}) of a compound.

1.2 Literature research

The literature search focused on peer-reviewed publications, publications by public institutions, and other relevant documents related to specific subject areas. The search was conducted using the internet search engine "Google," the collection of the University Library of Kiel, and several online citation and literature databases. These included databases such as "Web of Science", "Google Scholar", "ScienceDirect", "Scopus,", and the "Environmental Discovery System." The search was focused on publications and documents published after the year 2000. Literature published prior to 2000 was partially included, as the literature cited in Sturm et al. (2006) and Schmidt (2006) given in Exposit 3.02 (UBA 2018). Keywords were used in both German and English across various databases. These terms covered not only PPPs and their transformation products but also compounds exhibiting similar environmental behaviors to pharmaceuticals and their metabolites. Some examples of the keywords used are "pesticide", "pharmaceutical", "transformation products". Additionally, terms describing the spatial characteristics of bank filtration, e.g., "river bank", "stream", "sediment", were employed. Keywords encompassing various processes of bank filtration such as "filtration", "passage", "recharge", were also used (see Appendix A.1 for full list of keywords). Besides the terms already mentioned, other terminology potentially associated with bank filtration was utilized. To further optimize the search results, combinations of these terms were also entered into the databases, for example, "(((TS=(riverbanks)) OR TS=(river bank)) AND TS=(filtration)) AND TS=(pesticides)". The relevant hits from the databases were transferred to the reference management program "Zotero." The search initially focused on the titles and keywords of the identified publications and documents, resulting in a large number of articles being found. The next step was to further refine the database created in Zotero. This involved removing duplicate entries in the database and reducing the number of articles by taking a more detailed examination of the abstracts and summaries; in certain cases, the entire articles were reviewed. All publications were then read in their entirety and further literature was obtained manually from the references. The complete reading process also made it possible to identify unsuitable articles. This analysis helped ensure a selection of literature that met the requirements of work packages 1 to 2. In total, 174 journal articles, manuscripts, reports, and book chapters were identified that contributed to the processing of these work packages. The procedure of the literature research is displayed in Figure

1. The literature review description for the assessment of the model Exposit (UBA 2018) and recommendations for improvement (WP3) are described in section 0.

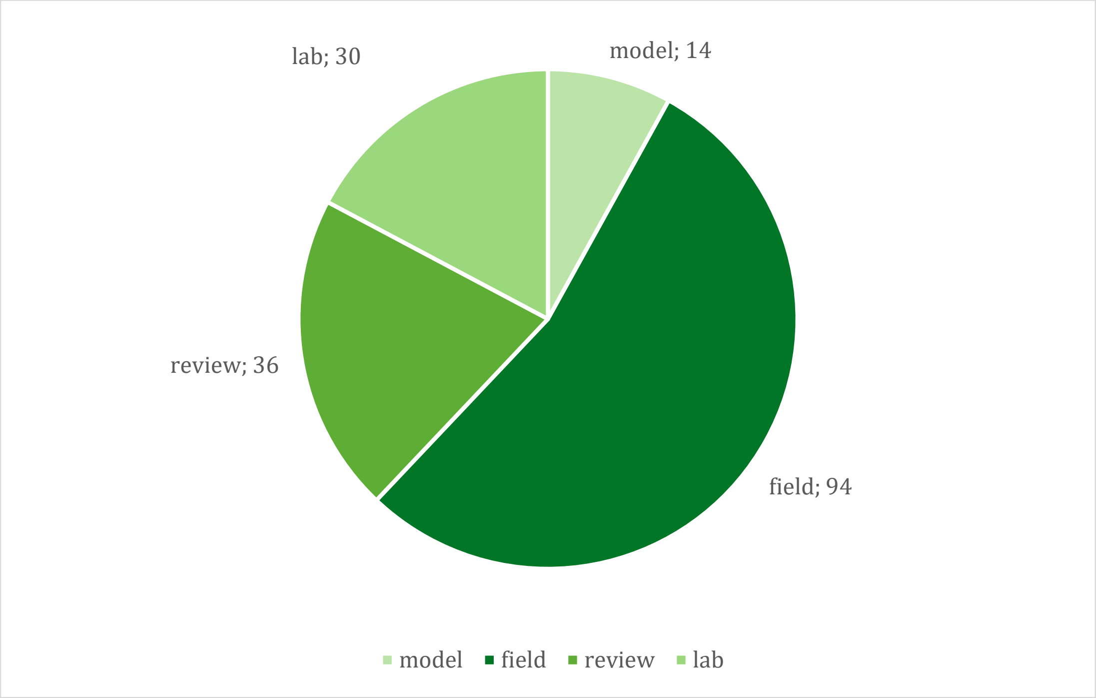
Figure 1: Procedure for the literature search



Source: own illustration, INR

The majority of the publications found were field studies. To a lesser extent, publications on laboratory and modeling studies were found (Figure 2). In addition, several reviews were found that examined bank filtration. Some studies could also be assigned to more than one category, e.g., lab and field, as both were examined.

Figure 2: **Distribution (n = number of studies) of final findings by laboratory, modeling, review, and field studies (own illustration, Institute of Natural Resource Conservation, CAU Innovation GmbH)**



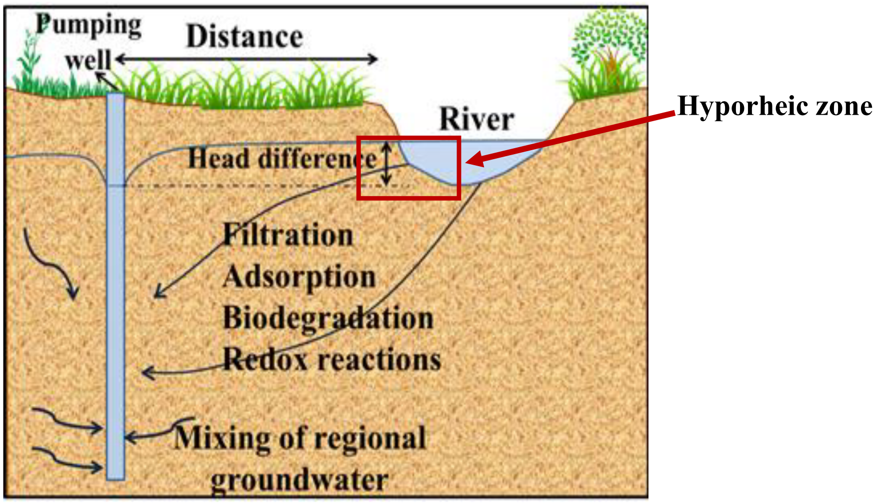
Source: own illustration, INR

The studies identified in the meta-analysis examined bank filtration of a wide range of compounds. These included compounds from industrial production or combustion processes like polycyclic aromatic hydrocarbons and agriculture (PPPs and nutrients), as well as heavy metals. The majority of studies focused on compounds from domestic wastewater such as pharmaceuticals, as well as pathogens. When examining the study ratio of pharmaceuticals to PPPs of 124:91, a data/knowledge gap in the field of PPPs becomes evident. This gap is particularly pronounced in the context of natural bank filtration, where only one study was identified (Wang and Squillace 1994). Therefore, studies on bank filtration of pharmaceuticals were also considered in the review. It is assumed that pharmaceuticals received more attention in studies because water from bank filtration is often used as raw water for drinking water production in densely populated areas, where the influence of wastewater treatment plant effluents and the percolation of treatment plant effluents for groundwater recharge is applied.

2 Current state of the art on the bank filtration pathway

When water containing dissolved and particulate matter infiltrates from the surface water into the subsurface, natural purification processes occur during this passage. These processes reduce the concentration of compounds through mechanisms such as physical filtering, sorption to the subsurface, microbial degradation, and dilution by uncontaminated groundwater (Ray et al. 2002a; Eckert and Irmscher 2006; Jeyakumar et al. 2017; Kruc-Fijalkowska et al. 2022) (Figure 3).

Figure 3: Processes during bank filtration of an active ingredient



Source: Jeyakumar et al. (2017, altered)

The decrease of an active compound concentration during the transport from surface water to groundwater is defined as BFR [%]. The BFR is influenced by several factors governing the processes during bank filtration (Table 1), which will be discussed in section 3.

Table 1: Factors influencing the bank filtration of active ingredients

	Site characteristics: transport, biological degradation	**Subsurface properties: infiltration, transport, sorption, biological degradation**	**Hydrometeorological factors: infiltration, transport, sorption, biological degradation**	**Compound properties: infiltration, transport, sorption, biological degradation**
Factors	Distance surface water-groundwater	Soil type	Discharge regime	Functional groups, pos/neg. charge
	Redox conditions	Hydraulic conductivity	Water level in surface water and groundwater	Concentration of compound in feed water
	Temperature	Porosity	----	Adsorption coefficient (K_{oc})
	Microbial activity during pathway	Organic carbon content (C_{org}), dissolved organic carbon (DOC), total	----	Persistence ($DT_{50,\ water\text{-}sediment}$)

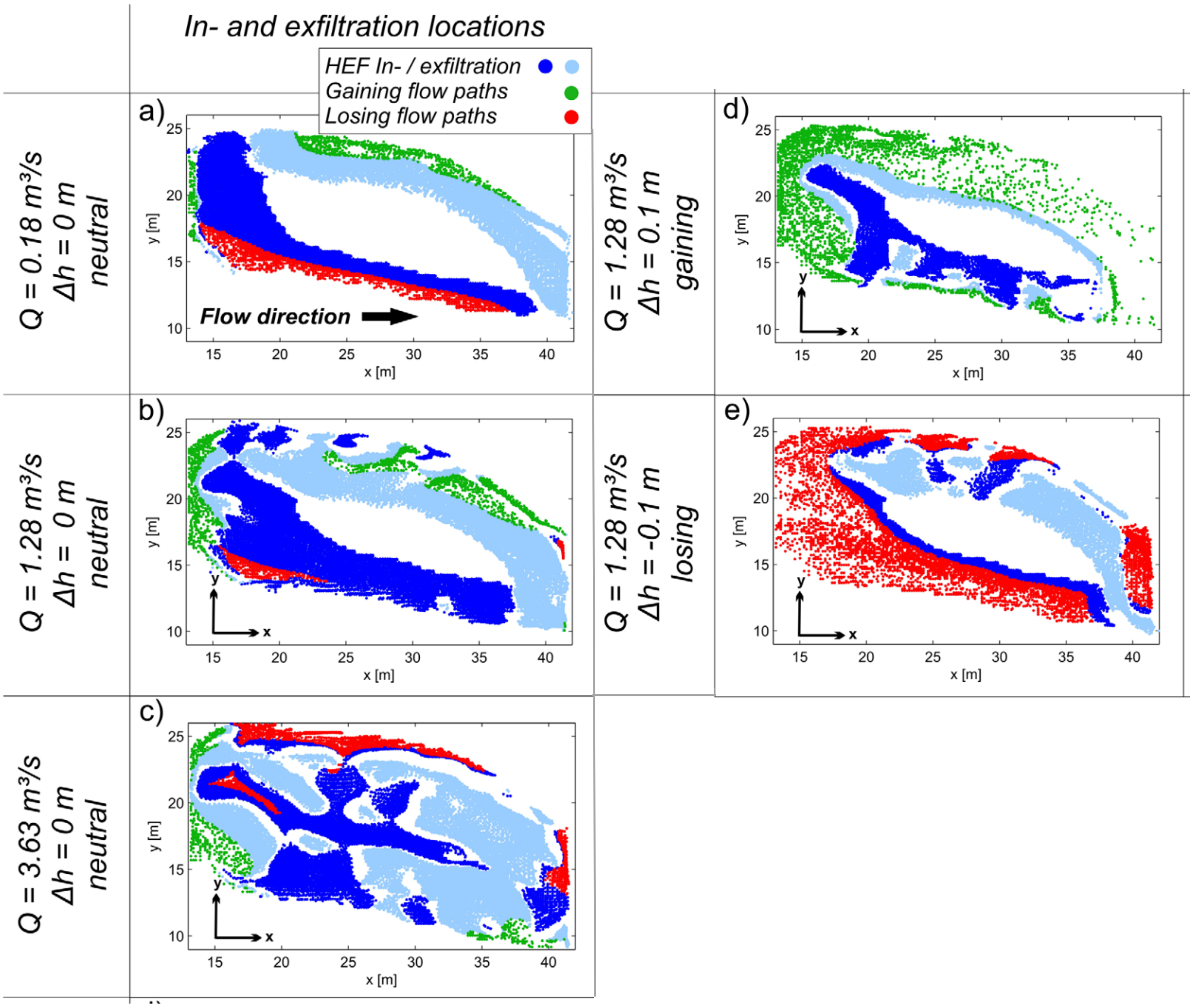
	Site characteristics: transport, biological degradation	Subsurface properties: infiltration, transport, sorption, biological degradation	Hydrometeorological factors: infiltration, transport, sorption, biological degradation	Compound properties: infiltration, transport, sorption, biological degradation
		organic carbon (TOC), clay minerals		

2.1 Processes during the bank filtration pathway

2.1.1 Infiltration

During bank filtration, water infiltrates from a surface water body into the subsurface due to a hydraulic gradient between the water levels of the surface water and the groundwater. It enters through the typically fine-grained infiltration zone of clays and silts at the riverbed (hyporheic zone) and passes through the generally coarser sediments of the aquifer (Marschke et al. 2006; Massmann et al. 2009). The bank filtration transport pathway is only active when the hydraulic gradient is directed toward the groundwater, i.e., when the water level in the surface water is higher than the groundwater level (Epting et al. 2018). This situation predominantly occurs in spring and summer, when groundwater levels decline due to lower precipitation and higher evapotranspiration. Therefore, this is a temporal transport pathway (Wang and Squillace 1994; Epting et al. 2018; Willkommen et al. 2022; Loose et al. 2024). Groundwater and surface water interact on different scales, ranging from entire riparian areas controlled mainly by the geological properties of the catchment, to exchange processes in the hyporheic zone governed by hydraulic gradients, properties, and topography of the river bottom (Dahl et al. 2007; Trauth et al. 2018). The examples in Figure 4 illustrate how areas of surface water infiltration into groundwater and exfiltration of groundwater into surface water vary spatially at a specific site, depending on the hydraulic conditions.

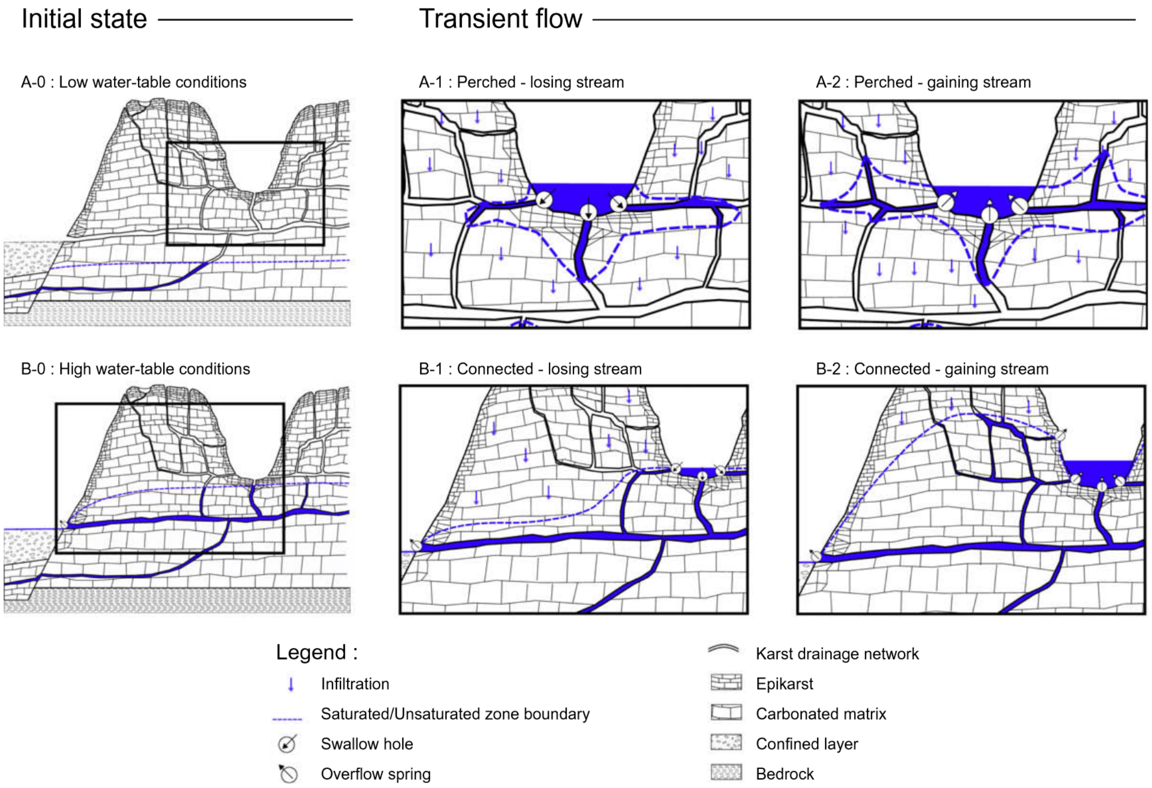
Figure 4: **Infiltration and exfiltration locations at the riverbed (infiltration: dark blue, exfiltration: light blue), gaining flow paths (green), and losing flow paths (red). Low, moderate, and high stream discharges (a–c) under neutral conditions (Δh and gaining and losing conditions (d and e) for constant stream discharge**



Source: Trauth et al. (2015 altered)

Numerous experimental and model-based studies conducted in recent decades have aimed to understand the extent and variability of groundwater and surface water interaction, revealing high spatial and temporal variability in exchange processes (Bailly-Comte et al. 2009; Trauth et al. 2015, 2018). The variability of infiltration/exfiltration is particularly pronounced in highly karstified watersheds due to the specific karst drainage network (Figure 5). This network makes it difficult to estimate the spatial extent of water transport in the subsurface and poses an increased risk that pollutants can quickly spread over large areas, depending on the hydraulic conditions (Bailly-Comte et al. 2009).

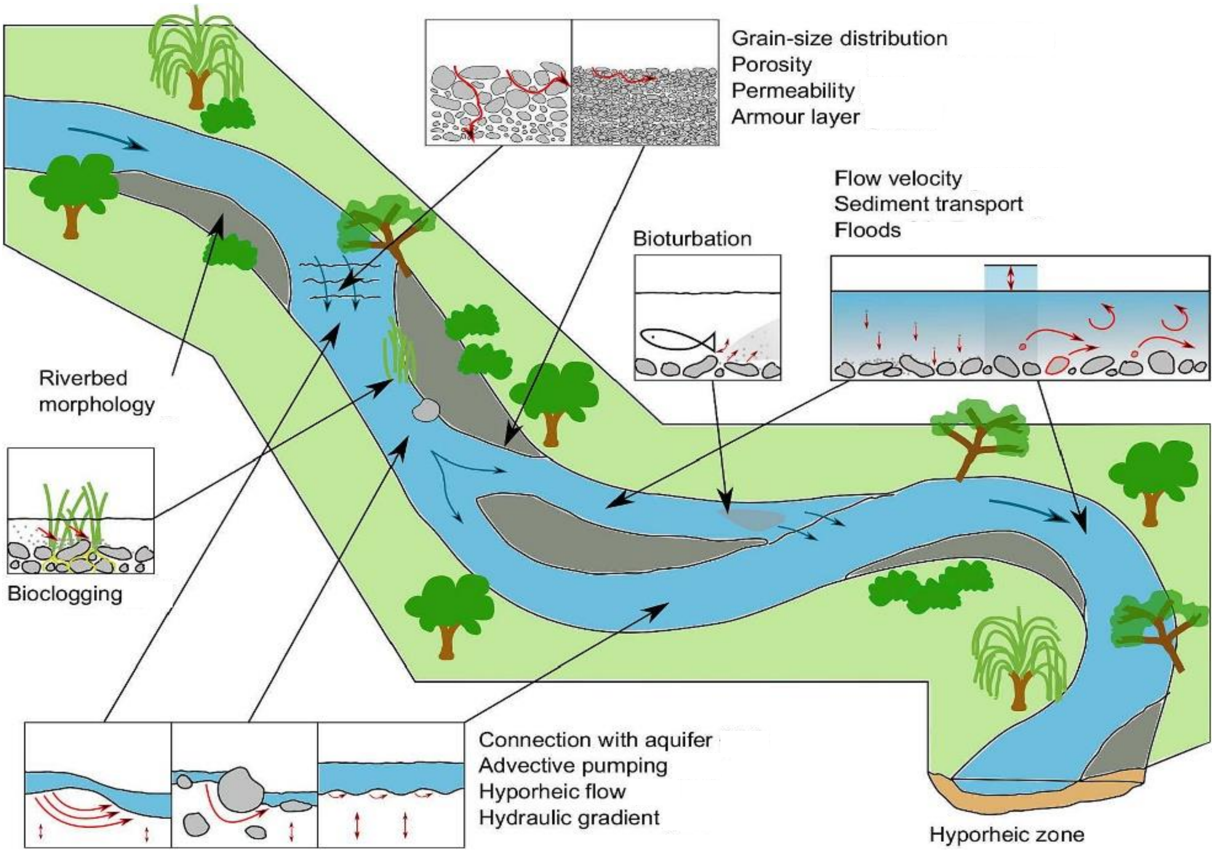
Figure 5: **Conceptualization of gaining/losing connected/perched stream in case of a karst aquifer Coulazou River/France**



Source: Bailly-Comte et al. (2009)

The hydraulic potential gradient can be of natural origin, during floods or related to topographical features such as river meanders. However, a potential gradient can also be artificially generated and controlled by impounding the surface water or by lowering the groundwater level through groundwater extraction (Marschke et al. 2006). The hydraulic gradient is highly variable and increases with rising water level in the surface water, e.g., seasonal variations, after rainfall events or snow melt (Massmann et al. 2009; Willkommen et al. 2022, Kondor et al. 2024). With rising hydraulic gradient, the infiltration into groundwater increases (Epting et al. 2018). Furthermore, the infiltration depends on the characteristics of the hyporheic zone, especially the grain size distribution since this layer acts as a filter (Massmann et al. 2009; Epting et al. 2018). Certain passages of the hyporheic zone of a surface water can be clogged (colmation) due to sedimentation of carbonates, iron or manganese compounds, microorganisms, colloids or suspended sediments and therefore reduce infiltration (Massmann et al. 2009; Gutiérrez et al. 2018; de Carvalho Filho et al. 2022) (Figure 6). During floods with high hydraulic energy, the riverbed can be altered, and the colmation layer can be eroded (Hiscock and Grischek 2002).

Figure 6: Main factors affecting the clogging of the riverbed by fine sediments



Source: Dubuis and De Cesare (2023)

The potential for clogging is higher at point bar locations along river banks, where the flow velocity is reduced, while the flow velocity is sufficiently high in the middle of the riverbed and at cut banks to either remove or prevent clogging (Schubert 2003; Marschke et al. 2006). Though this colmation can reduce the yield of bank filtration wells, its formation can generally be considered beneficial. Due to its higher content of fine-grained material and/or organic carbon, it potentially increases the residence time of bank filtrate in the subsurface and is more effective at retaining contaminants (Massmann et al. 2009; Handl 2023). The extent of this zone can differ from several decimeters to 30 m (Jüttner 1999; Ziegler 2001) and is followed by a subsurface passage characterized by lower retention potential and increased mixing of bank filtrate with groundwater (Grischek 2003; Eckert and Irmscher 2006; Massmann et al. 2009).

2.1.2 Transport

A main basis for compound transport during infiltration and subsurface passage is the flow process. The extent of water movement depends on the driving potential gradient and the permeability of the aquifer (Schmidt and Lange 2006). Hydrodynamic dispersion is mainly responsible for the spatial distribution of compounds dissolved in water, based on molecular diffusion and mechanical dispersion. Molecular diffusion caused by Brownian motion transports compounds from high to low concentration areas, independent of flow velocity and direction. Mechanical dispersion occurs because water molecules do not move along straight paths but flow around substrate grains, taking different paths from the same starting point. Additionally, flow velocities vary due to different pore sizes and geometries resulting in the spreading of the concentration peak (Wernli 2011). The hydrodynamic dispersion depends on the porosity/hydraulic conductivity of the aquifer (Geiges 2002; Schmidt and Lange 2006). Distance between surface water and groundwater as well as travel time of the compound are additional factors influencing BFR (Jaramillo et al. 2019). Nagy-Kovács et al. (2018) point out the challenge to assess whether the travel distance or the travel time is more responsible for the attenuation. Several studies show that with increasing distance, the BFR rises (Hollender et al. 2018; Kruc-Fijalkowska et al. 2022; Handl 2023). The travel time does not necessarily increase with greater distance, as the hydraulic conductivity of the subsurface significantly influences transport velocity. Short distances in a highly impermeable subsurface can result in longer travel times compared to longer distances in a subsurface with high permeability (Hollender et al. 2018; Abdelrady et al. 2020; Handl 2023). Dragon et al. (2018) investigated that with increasing distance between surface water and groundwater, the potential for dilution of the compound's surface water concentration by clean groundwater rises resulting in a higher BFR. In wells located 5 m to 82 m distant to the river, 65–85% of the water originated from bank filtration, whereas in a well approximately 680 meters away from the river, this percentage was around 40%. In further studies of the review, the proportion of bank filtrate in the abstracted raw water from wells ranged from 21% to 100% (Massmann et al. 2006b; Sprenger et al. 2017). Schmidt and Lange (2006) assessed the effect of dilution by clean groundwater as one of the main reasons for concentration decrease from surface water to groundwater. Besides aforementioned factors, the organic carbon content of the subsurface and the compound's adsorption coefficient K_{oc} alter the transport and hence BFR by sorption processes (Loffredo and Senesi 2008; Storck 2012; Malaguerra et al. 2013) (see Section 2.1.3). The persistence of a compound displayed as DT_{50} is a further factor modifying its transport and hereby its BFR due to biological degradation (Stuyfzand et al. 2007; Trinh et al. 2012; Kondor 2020) (see Section 2.1.4).

2.1.3 Sorption processes

Solid subsurface materials can remove organic trace compounds from bank filtrate through sorption, which involves transferring compounds from the aqueous phase to the solid phase. The infiltration layer and aquifer contain organic and inorganic materials such as algae, bacteria, clays, and oxides (Delle Site 2001; Schmidt and Lange 2006). The complex composition of sediment particles with their diverse chemical-physical surface properties allows a variety of sorption mechanisms that can reduce the concentration of trace compounds in the aqueous phase. Subsurface material continuously regenerates and provides various sorption mechanisms, including hydrophobic interactions, hydrogen bonding, electrostatic interactions, and chemisorption (Schmidt and Lange 2006). Schaffer and Licha (2015) identified two main sorption processes: hydrophobic and ionic sorption. Hydrophobic sorption involves nonpolar, neutral compounds that attach to uncharged sites on organic matter, which is effective due to its large specific surface area (Delle Site 2001). Ionic sorption involves polar, ionized compounds that interact with charged sites on clay minerals, organic matter, and metal oxides through mechanisms such as ion exchange and hydrogen bonding (Delle Site 2001). Depending on the nature and extent of the interactions, sorbed compounds can be completely or partially desorbed or irreversibly fixed (Schmidt and Lange 2006). During bank filtration, the riverbed or hyporheic zone is identified as the zone with the highest sorption potential due to its high organic matter content (Wang and Squillace 1994; Abogabal et al. 2020). With increasing distance from the riverbed, the sorption potential decreases, influenced by the characteristics of the aquifer (Jüttner 1999; Ziegler 2001; Ray et al. 2002a).

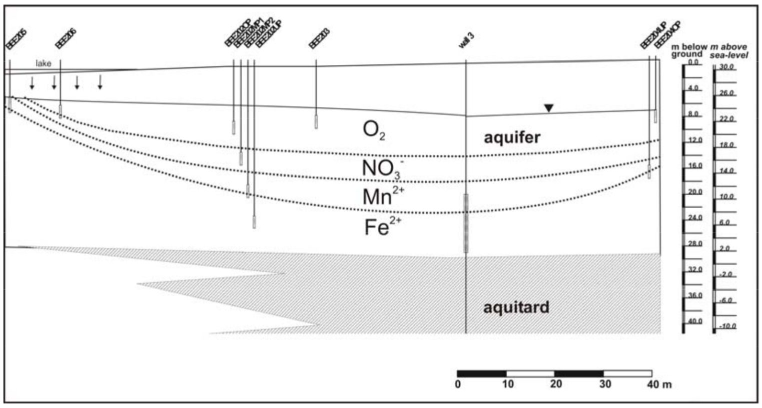
2.1.4 Microbial degradation

Aquatic ecosystems host diverse communities of organisms (biocenoses) that constantly interact with their abiotic environment. The chemical and physical properties of water and the subsurface determine site-specific conditions, influencing the type and abundance of microorganisms. Microbial metabolic activities, utilizing available organic and inorganic compounds, modify these conditions, often favoring different, better-adapted microbial communities (metabiosis). In particular, the hyporheic zone, with its fine-grained sediments and high organic carbon content, provides optimal conditions for the settlement and growth of microorganisms, resulting in a high potential for compound degradation and thus water purification (Trinh et al. 2012; Lewandowski et al. 2019; Höhne et al. 2022).

A key aspect of these ecological interactions is biocenotic succession, the temporal or spatial sequence of microbial communities within a habitat. Important environmental indicators, including redox potential (EH value) and oxygen content, both influence and are influenced by hydrochemical and microbially mediated processes during bank filtration. The input of biodegradable organic matter, serving as an electron donor in microbial metabolism, can lead to significant oxygen depletion, potentially resulting in anaerobic conditions in the subsurface passage (Eckert and Irmscher 2006; Massmann et al. 2008b). Microbial communities adapt to these changing conditions by using alternative, less efficient electron acceptors (e.g., nitrate, manganese (IV), iron (III), sulfate, and carbon dioxide) to continue the breakdown of organic compounds (Marschke et al. 2006; Schmidt and Lange 2006; Massmann et al. 2008b).

The microbial activity causes a gradual decrease in redox potential. Thus, redox potential significantly influences hydrochemical conditions and the transformation of compounds along the flow path. At the same time, microbial activity considerably alters chemical and physical conditions, often creating a sequence of redox zones. These zones can range from a few centimeters to several hundred meters, depending on sediment thickness, carbon content, and other hydrochemical, biological, and hydraulic conditions and show that the main microbial transformations of dissolved electron acceptors occur primarily in the infiltration area (Bradley 2014; Henzler et al. 2016; Kovačević 2017) (Figure 7).

Figure 7: **Approximate redox zoning as indicated by oxygen (O_2), nitrate (NO_3), manganese (Mn) and iron (Fe) presence in Lake Wannsee, Berlin**

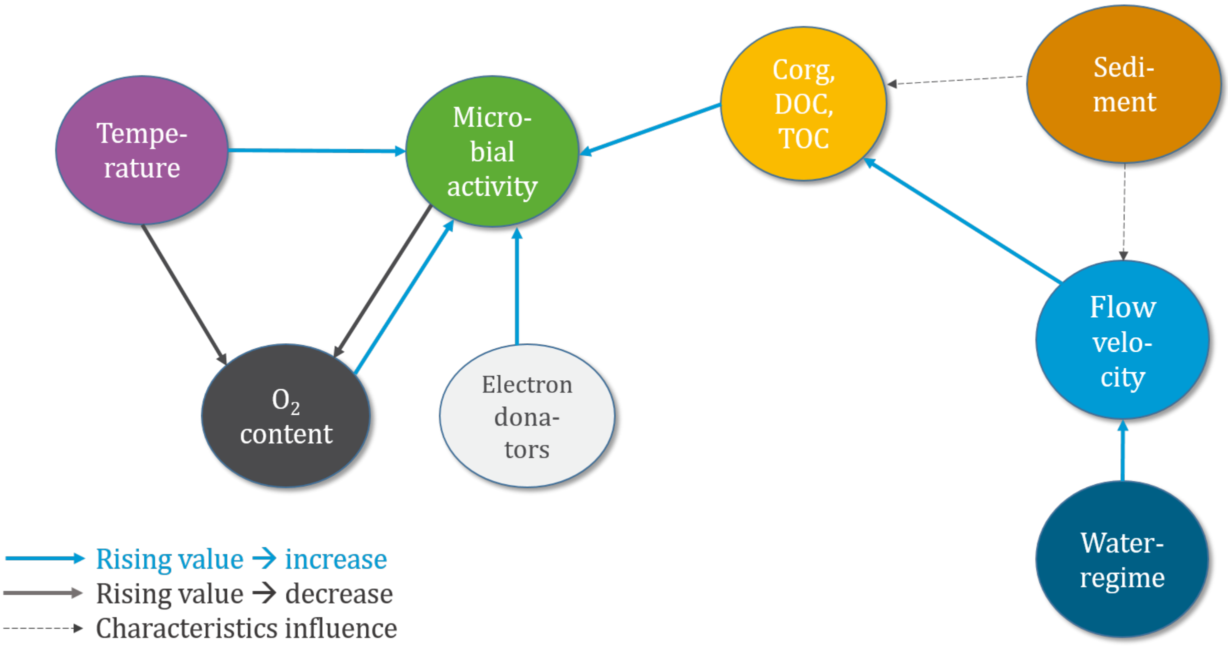


Source: (Massmann et al. (2006b)

The biodegradation of compounds is highly dependent on their interaction with the microbial community. Microorganisms tend to degrade compounds more efficiently when these compounds are present in high concentrations or when the microbial metabolism is specifically adapted to target them. When concentrations of C_{org} are high and compound concentrations are low, microorganisms preferentially use C_{org} as their energy source, reducing their focus on degrading the other compounds (Helbling 2015).

Overall, the complex interactions between biotic and abiotic components related to microbial degradation of compounds in aqueous matrices are influenced by various environmental factors, which are closely connected and have to be considered in combination. Figure 8 illustrates the strong linkage between temperature, oxygen content/electron donors, and available energy sources to microbial activity (Massmann et al. 2009; Henzler et al. 2016).

Figure 8: Interaction of biotic and abiotic factors related to microbial degradation of compounds in aqueous matrices

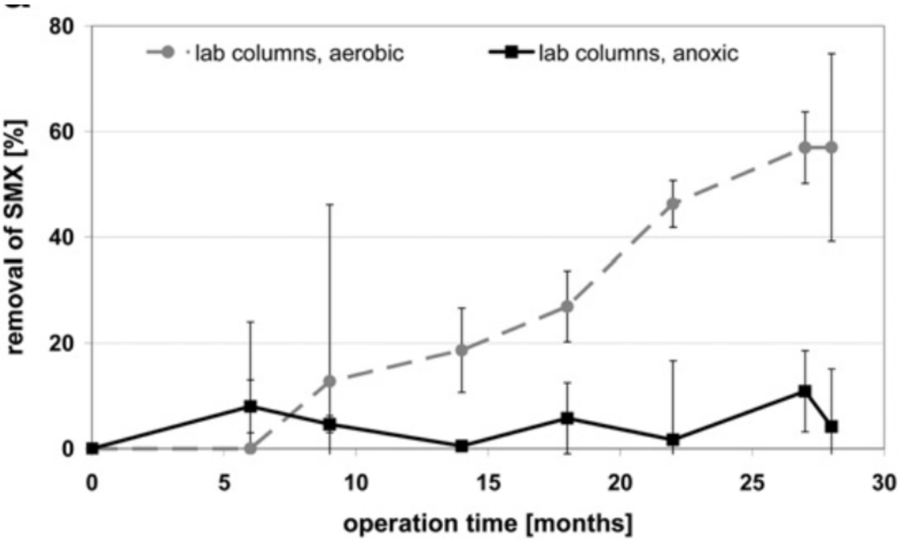


Source: own illustration, INR

3 Bank filtration rates

This section describes in detail BFR values and the factors influencing them, as mentioned in Table 1. A wide variety of study types, study designs, site conditions, and investigated compounds were observed in the reviewed literature, resulting in BFR data with broad ranges for the same compound, as presented in the following sections 3.1-3.3 and appendix A.2. Exemplarily, Figure 9 reveals clearly how BFR values can differ depending on one factor of the study design, e.g., on the length of the study period. The BFR of sulfametoxazole would be close to 0% in the first months and increases to almost 60% after 28 months under aerobic conditions. This raises the question: which value is the most representative one?

Figure 9: Relative removal of sulfamethoxazole in laboratory columns (0.25 ± 0.08 mg/L, travel time 14 d (arithmetic means with standard deviation of two parallel columns)



Source: Baumgarten (2011, altered)

To ensure that comparisons are meaningful, a distinction is made between field studies/modeling and laboratory studies, with only the study by Wang & Squillace (1994) considering natural bank filtration of compounds in a field study. Since environmental conditions in field studies can be varied only within a narrow range (e.g., in distance), the conclusions from these studies are primarily qualitative, often providing data for individual influencing factors only. In laboratory studies, at least one influencing factor was typically varied, allowing for some semi-quantitative statements.

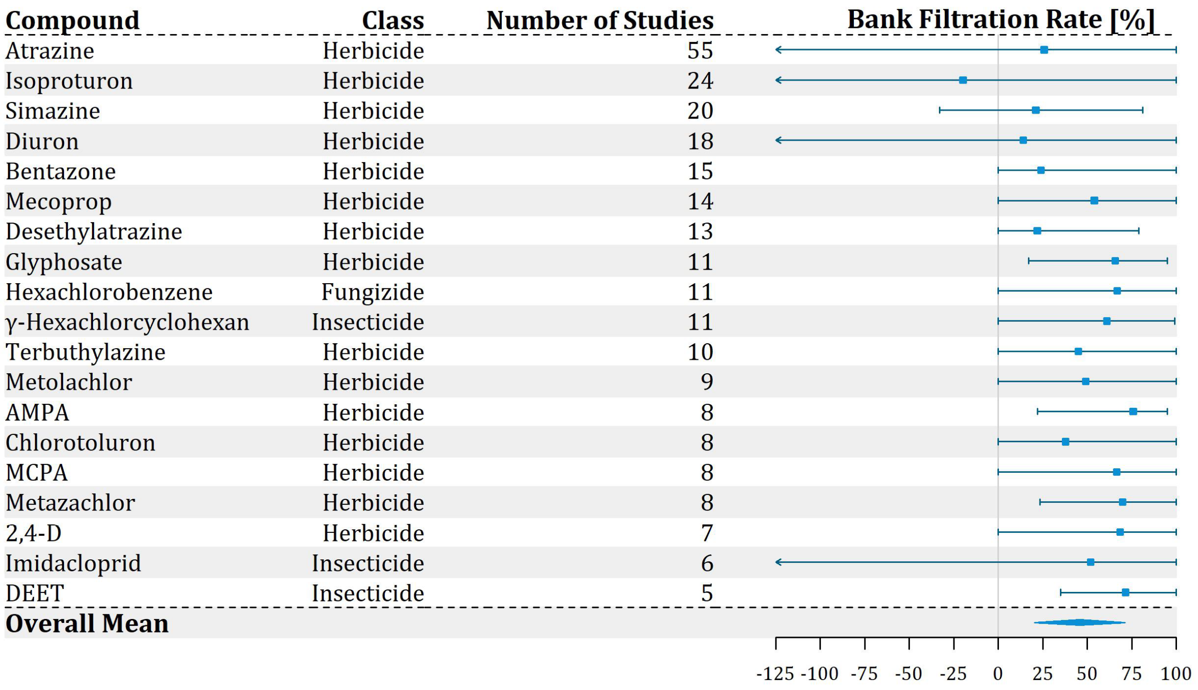
3.1 Bank filtration rates identified in the studies

In total, 705 data sets reporting a BFR were extracted. 91 PPPs were among the 215 compounds. The complete data set is shown in Appendix A.2. Exemplarily, the BFR of PPPs and pharmaceuticals, which were the most frequently observed in the literature review, are displayed in Figure 10 and Figure 11.

Some field studies reported negative BFR with values up to -1375% (e.g., Bruchet et al. 2012; Hollender et al. 2018; Oberleitner et al. 2020). Negative values can arise when the ambient groundwater contains higher concentrations of the specific compounds than the bank filtrate (Ziegler 2001) or when desorption processes of these compounds occur along the bank filtration pathway (Brauch et al. 2000). Negative values are still included in the list of BFR found in the literature (Appendix A.2).

When comparing the BFR, the range for the same compound varies from 10% (e.g., Iopromide, DEET) to 100% (Diuron). The results originate from divers types of study (field, modeling and laboratory) where conditions vary considerably or can only be partially replicated in terms of scale and process complexity (Onesios et al. 2009; Burke et al. 2014; Banzhaf and Hebig 2016). Variability arises due to differing conditions such as compound concentrations of infiltrating surface water, subsurface substrate characteristics, microbiome composition/amount at the study site, and the distance between surface water and groundwater. In laboratory studies, the incubation period required for microorganisms to adapt to the experimental conditions can be another contributing factor (Burke et al. 2014).

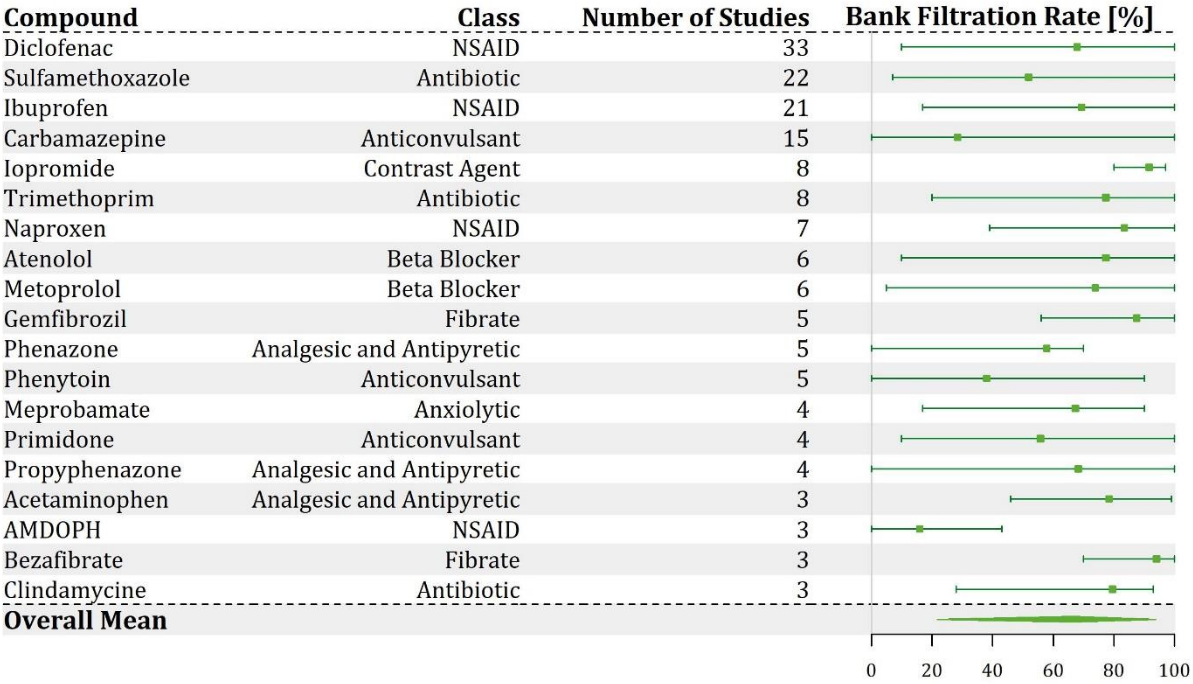
Figure 10: Bank filtration rates [%] of the PPPs most frequently observed in the studies of the literature review; blue dots = arithmetic mean value, blue lines = full range of BFRs (minimum to maximum values)



Compound	Class	Number of Studies
Atrazine	Herbicide	55
Isoproturon	Herbicide	24
Simazine	Herbicide	20
Diuron	Herbicide	18
Bentazone	Herbicide	15
Mecoprop	Herbicide	14
Desethylatrazine	Herbicide	13
Glyphosate	Herbicide	11
Hexachlorobenzene	Fungizide	11
γ-Hexachlorcyclohexan	Insecticide	11
Terbuthylazine	Herbicide	10
Metolachlor	Herbicide	9
AMPA	Herbicide	8
Chlorotoluron	Herbicide	8
MCPA	Herbicide	8
Metazachlor	Herbicide	8
2,4-D	Herbicide	7
Imidacloprid	Insecticide	6
DEET	Insecticide	5
Overall Mean		

Source: own illustration, INR

Figure 11: **Bank filtration rates [%] of the pharmaceuticals most frequently observed in the studies of the literature review; green dots = arithmetic mean value, blue lines = full range of BFRs (minimum to maximum values)**



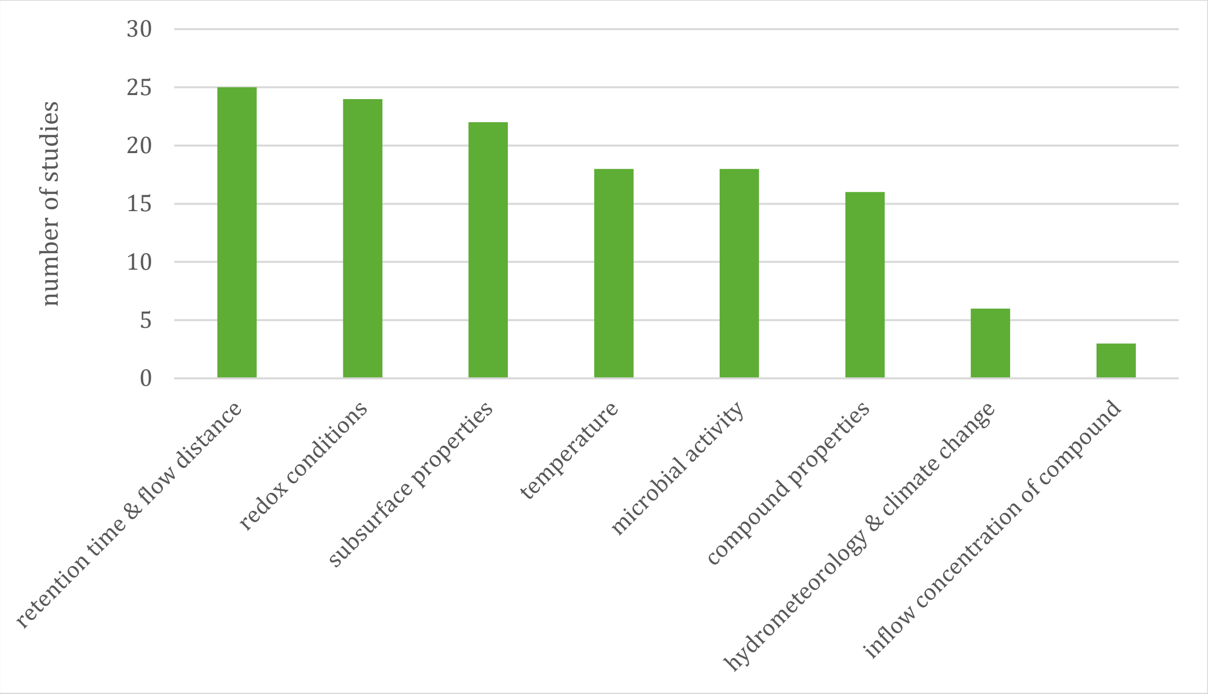
Compound	Class	Number of Studies
Diclofenac	NSAID	33
Sulfamethoxazole	Antibiotic	22
Ibuprofen	NSAID	21
Carbamazepine	Anticonvulsant	15
Iopromide	Contrast Agent	8
Trimethoprim	Antibiotic	8
Naproxen	NSAID	7
Atenolol	Beta Blocker	6
Metoprolol	Beta Blocker	6
Gemfibrozil	Fibrate	5
Phenazone	Analgesic and Antipyretic	5
Phenytoin	Anticonvulsant	5
Meprobamate	Anxiolytic	4
Primidone	Anticonvulsant	4
Propyphenazone	Analgesic and Antipyretic	4
Acetaminophen	Analgesic and Antipyretic	3
AMDOPH	NSAID	3
Bezafibrate	Fibrate	3
Clindamycine	Antibiotic	3
Overall Mean		

Source: own illustration, INR

3.2 Influencing factors in field studies and modeling

The field studies varied greatly in terms of study design and the factors influencing bank filtration that were recorded. Nevertheless, numerous studies provided information on important influences on bank filtration. The field studies most frequently investigated the retention time and flow distance, redox conditions and subsurface properties as influencing factors for bank filtration processes (Figure 12).

Figure 12: Literature review analysis of factors influencing BFR in field studies



Source: own illustration, INR

3.2.1 Influence of subsurface properties on bank filtration

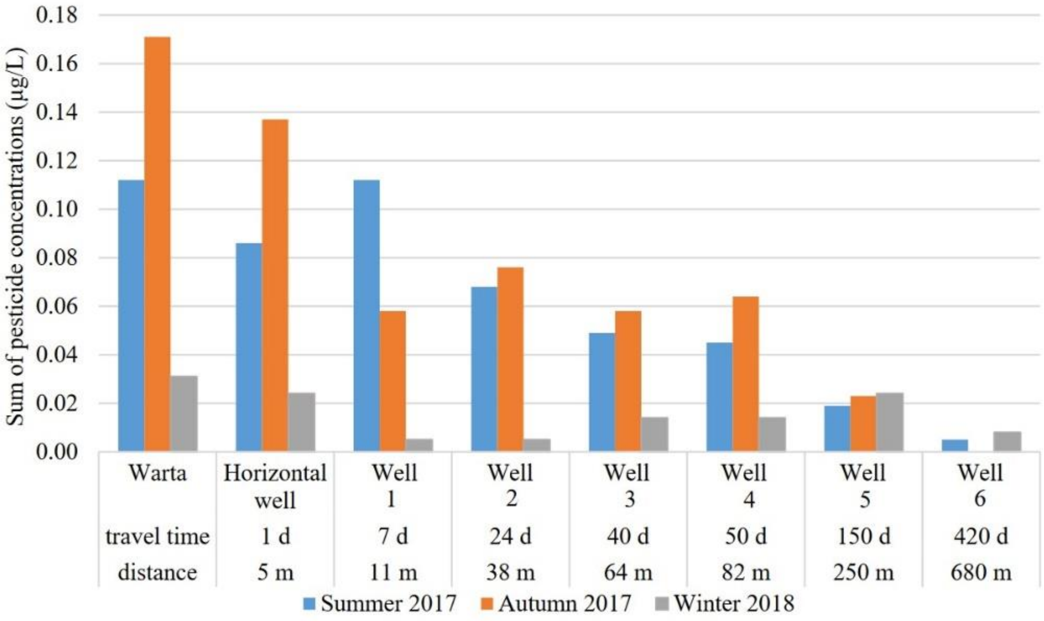
Subsurface properties such as organic matter content, clay content, and texture considerably influence BFR. High content of clay and organic matter improve pollutant removal by increasing adsorption and biodegradation rates, while sandy soils with low organic matter content may allow greater herbicide transport to the groundwater due to higher permeability (Wang and Squillace 1994; Hrkal et al. 2018; Abogabal et al. 2020). The hyporheic zone's biological activity, influenced by temperature, fine sediments, and microbial communities, plays a crucial role in compound attenuation and nutrient cycling, although excessive biological activity can lead to anoxic conditions that reduce degradation rates (Massmann et al. 2009; Bertrand 2021; Handl 2023). Hydraulic gradients, influenced by streamflow and aquifer properties, drive the movement of contaminants into groundwater. The aquifer's hydraulic conductivity and thickness further modulate the filtration process, highlighting the complexity of interactions between soil properties and BFR (Ray et al. 2002b; Malaguerra et al. 2013; Kondor 2020; Oberleitner et al. 2020). Physical deposition and biological growth can lead to clogging and affect BFR (Wang and Squillace 1994; Epting et al. 2018; de Carvalho Filho et al. 2022). Cation exchange capacity, pH, and salinity further impact adsorption efficiency, with specific combinations of these factors affecting the removal of different compounds (Kodešová et al. 2011; Greskowiak 2017).

3.2.2 Influence of subsurface retention time and distance on bank filtration

Subsurface retention time, referred to as hydraulic retention time, plays a crucial role in the removal of compounds through bank filtration. BFR can be impaired by factors like short flow paths and high flow velocities, requiring additional post-treatment in certain cases (Weiss et al. 2003a; Hu et al. 2016). Effective compound attenuation often requires longer hydraulic retention time, with minimum times of 0.5 to 1 day recommended for trace organic chemicals, and significantly better water quality observed with groundwater residence times of at least six months (Górski 2011; Filter et al. 2021). Longer flow paths and increased travel times not only facilitate higher removal rates of specific compounds like pharmaceuticals but also allow for the accumulation of beneficial microbial communities that contribute to the biotransformation of contaminants (Grünheid et al. 2005; Glorian et al. 2018; Dragon et al. 2019; Handl 2023). The location of wells relative to the river significantly affects BFR; wells placed 150-250 m from the river benefit from both longer travel times and better mixing with ambient groundwater, which helps in reducing compound concentrations (Ziegler 2001; Ahmed and Marhaba 2017; Dragon et al. 2019; Kruć et al. 2019). The shortest distance reported in the field studies was 5 m (Wang and Squillace 1994; Schmidt et al. 2004; Dragon et al. 2018).

Increased travel times also enhance the attenuation of persistent compounds by allowing more time for sorption processes and microbial activity, though the underlying redox conditions can have a more pronounced effect than the residence time alone (Schmidt et al. 2004; Storck 2012; Obeid et al. 2023). Overall, strategic positioning of wells and controlling the hydraulic conditions of the aquifer, including well operation and pumping rates, are essential for maximizing the efficiency of bank filtration systems. Dragon et al. (2018) were able to show the decrease of the pesticide sum concentrations with increasing distance from the Warta River to well 6 and longer residence time in the subsurface (Figure 13).

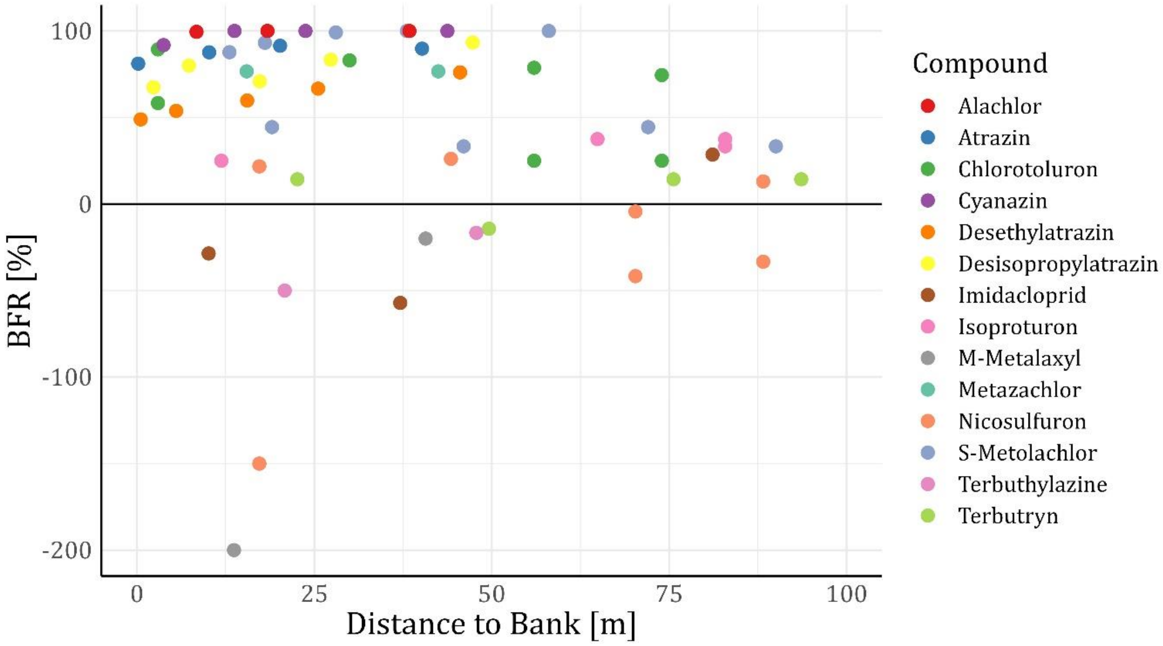
Figure 13: The sum of PPP concentrations [µg/L] along a flow path with respective travel time from the river Warta to different sampling wells in three seasons from summer 2017 to winter 2018



Source: Dragon et al. (2018, altered)

Observing the decrease of BFR of single PPPs along the flow path, variations can be exhibited. While certain studies predominantly show positive BFR, including those conducted by Wang and Squillace (1994) and Dragon (2019) (Figure 14), there are also several compounds with negative BFRs as well as high fluctuations. For instance, alachlor shows mostly high BFRs even in short distances to the bank, whereas chlorotoluron’s BFRs decrease with increasing flow path lengths. In contrast, certain compounds such as nicosulfuron show high variation and no reduction in the BFR at greater distances from the bank. The BFRs range from -200% to 100% across distances from a few meters up to 100 meters.

Figure 14: **BFR [%] and distance [m] to bank from the field studies of Wang and Squillace (1994) and Dragon et al. (2019)**



Source: own illustration, INR

3.2.3 Influence of hydrometeorology and climate change on bank filtration

Climate change and hydrometeorological events significantly influence bank filtration by altering water quantity, travel time, and compound levels. Extreme conditions such as floods and droughts can shorten travel times of bank filtrate, reducing residence time and leading to potential contamination by organic micropollutants (Sharma et al. 2012a; Essl 2014). High river discharge events increase the presence of sewage and agricultural runoff in rivers, subsequently elevating organic micropollutant concentrations in groundwater, necessitating adaptive management or enhanced water treatment (Epting et al. 2018). Conversely, droughts promote anaerobic conditions, while low-flow conditions extend residence times, enhancing pollutant degradation (Sprenger et al. 2011; Sharma et al. 2012a). The formation and removal of colmation layers, influenced by low and high water levels respectively, affect the availability of water at bank filtration sites and the efficiency of biological compound breakdown (Handl et al. 2020). Additionally, climate change impacts such as temperature variations and changes in organic matter composition further influence redox conditions and the overall quality and quantity of water obtained through bank filtration (Hu et al. 2016).

3.2.4 Influence of compound concentration in infiltrating water on bank filtration

The initial concentration of compounds can influence their removal during the bank filtration process, although this effect is seldom mentioned in studies. Storck (2012) indicates that higher initial concentrations enhance the biodegradation rate of certain pharmaceuticals and reduce the lag time for easily biodegradable compounds. Similarly, Ziegler (2001) notes that the elimination of organic compounds depends on the initial concentration and other environmental factors, with approximately 30 to 50% of dissolved organic compounds being removed through bank filtration and artificial groundwater recharge. Furthermore, Ray et al. (2002b) demonstrate that the removal efficiency of organic compounds, including aromatic amines, is directly related to their biodegradability and initial concentrations.

3.2.5 Influence of temperature on bank filtration

Temperature considerably influences bank filtration by affecting microbial activity, redox conditions, and the degradation of pollutants. Higher temperatures enhance microbial growth and increase the adsorption efficiency of hydrophilic compounds, leading to greater attenuation of pollutants (Sharma et al. 2012a; Abogabal et al. 2020). Higher temperatures (>14°C) promote higher microbial activity and faster biodegradation rates but also create anoxic conditions due to higher oxygen demand of aerobic microorganisms. Lower temperatures (<14°C) support oxic conditions and slower pollutant removal (Diaz-Cruz and Barceló 2008; Ahmed and Marhaba 2017). The degradation rates of certain organic micropollutants increase with temperature, with compounds like Iopromide showing more tolerance to temperature changes compared to others (Grünheid et al. 2008). Seasonal temperature variations can lead to significant changes in redox conditions and oxygen levels due to lower potential of warm water to dissolve oxygen and due to microbial respiration, affecting the overall BFR (Gross-Wittke et al. 2010; Sharma et al. 2012a). Although temperature increases generally enhance the degradation of pollutants, the specific impacts can vary depending on the site and the type of compounds present (Munz et al. 2019; Handl et al. 2020).

3.2.6 Influence of redox conditions on bank filtration

The influence of oxygen content on bank filtration varies significantly and plays a crucial role in the effectiveness of compound removal, as oxygen levels impact microbial activity and redox conditions. Most organic compounds are attenuated within the first meters of infiltration, and removal efficiencies vary widely depending on redox conditions, which shift from oxic to anoxic during subsurface passage (Maeng et al. 2011; Hollender et al. 2018). Oxic conditions generally promote the degradation of most pharmaceuticals, except for specific compounds like carbamazepine, which is more effectively removed under anoxic conditions (Rauch-Williams et al. 2009; Kovacevic et al. 2017; Schaper et al. 2018). The transient nature of redox indicators at bank filtration sites, which varies greatly in both space and time, affects the removal efficiencies of organic micropollutants (Schmidt et al. 2004; Henzler et al. 2016). High oxygen consumption can negatively impact the removal rate of redox-sensitive organic micropollutants by creating an oxygen deficit that limits microbial degradation processes (Eckert et al. 2008; Filter et al. 2017). Seasonal and spatial variations in oxygen concentration influence the microbial activity, which can lead to shifts from aerobic to anaerobic conditions affecting the degradation potential within the aquifer (Eckert and Irmscher 2006; Massmann et al. 2008b, 2009; Muellegger et al. 2013). Overall, the availability of oxygen and the resulting redox conditions within the bank filtration system are critical for determining the BFR of various compounds, highlighting the need for site-specific management strategies to optimize filtration outcomes (Sprenger et al. 2011; Storck 2012).

3.2.7 Influence of microbial processes on bank filtration

Microbial processes are essential for the degradation and removal of compounds during bank filtration, with biodegradation being a primary mechanism influenced by temperature, oxygen levels, and organic carbon composition (Li et al. 2013; D'Alessio et al. 2015). The hyporheic zone, with its fine sediments and high organic carbon content, creates ideal conditions for microbial colonization and growth, playing a key role in the attenuation of compounds (Massmann et al. 2009; Bertrand 2021; Handl 2023). Microbial competence in river sediments plays a considerable role in the degradation of compounds, e.g., for isoproturon, indicating that opportunities for degradation are higher in sediments than in river or groundwater (Trinh et al. 2012). Higher biomass quantities enhance biodegradation rates, and the specific composition of organic carbon in river water compared to wastewater significantly shapes the responsible microbial communities (Li et al. 2013; Alidina et al. 2014). Microorganisms adapt over time to various pollutants, leading to more efficient degradation in natural settings compared to lab environments (Storck 2012; Epting et al. 2018). Strong binding of chemicals to subsurface such as with DDT (dichlorodiphenyldichloroethane) can hinder biodegradation, highlighting the importance of subsurface composition and organic matter in microbial processes (Linde 1994; Loffredo and Senesi 2008). The fate and persistence of pharmaceuticals are significantly affected by microbial activity, which can transform or adsorb molecules differently in natural environments (Kondor 2020).

3.2.8 Influence of compound properties on bank filtration

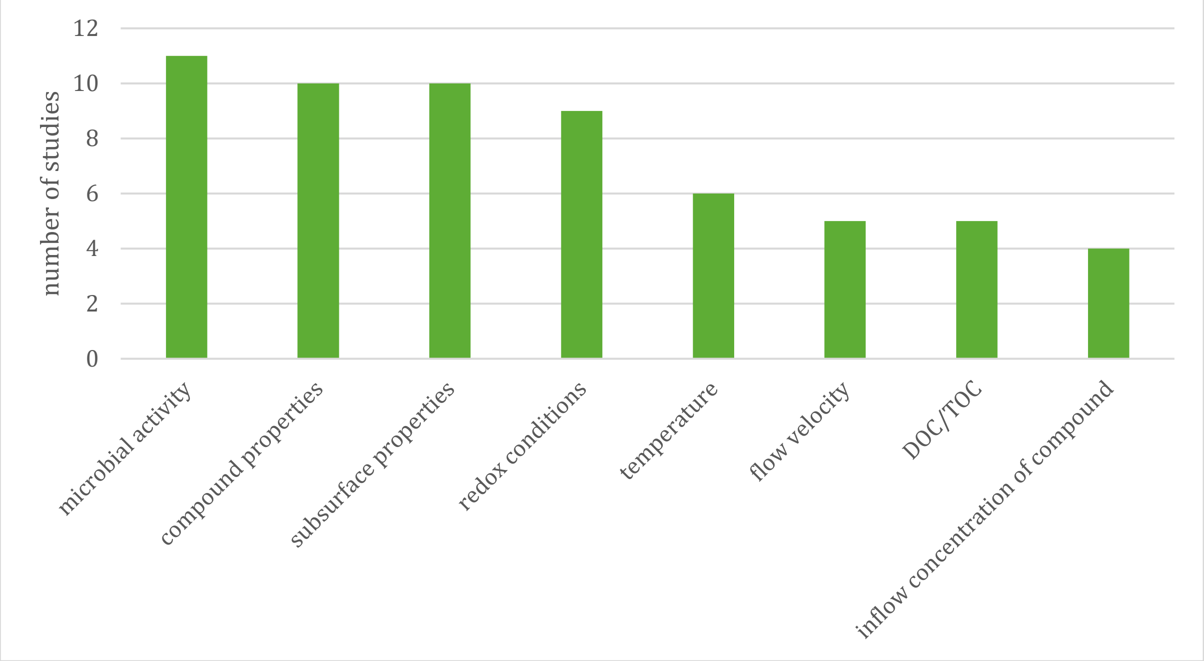
Persistence and removal of compounds in river bank filtration depend on various factors, including compound properties and environmental conditions (Henzler et al. 2016; Huntscha et al. 2013; Jaramillo et al. 2019; Maeng et al. 2010). Polar and water-soluble compounds, e.g. many pharmaceuticals and PPP transformation products, tend to be more problematic in bank filtration due to their persistence and mobility, with some compounds like carbamazepine and sulfamethoxazole showing high resistance to degradation (Heberer 2002; Postigo and Barceló 2015; Hamann et al. 2016). Nagy-Kovács et al. (2018) mention as an example metazachlor and metolachlor, which rapidly degrade into oxanilic acid (OA), ethane sulfonic acid (ESA), and related transformation products. These transformation products exhibit low adsorption to soil, resulting in high mobility. Consequently, the OA and ESA derivatives of metazachlor and metolachlor are among the most common and concentrated pollutants found in water. Contrary, highly sorbable and degradable compounds lead to low concentrations in groundwater (Malaguerra et al. 2013). Sorption capacity and degradability are also influenced by molecular structure, functional groups, and environmental conditions like pH, redox potential, and temperature, which affect the interaction between compounds and subsurface organic matter (Kolpin et al. 1998; Loffredo and Senesi 2008). Anionic compounds, being repelled by negatively charged matrices, rely more on biological degradation for removal, which necessitates carbon sources as C_{org} (Schwarzenbach et al. 1983). Overall, the fate and transport of compounds during bank filtration are governed by a complex interplay of their chemical properties and the prevailing environmental conditions (Henzler et al. 2016).

3.3 Influencing factors in laboratory studies

When comparing BFRs, it should be considered that column experiments are limited in their applicability to real-world conditions due to experimental constraints including scale limitations and the exclusion of several parameters in the laboratory column setup (Burke et al. 2014; Banzhaf and Hebig 2016). These limitations prevent the full representation of natural processes that occur simultaneously in the environment. Nevertheless, the primary aim of column experiments is not necessarily to produce results that can be directly transferred to real-world scenarios but to enhance the overall understanding of the behavior of organic compounds and how various boundary conditions influence this behavior (Burke et al. 2014; Banzhaf and Hebig 2016).

In the 30 laboratory studies included in this review, the main influencing factors examined were redox conditions and compound properties (Figure 15). Although soil material was frequently used to interpret the BFR, the laboratory experiments predominantly used sandy soils, meaning that the differences between the soils used in the studies, or within a single study, were minimal. No studies were found that varied more than two influencing factors. The pH during the experiment was documented in several studies, but its effects were not investigated. Similarly, while compound properties such as molecular weight and persistence (DT_{50}) were not explicitly examined, sorption potential was considered in terms of logPow, logD, or $\log K_{ow}$ rather than K_{oc}, which is more commonly used in the environmental fate assessment of PPPs.

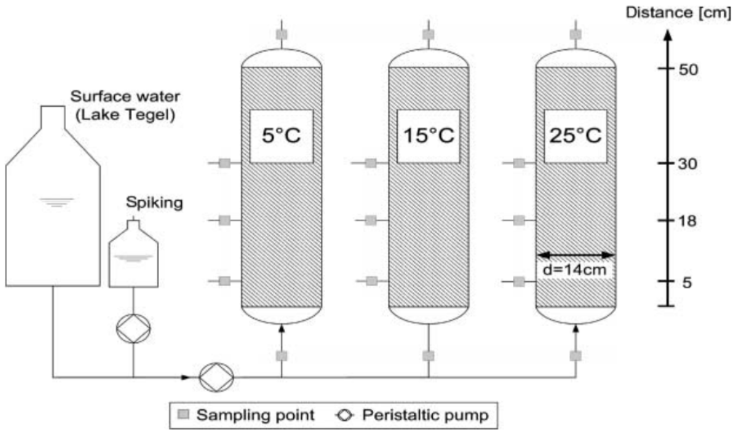
Figure 15: Literature review analysis of factors influencing BFR in laboratory studies



Source: own illustration, INR

The experimental design of the individual studies included columns varying in length from 5 m to 100 cm (one column was 366 cm long). The columns used were predominantly filled with sand. Generally, the columns were permeated from top to bottom. In some studies, the columns were permeated in both directions or only from bottom to top to prevent the formation of air bubbles. The hydraulic conductivity of the columns ranged from 0.000005 to 0.0001 m/s. Several studies incorporated a multi-month adaptation phase to establish the microbiome in the columns and enable better simulation of microbial processes. The duration of the experiments ranged from a few hours to four years, depending on the specific goals and variables of the study. Some experiments involved the use of series-connected columns, where a specific influencing factor was varied. This allowed for an analysis of the interactions and behavior of different compounds under controlled but variable conditions (Figure 16).

Figure 16: Schematic set-up of a temperature controlled soil column system



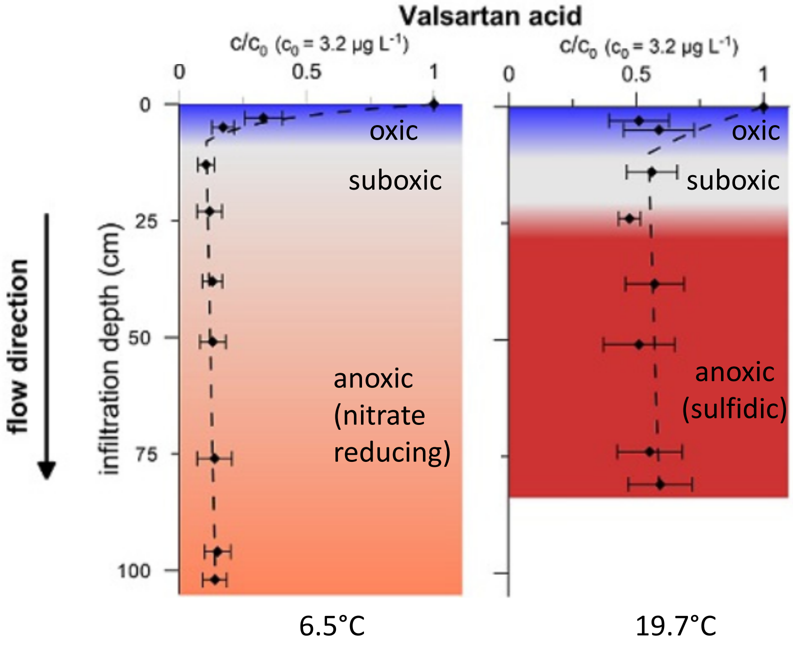
Source: Grünheid et al. (2008)

The summarized key findings from the laboratory studies overlap partly with those from field studies/modeling, but are still mentioned here for better clarity on the results from the laboratory studies.

3.3.1 Influence of subsurface properties and infiltrating water on bank filtration

The assessment of the impact of subsurface properties on BFR is discussed in contrast. When comparing two soil types with differing clay (0.5% vs. 3.7%), silt (0.5% vs. 3.6%), and sand content (99% vs. 93%), as well as variations in C_{org} content (0.3% vs. 0.9%), the observed degradation rates [1/d] for several pharmaceuticals and the PPPs Diuron, Triclopyr, Simazine, and Atrazine showed no statistically significant differences. Consequently, the authors concluded that the composition of the soil types considered in this study is not a crucial factor influencing the BFR (Bertelkamp et al. 2015). This finding is supported by another study, which observed no significant difference in removal in sediments containing 97% sand and 2.1% gravel compared to those with 86% sand and 13% gravel (Tuxen et al. 2000). Contrary, Burke et al. (2018) investigated two sediments for compound removal, one with approx. 90% fine sand, 10% medium to coarse grained sand and approx. 4% loss of ignition over the upper 40 cm. The second sediment can be described with varying amount (approx. 60-85%) of fine sand and medium to coarse sand (approx. 15-40%) and a loss of ignition value of 4.5% in the uppermost 10 cm, decreasing to 1.5% at 10-30 cm depths. The different composition of the sediments caused different zones of redox conditions resulting in varying half-life times of valsartan acid (Burke et al. 2018) (Figure 17).

Figure 17: **Concentration depth profiles for valsartan acid; black circles = arithmetic mean of measured concentrations (n = 3); standard deviations = error bars; removal curves (dashed lines) assume 1st order degradation**



Source: Burke et al. (2018, altered)

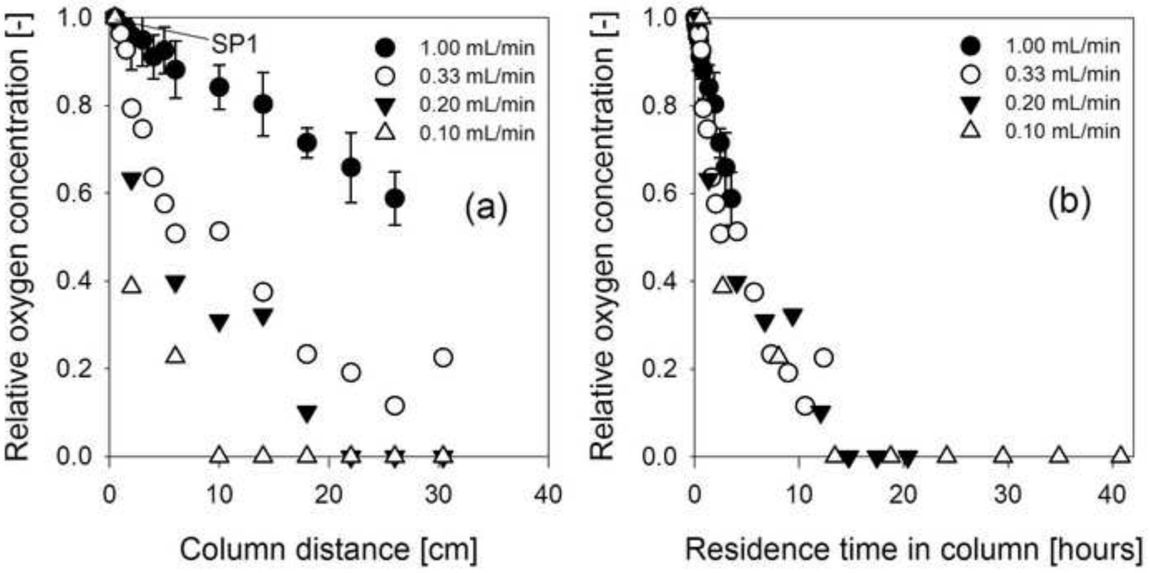
Similar to Burke et al. (2018) and field studies, a redox zonation was observed in columns with an oxic zone present only in the upper centimeters (20 cm in a 100 cm column (Massmann et al. 2008a)) followed by suboxic and anoxic layers. The thickness of these layers varies considerably, making compounds biodegradable under oxic conditions most efficiently eliminated in the upper centimeters (Massmann et al. 2008a; Burke et al. 2014, 2018). Low organic matter content and a low cation exchange capacity in the subsurface reduce the potential for adsorption of compounds with high K_{oc} values. Conversely, high organic matter content in form of humid acids can enhance the retention of compounds (Bajeer et al. 2012). When biodegradation is limited due to low temperatures and low oxygen concentrations, humic acids can act as electron donors providing energy for microorganisms (D'Alessio et al. 2015). The pH value in the column systems was reported in only few studies, ranging from 6.4 to 8.5 (e.g., Tuxen et al. 2000; Bajeer et al. 2012; Hoppe-Jones et al. 2012). However, none of the studies was conducted under varying pH conditions.

Bertelkamp et al. (2014, 2015) hypothesize that organic matter quantity in the water phase, rather than in the subsurface phase, governs the microbial activity and compound degradation, which is supported by Hoppe-Jones et al. (2012). In a batch study, the DOC concentrations of 4.1 and 10.3 mg/L in the influent led to an increase of the BFR in the range of 0 to 10% depending on the compound. For atrazine and isoproturon, BFR increased by up to approximately 25%, likely due to an enhanced potential for microbial degradation. This increased effectiveness of microbial processes may be attributed to the presence of sufficient energy sources such as DOC (Abdelrady et al. 2019). The effect of particulate organic matter is assed differently: while Filter et al. (2017) assume that particulate organic matter in the uppermost subsurface layer causes anoxic conditions, hampering the removal of redox-sensitive compounds, particulate organic matter in combination with natural sand can act as a relevant electron donor, sustaining aerobic conditions according to von Rohr et al. (2014).

3.3.2 Influence of flow velocity/travel time on bank filtration

Carpenter and Helbling (2017) varied the flow velocity in their study between 0.000028 m/s and 0.00011 m/s. Higher flow velocities increase the time for microorganism establishment but also allow microorganism presence and hereby compound degradation in greater depth. However, higher flow velocities provide less time for biodegradation and reduce the compound removal. For four out of nine compounds, the BFR decreased significantly with increasing flow velocity. Further, the flow rate impacts the redox zonation of the profile. At high flow rates of 1mL/min, oxic conditions persist whereas low flow rates of 0.2 mL/min cause anoxic conditions starting from 20 cm depth. Lower flow rates extend the hydraulic residence time, resulting in increased oxygen consumption within the same column zone and leading to anoxic conditions (von Rohr et al. 2014) (Figure 18). Grünheid et al. (2005) assessed very generally the travel time as most important design parameter for BFR in their study. Based on measured data in a column experiment, the length of the column was simulated until the concentration fell below the European threshold for drinking water of 0.1 µg/L (Directive (EU) 2020/2184 2020) (Litz et al. 2011). For glyphosate concentrations of 3.5 µg/L and 11.6 µg/L, the column length was determined to be 2.75 m and 3.75 m, respectively, while the column length was 1.0 m during the experiment (Litz et al. 2011).

Figure 18: **Profiles of relative oxygen concentration (normalized to inflow SP1) as function of (a) infiltration distance and (b) residence time at flow rates of 0.10 (n=1), 0.20 (n=1), 0.33 (n=1) and 1.00 (n=13) mL/min at 20°C**



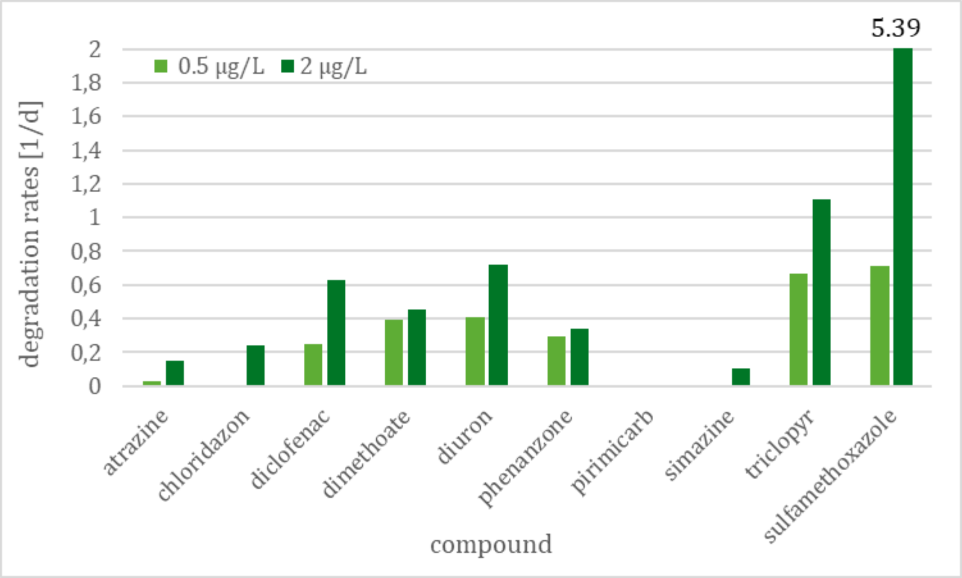
Source: von Rohr et al. (2014)

3.3.3 Influence of compound concentration in infiltrating water on bank filtration

Compound concentrations in the infiltrating water considerably influence the BFR (Baumgarten 2011): In a long-term experiment of 24 months, elevated concentrations of 4 mg sulfamethoxazole/L led to faster microbial adaptation (3-12 months) and more effective relative removal of 95% compared to concentrations of 0.25 µg sulfamethoxazole/L, where adaptation continued to increase during the second year. At higher concentration levels, sulfamethoxazole was removed even under anaerobic conditions by 51% and anoxic conditions by 27%. It is assumed that sulfamethoxazole degradation occurs only above a threshold concentration, where the adaptation process of microorganisms for sulfamethoxazole becomes beneficial for them (Baumgarten 2011).

The observation that degradation rates increase with higher compound concentrations in inflowing water has been corroborated as well by Bertelkamp et al. (2016a) (Figure 19). In contrast, a study with continuous glyphosate inputs of 3.5 and 11.6 µg/L simulated a decreased retardation factor of 25 and 18, respectively. This effect was attributed to altered adsorption behavior depending on the concentration (Litz et al. 2011).

Figure 19: Degradation rates of selected compounds at two different influent concentrations based on selected data of Bertelkamp et al. (2016a)

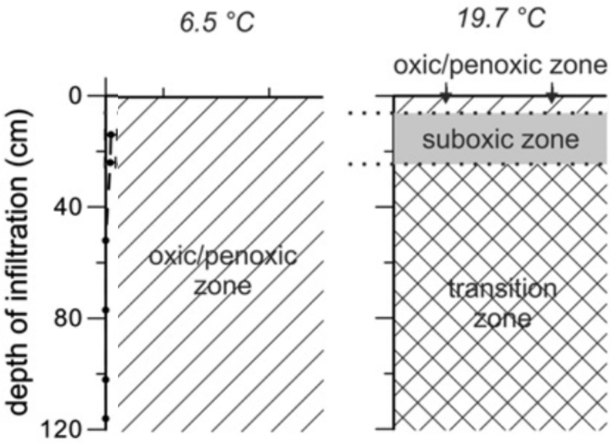


Source: own illustration, INR

3.3.4 Influence of temperature on bank filtration

The temperature applied in the laboratory studies was in the range of 5-30°C (Burke et al. 2014; von Rohr et al. 2014; Abdelrady et al. 2019). Due to the strong relation between temperature and microbial activity, biodegradation increases with rising temperatures by enhanced microbial growth, which is beneficial for the removal of biodegradable hydrophilic compounds (Grünheid et al. 2008; Abdelrady et al. 2019; Abogabal et al. 2020). Besides microbial growth, also the adsorption efficiency for hydrophobic compounds increases (Abdelrady et al. 2019). Burke et al. (2014) determined an increase of BFR for metropolol by 32%, for acesulfam of 24%, and for tolytriazole of 32% when temperature rises from 6.5-19.7°C (Figure 20). At the same time, the removal of diclofenac decreased from 89% to 65% under these conditions. BFR increased by factor 10 for Iopromide when temperature changed from 5-15°C (Grünheid et al. 2008) and to rates of 95% for hydrophilic compounds (Abdelrady et al. 2019). The results reveal the high individuality of BFR, which is closely connected not only to one factor but a set of factors such as compound characteristics, temperature, and microbial activity. The microbial growth enhanced by higher temperatures leads to higher oxygen consumption due to respiration. As a result, oxygen concentrations are depleted already within the upper layers of the column and suboxic/anoxic zones follow where the BFR of compounds biodegradable under oxic conditions decreases (Burke et al. 2014; von Rohr et al. 2014; Burke et al. 2018).

Figure 20: Redox zonation in the column as influenced by temperature



Source: Burke et al. 2014, altered)

3.3.5 Influence of redox conditions on bank filtration

Redox conditions play a crucial role in determining the BFR for various pollutants, with biodegradation being a key factor. Oxic conditions favor aerobic microbial activity increasing BFR of compounds removed under oxic conditions. Biodegradation rates of selected PPPs are reported in Table 2, showing the compound specific behavior according to the redox conditions. These degradation rates are limited to similar experimental conditions.

Table 2: Biodegradation rates [1/d] of selected PPPs for oxic, suboxic and anoxic pilots (Bertelkamp et al. 2016b adapted)

	Oxic pilot	Suboxic pilot	Anoxic pilot
	Oxic conditions	**NO3 reducing conditions**	**Complete NO3 removal**
PPP	**Biodegradation rate [1/d]**	**Biodegradation rate [1/d]**	**Biodegradation rate [1/d]**
Atrazine	0	0	0
Chloridazon	2.77[a]	not determined	not determined
Dimethoate	0.39[a]	0.06	0.11
Diuron	0.52	0.09	0.11
Pirimicarb	0.06	0.04	0.08 [b]

[a] Show increase in organic micorpollutant biodegradation rate over time, adapted biodegradation rate is presented

[b] Biodegradation rate of pirimicarb in the anoxic pilot is statistically not significant (confidence interval is going through zero).

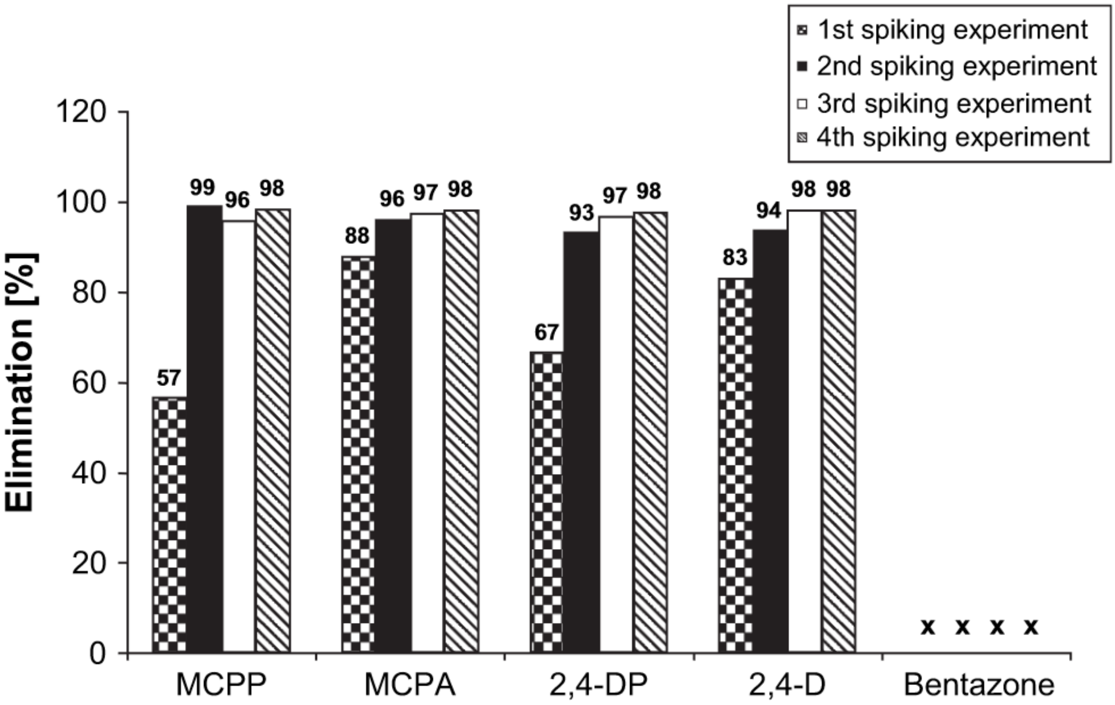
Oxic conditions are particularly favorable for the removal of organic compounds, underscoring the significance of maintaining oxygenated environments for effective pollutant degradation (Abogabal et al. 2020). Conversely, certain compounds like sulfonamides show higher degradability under anoxic conditions compared to oxic and suboxic conditions, indicating that redox conditions can differentially impact the degradation of specific pollutants (Bai et al. 2019). Anoxic conditions can also result from low infiltration rates, which lead to greater oxygen consumption over a given infiltration distance, potentially causing anoxic conditions. During future summer conditions, the combined effect of high temperatures (≥20°C) and low infiltration rates (≤0.01 m/h) due to low water levels could lead to temporary anoxic conditions (von Rohr et al. 2014). Combining high temperatures with different redox states, highest removal rates of pharmaceuticals were observed under conditions of high temperatures with oxic, penoxic, or suboxic redox states (Burke et al. 2014). In contrast, cold oxic/penoxic conditions showed removal rates about an order of magnitude lower than their warm counterparts. Consequently, pollutant attenuation is most efficient in summer when oxic conditions dominate during the initial stages of infiltration (Burke et al. 2014). However, the enlargement of the oxic zone in colder conditions can offset lower removal rates through longer residence times, potentially maintaining or even enhancing overall attenuation efficiency (Massmann et al. 2006a). Banzhaf et al. (2012) focused on redox conditions under varying nitrate concentrations. They observed that denitrifying or nitrate-reducing redox conditions can affect BFR when compounds are sensitive to specific nitrogen-related redox conditions, which counts especially for sulfamethoxazole.

3.3.6 Influence of microbial processes on bank filtration

The previous sections illustrate the interplay of temperature, redox conditions, organic matter content and microbial activity. Microorganisms play an important role in the bank filtration process, significantly influencing the removal of pollutants under various redox conditions. To display natural conditions in laboratory studies, a lag period for microorganisms is often required to acclimate and start degrading new compounds (González et al. 2006; Baumgarten 2011; Bertelkamp et al. 2016b). Hoppe-Jones et al. (2012) investigated the combined effect of adapted/non-adapted microorganisms and varying concentrations of biodegradable DOC on BFR. Under conditions characterized by low levels of biodegradable DOC and non-adapted microorganisms, the reduction of biodegradable compounds was minimal, at less than 15%. However, after a three-month period allowing for adaptation, BFRs increased considerably, exceeding 80%. This implies that adaptation may stimulate enzyme production, facilitating compound degradation even in environments with limited biodegradable DOC. In scenarios involving both stressed (non-adapted) and adapted conditions, where biodegradable DOC concentrations were higher and travel times were around 7 days, BFRs varied but generally exceeded 25%. This suggests that maintaining biodegradable DOC levels above 1.6 mg/L can create favorable conditions for microbial activity, promoting removal even in systems that have not yet adapted (Hoppe-Jones et al. 2012).

Infiltration site sand exhibited significantly higher removal rates for sulfamethoxazole of 98% under aerobic conditions and 67% under anoxic conditions, compared to 'technical' sand, which showed removal rates of 23% and 3%, respectively (Baumgarten 2011). This highlights the substantial impact of differently adapted microbial communities on bank filtration rates. In a membrane bioreactor, microorganisms adapted to the influent water or the microbiome composition changed after the first spiking experiment. Depending on the compound, an increase in the BFR of 11% for 2,4-Dichlorophenoxyacetic acid (2,4 D) and of 42% for 2-methyl-4-chlorophenoxyacetic acid (MCCP) was observed from first to second spiking event (González et al. 2006) (Figure 21).

Figure 21: Elimination rate (%) of spiked compounds in a membrane bioreactor after the first day of spiking, with MCPP=methylchlorophenoxypropionic acid; MCPA=2-methyl-4-chlorophenoxyacetic acid; 2,4-DP=dichlorprop; 2,4-D=2,4-dichlorophenoxyacetic acid



Source: González et al. (2006)

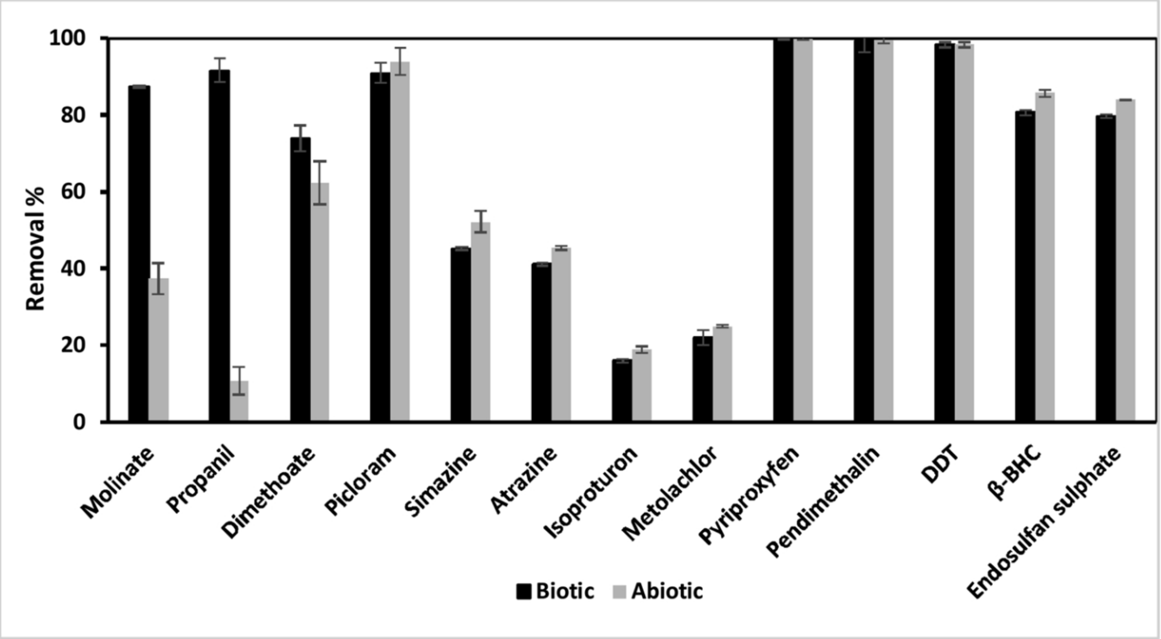
Carpenter and Helbling (2017) attribute the BFR during the initial phase (<171 d) of their study to the development of microorganisms, while the BFR observed after 171 d is linked to changes in microbial community activity. Microbial communities can adapt to new compounds through genetic changes, enzyme induction, and population changes (Spain et al. 1980; Spain and Van Veld 1983; Hoppe-Jones et al. 2012).

For hydrophilic compounds such as molinate, propanil, and dimethoate, removal efficiencies are significantly lower under abiotic conditions, remaining below 40%, but increase to over 70% under biotic conditions, indicating the importance of microbial activity in their attenuation (Abdelrady 2019; Abogabal et al. 2020). Optimal removal of these compounds occurs at temperatures around 25°C, emphasizing the influence of temperature and biodegradable organic matter on microbial processes (Abdelrady et al. 2019).

For optimal microbial activity, several requirements are beneficial: suitable temperatures enable optimal biomass growth, C_{org} or DOC/TOC are crucial energy sources for microorganisms, a minimum concentration of the compound to be degraded and sufficient oxygen or electron donors (or anoxic environments) are needed for effective microbial activity (see Sections 3.3.3-3.3.5). However, systems are flexible and the expansion of the oxic zone at lower temperatures can compensate for lower removal rates with longer residence times, as observed in some studies (Massmann et al. 2006a).

Microbial degradation can occur under both oxic and anoxic conditions, but the efficiency may vary. For example, aerobic conditions are particularly favorable for the removal of organic compounds (Abogabal et al. 2020) (see Sections 3.3.3-3.3.5), while some compounds like sulfonamides show higher degradability under anoxic conditions (Bai et al. 2019). Examples are presented in Figure 22. Baumgarten et al. (2011) observed a BFR for sulfamethoxazole of 98% under oxic and of 67% under anoxic conditions.

Figure 22: Removal of compounds under biotic and abiotic conditions at 20 °C for Nile River influent water



Source: Abdelrady et al. (2019)

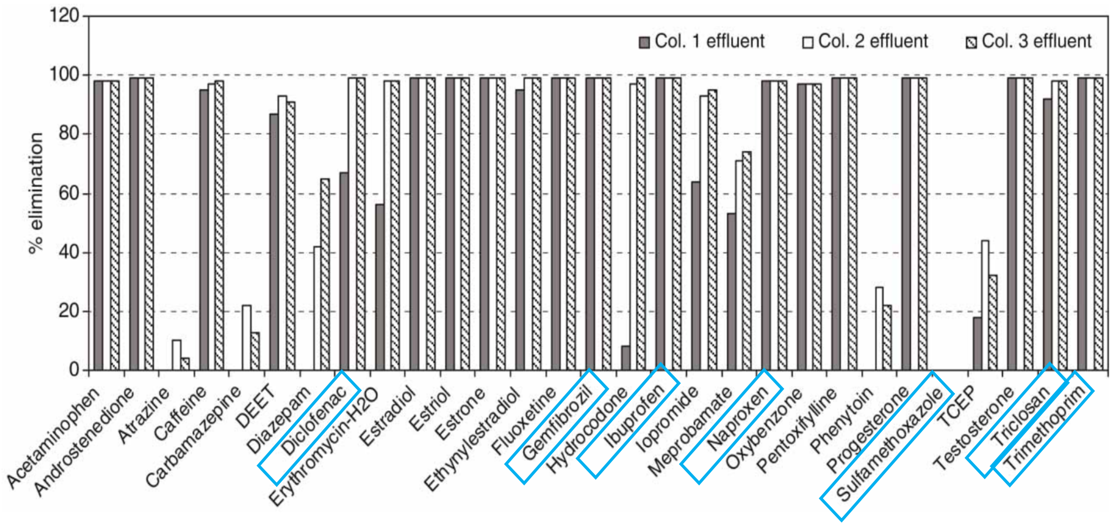
In terms of environmental conditions, higher temperatures and the presence of organic matter enhance the removal of certain persistent compounds through adsorption and microbial activity (Abdelrady et al. 2019). The presence of a heterotrophic biofilm enhances the degradation of compounds, underscoring the importance of microbial biomass and activity in OMP removal (Sanchez-Perez et al. 2013). The ability of the microbial community to degrade the compounds depends on its potential to adapt to specific compounds (Spain et al. 1980; Spain and Van Veld 1983) and elevated concentrations of certain compounds can shorten adaptation times and increase removal rates even under less favorable conditions (Baumgarten et al. 2011).

3.3.7 Influence of compound characteristics on bank filtration

Compound characteristics considerably govern their fate during bank filtration. Several attempts have been made to relate compound properties and molecule structures to their removal. Highly hydrophobic compounds (representing also non-polar and sorptive properties) are effectively removed by adsorption, whereas less hydrophylic (representing also polar and less-sorptive properties) compounds depend more on biodegradation processes (Abdelrady et al. 2019; Abogabal et al. 2020). Benotti et al. (2012) used the octanol-water partition coefficient $\log K_{ow}$ as property reflecting the sorption potential. The concentration of compounds with $\log K_{ow}$ values ≥ 3.7 decreased in the column system below the detection limit, suggesting a removal was at least partly governed by sorption. Based on the compound's sorption potential expressed with different parameters such as partition coefficients $\log D/\log P_{ow}$ or dissociation constant pK_a – particularly since many studies focus on pharmaceuticals where K_{oc} values are rarely available – authors assess whether sorption (as $\log K_{ow}$) or microbial degradation processes (as λ) are primarily responsible for their removal (Maćerak 2018). Only one study considered the solubility of a compound as logS value for the environmental behavior of the compound. Atrazine, simazine, isoproturon, and metolachlor with logarithm of solubility ranges between -2.5 and -4 were assessed to be retained by adsorption (Benotti et al. 2012). Additional clear statements related to defined values of the property are missing. The persistence expressed as DT_{50} was not considered in the laboratory studies. Instead, half lifes under varying site conditions were determined in the study either by measurement or calculation/modelling (Baumgarten et al. 2011; Maćerak 2018).

Going further into details, cationic compounds are removed more rapidly than anionic compounds due to strong adsorption to negatively charged soil matrices like clay and organic matter. BFRs higher than 80% were determined for neutral and cationic pharmaceuticals in a study by Im et al. (2016). Adversely, anionic compounds, being repelled by negatively charged matrices, rely more on biological degradation for removal, which necessitates carbon sources (Benotti et al. 2012; Bertelkamp et al. 2014; Im et al. 2016). Non-charged compounds are primarily removed through sorption based on their lipophilicity values (log D, $\log P_{ow}$), which influence their ability to penetrate microbial cells and undergo degradation (Bertelkamp et al. 2014). The study by Benotti et al. (2012) observed the elimination of 29 compounds, without positively-charged compounds but including seven negatively-charged and 22 non-charged compounds. It reveals that both the sorption potential and the charge of a compound influence its removal. The combination of these properties, like a high sorption potential coupled with a positive charge or other variations, also plays a crucial role (Figure 23).

Figure 23: Removal of pharmaceuticals and endocrine disrupting compounds by pilot-scale consisting of three subsequent columns (Col. 1-Col. 3); blue frame=negatively charged compound



Source: Benotti et al. (2012, altered)

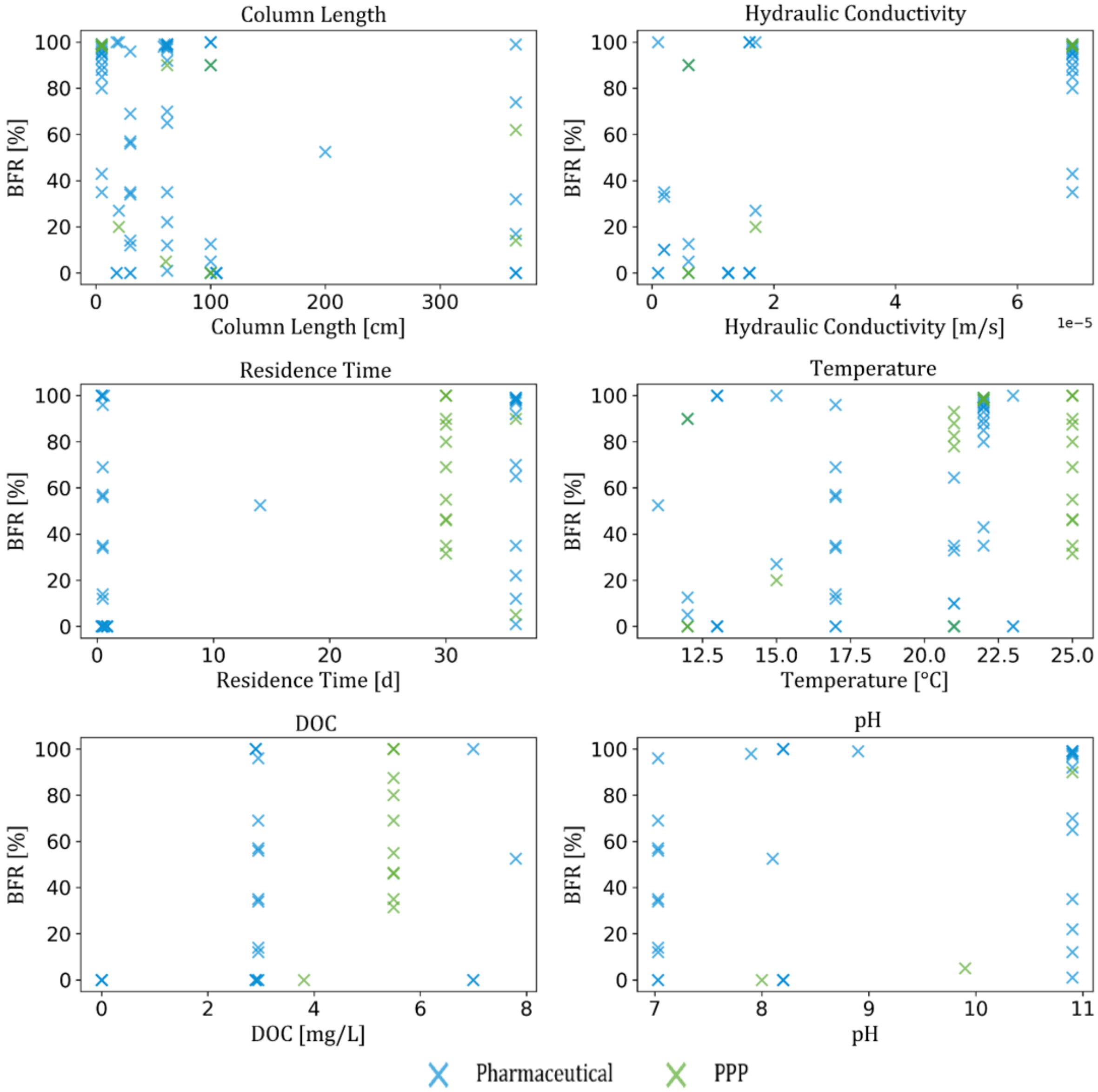
Considering functional groups, compounds with ethers and carbonyl groups exhibit higher biodegradability, while those with amines, ring structures, aliphatic ethers, and sulfur are less biodegradable and harder to degrade (Bertelkamp et al. 2014, 2016b). Despite of these results, Bertelkamp et al. (2014, 2016b) investigated whether the redox dependency of compounds or the ability of microorganisms to adapt to their degradation can be related to the physical-chemical properties of the compounds. No statistically significant correlation was found between properties such as hydrophobicity, charge, and molecular weight with redox dependency or biodegradability. However, slight trends were observed for compounds containing ethers, sulfur, primary, and secondary amines groups, with biodegradation rates increasing after a period of microbial adaption. Several studies in the review attempted to relate physical-chemical properties of compounds to their BFR, but most focused on the molecule's structure, specifically functional groups or charge, and their impact on BFR.

Compounds undergo chemical or microbial transformation processes in the environment and form transformation products (Fenner et al. 2013). One study observed the formation of transformation products of pharmaceuticals during bank filtration. Specifically, five, three, and two transformation products were identified for trimethoprim, valsartan, and propachlor, respectively. In each case, one transformation product emerged as the dominant compound, constituting approximately 80% of the peak area of all transformation products (Carpenter and Helbling 2017). Jaramillo et al. (2019) in general recommend to include transformation products in the studies as they can be more persistent and mobile than their parent compound (Reemtsma et al. 2013; Ulrich et al. 2021). These studies reveal that the formation of transformation products during bank filtration has to be considered as a further potential source for groundwater contamination.

3.3.8 Analysis of factors influencing BFR in laboratory studies

A correlation analysis was conducted to investigate whether the BFR depends on certain influencing factors. This analysis is limited to data from laboratory studies, as they provide a higher number of precise values for the factors compared to field studies (see also Section A.4). The scatter plots (Figure 24) illustrate the relationship between BFR and various experimental factors from laboratory studies such as column length, hydraulic conductivity, residence time, temperature, DOC, and pH (please note, the influence of pH was not investigated but documented). The data differentiates between pharmaceuticals and PPPs. Across all factors, BFRs show significant variability. There are no clear trends in the correlations between BFR of pharmaceuticals/PPPs and the aforementioned parameters. This suggests that both high and low BFRs can occur across the full range of these parameters. Exemplarily, column length underlines this variability: BFRs range from 0% to 100% for both short and long columns.

Figure 24: **Scatter plots showing the BFRs and experimental parameters (column length, hydraulic conductivity, residence time, and temperature) from laboratory studies. The data distinguishes between pharmaceuticals (blue markers) and PPP (green markers)**



Source: own illustration, INR

The data sets for the factors typically contain a limited number of measurements, with some factors, like temperature, being studied more extensively across several studies, while others, like DOC, are less frequently examined. Additionally, some studies provided only qualitative descriptions, e.g., for microbial activity or redox conditions, without giving specific values. Especially for PPP compounds, the database is lacking. Furthermore, the data often exhibit variations and do not follow a normal or other distribution, as can be seen for the residence time. Additionally, the plots aggregate results from multiple studies with differing experimental setups. These factors complicate the statistical evaluation of the laboratory data and raise questions about the reliability of potential correlations.

3.4 Challenges assessing the BFR

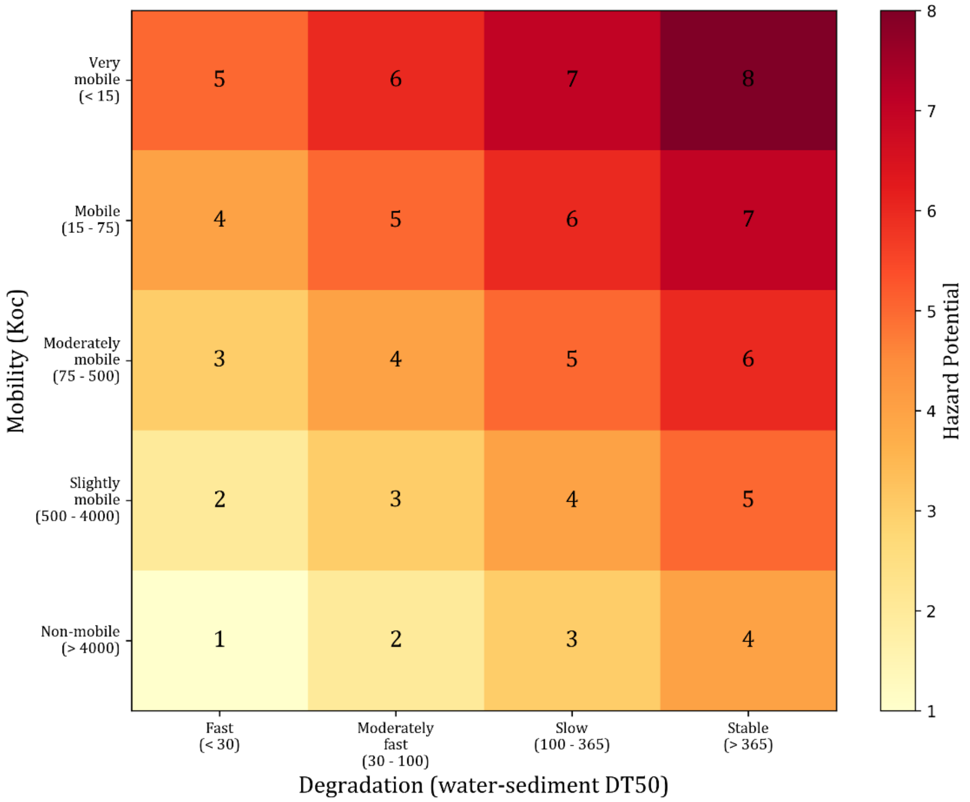
The literature review on BFR for PPPs reveals several significant challenges, particularly regarding the scarcity and variability of data and methodologies, which complicate the reliable assessment and comparison of BFR values. One of the primary challenges is the lack of data for PPPs, especially those currently used frequently in Germany like glyphosate, prosulfocarb, chlormequat, and others (BVL 2024). This data gap limits comprehensive assessments and predictions about the effectiveness of bank filtration in removing these compounds. Additionally, field and laboratory studies on bank filtration are not standardized, leading to considerable variations in environmental and laboratory conditions, adaptation time for microorganisms (in laboratory studies), observation of different compounds, and duration of the studies. This lack of standardization hampers the ability to compare results across different studies. Moreover, important information about these conditions is often incomplete, further complicating the interpretation and comparison of results. In addition, precise data are frequently missing, as results are often displayed in figures with few values explicitly mentioned in the text. As a result, qualitative assessments prevail in the literature. Expressions such as “compounds … were eliminated more efficiently under oxic conditions” (e.g., Massmann et al. 2008a) are common, while quantitative comparisons, like “an order of magnitude lower,” (Burke et al. 2014) are rare. When quantitative statements are made, they are usually included in laboratory studies where a single parameter is varied but field studies seldom provide such detailed quantitative data. Laboratory studies tend to focus on a single parameter and its effect on BFR in a controlled environment. While these studies provide detailed insights into processes during bank filtration, their transferability to field scale includes a high degree of uncertainty since the complexity of natural conditions cannot be represented under laboratory conditions (Onesios et al. 2009; Burke et al. 2014; Banzhaf and Hebig 2016). The variability in study designs and site conditions means that BFR values for the same compound can differ considerably in the order of several magnitudes between studies, making a reliable assessment challenging (see Figure 10 and Figure 11). This clearly indicates the relevance of including all data of the environmental site conditions into reports or better to conduct experiemnts under standardized conditions. The complexity of processes during bank filtration is further compounded by the fact that several factors affecting BFR are strongly interconnected such as temperature, redox potential, and carbon source with microbial activity, and C_{org} also with sorption potential. These interconnections make it difficult to isolate the effect of a single factor on BFR. Therefore, assessing the impact of individual parameters requires careful consideration of these complex interactions. Studies rarely rank factors according to their relevance in contributing to BFR. When such rankings are provided, they are often compound-specific, preventing generalizations across different PPPs (D’Alessio et al. 2015; Burke et al. 2018). Therefore, the challenges in assessing bank filtration rates for PPPs are manifold, stemming from insufficient data, non-standardized methodologies, inconsistent reporting, and the complex interplay of various factors. Addressing these challenges requires a concerted effort to standardize study designs, improve data reporting practices, and better understand the interactions between different environmental parameters, which is essential for achieving more reliable and comprehensive assessments of bank filtration rates for PPPs.

3.5 Groundwater hazard potential classification based on compound properties

Several studies have explored the impact of compound properties on BFRs, with a consensus that mobility and persistence are critical factors (Sections 3.2.8 and 3.3.7). Investigations into molecular structure have sought to explain how charges or functional groups influence a compound’s persistence or mobility (Kolpin et al. 1998; Maeng et al. 2011; Benotti et al. 2012; Im et al. 2016). Compounds with high sorption potential tend to be retained or delayed by adsorption to the soil matrix during bank filtration. Conversely, low-sorbing, polar compounds are quickly transported in soil water and are more prone to microbial degradation than to long-term sorption (Abdelrady et al. 2019; Abogabal et al. 2020). Mobility and persistence are typically reported using various metrics such as $\log P_{ow}$, $\log K_{ow}$, or logD for mobility, and degradation rate constants, breakthrough curves, or simulations for persistence. This variety of units complicates data comparison, and when comparisons are made, they are usually limited to the compounds investigated within a specific study. This limits the ability to generalize the findings due to the unique study design.

A categorization can provide a preliminary estimate of a compound's environmental behavior in the absence of concrete measured data. For the classification of PPPs, a decision matrix was developed based on their mobility (K_{oc}) and persistence ($DT_{50,\text{ water-sediment}}$) (Figure 25). The half-life DT_{50} according to OECD guidelines (e.g., 307 (2002) for soil or 308 (2002) for sediment) indicates the period of time within which the concentration of a compound has decreased by 50% due to biodegradation. In terms of bank filtration, it is important to apply the $DT_{50,\text{ water-sediment}}$, since studies reveal that the highest potential of biodegradation is in the hyporheic zone (Lewandowski et al. 2020; Massmann et al. 2009; Bertrand 2021; Handl 2023; Höhne 2022). Both, the categories within the matrix and the compound property values, are defined by specific ranges for K_{oc} and $DT_{50,\text{ water-sediment}}$ according to the Pesticide Properties Database(PPDB) (Lewis et al. 2016). This segmentation groups PPPs based on how long they persist and how easily they move through the water-sediment system, reflecting their potential environmental risk. This approach resulted in the creation of eight groundwater hazard potential classes, which are used to evaluate the potential risk that PPPs pose.

Figure 25: Categorization of PPPs based on their mobility (K_{oc}) [mL/g] and degradation [d]



Source: own illustration, INR

To test the decision matrix, a comparison was made between the groundwater hazard potential classes and BFRs from the reviewed literature for the eight PPPs with the highest number of BFRs (Table 3). The reviewed literature includes classifications based on K_{oc} and DT_{50}, but specifically omits $DT_{50,\ \text{water-sediment}}$ (Malaguerra et al. 2013; Abdelrady et al. 2019; Abogabal et al. 2020). Despite this omission, further discrepancies exist between the groundwater hazard potential classification and literature-based BFR data. For instance, atrazine, simazine, and MCPA, the mean BFR from the literature ranges from 21.1% to 66.3%, showing a variation of over 100% within the same class. Additionally, glyphosate, assessed for class 1, and MCPA, for class 4, have mean BFRs of 65.5% and 66.3% respectively, which do not reflect the significant differences in their groundwater hazard potential classes based on K_{oc} and $DT_{50,\ \text{water-sediment}}$.

The comparison indicates that PPPs cannot be reliably classified based on their properties alone for predicting high or low BFRs. To enable such classification, the impact of compound properties needs to be investigated under a standardized study design and study conditions. The study results used for this comparison include BFR data from various field sites and laboratory experiments, conducted under different conditions, making them inadequate for drawing conclusions based solely on compound properties. Various factors beyond K_{oc} and DT_{50} values, including site conditions, significantly influence a compound's BFR (e.g., Sturm et al. 2006; Górski 2011; Maeng 2013; Kondor 2020).

Table 3: Comparison of groundwater hazard potentials ($DT_{50,\ \text{water-sediment}}$ and K_{oc} from the Pesticides Properties Data Base (PPDB) (Lewis et al. 2016)) with literature-based BFR data for selected PPPs

PPP	Water-Sediment DT50 [d]	Koc [mL/L]	Hazard Potential	Min BFR [%]	Max BFR [%]	Mean BFR [%]	Number of studies/data
Atrazine	80.0	100.0	4	-246	100	25.7	55
Simazine	33.0	130.0	4	-33	81	21.1	20
Diuron	48.0	680.0	3	-566	100	14.0	18
Glyphosate	20.8	1424	1	17	95	65.5	11
Mecoprop	50.0	47.0	5	0	100	54.0	14
Metolachlor	365.0	120.0	5	0	70	52.4	9
Bentazone	716.0	55.3	7	0	100	23.9	15
MCPA	17.0	73.9	4	0	100	66.3	8

3.6 Relevance of bank filtration for the contamination risk of groundwater

The relevance of bank filtration can be evaluated from various perspectives, which will be discussed in the following.

Differences between natural and technically initiated bank filtration

Under natural conditions, dissolved or particulate matter can only be transported from surface water into groundwater where surface water infiltrates through the riverbed/banks into adjacent groundwater aquifers due to naturally occurring hydraulic gradients. As described in section

2.1.1, the volume of infiltrating water and the purification efficiency of the site heavily depend on the natural geological and hydrological conditions, which can vary seasonally and spatially (Ray et al. 2002b; Hiscock 2005). Technically induced bank filtration is employed to enhance surface water infiltration into groundwater aquifers. This is achieved through methods such as pumping, creating artificial recharge zones, or modifying riverbeds and can overcome natural hydraulic gradients from groundwater to surface water. In technical bank filtration, especially with pumping, the volume of infiltrating water can be controlled and is therefore more consistent than during natural bank filtration, making it independent of natural geological and hydrological conditions (Ray et al. 2002b; Hiscock 2005). The literature search revealed only two studies on natural bank filtration (Wang and Squillace 1994; Massmann et al. 2006b). While Massmann et al. (2006b) investigated hydrogeological-hydrogeochemical processes, Wang and Squillace (1994) focused on BFR of selected compounds at the Cedar River/USA. Massmann et al. (2006b) compared artificial recharge (AR) and bank filtration at Lake Tegel. They identified as major differences

- thicker clogging layers at bank filtration, since these layers are removed at AR,
- vertical age stratifications were observed at AR but not at bank filtration,
- shorter travel times at AR compared to bank filtration can be expected,
- more reducing redox conditions at bank filtration,
- preferential degradation of compounds that are subject to anaerobic degradation.

These differences suggest that the underlying processes may vary depending on whether the conditions are technically induced or naturally occurring. A clear comparison of the quantity of water transported via natural and technically induced bank filtration cannot be made due to a lack of data for both types. It is hypothesized that natural bank filtration occurs across the landscape in small amounts, while technically induced filtration is concentrated at specific sites such as raw water production facilities and agricultural regions, where it involves the abstraction of larger volumes of water. Table 4 presents a comparison between BFR data from natural bank filtration and data from technically initiated bank filtration found in the literature. However, the limited data on natural bank filtration (only a single dataset) do not allow for a definitive conclusion regarding its relevance, or whether it is more effective than technically initiated filtration in mitigating compound contamination.

Table 4: Comparison of BFRs under natural and technical conditions; n=number of studies

PPP	Natural, 50 m distance	Technically initiated, 5 – 680 m distance	
	Wang & Squillace (1994)	Mean value; range [%]; n	Citation
Alachlor	100	75; 75-76; 1	Verstraeten et al. (2002)
Atrazine	88	25; -246-100; 39	Oberleitner et al. (2020) Benotti et al. (2012) Hollender et al. (2018) Bruchet et al. (2012) Regnery et al. (2015) Verstraeten (2002)

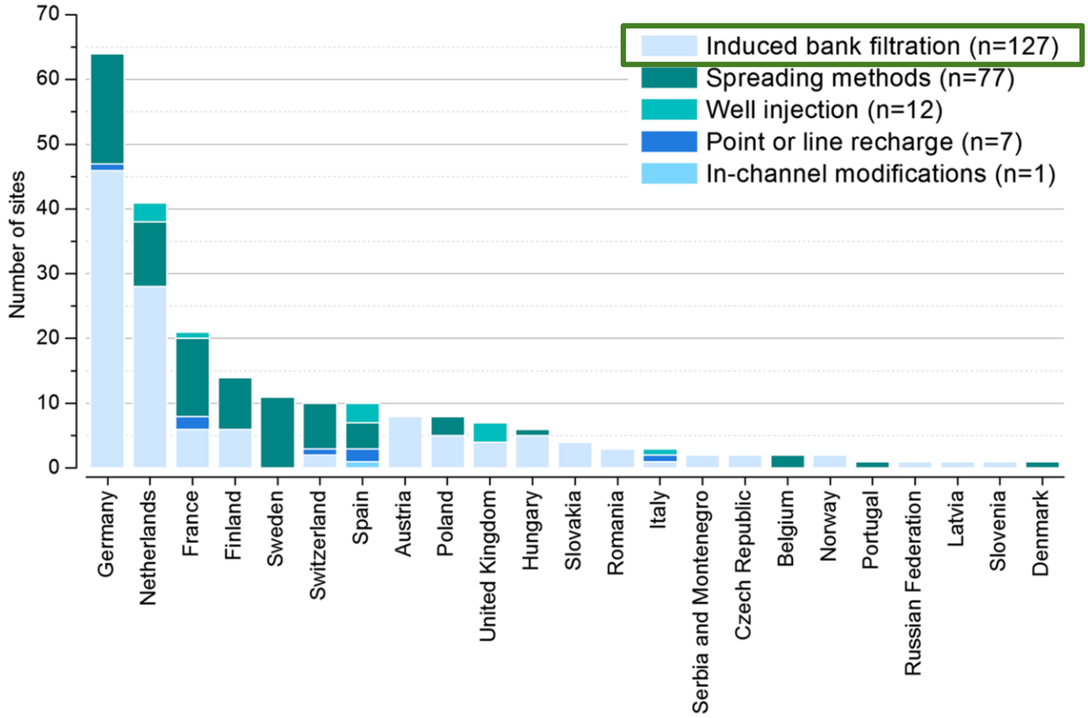
PPP	Natural, 50 m distance	Technically initiated, 5 – 680 m distance	
	Wang & Squillace (1994)	Mean value; range [%]; n	Citation
			Díaz-Cruz and Barceló (2008) Köck-Schulmeyer et al. (2013) Oberleitner et al. (2020) Zullei-Seibert (1996) cited in Schmidt et al. (2003) Schmidt (2006)
Cyanazine	100	20; 1-71; 1	Verstraeten et al. (2002)
Desethylatrazine	76	20; 0-62; 9	Köck-Schulmeyer et al. (2013) Oberleitner et al. (2020) Schmidt (2006)
Desisopropylatrazine	90	7.5; 0-15; 1	Schmidt (2006)
Metolachlor	100	45.5; 0-70; 5	Dragon et al. (2018) Verstraaten (2002) Schmidt (2006)

Technically initiated bank filtration applications

This approach is often applied to collect raw water for drinking water production. Water abstraction near surface water can reverse hydraulic gradients, causing surface water to flow into groundwater where it would not naturally occur, thereby enhancing the relevance of bank filtration. This effect can be particularly observed in wells closely located to surface water such as those used for agricultural irrigation (Eckert and Irmscher 2006; Handl 2023; Heinrich-Böll-Stiftung 2023).

Bank filtration has a long history in Europe for producing drinking water. Up to 10% of drinking water was sourced from bank filtration in the last century with variations across different countries (Eckert and Irmscher 2006; Sprenger et al. 2017) (Figure 26).

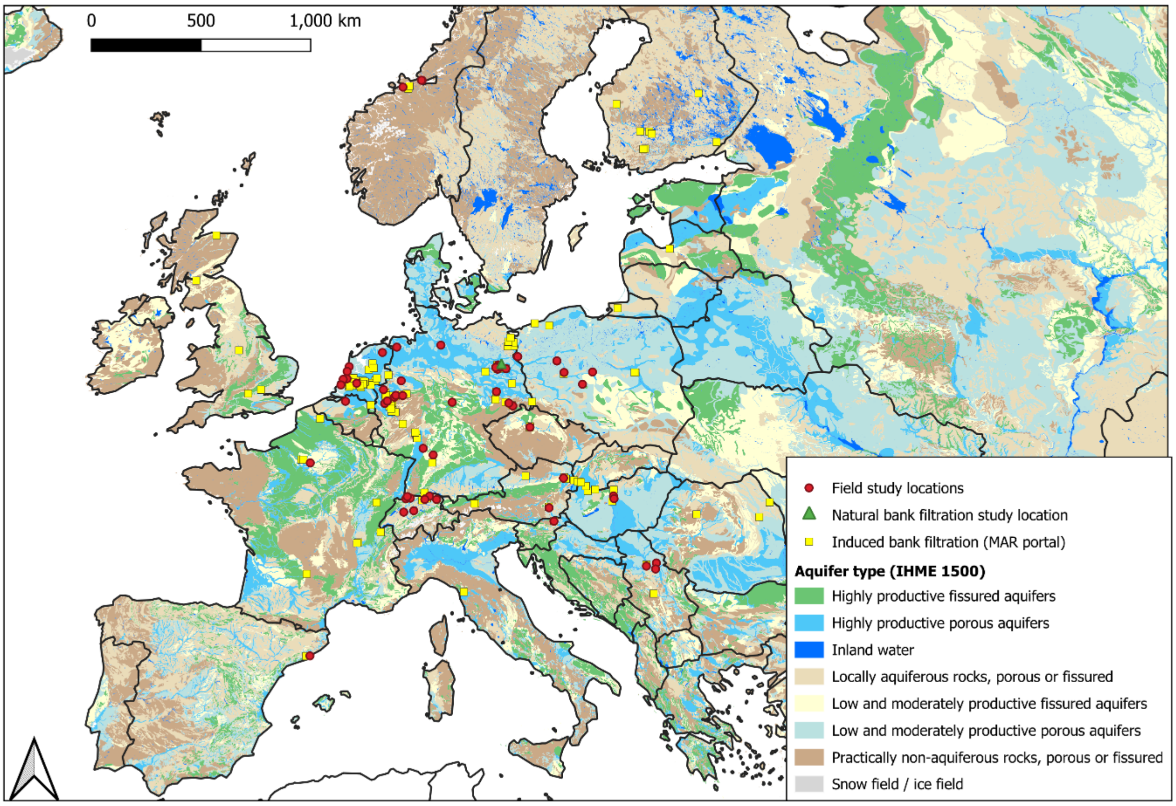
Figure 26: **Number of induced bank filtration sites within manual aquifer recharge (MAR) sites in European countries (only MAR sites active in 2013 are shown)**



Source: Sprenger et al. 2017)

The literature review and the Manual Aquifer Recharge Portal identified bank filtration sites in 18 different European countries (n=80), the USA (n=22), eastern China (n=9), northern/western India (n=13), and Egypt (n=5). The locations of the European bank filtration sites are shown in Figure 27. In Germany, 47 sites, primarily located in the eastern and western regions, use bank filtration for drinking water production. These sites are often found near densely populated areas (e.g., the Ruhr area, Berlin and its surroundings, Stuttgart) (MAR Portal 2024).

Figure 27: **Locations of field studies (literature review), natural bank filtration and induced bank filtration (MAR portal) including aquifer types according to IHME**



Source: (International Hydrogeological Map of Europe 1500)

Most study and induced bank filtration sites, not all of which are still in operation, can be found in two aquifer types: the "highly productive porous aquifers" and the "low and moderately productive porous aquifers" (Figure 27). Highly productive porous aquifers have high porosity and permeability, enabling them to store and transmit large volumes of groundwater efficiently. These aquifers, often composed of well-sorted sands and gravels, are crucial for municipal, agricultural, and industrial water supplies due to their significant yield (Struckmeier and Margat 1995; BGR 2023).

In Germany, approximately 16% of raw water for drinking water production is sourced through bank filtration (BDEW 2022). With an annual drinking water production of 5.4 billion m^3 in 2019, this corresponds to a volume of 0.92 billion m^3 produced from bank filtration (BDEW 2022). Due to the shorter soil passage, the risk of contamination of raw water obtained from bank filtration is higher compared to raw water sourced from groundwater (63% of drinking water production). Although karst aquifers are not typically used for raw water production, natural bank filtration can also occur in these areas. Karst regions are quite common; in Germany, they are primarily located in the central and southern regions. In Europe, additional karst areas are found particularly in the Austrian and Swiss Alps, as well as in most other European countries (BGR 2024).

Bank filtration in the hydrological context

Bank filtration is limited to periods when the hydraulic gradient directs water from surface water toward groundwater. This typically occurs when surface water levels are higher than groundwater levels, a condition more common during drier periods in spring and summer. As a result, bank filtration is not constant but varies and is restricted to specific times of the year (Wang and Squillace 1994; Epting et al. 2018; Willkommen et al. 2022; Loose et al. 2024). None of the studies calculated the water balance of their study site or system. However, by assessing the water balance of a surface water body, it is possible to estimate the volume of water infiltrating from surface water into groundwater, known as the bank filtration volume. Although this process exhibits temporal and spatial variations, calculations would provide valuable insight into the magnitude of infiltration (Epting et al. 2018; Willkommen et al. 2022; Loose et al. 2024). Given that the infiltration of surface water into groundwater is a natural process, it is hypothesized that this process occurs across the landscape, albeit in smaller amounts compared to other transport pathways within the water balance.

Specific protection of the groundwater resource

Groundwater as a resource is especially protected due to its high value for humans and the environment. This is reflected in the legislation, as established by the limit value in the Plant Protection Regulation (Regulation (EC) No 1107/2009 2009) of 0.1 µg/L for PPPs and relevant metabolites. The Groundwater Directive (Directive 2006/118/EC 2006) establishes groundwater quality standards of 0.1 µg/L for active substances in pesticides including their relevant metabolites, along with a cumulative limit of 0.5 µg/L for the sum of all individual pesticides including their relevant metabolites. Additionally, a European threshold for drinking water of 0.1 µg/L for PPPs and their relevant metabolites (Directive (EU) 2020/2184 2020) underscores the importance of maintaining uncontaminated groundwater.

Risk of groundwater contamination by PPPs via bank filtration

The examined studies reported high variations of a compound's BFR due to environmental conditions and compound properties (see Section 3 and Appendix A.2). These variations hamper a thorough assessment of the efficiency of bank filtration for a specific compound. Across all studies, a mean BFR of 100% was observed for only 9 out of 91 PPPs, while mean BFRs below 25% were reported for 44 PPPs and below 10% for 24 PPPs (Appendix A.2). Therefore, a total purification of PPPs through bank filtration cannot be assumed in general. Groundwater contamination cannot be ruled out, and the threshold value of 0.1 g/L for groundwater (Directive 2006/118/EC 2006) may possibly be exceeded. Schmidt et al. (2005) highlight the potential risk of PPP concentrations exceeding 0.1 µg/L in groundwater, attributing most findings to surface water entry into shallow groundwater in monitoring wells located close to surface water bodies. According to the precautionary principle of the authorization process, bank filtration can be considered a potential mitigation measure to reduce PPP concentrations from surface water to groundwater, though it cannot fully protect groundwater from all compounds according to the high variability of BFR found in the literature. Additionally, deep groundwater can be impacted by the long-term leaching of these compounds through cracks in low-permeability subsurface layers, leading to contamination of groundwater that may be used directly for raw water (Foster and Chilton 2003).

Summing up the aforementioned perspectives of the relevance of bank filtration to groundwater contamination risk, it is evident that compounds are seldom retained completely during this transport, thereby posing a risk to groundwater. This is particularly important given the high value of groundwater as a resource and the fact that raw water collection through bank filtration across Europe provides drinking water to a large population. However, based on the comprehensive literature review, a concise conclusion regarding the extent of groundwater risk by bank filtration remains elusive due to the studies' variability in terms of study design, site characteristics, subsurface properties, hydrometeorological conditions, and investigated compounds. Although bank filtration can be limited both spatially and temporally, quantifying the volume of water transported through this subsurface passage would enhance our understanding. A focused literature review or targeted field studies on this aspect would be beneficial.

4 Approaches to optimize the Exposit 3.02 model

In Germany, the model Exposit 3.02 (UBA 2018) is applied in the PPP authorization process (Regulation (EC) No 1107/2009 2009; PflSchG 2012) to estimate the predicted environmental concentration in groundwater through bank filtration. In the following sections, the model's applicability in terms of bank filtration is evaluated, and suggestions for improving its representativity are provided.

4.1 Description and evaluation of the bank filtration rate calculation in the Exposit 3.02 model

To determine the BFR of a specific PPP, Exposit 3.02 first calculates the initial concentration in a surface water body (PEC $ini_{surface\ water}$) [µg/L] based on PPP inputs via surface runoff ($PECini_{runoff}$) [µg/L] and drainage ($PECini_{ditch}$) [µg/L]. These inputs are considered to be diluted at a ratio of 1:12.5 in the receiving surface water body. The $PECini_{surface\ water}$ is the starting point for the assessment of the bank filtration pathway since this type of water infiltrates into the subsurface.

For the subsurface passage, Exposit 3.02 uses the compound properties solubility L_{H2O}, half-life in soil under aerobic conditions $DT_{50,\ soil}$, and the adsorption constant K_{oc} to assess the elimination of a PPP. These parameters are not directly but indirectly incorporated through so-called groundwater risk groups (risk groups 1-4, Table 5). Each of the four defined groundwater risk groups is subsequently assigned a BFR, which defines the BFR of the considered PPPs. For 13 PPPs, an individual BFR is applied based on the data of Sturm et al. (2006) and Schmidt (2006).

Table 5: Groundwater risk groups for PPPs in Exposit 3.02 (UBA 2018)

Risk group	I (low)	II (moderate)	III (significant)	IV (high)
L_{H2O} [mg/L]	<1	<100	>>100	>>100
K_{oc} [L/kg]	>>500	<500	<<500	<100
$DT_{50,\ soil}$ [d]	>100	>21	<21>	<<21
BFR [%]	100	75	90	100

Looking at the compound properties considered in Exposit 3.02, the importance of a compound’s sorption potential for the assessment of its BFR is in general validated by the results of the literature review (e.g., Malaguerra et al. 2013; Abdelrady et al. 2019; Abogabal et al. 2020). The K_{oc} reflects the degree of hydrophobicity, polarity, and sorption potential of a compound, parameters considered in the studies (e.g,. Bertelkamp et al. 2014; Hamann et al. 2016; Abdelrady et al. 2019) and provides information about the compound’s sorption potential. DT_{50}, determined according to OECD guidelines (e.g., test 307 (2002) for soil or 308 (2002) for aquatic sediment systems), provides information about the aerobic and anaerobic transformation of a compound. The Exposit 3.02 calculation of the BFR considers $DT_{50,\ soil}$ under aerobic conditions (OECD 2002a) while the studies of the review lack precise information about which DT_{50} value was considered. Nevertheless, $DT_{50,\ water\text{-}sediment}$ determined according to OECD Test 308 (OECD 2002b) is more appropriate than $DT_{50,\ soil}$, since several studies pointed out that the hyporheic zone at the sediment of the surface water body contributes considerably to microbial degradation of PPPs rather than the soil surface (e.g., Massmann et al. 2009; Bertrand 2021; Handl 2023). A compound’s solubility is not very appropriate to estimate its environmental behavior (Bach et al. 2017). It only indicates the amount of compound at which a saturated solution occurs. In case of PPP contamination, the concentrations in the environment are typically in the ng/L and low µg/L range while the solubility of PPPs is in the range of mg/L to g/L (Lewis et al. 2016). Although high solubility suggests a low sorption potential, this is more accurately indicated by the K_{oc} (Bach et al. 2017).

According to the groundwater risk groups, a PPP with a high K_{oc} >>500 L/kg is retained 100% during bank filtration. The same applies to a PPP with a half-life of <<21 d. It cannot be assessed if or to what extent the three compound properties are weighted, or if they have a relative importance, even though these properties are critical for determining the BFR in groundwater risk groups II and III. Based on the literature cited in Exposit 3.02, it is not possible to determine whether K_{oc}, $DT_{50, soil,}$ or L_{H2O} is the more significant factor influencing retention. The conclusions in the studies are often too generalized or vary depending on the specific compound being examined, even within the same study.

The classification of groundwater risk groups in Exposit 3.02 could benefit from increased transparency. L_{H2O}, K_{oc}, and DT_{50}, as key parameters, are not comprehensively represented across their entire range of values (Bach et al. 2017). Specifically, thresholds of 1 mg/L and 100 mg/L for L_{H2O}, 500 L/kg and 100 L/kg for K_{oc}, as well as 21 days and 100 days for $DT_{50, soil}$ are used to define these groundwater risk groups. The rationale behind the selection of these value ranges for each groundwater risk group remains unclear. The PPDB (Lewis et al. 2016) offers a more detailed classification for K_{oc} values, encompassing more categories with a finer resolution, especially at the lower end of the spectrum (Table 6). Similarly, $DT_{50, water-sediment}$ values are categorized into four groups, similar to the Exposit 3.02 classification, but with a broader range (Table 7).

Table 6: Classification of adsorption coefficient (K_{oc}) according to PPDB (Lewis et al. 2016)

Classification	Very mobile	Mobile	Moderately mobile	Slightly mobile	Non-mobile
Range [mL/g]	< 15	15-75	75-500	500– 4000	> 4000

Table 7: Classification of persistence ($DT_{50, water-sediment}$) according to PPDB (Lewis et al. 2016)

Classification	Non-persistent	Moderately persistent	Persistent	Very persistent
Range [d]	< 30	30-100	100-365	>365

The literature review identified site properties as significant factors influencing the BFR. Numerous studies have examined the impact of redox conditions on the retention of compounds during bank filtration (Massmann et al. 2008b, 2009; Maeng et al. 2013). Additionally, the flow distance and subsurface characteristics affecting flow velocity (e.g., porosity) (Górski 2011; Glorian et al. 2018; Kruć et al. 2019; Handl 2023) as well as microbial activity (Li et al. 2013; Epting et al. 2018; Kondor 2020) contribute to BFR value. In Exposit 3.02, none of the site characteristics are considered. Sturm et al. (2006) argue that BFR can only be accurately assessed when site characteristics are included in the BFR determination. The authors critically note that processes during bank filtration are overly simplified in Exposit 3.02 and that a minimum BFR of 75%, as considered in Exposit 3.02 in groundwater risk group 4 (except for the 13 PPPs, where BFR from literature is used), is overestimated. When comparing the specific BFR for the 13 selected PPPs defined in Exposit 3.02 with literature values published up to 2005, Schmidt and Lange (2006) showed that BFR literature values indicate lower efficiencies than those in Exposit 3.02. Table 8 compares the specific BFR for the 13 selected PPPs defined in Exposit 3.02 with those collected in the literature review (summarized in Appendix A.2). Considering only the minimum BFR from literature for each PPP for comparing the specific rates, eleven PPPs have a higher BFR in Exposit 3.02 compared to the minimum BFR from literature and two PPP have the same minimum BFR comparing the values in Exposit 3.02 and the minimum BFR from literature (Table 8).

Table 8: Comparison of bank filtration rates applied in Exposit 3.02 (UBA 2018) and those from literature review (Appendix A.2)

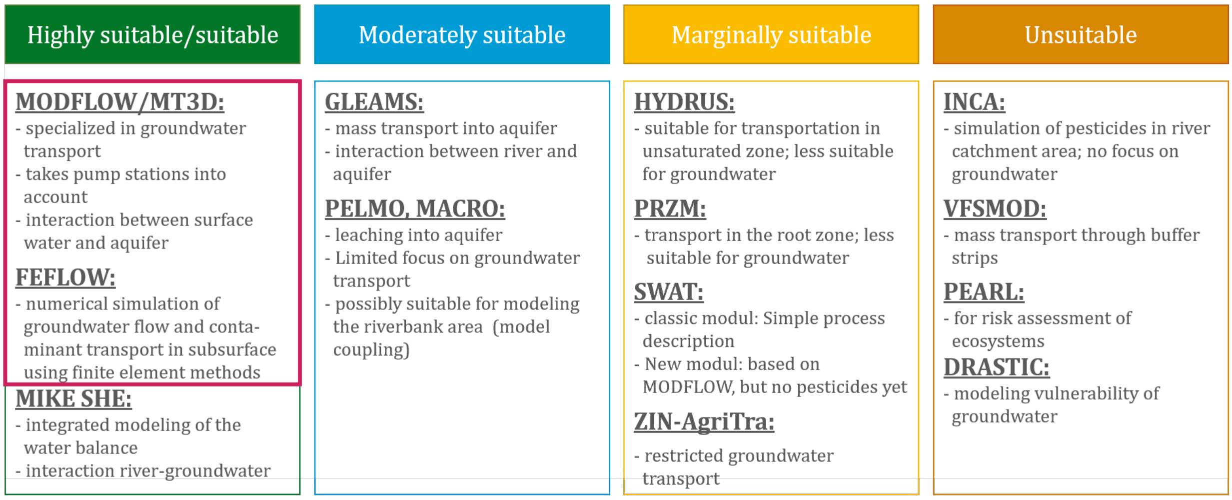
PPP	Bank filtration Rate [%] Exposit	Bank filtration Rate [%] Literature			
		Min	Max	Mean	Number of data sets
2,4 D	91.4	0	100	68.5	7
Bentazone	5	0	100	23.9	15
Dichlorprop	30	30	100	68.3	3
Diuron	20.3	-566	100	14	18
Flufenacet	63	63	63	63	1
Glyphosate	23.5	17	95	65.6	11
Isoproturon	21.6	-1375	100	-23.9	24
MCPA	74	0	100	66.4	8
Mecoprop	20	0	100	54	14
Metalaxyl	75	1.4	75	30.9	3
Metazachlor	73.6	23.3	100	69.8	8
Metolachlor	38	0	70	52.2	9
Terbuthylazine	27.5	0	100	45	10

Table 8 highlights the high variability of BFR, making an accurate assessment of the transport via bank filtration into groundwater difficult, and prevailing mean BRF <75%. More studies reveal a broader range of BFR for most of the defined BFR in Exposit 3.02, demonstrating the high variability depending on compound and site characteristics, and thereby the high uncertainty of BFR values as well as the difficulty to define representative BFR values. However, the assumption that PPPs are in general retained at >75% during bank filtration as defined in Exposit 3.02, except for the 13 PPPs mentioned above, represents a "best-case" scenario rather than a precautionary "worst-case" approach. Therefore, determining the specific BFR of selected PPPs or compound groups is a step in a more precautionary risk assessment. A standardized method to determine individual BFRs for all PPPs would provide a more realistic representation of the groundwater hazard potential.

4.2 Models considering the bank filtration path

Exposit 3.02 is a model which displays bank filtration in a very simplified way. In order to gain knowledge about the representation of this transport pathway in more complex models, another literature research was conducted. The search terms "groundwater quality model review pesticide" were used in the "Web of Science", and the terms "river bank filtration", "groundwater surface water interactions", "model", "contamination", "pesticide", and "organic micropollutants" were used in Google Scholar and with ChatGPT. From 1,224 publications, 65 models were identified, of which 21 provided sufficient documentation of the calculation methods for pesticide transport. These models were then classified based on their suitability for representing the transport of pesticides through this pathway into categories of "highly suitable/suitable", "moderately suitable", "marginally suitable," and "unsuitable" (Figure 28).

Figure 28: Model suitability for modeling the entry of PPPs into groundwater via bank filtration



Highly suitable/suitable	Moderately suitable	Marginally suitable	Unsuitable
MODFLOW/MT3D: - specialized in groundwater transport - takes pump stations into account - interaction between surface water and aquifer **FEFLOW:** - numerical simulation of groundwater flow and contaminant transport in subsurface using finite element methods **MIKE SHE:** - integrated modeling of the water balance - interaction river-groundwater	**GLEAMS:** - mass transport into aquifer - interaction between river and aquifer **PELMO, MACRO:** - leaching into aquifer - Limited focus on groundwater transport - possibly suitable for modeling the riverbank area (model coupling)	**HYDRUS:** - suitable for transportation in unsaturated zone; less suitable for groundwater **PRZM:** - transport in the root zone; less suitable for groundwater **SWAT:** - classic modul: Simple process description - New modul: based on MODFLOW, but no pesticides yet **ZIN-AgriTra:** - restricted groundwater transport	**INCA:** - simulation of pesticides in river catchment area; no focus on groundwater **VFSMOD:** - mass transport through buffer strips **PEARL:** - for risk assessment of ecosystems **DRASTIC:** - modeling vulnerability of groundwater

Source: own illustration, INR

The combination of the freely available models MT3D/MODFLOW (Bedekar et al. 2016) proved to be the most suitable for the considered question. MT3D uses the advection-dispersion-reaction equation under generalized hydrogeological conditions (Parker and Van Genuchten 1984; Toride et al. 1995; Bjerg et al. 1996) to calculate the transport of PPPs in groundwater. This equation is a fundamental mathematical calculation used to describe the transport of compounds in groundwater and considers three important processes:

Advection describes the transport of PPPs in groundwater due to the flow velocity of the water. This process helps to transport PPPs with the groundwater flow.

Dispersion refers to the spread and mixing of PPPs due to differences in flow velocity and pore sizes in the aquifer. These differences cause the PPPs to not only move along a straight line but also spread laterally.

Additionally, degradation and sorption reactions in groundwater, which affect the retention of PPPs in bank filtrate, as can be considered.

In addition to MT3D/MODFLOW, the studies of Schmidt and Lange (2006) and Tuxen et al. (2000) also described the distribution of compounds along a subsurface passage mathematically using the classical advection-dispersion-equation for aquifers under generalized hydrogeological conditions (Parker and Van Genuchten 1984; Toride et al. 1995; Bjerg et al. 1996):

$$\frac{\partial C}{\partial t} = D_{\mathrm{L}} \frac{\partial^2 C}{\partial x^2} - v_{\mathrm{p}} \frac{\partial C}{\partial x} - \frac{\rho_{\mathrm{b}}}{\theta} \frac{\partial S}{\partial t} - E, \tag{1}$$

with

c = concentration of the PPP [µg/L]

x = distance from inlet [m]

t = time [d]

v_p = flow velocity of porewater [m/d]

DL = sum of longitudinal dispersion and diffusion [m^2/s]

ρ_b = bulk density [g/cm^3]

θ = porosity of aquifer [-]

E = source-sink due to degradation [µg/L]

S = source-sink due to sorption [µg/L]

4.3 Optimizing the Exposit model

Complex models like MODFLOW/MT3D or MIKE SHE/FEFLOW offer a more realistic representation of PPP transport by considering a variety of relevant processes. Incorporating environmental parameters and compound-specific behavior allows for a more precise prediction of transport and retention via bank filtration. However, using complex models entails higher efforts in terms of implementation, validation, and model updating. Therefore, simplified models that neglect advection and dispersion, while focusing on compound and site characteristics, may be considered, as validated by the results of the reviewed studies. The degree of simplification could range from creating a model in Python or R-based languages to improve the Exposit approach in Excel. This simplification enables easier handling but provides a less accurate representation of natural processes and thus lower simulation result accuracy compared to complex models. The determination of the BFR could be approximated using simplified equations rooted in MODFLOW/MT3D (Bedekar et al. 2016) and applied by Schmidt and Lange (2006) and Tuxen et al. (2000), which are based on the advection-dispersion-equation (1) (Parker and Van Genuchten 1984; Toride et al. 1995; Bjerg et al. 1996) in a 5 steps procedure:

1. Calculation of retardation R_d [-]

$$R_d = 1 + \frac{\rho_b K_d}{\theta} \tag{2}$$

with

ρ_b = bulk density [g/cm^3]
K_d = sorption coefficient [mL/g]
θ = porosity of aquifer [-]

with

$$K_d = K_{oc} * \frac{C_{org}}{100} \tag{3}$$

K_d = sorption coefficient [mL/g]
K_{oc} = adsorption coefficient [mL/g]
C_{org} = organic carbon content [%]

The K_d value describes the ratio of the concentration of the PPP bound to the soil matrix to the dissolved concentration in the soil water and can be determined using the soil organic matter C_{org} and the K_{oc}.

2. Calculation of residence time t [d] during bank filtration

$$t = \frac{v_p}{R_d} * x \quad (4)$$

with

v_p = flow velocity of porewater [m/d]
R_d = retardation [-]
x = distance [m]

3. Calculation of degradation rate λ [1/d]

$$\lambda = \frac{ln\,2}{DT_{50,water-sediment}} \quad (5)$$

The degradation rate is calculated with the $DT_{50,\text{ water-sediment}}$ according to PPDB values (Lewis et al. 2016) and considers only simple first order kinetics.

4. Calculation of concentration C_1 after certain bank filtration distance [µg/L]

$$C_1 = C_0 * exp^{-\lambda * t} \quad (6)$$

with

C_0 = concentration in surface water [µg/L]
λ = degradation time [1/d]

5. Calculation of BFR [%]

$$BFR = \frac{C_0 - C_1}{C_0} * 100 \quad (7)$$

The literature review identified additional factors influencing BFR such as redox conditions, microbial activity, and temperature, which are not accounted for in the simplified calculations presented. Incorporating all these factors and their variability into a model poses significant challenges, as none of the models discussed in section 4.2 takes factors besides compound and subsurface properties into account.

4.4 Creation of environmental scenarios

The creation of environmental scenarios offers a valuable opportunity to assess the transport of PPPs from surface water to groundwater with various subsurface properties. By simulating different scenarios, the compound-specific contamination patterns can be more meaningfully assessed based on individual combinations of compound and site conditions.

Based on the studies, greatest risk in terms of subsurface properties is related to sandy aquifers, where short flow paths and high flow velocities impair high BFR (Wang and Squillace 1994; Hu et al. 2016; Ahmed and Marhaba 2017; Handl 2023). Furthermore, a low C_{org} offers only reduced sorption potential for compounds (Wang and Squillace 1994; Abogabal et al. 2020). Since the studies do not provide sufficient details of the subsurface, typical properties of a sandy aquifer were collected from external literature (Table 9). The realistic worst-case scenario will therefore incorporate the aquifer characteristics listed in Table 9, along with a short distance of 5 meters between surface water and groundwater. Considering a 5 m distance is a pragmatic approach, as it reflects the shortest distance reported in the field studies (Wang and Squillace 1994; Schmidt et al. 2004; Dragon et al. 2018). If suitable data on flow velocity are not available, values of hydraulic conductivity and hydraulic gradients can be used, as flow velocity is influenced by both the hydraulic conductivity and the hydraulic gradient.

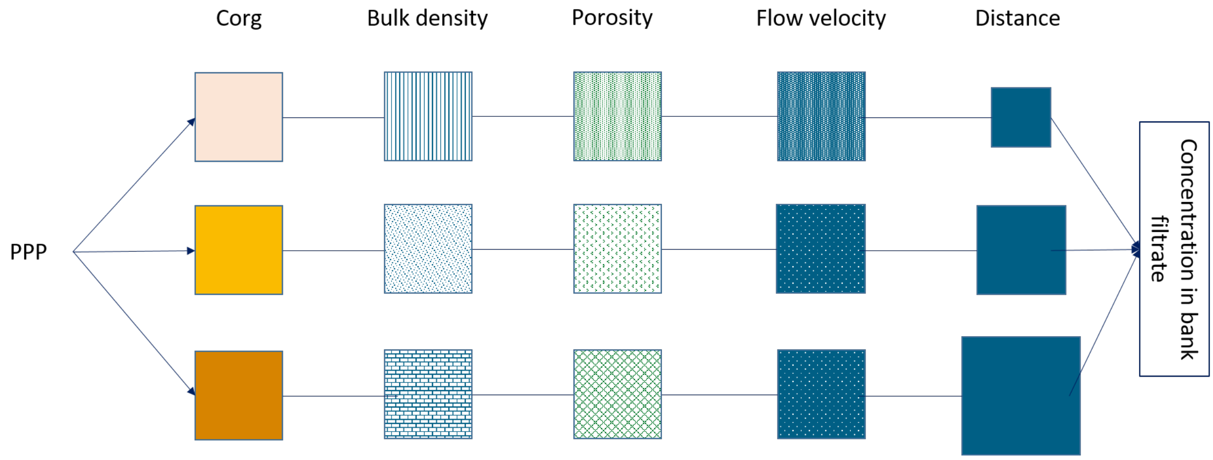
Table 9: Properties of sandy aquifers from external literature

Property	Value	Source
Organic carbon content [%]	0.02-1	Domenico and Schwartz (1998)
Hydraulic conductivity [m/s]	0.00001-0.1	Freeze and Cherry (1979)
Bulk density [g/cm^3]	1.67-1.19	Hartge et al. (2014)
Porosity [-]	0.25-0.35	Hölting and Coldewey (2013)

It has to be pointed out that the passage from surface water to groundwater consists of several zones such as the river sediment and the aquifer and probably a transition zone. These zones have different properties, which cannot be considered individually in this context. Instead, only the properties of the aquifer are used for the passage.

Therefore, when creating environmental scenarios, different conditions should be considered (Figure 29). All parameters displayed in Figure 29 are included in the calculations of equations 2-7 and can therefore be varied. As an option, a dilution factor due to inflow of ambient uncontaminated groundwater can be considered as well.

Figure 29: Variations in site conditions under different bank filtration scenarios



Source: own illustration, INR

Potential scenarios could consider variations in the subsurface properties outlined in Table 9 for the realistic worst-case scenario. By altering individual site conditions (e.g., minimum, maximum or mean flow velocity), it is possible to determine the range of the BFR for the same compound and potentially identify, which factors have a greater influence on the final result compared to others. It is important to note that the representativity of these scenario calculations must be tested with an appropriate data set, ideally originating from field studies with natural bank filtration.

5 Recommendations for Action

The current state of research highlights the complexity of bank filtration as an entry pathway for PPPs from surface water into groundwater, influenced by multiple factors. Individual processes such as sorption and microbial degradation are understood, but data demonstrating the impact of individual factors and particularly their interactions are still insufficient. Clear statements on this matter are further complicated by the close interconnection of compound and site data, resulting in a high variability of statements. The following sections outline the research deficits.

5.1 Knowledge deficits derived from literature review

- The literature review identified a total of 174 studies focusing on bank filtration and BFR in the form of field studies, laboratory experiments or modeling. There was only one study that examined natural bank filtration at field scale, while all other studies at field scale involved technically initiated bank filtration by pumping. Hence, the knowledge is very limited how compounds are removed along the bank filtration pathway under natural conditions.
- There are notably more studies on pharmaceuticals than on PPPs (ratio approximately 124:91). The BFR of pharmaceuticals is often higher than that of PPPs, except for persistent pharmaceuticals that are not eliminated regardless of environmental conditions. An explanation for this discrepancy has not yet been found. A broader database for the BFR of PPPs is necessary for a better understanding of their behavior during bank filtration.
- The relevance of the bank filtration entry pathway for the contamination potential of groundwater in Germany/Europe includes several perspectives and cannot be conclusively assessed. It becomes evident that compounds are seldom fully retained during this process, posing a risk to groundwater. This issue is crucial given groundwater's value and its role in providing drinking water across Europe. However, the variability in study design, site characteristics, and other factors make it difficult to draw definitive conclusions about the extent of the contamination risk. Understanding the contribution of bank filtration to the overall water balance of a site requires data from a sufficient number of sites to enable statistical analyses. This would enhance our understanding and provide the necessary information to assess its importance, especially in comparison to technically induced bank filtration.
- The study design, especially for field experiments, is geared toward pharmaceuticals and raw water production. Groundwater enrichment through the percolation of treated domestic wastewater rather than bank filtration is often considered. Additionally, water is pumped at a specific flow rate/pumping rate rather than controlled by the hydraulic gradient. This can result in different flow rates and residence times for the compounds causing different values of BFR. This study design is not suitable for the assessment of PPP removal during natural bank filtration and needs to be adapted.
- In the context of environmental fate of PPPs and the Exposit 3.02 model, compound properties like K_{oc} and DT_{50} are mainly considered. However, the reviewed field and laboratory studies, which more frequently considered pharmaceuticals, evaluate compound properties using parameters more common in the context of pharmaceuticals (e.g. $\log P_{ow}$, logD, $\log K_{ow}$ for the sorption potential), and persistence as DT_{50} is not considered. Therefore, the study design should be adjusted to incorporate the environmental fate properties specific to PPPs, ensuring better alignment with calculations and modeling purposes in this context.

- In several sections of the report, the high variability of study design and conditions is highlighted. There is no standardized procedure for evaluating the BFR in either field or laboratory studies. Due to significant variations in study design both between and within field and laboratory studies, comparability of the obtained values is lacking.
- Many studies, especially field studies, provide primarily qualitative statements (e.g., higher temperatures lead to increased microbial activity). Quantitative statements can be made more reliably in laboratory studies when individual influencing factors are systematically varied and the effect can be measured. However, few studies offer such precise information, allowing for comparison with similarly designed studies. This indicates the need for studies with targeted variation of influencing factors and quantitative statements.
- In some laboratory studies, study designs or chosen parameter ranges only partially correspond to natural environmental conditions. Studies were found where flow velocity ranged from 0.02 m/d to 9.5 m/d and temperature varied between 5°C and 30°C. While this range of experimental conditions allows for observing the fundamental effects of factors like temperature on the BFR, it is uncertain to what extent these influences can be observed within the more typical real-world temperature fluctuations of 2°C to approximately 20°C. In laboratory studies on the influence of redox potential on the BFR, the information in the variants was often qualitative and rarely quantitative. A more differentiated approach would be desirable. Additionally, it was not clearly evident from existing studies, to what extent one influencing factor had a stronger effect on the BFR when more than one influencing factor was varied. Either this was compound-dependent and varied significantly, or a clear statement was not made. These observations indicate that a better systematic approach to experimental design is necessary in laboratory studies, enabling not only qualitative but also quantitative statements.

5.2 Recommendations for Research

The reviewed studies indicate the necessity for a standardized study design for both laboratory and field studies to enable the comparison of results and draw further conclusions based on the generated data. Therefore, the following recommendations are summarized to establish a suitable database that can be used to better understand the impact of site conditions and compound properties on the BFR.

For a standardized procedure, laboratory studies should be conducted with a defined column size. The prevalent length of columns used in the studies was 1 m. Initially, a standardized material (probably the same which is used for OECD Test 308 (2002)) representing a typical aquifer should be used, with consistent subsurface properties C_{org}, bulk density, porosity, and hydraulic conductivity. This setup allows for the isolated investigation of each factor that reflects additional site conditions, including temperature, redox potential, DOC concentrations in influent water, and microbial processes. These factors can be varied in their value range. To observe microbial processes effectively, it is important to implement an adaptation phase prior to the start of the experiment to establish a natural microbiome in the columns. Depending on the desired complexity of the study design, initial investigations can be carried out with a single PPP, followed by studies involving PPPs with different K_{oc} and $DT_{50,\text{ water-sediment}}$ values. This approach may provide insights into the environmental behavior during bank filtration based solely on compound properties and could therefore help testing the groundwater hazard potential classification proposed in section 3.5. In subsequent experiments, multiple factors can be varied simultaneously to assess the interrelations of the influencing factors, and the subsurface material can be altered. The results would potentially allow for the assessment of the relevance of individual factors influencing the BFR and indicate whether the study findings are transferable or highly compound-dependent. Further, the interaction among these factors and how they affect each other as a function of their value is not yet understood and should be investigated.

- Field studies have to be conducted to validate the results of laboratory studies, since laboratory studies cannot mimic the complexity of a natural site. Bank filtration can occur in general at each location wherever a surface water body loses water to the subsurface, independent of technically initiated pumping. Currently, there is almost no data, and certainly no comprehensive database, of PPP-BFRs under natural conditions. Therefore, the field studies should be conducted under natural hydraulic gradients and flow velocities. Flow distance and retention time of the compounds have been shown to have an impact on the BFR but the relevance of the site conditions temperature, redox potential, DOC concentrations of influent water, and microbial processes on BFRs has not been examined under natural conditions. Field scale experiments can help to fill this knowledge gap. Given the diversity of study sites, conditions can be varied only to a limited extent (e.g., hydraulic gradient, temperature, subsurface properties). It is crucial that these conditions are described in great detail. Data gained from field studies under natural conditions are essential because they will form the basis for BFR assessment using the Exposit model 3.02 in the current version and with the suggested alterations.

- In both laboratory and field studies, several factors influencing the BFR were investigated more frequently than other factors. These include retention time, flow distance, redox conditions, and subsurface properties in field studies. Microbial processes, redox conditions, and subsurface properties were more frequently observed in laboratory studies. Retention time and flow distance in field studies consistently show improved removal with increasing values. However, it is not possible to quantify that the BFR increases by a specific percentage with each additional meter of distance or hour of retention time. It remains uncertain whether such precise quantifications can be achieved in field studies. Though laboratory studies often provide quantified results, a more systematic approach is needed to investigate the impact of each specific influencing factors as well as their interactions on individual compounds. The data analysis from these studies indicates that the current database is insufficient for making reliable conclusions in this context (Section 3.3.8), highlighting the need for further research as outlined in the previous bullet points.

- It is important to assess the relevance of bank filtration in the hydrological context. The water balance of a water body system provides information on gaining and losing water from the surface water body. Based on water level measurements in the surface water body and the surrounding groundwater, the application of salt or/and dye tracers, and isotope concentration measurements, the water balance of the system can be determined. In this frame, the bank filtration volume can be quantified at field scale. Including PPP analysis into such a study, PPP loads can be calculated for all transport pathways and the relevance of bank filtration can be assessed. For the calculation of the water balance and herewith the bank filtration share at catchment scale, more complex hydrological models (e.g., Soil Water Assessment Tool SWAT (Arnold et al. 1998)) have to be used.

- In the last decade, the occurrence of PPP transformation products in the environment has drawn the attention of authorities, regulators, and the science community. Degradation processes, which also occur during bank filtration, alter the molecule structure of the PPP. Therefore, the potential transformation during bank filtration should be assessed, as these transformation products could be more persistent and pose a higher risk to the environment than their parent compounds. This can be accomplished by incorporating potential transformation products of the investigated PPPs into the chemical analysis during laboratory and field studies.

5.3 Recommendations for the Exposit 3.02 model

The model Exposit 3.02 was evaluated for its suitability to represent realistic BFR of PPPs. Based on the reviewed literature, subsurface and compound properties play an important role influencing the BFR. The analysis revealed the Exposit 3.02 model does not explicitly consider subsurface properties, and only indirectly incorporates compound properties via groundwater groundwater risk groups. For 13 PPPs, an individual BFR is applied from literature (Sturm et al. 2006; Schmidt 2006). Based on the advection-dispersion-equation for aquifers, a simple improvement to the model is proposed in section 4.2 by directly integrating compound properties such as K_{oc} and $DT_{50,\text{ water-sediment}}$, along with subsurface characteristics. A simplified calculation of retardation, residence time, degradation rate, and concentration after bank filtration of a specific PPP (equations 2-7) allows for a more realistic estimation of the BFR compared to the current model, without significantly increasing the effort for applicants or regulatory authorities. This proposal enables the variation of the subsurface including organic matter content, bulk density, hydraulic conductivity, and flow path length, optionally considering a dilution factor through groundwater. Realistic worst-case conditions for elimination of PPPs during bank filtration would entail low C_{org} content and bulk density, high porosity and flow velocity as well as a short flow path length. The calculation of further scenarios should be considered to assess the variability of the BFR under different subsurface conditions.

It must be noted that the proposed simplified calculation cannot capture the full complexity of the environmental processes during bank filtration. Redox conditions, temperature, microbial processes as site conditions and their impact on the BFR are not considered due to the high degree of interrelation among each other, with the subsurface material and the compounds. Even in complex models simulating matter transport in the subsurface such as Modflow/MT3D, FEFLOW or MIKE SHE, site characteristics are not represented. Further, the bank filtration pathway includes both the hyporheic zone and the subsurface, which can differ considerably in terms of their C_{org}, hydraulic conductivity, porosity, and microbial activity. For simplification, the proposed calculations are based on the properties of the subsurface and neglect those of the hyporheic zone.

5.4 Requirements for implementing a suitable model-based approach at EU level

So far, Germany is the only EU member state, which considers bank filtration as a pathway for groundwater contamination by PPPs in the authorization process for PPPs. The exposure assessment of groundwater due to bank filtration in the model Exposit 3.02 is generally based on three BFRs, 100%, 90 % and 75 %. For a limited number of PPPs, lower BFRs are assigned. In the reviewed studies BFRs show a broad value range for the same PPP and mean BFR values lower than 50% are often determined. Hence, there is concern that groundwater can be harmed by PPPs via bank filtration. Nevertheless, some issues have to be clarified before implementing a suitable model-based approach at the EU level.

It is recommended that the EU member states should reach a consensus if and how the bank filtration pathway should be incorporated into the approval process. Additional data collected within the EU could help to make more informed decision regarding the spatial, temporal, and quantitative occurrence of bank filtration as a pathway for groundwater contamination within the EU.

It becomes evident that a standardized method for conducting studies to determine BFRs is needed. Particularly, a standardized study design and documentation of site characteristics, subsurface properties, and hydrometeorological conditions would be beneficial to better understand the dependency of a compound's BFR and ensure consistency and comparability of results across different regions and research contexts. Initially, such a database can originate from laboratory studies but should be extended to field studies.

A centralized database that compiles data from both field and laboratory studies on bank filtration rates and influencing factors would be beneficial. BFR data for PPPs from studies conducted in Europe could offer improved insights into the spatial variability of a compound's BFR within the EU. This resource will support researchers and regulators in making informed decisions and improving model accuracy.

If the proposed 5-step calculation for Exposit 3.02 is used for BFR assessment in the authorization process, it will be essential that this method is validated by data obtained from field studies conducted under natural conditions. This will allow for a comparison between the calculated values based on subsurface and PPP properties from literature and the actual field data. In these field studies, the subsurface properties should match those intended for use in Exposit 3.02. For instance, if the BFR of a compound is to be tested under the realistic worst-case scenario defined in section 3.5, the subsurface properties at the site should include a C_{org} content of 0.02-1%, a porosity of 0.25-0.35, a bulk density of 1.19-1.67 g/cm^3, a kf range of 0.00001-0.1 m/s, and the distance between the surface water body and well should be 5 meters. The same study can be conducted under different site conditions and with other PPPs, but all relevant data for the 5-steps calculation must be documented to enable accurate calculation.

The Exposit model 3.02 considers compound properties indirectly by integrating them into groundwater risk groups, to which specific BFRs are assigned. A more direct approach is proposed, incorporating the compound's mobility (K_{oc}) and persistence ($DT_{50,\ water\text{-}sediment}$) into an 8-class groundwater hazard potential classification, aiming to better estimate BFRs based on compound properties. However, the high variability of study conditions in the literature makes it difficult to validate this classification concept. If this concept is to be applied in the future, its reliability needs to be demonstrated with data from studies that focus on the effect of compound properties on BFRs while keeping subsurface properties and environmental conditions constant. This validation is assumed to be more feasible under laboratory conditions. Studies conducted using standardized methods will help to understand the impact of compound properties on BFRs compared to other influencing factors, thereby evaluating the proposed groundwater hazard potential classification.

Several factors influence bank filtration processes and the removal of compounds during this passage. Expertise from various disciplines, including soil science, (hydro-)geology, hydrology, chemistry, and microbiology, is essential for conducting meaningful studies and analyzing results. Collaborative and interdisciplinary research should be initiated to address existing research gaps, thereby supporting regulators, producers, and the scientific community.

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A Appendix

A.1 Keywords for literature review

Compounds	Bank filtration process	Environmental context	Others
Pesticide	Bank filtration	River bank / Riverbank	Water purification
Agrochemicals	Filtration	River	Drinking water
Herbicides	Passage	Stream	Contaminant transport
Insecticides	Recharge	Lake	Water quality
Fungicides	Aquifer recharge	Soil	Aquifer recharge
Pharmaceutical	Managed aquifer recharge	Sediment	Environmental fate
Metabolite	Natural attenuation	Aquifer	Environmental monitoring
Transformation products	Sorption	Groundwater	Analytical methods
Drug residues	Adsorption	Riparian zone	Sampling techniques
Degradation products	Biodegradation	Hyporheic zone	Risk assessment
Micropollutants	Chemical transformation	Watershed	Water purification
	Hydraulic conductivity	Floodplain	
	Hydrological connectivity	Water table	
	Groundwater surface water interaction		

A.2 Bank filtration rates [%]

Bank filtration rates were extracted from literature with focus on publications from 2000-2014 including studies cited in the Exposit model 3.02 with K_{oc} and DT_{50}, water-sediment data for PPPs from PPDB (Lewis et al. 2016). If only one BFR value is provided for a compound in the study, this value is reported as the mean value. Some filtration rates are based on secondary citations as reported in review articles; original sources were nor accessible. In cases, where original publications were not accessible, data are cited as reported by review articles that referenced the original studies.

Compound	Class	Min. bank filtration rate [%]	Max bank filtration rate [%]	Arithmetic mean bank filtration rate [%]	Type of study	Reference	K_{oc} [mg/L]	$DT_{50, water-sediment}$ [d]
1,3,6-NTS	Pharma			10	fixed-bed reactor	Storck et al. (2012)		
1,5-NDS	Pharma			10	fixed-bed reactor	Storck et al. (2012)		
17a-Ethinylestradiol (EE2)	Pharma	20.2	100	60.1	batch	Onesios et al. (2009)		
17-α-Ethynilestradiol	Pharma			80	fixed-bed reactor	Storck et al. (2012)		
2,4,5-T (2,4,5-Trichlorphenoxy acidic acid)	Herbicide			90	field	Schmidt (2006)	10	-
2,4,5-T (2,4,5-Trichlorphenoxy acidic acid)	Herbicide			70	pilot	Schmidt (2006)	10	-
2,4,5-T (2,4,5-Trichlorphenoxy acidic acid)	Herbicide			10	pilot	Schmidt (2006)	10	-
2,4,5-T (2,4,5-Trichlorphenoxy acidic acid)	Herbicide			40	column	Schmidt (2006)	10	-
2,4,5-T (2,4,5-Trichlorphenoxy acidic acid)	Herbicide			0	column	Schmidt (2006)	10	-

Compound	Class	Min. bank filtration rate [%]	Max bank filtration rate [%]	Arithmetic mean bank filtration rate [%]	Type of study	Reference	K_{oc} [mg/L]	$DT_{50, \text{water-sediment}}$ [d]
2,4-D	Herbicide	42.32	56.58	49.5	batch	Boivin et al. (2005)	39.3	18.2
2,4-D	Herbicide			86	field	Schmidt (2006)	39.3	18.2
2,4-D	Herbicide			97	field	Schmidt (2006)	39.3	18.2
2,4-D	Herbicide			87	pilot	Schmidt (2006)	39.3	18.2
2,4-D	Herbicide	60	100	80	column	Schmidt (2006)	39.3	18.2
2,4-D	Herbicide			80	column	Schmidt (2006)	39.3	18.2
2,4-D	Herbicide			0	column	Schmidt (2006)	39.3	18.2
2,4-dichlorophenol	Phenol			54.92	pilot	Ma et al. (2010)	39.3	18.2
2,4-dichlorophenol	Phenol			90	pilot	Yang et al. (2010)	39.3	18.2
2,4-DP	Herbicide	67	98	82.5	pilot	Gonzalez et al. (2006)	39.3	18.2
2,4-DP	Herbicide	83	98	90.5	pilot	Gonzalez et al. (2006)	39.3	18.2
4-AAA	Pharma			91.2	field	Kovacevic et al. (2017)		
4-Chloro-m-cresol	Pharma			99	batch	Onesios et al. (2009)		
4-FAA	Pharma			70	field	Kovacevic et al. (2017)		
5-Fluorouracil	Pharma			70	batch	Onesios et al. (2009)		

Compound	Class	Min. bank filtration rate [%]	Max bank filtration rate [%]	Arithmetic mean bank filtration rate [%]	Type of study	Reference	K_{oc} [mg/L]	$DT_{50,\ water\text{-}sediment}$ [d]
AAA	Pharma			96	field	Massmann et al. (2006a)		
AAA	Pharma	45	90	67.5	column	Massmann et al. (2008a)		
Acesulfame	Sweetener	71	85	78	field	Hrakl et al. (2023)		
Acesulfame	Pharma	27	40	33.5	field	Nagy-Kovacs et al. (2018)		
Acetaminophen	Pharma			90	pilot	Benotti et al. (2012)		
Acetaminophen	Pharma			46	biofiltration	Carpenter and Helbling (2017)		
Acetaminophen	Pharma			99	batch	Onesios et al. (2009)		
Acetamiprid	Insecticide	64	88	76	field	Glorian et al. (2018)	200	-
Acetamiprid	Insecticide			21.4	column	Pietrzak et al. (2020)	200	-
Acetochlor	Herbicide	0	20	10	field	Schmidt (2006)	156	19.7
Acetochlor	Herbicide			72	field	Schmidt (2006)	156	19.7
Acetyl-Sulfamethoxazole	Pharma			100	field	Heberer et al. (2008)		
Alachlor	Herbicide	93	100	96	field	Wang and Squillace (1994)	335	2
Alachlor	Herbicide			76	field	Schmidt (2006)	335	2
Aldrin	Herbicide	82	100	91	pilot	Schmidt (2006)	17500	50.1

Compound	**Class**	**Min. bank filtration rate [%]**	**Max bank filtration rate [%]**	**Arithmetic mean bank filtration rate [%]**	**Type of study**	**Reference**	**K_{oc} [mg/L]**	**$DT_{50, water-sediment}$ [d]**
Aldrin	Herbicide			98	pilot	Schmidt (2006)	17500	50.1
AMDOPH	Pharma			5	field	Massmann et al. (2006a)		
AMDOPH	Pharma			43	field	Massmann et al. (2007)		
AMDOPH	Pharma			0	column	Massmann et al. (2008a)		
Ametryn	Herbicide			84	column	Jaramillo et al. (2016)	316	-
Ametryn	Herbicide	0	20	10	field	Schmidt (2006)	316	-
Amidosulfuron	Herbicide	8.2	26	17.1	column	Schmidt (2006)	29.3	50.1
Amidosulfuron	Herbicide			37	column	Schmidt (2006)	29.3	50.1
AMPA	Herbicide	46	87	66.5	field	Schmidt (2006); EC (2021)	2002	132
AMPA	Herbicide	85	94	89.5	field	Schmidt (2006)); EC (2021)	2002	132
AMPA	Herbicide			90	field	Schmidt (2006)); EC (2021)	2002	132
AMPA	Herbicide			22	field	Bruchet et al. (2012)	2002	132
AMPA	Herbicide	25	95	60	field	EC (2021)	2002	132
AMPA	Herbicide			90	field	Post et al. (2000) from EC (2021)	2002	132

Compound	Class	Min. bank filtration rate [%]	Max bank filtration rate [%]	Arithmetic mean bank filtration rate [%]	Type of study	Reference	K_{oc} [mg/L]	$DT_{50, \text{water-sediment}}$ [d]
AMPA	Herbicide		95	95	field	Schlett et al. (2005) from EC (2021)	2002	132
AMPA	Herbicide	89		89	sand filter	Schlett et al. (2005) from EC (2021)	2002	132
AMPA	Herbicide		94	94	sand filter	Hopman et al. (1995) from EC (2021)	2002	132
Androstenedione	Pharma			90	pilot	Benotti et al. (2012)		
Anhydroerythromycin	Antibiotics			98	field	Heberer et al. (2008)		
Anhydroerythromycin	Pharma	90	98	94	field	Heberer et al. (2008)		
Ascesulfame	Pharma			17	column	Trussel et al. (2018)		
Atenolol	Pharma			90	pilot	Benotti et al. (2012)		
Atenolol	Pharma			10	biofiltration	Carpenter and Helbling (2017)		
Atenolol	Pharma			90	field	Regnery et al. (2015)		
Atenolol	Pharma			100	field	Postigo und Barcelo (2015)		
Atenolol	Pharma			97	fixed-bed reactor	Storck et al. (2012)		
Atenolol	Pharma			77	column	Trussel et al. (2018)		
Atrazine	Herbicide				field	Schmidt (2006)	100	80

Compound	Class	Min. bank filtration rate [%]	Max bank filtration rate [%]	Arithmetic mean bank filtration rate [%]	Type of study	Reference	K_{oc} [mg/L]	$DT_{50, water-sediment}$ [d]
Atrazine	Herbicide	0	20	10	field	Schmidt (2006)	100	80
Atrazine	Herbicide			50	field	Schmidt (2006)	100	80
Atrazine	Herbicide			28	field	Schmidt (2006)	100	80
Atrazine	Herbicide			14	field	Schmidt (2006)	100	80
Atrazine	Herbicide	40	60	50	field	Schmidt (2006)	100	80
Atrazine	Herbicide	0	20	10	field	Schmidt (2006)	100	80
Atrazine	Herbicide			16	field	Schmidt (2006)	100	80
Atrazine	Herbicide			25	field	Schmidt (2006)	100	80
Atrazine	Herbicide			20	field	Schmidt (2006)	100	80
Atrazine	Herbicide			18	field	Schmidt (2006)	100	80
Atrazine	Herbicide	0	10	5	field	Schmidt (2006)	100	80
Atrazine	Herbicide			90	field	Schmidt (2006)	100	80
Atrazine	Herbicide			25	field	Schmidt (2006)	100	80
Atrazine	Herbicide			35	field	Schmidt (2006)	100	80
Atrazine	Herbicide			50	field	Schmidt (2006)	100	80
Atrazine	Herbicide	0	20	10	field	Schmidt (2006)	100	80
Atrazine	Herbicide			70	field	Schmidt (2006)	100	80

Compound	Class	Min. bank filtration rate [%]	Max bank filtration rate [%]	Arithmetic mean bank filtration rate [%]	Type of study	Reference	K_{oc} [mg/L]	$DT_{50,\ water\text{-}sediment}$ [d]
Atrazine	Herbicide			86	field	Schmidt (2006)	100	80
Atrazine	Herbicide	48	80	64	field	Schmidt (2006)	100	80
Atrazine	Herbicide			12	field	Schmidt (2006)	100	80
Atrazine	Herbicide	16	23	19.5	field	Schmidt (2006)	100	80
Atrazine	Herbicide			20	field	Schmidt (2006)	100	80
Atrazine	Herbicide	50	85	67.5	field	Schmidt (2006)	100	80
Atrazine	Herbicide	5	23	14	pilot	Schmidt (2006)	100	80
Atrazine	Herbicide			0	field	Schmidt (2006)	100	80
Atrazine	Herbicide			0	field	Schmidt (2006)	100	80
Atrazine	Herbicide			0	field	Schmidt (2006)	100	80
Atrazine	Herbicide			0	field	Schmidt (2006)	100	80
Atrazine	Herbicide			0	field	Schmidt (2006)	100	80
Atrazine	Herbicide			0	field	Schmidt (2006)	100	80
Atrazine	Herbicide			0	column	Schmidt (2006)	100	80
Atrazine	Herbicide			0	pilot	Schmidt (2006)	100	80
Atrazine	Herbicide			45	column	Schmidt (2006)	100	80

Compound	Class	Min. bank filtration rate [%]	Max bank filtration rate [%]	Arithmetic mean bank filtration rate [%]	Type of study	Reference	K_{oc} [mg/L]	$DT_{50, water-sediment}$ [d]
Atrazine	Herbicide	-246	100	-73	field	Oberleitner et al. (2020)	100	80
Atrazine	Herbicide	-29	47	9	field	Benotti et al. (2012)	100	80
Atrazine	Herbicide			20	column	Benotti et al. (2012)	100	80
Atrazine	Herbicide	-109	79	-15	field	Hollender et al. (2018)	100	80
Atrazine	Herbicide	-5	30	12.5	field	Bruchet et al. (2012)	100	80
Atrazine	Herbicide			25	field	Regnery et al. (2015)	100	80
Atrazine	Herbicide	14	84	49	field	Verstraeten et al. (2002)	100	80
Atrazine	Herbicide			45	batch	Abdelrady et al. (2019)	100	80
Atrazine	Herbicide			0	column	Bertelkamp et al. (2016)	100	80
Atrazine	Herbicide			5	pilot	Patterson et al. (2002)	100	80
Atrazine	Herbicide	0.47	56.4	28.435	pilot	Rodriguez-Cruz et al. (2007)	100	80
Atrazine	Herbicide			80	bench	Vieira Dos Santos et al. (2017)	100	80
Atrazine	Herbicide	84.4	97.8	91.1	batch	Boivin et al. (2005)	100	80

Compound	Class	Min. bank filtration rate [%]	Max bank filtration rate [%]	Arithmetic mean bank filtration rate [%]	Type of study	Reference	K_{oc} [mg/L]	$DT_{50, water-sediment}$ [d]
Atrazine	Herbicide			0	biofiltration	Carpenter and Helbling (2017)	100	80
Atrazine	Herbicide			10	field	Diaz-Cruz & Barcelo (2008)	100	80
Atrazine	Herbicide			97	column	Jaramillo et al. (2016)	100	80
Atrazine	Herbicide			50	field	Köck-Schulmeyer et al. (2013)	100	80
Atrazine	Herbicide			50	field	Oberleitner et al. (2020)	100	80
Atrazine	Herbicide			2	column	Patterson et al. (2002)	100	80
Atrazine	Herbicide			10	field	Zullei-Seibert (1996) in Schmidt et al. (2003)	100	80
Atrazine	Herbicide	54	88	71	field	Wang and Squillace (1994)	100	80
Atrazine	Herbicide			0	fixed-bed reactor	Storck et al. (2012)	100	80
Azithromycin	Pharma	0.4	0.5	0.45	batch	Onesios et al. (2009)		
Bentazone	Herbicide			60	field	Heberer et al. (2004)	55.3	716
Bentazone	Herbicide	92.6	100	96.9	batch	Boivin et al. (2005)	55.3	716
Bentazone	Herbicide			27	pilot	Gonzalez et al. (2006)	55.3	716

Compound	Class	Min. bank filtration rate [%]	Max bank filtration rate [%]	Arithmetic mean bank filtration rate [%]	Type of study	Reference	K_{oc} [mg/L]	$DT_{50, \text{water-sediment}}$ [d]
Bentazone	Herbicide	70	100	85	field	Oberleitner et al. (2020)	55.3	716
Bentazone	Herbicide	0	30	15	field	Schmidt (2006)	55.3	716
Bentazone	Herbicide	30	60	45	field	Schmidt (2006)	55.3	716
Bentazone	Herbicide			0	field	Schmidt (2006)	55.3	716
Bentazone	Herbicide			0	field	Schmidt (2006)	55.3	716
Bentazone	Herbicide			0	field	Schmidt (2006)	55.3	716
Bentazone	Herbicide			0	field	Schmidt (2006)	55.3	716
Bentazone	Herbicide			0	pilot	Schmidt (2006)	55.3	716
Bentazone	Herbicide			0	column	Schmidt (2006)	55.3	716
Bentazone	Herbicide			0	column	Schmidt (2006)	55.3	716
Bentazone	Herbicide	13	15	14	column	Schmidt (2006)	55.3	716
Bentazone	Herbicide	5	27	16	column	Schmidt (2006)	55.3	716
Benzotriazol	other	88	100	94	field	Hrakl et al. (2023)		
Bezafibrat	Pharma			97	field	Massmann et al. (2007)		
Bezafibrat	Pharma	70	100	85	field	Oberleitner et al. (2020)		

Compound	Class	Min. bank filtration rate [%]	Max bank filtration rate [%]	Arithmetic mean bank filtration rate [%]	Type of study	Reference	K_{oc} [mg/L]	$DT_{50,\ water\text{-}sediment}$ [d]
Bezafibrate	Pharma			100	batch	Onesios et al. (2009)		
Biosol	Pharma			80	batch	Onesios et al. (2009)		
Biphenylol	Pharma			99	batch	Onesios et al. (2009)		
BPA	Pharma			98	column	Trussel et al. (2018)		
Bromoxynil	Herbicide	78	99	88.5	column	Schmidt (2006)	302	13
Bromoxynil	Herbicide	83	96	89.5	column	Schmidt (2006)	302	13
Candesartan	Pharma			20	field	Burke et al. (2018)		
Carbamazepine	Pharma			20	pilot	Benotti et al. (2012)		
Carbamazepine	Pharma	1	4	2.5	biofiltration	Carpenter and Helbling (2017)		
Carbamazepine	Pharma	20	60	40	field	Schmidt et al. (2007)		
Carbamazepine	Pharma			10	column	D´Alessio et al. (2015)		
Carbamazepine	Pharma	15	73	44	field	Glorian et al. (2018)		
Carbamazepine	Pharma	4	100	52	field	Hrakl et al. (2023)		
Carbamazepine	Pharma			27.2	field	Kondor et al. (2020)		
Carbamazepine	Pharma			65.4	field	Kovacevic et al. (2017)		

Compound	Class	Min. bank filtration rate [%]	Max bank filtration rate [%]	Arithmetic mean bank filtration rate [%]	Type of study	Reference	K_{oc} [mg/L]	$DT_{50, \text{water-sediment}}$ [d]
Carbamazepine	Pharma	0	51.8	25.9	field	Kruc et al. (2019)		
Carbamazepine	Pharma			0	field	Massmann et al. (2006a)		
Carbamazepine	Pharma			32	field	Massmann et al. (2007)		
Carbamazepine	Pharma	4	20	12	field	Nagy-Kovacs et al. (2018)		
Carbamazepine	Pharma	70	100	85	field	Oberleitner et al. (2020)		
Carbamazepine	Pharma			0	fixed-bed reactor	Storck et al. (2012)		
Carbaryl	Insecticide	3.3	17	10.15	biofiltration	Carpenter and Helbling (2017)	300	5.8
Carbaryl	Insecticide			90	field	Schmidt (2006)	300	5.8
Carbofuran	Insecticide			61	field	Romero et al. (2010)	-	9.7
Carbofuran	Insecticide			77	column	Jaramillo et al. (2016)	-	9.7
Carisoprodol	Pharma			81	column	Trussel et al. (2018)		
Cefepime	Pharma	37	46	41.5	field	Nagy-Kovacs et al. (2018)		
Celiprolol	Pharma			100	field	Hrakl et al. (2023)		
Chloramphenicol	Antibiotics			83	field	Yang et al. (2017)		

Compound	Class	Min. bank filtration rate [%]	Max bank filtration rate [%]	Arithmetic mean bank filtration rate [%]	Type of study	Reference	K_{oc} [mg/L]	$DT_{50,\ water\text{-}sediment}$ [d]
Chloramphenicol	Pharma			100	field	Hrakl et al. (2023)		
Chloridazon	Herbicide	70	98	84	field	Köck-Schulmeyer et al. (2013)	120	137
Chlorophene	Pharma			99	batch	Onesios et al. (2009)		
Chlorotoluron	Herbicide	70	100	85	field	Oberleitner et al. (2020)	308	-
Chlorotoluron	Herbicide			17	field	Dragon et al. (2018)	308	-
Chlorotoluron	Herbicide			100	field	Schmidt (2006)	308	-
Chlorotoluron	Herbicide			0	field	Schmidt (2006)	308	-
Chlorotoluron	Herbicide			0	field	Schmidt (2006)	308	-
Chlorotoluron	Herbicide			0	field	Schmidt (2006)	308	-
Chlorotoluron	Herbicide			100	field	Schmidt (2006)	308	-
Chlorotoluron	Herbicide			100	field	Schmidt (2006)	308	-
Chlorotoluron	Herbicide			0	column	Schmidt (2006)	308	-
Clarithromycin	Antibiotics			100	field	Heberer et al. (2008)		
Clarithromycin	Antibiotics			34	fixed-bed reactor	Storck et al. (2012)		
Clindamycine	Antibiotics			98	field	Heberer et al. (2008)		

Compound	Class	Min. bank filtration rate [%]	Max bank filtration rate [%]	Arithmetic mean bank filtration rate [%]	Type of study	Reference	K_{oc} [mg/L]	$DT_{50, water-sediment}$ [d]
Clindamycine	Pharma	28	93	60.5	field	Heberer et al. (2008)		
Clindamycine	Pharma			80	field	Schmidt et al. (2003)		
Clofibric acid	Pharma	26	30	28	column	Onesios et al. (2009)		
Clofibric acid	Pharma			79	field	Onesios et al. (2009)		
Clofibric acid	Pharma			90	field	Massmann et al. (2007)		
Clopyralid	Herbicide			16	bench	Rodrigo et al. (2018)	5	-
Clothianidin	Insecticide			100	field	de Souza et al. (2020)	123	56.4
Clotrimazole	Pharma	58	80	69	field	Kahle et al. (2008)		
Continie	Pharma			38	column	Trussel et al. (2018)		
Cotinine	other			100	field	Hrakl et al. (2023)		
Cyanazine	Herbicide			10	field	Schmidt (2006)	190	84
Cyanazine	Herbicide	0	10	5	field	Schmidt (2006)	190	84
Cyanazine	Herbicide	64	95	79.5	pilot	Schmidt (2006)	190	84
Cyanazine	Herbicide	78	100	89	field	Wang and Squillace (1994)	190	84
Cytarabine	Pharma	2	50	26	batch	Onesios et al. (2009)		

Compound	Class	Min. bank filtration rate [%]	Max bank filtration rate [%]	Arithmetic mean bank filtration rate [%]	Type of study	Reference	K_{oc} [mg/L]	$DT_{50,\ water\text{-}sediment}$ [d]
DDT	Insecticide			80	batch	Abdelrady et al. (2019)	151,000	-
DEET	Insecticide	80	100	90	field	Hrakl et al. (2023)	277	-
DEET	Insecticide			80	field	Postigo und Barcelo (2015)	277	-
DEET	Insecticide			62	column	Trussel et al. (2018)	277	-
DEET	Insecticide			90	pilot	Benotti et al. (2012)	277	-
DEET	Insecticide			35	field	Barnes et al. (2008)		
Dehydrato-erythromycine A	Antibiotics			80	field	Schmidt et al. (2003)		
Demeton-S-methyl	Herbicide	20	50	35	pilot	Schmidt (2006)	90	-
Desethylatrazine	Herbicide	0	10	5	field	Schmidt (2006)	110	-
Desethylatrazine	Herbicide	0	10	5	field	Schmidt (2006)	110	-
Desethylatrazine	Herbicide	0	20	10	field	Schmidt (2006)	110	-
Desethylatrazine	Herbicide			30	field	Schmidt (2006)	110	-
Desethylatrazine	Herbicide	0	20	10	field	Schmidt (2006)	110	-
Desethylatrazine	Herbicide	45	79	62	field	Schmidt (2006)	110	-
Desethylatrazine	Herbicide	0	10	5	pilot	Schmidt (2006)	110	-
Desethylatrazine	Herbicide			0	field	Schmidt (2006)	110	-

Compound	Class	Min. bank filtration rate [%]	Max bank filtration rate [%]	Arithmetic mean bank filtration rate [%]	Type of study	Reference	K_{oc} [mg/L]	$DT_{50, \text{water-sediment}}$ [d]
Desethylatrazine	Herbicide			0	field	Schmidt (2006)	110	-
Desethylatrazine	Herbicide			8	pilot	Schmidt (2006)	110	-
Desethylatrazine	Herbicide			50	field	Köck-Schulmeyer et al. (2013)	110	-
Desethylatrazine	Herbicide	28	70	49	field	Wang and Squillace (1994)	110	-
Desethylatrazine	Herbicide			50	field	Oberleitner et al. (2020)	110	-
Desisopropylatrazine	Herbicide			0	field	Schmidt (2006)	130	-
Desisopropylatrazine	Herbicide	57	90	74	field	Wang and Squillace (1994)	130	-
Desisopropylatrazine	Herbicide			15	field	Schmidt (2006)	130	-
Diatrizoate	Pharma			100	batch	Onesios et al. (2009)		
Diazepam	Pharma	20	80	50	pilot	Benotti et al. (2012)		
Diazinon	Insecticide			90	column	Rattier et al. (2014)	609	10.4
Diazinon	Insecticide			94	biofiltration	Carpenter and Helbling (2017)	609	10.4
Diazinon	Insecticide			50	field	Köck-Schulmeyer et al. (2013)	609	10.4
Dichlobenil	Herbicide	10	20	15	pilot	Schmidt (2006)	257	142

Compound	Class	Min. bank filtration rate [%]	Max bank filtration rate [%]	Arithmetic mean bank filtration rate [%]	Type of study	Reference	K_{oc} [mg/L]	$DT_{50, water-sediment}$ [d]
Dichlobenil	Herbicide	50	90	70	pilot	Schmidt (2006)	257	142
Dichlorprop	Herbicide	30	100	65	field	Tuxen et al. (2000)	74	12
Dichlorprop	Herbicide	30	50	40	field	Schmidt (2006)	74	12
Dichlorprop	Herbicide			100	field	Schmidt (2006)	74	12
Diclofenac	Pharma			90	pilot	Benotti et al. (2012)		
Diclofenac	Pharma	30	100	65	field	Bertrand et al. (2022)		
Diclofenac	Pharma			80	field	Schmidt (2006)		
Diclofenac	Pharma	25	90	57.5	field	Regnery et al. (2015)		
Diclofenac	Pharma	60	80	70	field	Diaz-Cruz & Barcelo (2008)		
Diclofenac	Pharma			90	column	Filter et al. (2017)		
Diclofenac	Pharma	39	100	58.5	field	Glorian et al. (2018)		
Diclofenac	Pharma	44	85	64.5	pilot	Gonzalez et al. (2006)		
Diclofenac	Pharma			17	field	Heberer et al. (2002)		
Diclofenac	Pharma			69	field	Heberer et al. (2002)		
Diclofenac	Pharma			100	field	Hrakl et al. (2023)		
Diclofenac	Pharma	14	69	41.5	batch and column	Im et al. (2016)		

Compound	Class	Min. bank filtration rate [%]	Max bank filtration rate [%]	Arithmetic mean bank filtration rate [%]	Type of study	Reference	K_{oc} [mg/L]	$DT_{50, water-sediment}$ [d]
Diclofenac	Pharma			85	field	Massmann et al. (2007)		
Diclofenac	Pharma	32	44	38	field	Nagy-Kovacs et al. (2018)		
Diclofenac	Pharma	50	100	75	field	Oberleitner et al. (2020)		
Diclofenac	Pharma			80	field	Postigo und Barcelo (2015)		
Diclofenac	Pharma	10	24	17	fixed-bed reactor	Storck et al. (2012)		
Diclofenac	Pharma	34	38	36	column	Onesios et al. (2009)		
Diclofenac	Pharma			30	batch	Onesios et al. (2009)		
Diclofenac	Pharma	70	100	81	field	Oberleitner et al. (2020)		
Diclofenac	Pharma	50	70	60	field	Oberleitner et al. (2020)		
Diclofenac	Pharma			80	field	Heberer et al. (2004)		
Diclofenac	Pharma			100	field	Hamann et al. (2016)		
Diclofenac	Pharma			100	field	Kruc et al. (2019)		
Diclofenac	Pharma			100	field	Van Driezum et al. (2019)		

Compound	Class	Min. bank filtration rate [%]	Max bank filtration rate [%]	Arithmetic mean bank filtration rate [%]	Type of study	Reference	K_{oc} [mg/L]	$DT_{50, \text{water-sediment}}$ [d]
Diclofenac	Pharma			93	field	Kondor et al. (2020)		
Diclofenac	Pharma			44	field	Nagy-Kovacs et al. (2018)		
Diclofenac	Pharma			32	field	Nagy-Kovacs et al. (2018)		
Dieldrin	Herbicide	7	42	24.5	pilot	Schmidt (2006)	12000	-
Dieldrin	Herbicide	80	98	89	pilot	Schmidt (2006)	12000	-
Dimenthenamid	Herbicide			9	field	Schmidt (2006)	-	-
Dimenthenamid	Herbicide	10	99	54.5	column	Schmidt (2006)	-	-
Dimethoate	Insecticide	13	18	15.5	batch	Abdelrady et al. (2019)	-	15.5
Diphenhydramine	Pharma			99	biofiltration	Carpenter and Helbling (2017)		
Disulfoton	Herbicide			95	column	Schmidt (2006)	1345	15
Diuron	Herbicide	37	91	64	field	Glorian et al. (2018)	680	48
Diuron	Herbicide	-55	100	22.5	field	Oberleitner et al. (2020)	680	48
Diuron	Herbicide	-566	76	-245	field	Hollender et al. (2018)	680	48
Diuron	Herbicide			-82	field	Bruchet et al. (2012)	680	48

Compound	Class	Min. bank filtration rate [%]	Max bank filtration rate [%]	Arithmetic mean bank filtration rate [%]	Type of study	Reference	K_{oc} [mg/L]	$DT_{50, water-sediment}$ [d]
Diuron	Herbicide			50	field	Bruchet et al. (2012)	680	48
Diuron	Herbicide			70	column	Jaramillo et al. (2016)	680	48
Diuron	Herbicide			50	field	Köck-Schulmeyer et al. (2013)	680	48
Diuron	Herbicide			90	field	Zullei-Seibert (1996) in Schmidt et al. (2003)	680	48
Diuron	Herbicide	60	95	77.5	batch	Stasinakis et al. (2009)	680	48
Diuron	Herbicide	40	50	45	field	Schmidt (2006)	680	48
Diuron	Herbicide			70	field	Schmidt (2006)	680	48
Diuron	Herbicide			12	field	Schmidt (2006)	680	48
Diuron	Herbicide			18	pilot	Schmidt (2006)	680	48
Diuron	Herbicide			0	field	Schmidt (2006)	680	48
Diuron	Herbicide			0	field	Schmidt (2006)	680	48
Diuron	Herbicide			0	field	Schmidt (2006)	680	48
Diuron	Herbicide			0	column	Schmidt (2006)	680	48
Diuron	Herbicide	0	20	10	column	Schmidt (2006)	680	48
DNOC	Herbicide	20	99	59.5	column	Schmidt (2006)	300	83

Compound	Class	Min. bank filtration rate [%]	Max bank filtration rate [%]	Arithmetic mean bank filtration rate [%]	Type of study	Reference	K_{oc} [mg/L]	$DT_{50, water-sediment}$ [d]
Endosulfan	Insecticide			80	batch	Abdelrady et al. (2019)	11,500	-
Endosulfan	Herbicide	80	90	85	field	Schmidt (2006)	11,500	-
Endosulfan	Herbicide	82	97	89.5	pilot	Schmidt (2006)	11,500	-
Erythromycin-H2O	Pharma			90	pilot	Benotti et al. (2012)		
Estradiol	Pharma			90	pilot	Benotti et al. (2012)		
Estriol	Pharma			90	pilot	Benotti et al. (2012)		
Estrone	Pharma			90	pilot	Benotti et al. (2012)		
Estrone	Hormon	80	100	90	field	Verstraeten et al. (2002)		
Ethynylestradiol	Pharma			90	pilot	Benotti et al. (2012)		
Exemestane	Pharma			80	batch	Onesios et al. (2009)		
FAA	Pharma			89	field	Massmann et al. (2006a)		
FAA	Pharma	36	72	54	column	Massmann et al. (2008a)		
Fenamiphos	Herbicide			5	pilot	Patterson et al. (2002)	446.2	5.8
Fenamiphos	Herbicide	11	21	16	column	Patterson et al. (2002)	446.2	5.8

Compound	Class	Min. bank filtration rate [%]	Max bank filtration rate [%]	Arithmetic mean bank filtration rate [%]	Type of study	Reference	K_{oc} [mg/L]	$DT_{50, water-sediment}$ [d]
Fenoprofen	Pharma			71	field	Onesios et al. (2009)		
Fluconazole	Pharma	0	100	50	field	Kruc et al. (2019)		
Flufenacet	Herbicide			63	field	Verstraeten et al. (2002)	401	81
Fluoxentine	Pharma			29	column	Trussel et al. (2018)		
Fluoxetine	Pharma			90	pilot	Benotti et al. (2012)		
Fluoxetine	Pharma			100	field	Postigo und Barcelo (2015)		
Gabapentin	Pharma	96	100	98	field	Hrakl et al. (2023)		
Gabapentin	Pharma	24.3	100	62.15	field	Kruc et al. (2019)		
Gabapentin	Pharma			90	batch	Onesios et al. (2009)		
Gemcitabine	Pharma	45	50	47.5	batch	Onesios et al. (2009)		
Gemfibrozil	Pharma			90	pilot	Benotti et al. (2012)		
Gemfibrozil	Pharma			100	field	Postigo und Barcelo (2015)		
Gemfibrozil	Pharma			56	fixed-bed reactor	Storck et al. (2012)		
Gemfibrozil	Pharma			92	column	Trussel et al. (2018)		
Gemfibrozil	Pharma			99	batch	Onesios et al. (2009)		

Compound	Class	Min. bank filtration rate [%]	Max bank filtration rate [%]	Arithmetic mean bank filtration rate [%]	Type of study	Reference	K_{oc} [mg/L]	$DT_{50, water-sediment}$ [d]
Glyphosate	Herbicide			90	field	Bruchet et al. (2012)	1424	20.8
Glyphosate	Herbicide			63	fixed-bed reactor	Storck et al. (2012)	1424	20.8
Glyphosate	Herbicide			30	field	Schmidt (2006); EC (2021)	1424	20.8
Glyphosate	Herbicide			17	field	Schmidt (2006); EC (2021)	1424	20.8
Glyphosate	Herbicide			95	column	Schmidt (2006); EC (2021)	1424	20.8
Glyphosate	Herbicide	70	80	75	sand filter	Litz et al. (2011) from EC (2021)	1424	20.8
Glyphosate	Herbicide	86	93	89.5	sand filter	Hedegaard & Albrechtsen (2014) from EC (2021)	1424	20.8
Glyphosate	Herbicide	20	95	57.5	field	Jönsson et al. (2013) from EC (2021)	1424	20.8
Glyphosate	Herbicide			50	field	Schlett et al. (2005) from EC (2021)	1424	20.8
Glyphosate	Herbicide			75	sand filter	Schlett et al. (2005) from EC (2021)	1424	20.8
Glyphosate	Herbicide			80	field	Krause et al. (2009) from EC (2021)	1424	20.8
Guanylurea	Pharma			100	field	Scheuer (2012)		

Compound	Class	Min. bank filtration rate [%]	Max bank filtration rate [%]	Arithmetic mean bank filtration rate [%]	Type of study	Reference	K_{oc} [mg/L]	$DT_{50,\ water-sediment}$ [d]
Heptachlor	Herbicide	96	98	97	pilot	Schmidt (2006)	24000	-
Heptachlor	Herbicide	77	90	83.5	pilot	Schmidt (2006)	24000	-
Hexachlorcyclohexane	Herbicide			50	field	Schmidt (2006)	1,270	394
Hexachlorcyclohexane	Herbicide			75	field	Schmidt (2006)	1,270	394
Hexachlorcyclohexane	Herbicide			67	pilot	Schmidt (2006)	1,270	394
Hexachlorcyclohexane	Herbicide			98	pilot	Schmidt (2006)	1,270	394
Hexachlorobenzene	Herbicide			92	field	Schmidt (2006)	50000	-
Hexachlorobenzene	Herbicide	52	97	74.5	field	Schmidt (2006)	50000	-
Hexachlorobenzene	Herbicide			94	field	Schmidt (2006)	50000	-
Hexachlorobenzene	Herbicide			20	pilot	Schmidt (2006)	50000	-
Hexachlorobenzene	Herbicide			33	pilot	Schmidt (2006)	50000	-
Hexachlorobenzene	Herbicide			94	pilot	Schmidt (2006)	50000	-
Hexachlorobenzene	Herbicide	23	69	46	pilot	Schmidt (2006)	50000	-
Hexachlorobenzene	Herbicide	97	100	98.5	pilot	Schmidt (2006)	50000	-
Hexachlorobenzene	Herbicide	0	48	24	pilot	Schmidt (2006)	50000	-
Hexachlorobenzene	Herbicide			99	column	Schmidt (2006)	50000	-
Hexachlorobenzene	Herbicide			60	pilot	Wan et al. (2010)	50,000	-

Compound	Class	Min. bank filtration rate [%]	Max bank filtration rate [%]	Arithmetic mean bank filtration rate [%]	Type of study	Reference	K_{oc} [mg/L]	$DT_{50, water-sediment}$ [d]
Hexachlorocyclohexane	Insecticide	50	75	62.5	field	Schwarzenbach et al. (1983)	1,270	394
Hydrochlorothiazide	Pharma			100	field	Hrakl et al. (2023)		
Hydrocodone	Pharma			90	pilot	Benotti et al. (2012)		
Iboprofen	Pharma	60	80	70	field	Diaz-Cruz & Barcelo (2008)		
Iboprufen	Pharma			80	field	Postigo und Barcelo (2015)		
Ibuprofen	Pharma			90	pilot	Benotti et al. (2012)		
Ibuprofen	Pharma	91	99	95	biofiltration	Carpenter and Helbling (2017)		
Ibuprofen	Pharma			79	pilot	Benotti et al. (2012)		
Ibuprofen	Pharma	19	74	46.5	field	Glorian et al. (2018)		
Ibuprofen	Pharma			100	field	Hrakl et al. (2023)		
ibuprofen	Pharma	35	57	46	batch and column	Im et al. (2016)		
Ibuprofen	Pharma	64	70	67	column	Onesios et al. (2009)		
Ibuprofen	Pharma	17	21	19	column	Onesios et al. (2009)		
Ibuprofen	Pharma	97	100	98.5	batch	Onesios et al. (2009)		
Ibuprofen	Pharma			99	field	Onesios et al. (2009)		

Compound	Class	Min. bank filtration rate [%]	Max bank filtration rate [%]	Arithmetic mean bank filtration rate [%]	Type of study	Reference	K_{oc} [mg/L]	$DT_{50, water-sediment}$ [d]
Ibuprofen	Pharma			80	field	Onesios et al. (2009)		
Ibuprofen	Pharma			71	field	Onesios et al. (2009)		
Ibuprofen	Pharma			62	field	Onesios et al. (2009)		
Ibuprofen	Pharma			52	field	Onesios et al. (2009)		
Ibuprofen	Pharma			17	field	Onesios et al. (2009)		
Ibuprofen	Pharma			80	field	Onesios et al. (2009)		
Ibuprofen	Pharma			52	field	Onesios et al. (2009)		
Ibuprofen	Pharma			51	field	Onesios et al. (2009)		
Ibuprofen-2-hydroxy	Pharma			100	field	Hrakl et al. (2023)		
Imidacloprid	Insecticide	22	89	55.5	field	Glorian et al. (2018)	-	129
Imidacloprid	Insecticide	-269	100	-84.5	field	Kruć-Fijałkowska et al. (2022)	-	129
Imidacloprid	Insecticide	94.13	96.53	95.33	column (soil)	Bajeer et al. (2012)	-	129
Imidacloprid	Insecticide	79.06	81.24	80.15	column (water)	Bajeer et al. (2012)	-	129
Imidacloprid	Insecticide			94	field	de Souza et al. (2020)	-	129
Imidacloprid	Insecticide			71	field	Dragon et al. (2018)	-	129
Indomethacin	Pharma			95	field	Massmann et al. (2007)		

Compound	Class	Min. bank filtration rate [%]	Max bank filtration rate [%]	Arithmetic mean bank filtration rate [%]	Type of study	Reference	K_{oc} [mg/L]	$DT_{50,\ water\text{-}sediment}$ [d]
Iohexal	Pharma			99	column	Trussel et al. (2018)		
Iohexol	Pharma			100	field	Hrakl et al. (2023)		
Iohexol	Pharma			0	fixed-bed reactor	Storck et al. (2012)		
Iomeprol	Pharma			80	field	Schmidt et al. (2003)		
Iomeprol	Pharma			100	field	Hrakl et al. (2023)		
Iomeprol	Pharma			0	fixed-bed reactor	Storck et al. (2012)		
Iopamidol	Pharma	40	60	50	field	Schmidt et al. (2003)		
Iopamidol	Pharma			35	fixed-bed reactor	Storck et al. (2012)		
Iopimide	Pharma			97	column	Trussel et al. (2018)		
Iopromide	Pharma			80	field	Schmidt et al. (2003)		
Iopromide	Pharma	82	89	85.5	field	Diaz-Cruz & Barcelo (2008)		
Iopromide	Pharma			100	field	Hrakl et al. (2023)		
iopromide	Pharma			80	batch and column	Im et al. (2016)		
Iopromide	Pharma			99	field	Jekel and Grünheid (2005)		

Compound	Class	Min. bank filtration rate [%]	Max bank filtration rate [%]	Arithmetic mean bank filtration rate [%]	Type of study	Reference	K_{oc} [mg/L]	$DT_{50, water-sediment}$ [d]
Iopromide	Pharma			100	field	Postigo und Barcelo (2015)		
Iopromide	Pharma	85	97	91	batch	Onesios et al. (2009)		
Iotalamic acid	Pharma			13	fixed-bed reactor	Storck et al. (2012)		
Ioxynil	Herbicide	25	28	26.5	column	Schmidt (2006)	-	4.6
Ioxynil	Herbicide	40	60	50	field	Schmidt (2006)	-	4.6
IPBC	Fungicide	70	98	84	field	Köck-Schulmeyer et al. (2013)	61	1.5
Irgfarol	Fungicide	70	98	84	field	Köck-Schulmeyer et al. (2013)	1569	-
Iso-Chloridazon	Herbicide			80	field	Schmidt (2006)	120	137
Iso-Chloridazon	Herbicide			80	field	Schmidt (2006)	120	137
Iso-Chloridazon	Herbicide			80	field	Schmidt (2006)	120	137
Isoproturon	Herbicide	-87.5	100	6.25	field	Kruć-Fijałkowska et al. (2022)	-	149
Isoproturon	Herbicide			-1375	field	Bruchet et al. (2012)	-	149
Isoproturon	Herbicide			45	batch	Abdelrady et al. (2019)	-	149
Isoproturon	Herbicide			100	batch	Trinh et al. (2012)	-	149

Compound	Class	Min. bank filtration rate [%]	Max bank filtration rate [%]	Arithmetic mean bank filtration rate [%]	Type of study	Reference	K_{oc} [mg/L]	$DT_{50, water-sediment}$ [d]
Isoproturon	Herbicide	66.2	85	75.6	batch	Boivin et al. (2005)	-	149
Isoproturon	Herbicide			50	batch	Bruchet et al. (2012)	-	149
Isoproturon	Herbicide			62.5	batch	Dragon et al. (2018)	-	149
Isoproturon	Herbicide			50	batch	Köck-Schulmeyer et al. (2013)	-	149
Isoproturon	Herbicide			20	field	Zullei-Seibert (1996) in Schmidt et al. (2003)	-	149
Isoproturon	Herbicide			70	field	Schmidt (2006)	-	149
Isoproturon	Herbicide			75	field	Schmidt (2006)	-	149
Isoproturon	Herbicide			28	field	Schmidt (2006)	-	149
Isoproturon	Herbicide			50	pilot	Schmidt (2006)	-	149
Isoproturon	Herbicide	9	70	39.5	column	Schmidt (2006)	-	149
Isoproturon	Herbicide	0	50	25	column	Schmidt (2006)	-	149
Isoproturon	Herbicide			99	column	Schmidt (2006)	-	149
Isoproturon	Herbicide			100	column	Schmidt (2006)	-	149
Isoproturon	Herbicide			0	field	Schmidt (2006)	-	149
Isoproturon	Herbicide			0	field	Schmidt (2006)	-	149

Compound	Class	Min. bank filtration rate [%]	Max bank filtration rate [%]	Arithmetic mean bank filtration rate [%]	Type of study	Reference	K_{oc} [mg/L]	$DT_{50,\ water\text{-}sediment}$ [d]
Isoproturon	Herbicide			0	field	Schmidt (2006)	-	149
Isoproturon	Herbicide			0	field	Schmidt (2006)	-	149
Isoproturon	Herbicide			0	field	Schmidt (2006)	-	149
Isoproturon	Herbicide			0	column	Schmidt (2006)	-	149
Isoproturon	Herbicide	0	8	4	column	Schmidt (2006)	-	149
Ketoprofen	Pharma	56	96	76	batch and column	Im et al. (2016)		
Ketoprofen	Pharma			99	batch	Onesios et al. (2009)		
Lamotrigine	Pharma	18	100	59	field	Hrakl et al. (2023)		
Lamotrigine	Pharma			41.3	field	Kondor et al. (2020)		
Lamotrigine	Pharma	0	100	50	field	Kruc et al. (2019)		
Lidocaine	Pharma			94.6	field	Kondor et al. (2020)	1270	394
Lindane	Insecticide			100	field	Diaz-Cruz & Barcelo (2008)	1270	394
Lindane	Insecticide			100	field	Zullei-Seibert (1996) in Schmidt et al. (2003)	1270	394
Malathion	Herbicide	50	95	72.5	pilot	Schmidt (2006)	1800	0.4
MCPA	Herbicide	88	98	93	pilot	Gonzalez et al. (2006)	73.88	17

Compound	Class	Min. bank filtration rate [%]	Max bank filtration rate [%]	Arithmetic mean bank filtration rate [%]	Type of study	Reference	K_{oc} [mg/L]	$DT_{50, water-sediment}$ [d]
MCPA	Herbicide			74	field	Huntscha et al. (2013)	73.88	17
MCPA	Herbicide	70	100	85	field	Oberleitner et al. (2020)	73.88	17
MCPA	Herbicide			74	field	Schmidt (2006)	73.88	17
MCPA	Herbicide			100	field	Schmidt (2006)	73.88	17
MCPA	Herbicide			0	column	Schmidt (2006)	73.88	17
MCPA	Herbicide			90	pilot	Schmidt (2006)	73.88	17
MCPA	Herbicide			15	column	Schmidt (2006)	73.88	17
Mecoprop	Herbicide	57	99	78	pilot	Gonzalez et al. (2006)	47	50
Mecoprop	Herbicide			33	field	Heberer et al. (2004)	47	50
Mecoprop	Herbicide			50	field	Köck-Schulmeyer et al. (2013)	47	50
Mecoprop	Herbicide	70	100	85	field	Oberleitner et al. (2020)	47	50
Mecoprop	Herbicide			80	field	Schmidt (2006)	47	50
Mecoprop	Herbicide			100	pilot	Schmidt (2006)	47	50
Mecoprop	Herbicide			85	pilot	Schmidt (2006)	47	50
Mecoprop	Herbicide			90	pilot	Schmidt (2006)	47	50

Compound	Class	Min. bank filtration rate [%]	Max bank filtration rate [%]	Arithmetic mean bank filtration rate [%]	Type of study	Reference	K_{oc} [mg/L]	$DT_{50,\ water\text{-}sediment}$ [d]
Mecoprop	Herbicide	60	100	80	column	Schmidt (2006)	47	50
Mecoprop	Herbicide	17	99	58	column	Schmidt (2006)	47	50
Mecoprop	Herbicide			0	field	Schmidt (2006)	47	50
Mecoprop	Herbicide			0	field	Schmidt (2006)	47	50
Mecoprop	Herbicide			0	field	Schmidt (2006)	47	50
Mecoprop	Herbicide			16	column	Schmidt (2006)	47	50
Meprobamate	Pharma	20	80	50	pilot	Benotti et al. (2012)		
Meprobamate	Pharma			90	pilot	Benotti et al. (2012)		
Meprobamate	Pharma	17	83	50	pilot	Benotti et al. (2012)		
Meprobamate	Pharma			79	column	Trussel et al. (2018)		
Metalaxyl	Herbicide	1.36	34.5	17.93	pilot	Rodriguez-Cruz et al. (2007)	162	56
Metalaxyl	Herbicide			75	field	Schmidt (2006)	162	56
Metalaxyl-M	Herbicide			0	field	Dragon et al. (2018)	-	32.1
Metazachlor	Herbicide			23.3	field	Dragon et al. (2018)	54	20.6
Metazachlor	Herbicide	50	70	60	field	Schmidt (2006)	54	20.6
Metazachlor	Herbicide	40	60	50	field	Schmidt (2006)	54	20.6

Compound	Class	Min. bank filtration rate [%]	Max bank filtration rate [%]	Arithmetic mean bank filtration rate [%]	Type of study	Reference	K_{oc} [mg/L]	$DT_{50, water-sediment}$ [d]
Metazachlor	Herbicide			80	field	Schmidt (2006)	54	20.6
Metazachlor	Herbicide			99	field	Schmidt (2006)	54	20.6
Metazachlor	Herbicide			99	field	Schmidt (2006)	54	20.6
Metazachlor	Herbicide	94	100	97	pilot	Schmidt (2006)	54	20.6
Metazachlor	Herbicide			50	column	Schmidt (2006)	54	20.6
Metformin	Pharma			100	field	Hrakl et al. (2023)		
Metformin	Pharma			100	field	Scheuer (2012)		
Methabenzthiazuron	Herbicide			100	field	Zullei-Seibert (1996) in Schmidt et al. (2003)	527	182
Methabenzthiazuron	Herbicide			70	field	Schmidt (2006)	527	182
Methabenzthiazuron	Herbicide			99	pilot	Schmidt (2006)	527	182
Methabenzthiazuron	Herbicide	20	40	30	pilot	Schmidt (2006)	527	182
Methoxychlor	Herbicide	93	100	96.5	pilot	Schmidt (2006)	80000	-
Methylparaben	other			100	field	Hrakl et al. (2023)		
Metolachlor	Herbicide	16	59	37.5	batch	Abdelrady et al. (2019)	120	365
Metolachlor	Herbicide			35	fixed-bed reactor	Storck et al. (2012)	120	365

Compound	Class	Min. bank filtration rate [%]	Max bank filtration rate [%]	Arithmetic mean bank filtration rate [%]	Type of study	Reference	K_{oc} [mg/L]	$DT_{50,\text{ water-sediment}}$ [d]
Metolachlor	Herbicide	84	100	92	field	Wang and Squillace (1994)	120	365
Metolachlor	Herbicide			52	field	Verstraeten et al. (2002)	120	365
Metolachlor	Herbicide			70	field	Schmidt (2006)	120	365
Metolachlor	Herbicide	30	60	45	field	Schmidt (2006)	120	365
Metolachlor	Herbicide	0	10	5	field	Schmidt (2006)	120	365
Metolachlor	Herbicide			50	column	Schmidt (2006)	120	365
Metolachlor-ESA	Herbicide	18	78	48	field	Nagy-Kovacs et al. (2018)	9	-
Metolachlor-ESA	Herbicide	33	62	47.5	field	Nagy-Kovacs et al. (2018)	9	-
Metolachlor-OA	Herbicide	0	25	12.5	field	Nagy-Kovacs et al. (2018)	17	-
Metoprolol	Pharma			5	biofiltration	Carpenter and Helbling (2017)		
Metoprolol	Pharma			80	field	Kim et al. (2009)		
Metoprolol	Pharma	78	100	89	field	Glorian et al. (2018)		
Metoprolol	Pharma			100	field	Hrakl et al. (2023)		
Metoprolol	Pharma	70	100	85	field	Oberleitner et al. (2020)		

Compound	Class	Min. bank filtration rate [%]	Max bank filtration rate [%]	Arithmetic mean bank filtration rate [%]	Type of study	Reference	K_{oc} [mg/L]	$DT_{50, water-sediment}$ [d]
Metoprolol	Pharma	83	85	84	fixed-bed reactor	Storck et al. (2012)		
Metoxuron	Herbicide			70	field	Schmidt (2006)	120	145
Metsulfuron-methyl	Herbicide	4.1	13	8.55	column	Schmidt (2006)	-	224.3
Molinate	Herbicide	11.35	12.65	12	batch	Abdelrady et al. (2019)	190	61
Naproxen	Pharma			90	pilot	Benotti et al. (2012)		
Naproxen	Pharma	89	99	94	biofiltration	Carpenter and Helbling (2017)		
Naproxen	Pharma			90	field	Regnery et al. (2015)		
Naproxen	Pharma	39	100	69.5	field	Glorian et al. (2018)		
Naproxen	Pharma			80	field	Postigo und Barcelo (2015)		
Naproxen	Pharma			90	fixed-bed reactor	Storck et al. (2012)		
Naproxen	Pharma	60	80	70	batch	Onesios et al. (2009)		
NDMA	Pharma	92	99.7	95.85	column	Trussel et al. (2018)		
Nicosulfuron	Herbicide			73.9	field	Dragon et al. (2018)	40	60.6
o,p`-DDT	Insecticide			50	field	Heberer et al. (2004)	-	-
o,p‘-DDT	Insecticide			96	pilot	Schmidt (2006)	-	-

Compound	Class	Min. bank filtration rate [%]	Max bank filtration rate [%]	Arithmetic mean bank filtration rate [%]	Type of study	Reference	K_{oc} [mg/L]	$DT_{50, water-sediment}$ [d]
Olmesartan	Pharma			20	field	Burke et al. (2018)		
Oxyfluorfen	Herbicide			80	bench	Vieira Dos Santos et a.l (2017)	-	-
Oxypurinol	other	0	63	31.5	field	Hrakl et al. (2023)		
Oxypurinol	Pharma	0	100	50	field	Kruc et al. (2019)		
p,p‘-DDT	Insecticide			50	field	Heberer et al. (2004)	151000	-
p,p‘-DDT	Herbicide			98	pilot	Schmidt (2006)	151000	-
p,p‘-DDT	Herbicide			97	pilot	Schmidt (2006)	151000	-
Paracetamol	Pharma	46	50	48	field	Glorian et al. (2018)		
Paracetamol	Pharma			100	field	Hrakl et al. (2023)		
Paraoxon-Äquivalente	Herbicide	0	26	13	column	Schmidt (2006)	7660	4.3
Paraoxon-Äquivalente	Herbicide	89	93	91	field	Schmidt (2006)	7660	4.3
Parathion-Äquivalente	Herbicide			96	field	Schmidt (2006)	7660	4.3
Parathion-Äquivalente	Herbicide			75	field	Schmidt (2006)	7660	4.3
Paraxanthine	other	25	100	62.5	field	Hrakl et al. (2023)		
p-Chloro-m-xylenol	Pharma			80	batch	Onesios et al. (2009)		
Pendimethalin	Herbicide	86.8	94	90.4	batch	Abdelrady et al. (2019)	17,491	16

Compound	Class	Min. bank filtration rate [%]	Max bank filtration rate [%]	Arithmetic mean bank filtration rate [%]	Type of study	Reference	K_{oc} [mg/L]	$DT_{50, water-sediment}$ [d]
Pentachlorphenol	Herbicide			47	field	Schmidt (2006)	30	-
Pentachlorphenol	Herbicide			82	field	Schmidt (2006)	30	-
Pentachlorphenol	Herbicide	10	30	20	field	Schmidt (2006)	30	-
Pentachlorphenol	Herbicide			17	pilot	Schmidt (2006)	30	-
PFOS	other	13	100	56.5	field	Hrakl et al. (2023)		
Phenazone	Pharma			91	field	Massmann et al. (2006a)		
Phenazone	Pharma	10	66	38	column	Massmann et al. (2008a)		
Phenazone	Pharma	50	70	60	field	Oberleitner et al. (2020)		
Phenazone	Pharma			100	field	Sharma et al. (2012a)		
Phenazone	Pharma			0	fixed-bed reactor	Storck et al. (2012)		
Phenobarbital	Pharma			80	batch	Onesios et al. (2009)		
Phenylharnstoffe	Herbicide			86	pilot	Schmidt (2006)		
Phenytoin	Pharma	20	80	50	pilot	Benotti et al. (2012)		
Phenytoin	Pharma			90	pilot	Benotti et al. (2012)		
Phenytoin	Pharma			0	biofiltration	Carpenter and Helbling (2017)		

Compound	Class	Min. bank filtration rate [%]	Max bank filtration rate [%]	Arithmetic mean bank filtration rate [%]	Type of study	Reference	K_{oc} [mg/L]	$DT_{50, \text{water-sediment}}$ [d]
Phenytoin	Pharma			0	pilot	Benotti et al. (2012)		
Phenytoin	Pharma			50	batch	Onesios et al. (2009)		
Picloram	Herbicide	84.5	95.7	90.1	batch	Abdelrady et al. (2019)	13	196.1
Primidon	Pharma			23	field	Massmann et al. (2007)		
Primidone	Pharma			90	pilot	Benotti et al. (2012)		
Primidone	Pharma	0	20	10	field	Regnery et al. (2015)		
Primidone	Pharma			100	field	Hrakl et al. (2023)		
Progesterone	Pharma			90	pilot	Benotti et al. (2012)		
Prometryn	Herbicide			83.3	field	Dragon et al. (2018)	400	38
Propanil	Herbicide	8.48	9	9.52	batch	Abdelrady et al. (2019)	149	1.25
Propazine	Herbicide	30	40	35	field	Schmidt (2006)	154	77
Propiconazole	Fungicide			20	field	Kahle et al. (2008)	1,086	561
Propylparaben	other			100	field	Hrakl et al. (2023)		
Propyphenazone	Pharma			100	field	Massmann et al. (2006a)		
Propyphenazone	Pharma			88	field	Massmann et al. (2007)		

Compound	Class	Min. bank filtration rate [%]	Max bank filtration rate [%]	Arithmetic mean bank filtration rate [%]	Type of study	Reference	K_{oc} [mg/L]	$DT_{50, \text{water-sediment}}$ [d]
Propyphenazone	Pharma	70	100	85	field	Oberleitner et al. (2020)		
Propyphenazone	Pharma			0	fixed-bed reactor	Storck et al. (2012)		
Pyriproxyfen	Insecticide	65.2	74.2	69.7	batch	Abdelrady et al. (2019)	-	6.5
Ranitidine	Pharma			48	biofiltration	Carpenter and Helbling (2017)		
Roxithrormycin	Pharma			100	field	Heberer et al. (2008)		
Sclindathromycin	Antibiotics			26	field	Heberer et al. (2008)		
Secobarbital	Pharma			70	batch	Onesios et al. (2009)		
Simazine	Herbicide	0	10	5	field	Schmidt (2006)	130	33
Simazine	Herbicide			30	field	Schmidt (2006)	130	33
Simazine	Herbicide	40	60	50	field	Schmidt (2006)	130	33
Simazine	Herbicide	0	20	10	field	Schmidt (2006)	130	33
Simazine	Herbicide			24	field	Schmidt (2006)	130	33
Simazine	Herbicide	20	40	30	field	Schmidt (2006)	130	33
Simazine	Herbicide	0	10	5	field	Schmidt (2006)	130	33
Simazine	Herbicide			70	field	Schmidt (2006)	130	33

Compound	Class	Min. bank filtration rate [%]	Max bank filtration rate [%]	Arithmetic mean bank filtration rate [%]	Type of study	Reference	K_{oc} [mg/L]	$DT_{50, water-sediment}$ [d]
Simazine	Herbicide	49	81	65	field	Schmidt (2006)	130	33
Simazine	Herbicide			13	pilot	Schmidt (2006)	130	33
Simazine	Herbicide			0	field	Schmidt (2006)	130	33
Simazine	Herbicide			0	field	Schmidt (2006)	130	33
Simazine	Herbicide	15	33	24	pilot	Schmidt (2006)	130	33
Simazine	Herbicide			35	pilot	Schmidt (2006)	130	33
Simazine	Herbicide			-33	field	Bruchet et al. (2012)	130	33
Simazine	Herbicide			40	field	Verstraeten et al. (2002)	130	33
Simazine	Herbicide			45	batch	Abdelrady et al. (2019)	130	33
Simazine	Herbicide			0	batch	Bertelkamp et al. (2016)	130	33
Simazine	Herbicide			17	batch	Bruchet et al. (2012)	130	33
Simazine	Herbicide	6.8	8.2	7.5	batch	Carpenter and Helbling (2017)	130	33
Simazine	Herbicide			14	column	Trussel et al. (2018)	130	33
S-Metolachlor	Herbicide			55.5	field	Dragon et al. (2018)	-	43.3
Sotalol	Pharma			80	field	Schmidt et al. (2003)		

Compound	Class	Min. bank filtration rate [%]	Max bank filtration rate [%]	Arithmetic mean bank filtration rate [%]	Type of study	Reference	K_{oc} [mg/L]	$DT_{50, \text{water-sediment}}$ [d]
Sotalol	Pharma	15	35	25	fixed-bed reactor	Storck et al. (2012)		
Sulfadiazine	Antibiotics	29.6	41.5	35.55	column	Bai et al. (2019)		
Sulfamethazine	Antibiotics	9	28.5	18.75	column	Bai et al. (2019)		
Sulfamethoxazole	Pharma	30	100	65	field	Hrakl et al. (2023)		
Sulfamethoxazole	Antibiotics			99	field	Heberer et al. (2008)		
Sulfamethoxazole	Antibiotics			100	field	Kovacevic et al. (2017)		
Sulfamethoxazole	Antibiotics	32.3	79.6	55.95	column	Bai et al. (2019)		
Sulfamethoxazole	Veterinary antibiotics			23	field	Barnes et al. (2008)		
Sulfamethoxazole	Veterinary antibiotics	27	90	58.5	column	Baumgarten et al. (2011)		
Sulfamethoxazole	Veterinary antibiotics			20	pilot	Benotti et al. (2012)		
Sulfamethoxazole	Antibiotics			57	column	Alidina et al. (2014)		
Sulfamethoxazole	Veterinary antibiotics	7	53	30	biofiltration	Carpenter and Helbling (2017)		
Sulfamethoxazole	Pharma	20	40	30	field	Schmidt et al. (2003)		
Sulfamethoxazole	Pharma	25	90	57.5	field	Regnery et al. (2015)		
Sulfamethoxazole	Pharma	20	50	35	field	Diaz-Cruz & Barcelo (2008)		

Compound	Class	Min. bank filtration rate [%]	Max bank filtration rate [%]	Arithmetic mean bank filtration rate [%]	Type of study	Reference	K_{oc} [mg/L]	$DT_{50,\ water\text{-}sediment}$ [d]
Sulfamethoxazole	Pharma	75	90	82.5	column	Filter et al. (2017)		
Sulfamethoxazole	Pharma	41	95	68	field	Glorian et al. (2018)		
sulfamethoxazole	Pharma	12	43	27.5	batch and column	Im et al. (2016)		
Sulfamethoxazole	Pharma	80	90	85	field	Jekel and Grünheid (2005)		
Sulfamethoxazole	Pharma	7.5	100	53.75	field	Kruc et al. (2019)		
Sulfamethoxazole	Pharma	9	30	19.5	field	Nagy-Kovacs et al. (2018)		
Sulfamethoxazole	Pharma	50	100	75	field	Oberleitner et al. (2020)		
Sulfamethoxazole	Pharma			20	column	Sanz-Prat (2020)		
Sulfamethoxazole	Pharma			8	fixed-bed reactor	Storck et al. (2012)		
Sulfamethoxazole	Pharma			75	field	Heberer et al. (2008)		
Sulfaquinoxaline	Veterinary antibiotics	39.2	49.1	44.15	column	Bai et al. (2019)		
TCPP	Pharma			80	field	Postigo und Barcelo (2015)		
Tebuconazole	Fungicide	0	100	50	field	Kruć-Fijałkowska et al. (2022)	-	365

Compound	Class	Min. bank filtration rate [%]	Max bank filtration rate [%]	Arithmetic mean bank filtration rate [%]	Type of study	Reference	K_{oc} [mg/L]	$DT_{50, water-sediment}$ [d]
Tebuconazole	Fungicide			100	field	Oberleitner et al. (2020)	-	365
Tebuconazole	Fungicide			20	field	Kahle et al. (2008)	-	365
Tebuconazole	Herbicide	70	100	85	field	Oberleitner et al. (2020)	-	365
Tebufenozide	Insecticide	70	98	84	field	Köck-Schulmeyer et al. (2013)	-	145.4
Telmisartan	Pharma	86	100	93	field	Hrakl et al. (2023)		
Telodrin	Herbicide	84	96	90	pilot	Schmidt (2006)	-	-
Terbuthylazine	Herbicide			0	field	Dragon et al. (2018)	-	70
Terbuthylazine	Herbicide			50	field	Köck-Schulmeyer et al. (2013)	-	70
Terbuthylazine	Herbicide	50	100	75	field	Oberleitner et al. (2020)	-	70
Terbuthylazine	Herbicide	10	50	30	field	Schmidt (2006)	-	70
Terbuthylazine	Herbicide	10	50	30	field	Schmidt (2006)	-	70
Terbuthylazine	Herbicide	20	40	30	field	Schmidt (2006)	-	70
Terbuthylazine	Herbicide			70	field	Schmidt (2006)	-	70
Terbuthylazine	Herbicide			0	field	Schmidt (2006)	-	70
Terbuthylazine	Herbicide			90	pilot	Schmidt (2006)	-	70

Compound	Class	Min. bank filtration rate [%]	Max bank filtration rate [%]	Arithmetic mean bank filtration rate [%]	Type of study	Reference	K_{oc} [mg/L]	$DT_{50, water-sediment}$ [d]
Terbuthylazine	Herbicide			75	field	Schmidt (2006)	-	70
Terbutryn	Herbicide			85.7	field	Dragon et al. (2018)	2,432	60
Terbutryn	Herbicide			84	field	Schmidt (2006)	2,432	60
Terbutryn	Herbicide			73	column	Schmidt (2006)	2,432	60
Thiacloprid	Insecticide			27.6	column	Pietrzak et al. (2020)	-	14.8
Thiamethoxam	Insecticide			85	field	de Souza et al. (2020)	56.2	40
Thifensulfuron-methyl	Herbicide			75	field	Schmidt (2006)	28.3	22.8
Thifensulfuron-methyl	Herbicide	13	46	29.5	column	Schmidt (2006)	28.3	22.8
Thiometon	Herbicide	0	21	10.5	column	Schmidt (2006)	579	-
Thiometon	Herbicide			95	column	Schmidt (2006)	579	-
Thrimetropin	Antibiotics			100	field	Kovacevic et al. (2017)		
Thrimetropin	Antibiotics			100	field	Yang et al. (2017)		
Tramadol	Pharma	54	100	77	field	Hrakl et al. (2023)		
Tramadol	Pharma			87.9	field	Kondor et al. (2020)		
Tramadol	Pharma	3.2	100	51.6	field	Kruc et al. (2019)		
Triazine	Herbicide			33	field	Verstraeten et al. (2002)	-	-

Compound	Class	Min. bank filtration rate [%]	Max bank filtration rate [%]	Arithmetic mean bank filtration rate [%]	Type of study	Reference	K_{oc} [mg/L]	$DT_{50,\ water\text{-}sediment}$ [d]
Triazine	Herbicide			49	pilot	Schmidt (2006)	-	-
Triclocarban	Pharma	21	97	59	field	Onesios et al. (2009)		
Triclocarban	Pharma			41	batch	Onesios et al. (2009)		
Triclocarban	Pharma	38	92	65	soil batch	Onesios et al. (2009)		
Triclosan	Pharma	93.5	95.5	94.5	biofiltration	Carpenter and Helbling (2017)		
Triclosan	Pharma			80	field	Postigo und Barcelo (2015)		
Trifluralin	Herbicide	8.8	25.8	17.3	batch	Boivin et al. (2005)	15,800	5.5
Trifluralin	Herbicide			51	field	Schmidt (2006)	15,800	5.5
Trimethoprim	Antibiotics			100	field	Heberer et al. (2008)		
Trimethoprim	Pharma			90	pilot	Benotti et al. (2012)		
Trimethoprim	Pharma	20	40	30	pilot	Benotti et al. (2012)		
Trimethoprim	Pharma			90	field	Regnery et al. (2015)		
trimethoprim	Pharma			81	batch and column	Im et al. (2016)		
Trimethoprim	Pharma			100	field	Kovacevic et al. (2017)		
Trimethoprim	Pharma			80	field	Postigo und Barcelo (2015)		

Compound	Class	Min. bank filtration rate [%]	Max bank filtration rate [%]	Arithmetic mean bank filtration rate [%]	Type of study	Reference	K_{oc} [mg/L]	$DT_{50, water-sediment}$ [d]
Trimethoprim	Pharma	25	70	47.5	batch	Onesios et al. (2009)		
Urotropine	Pharma	0	20	10	field	Schmidt et al. (2003)		
Valproic acid	Pharma			99	batch	Onesios et al. (2009)		
Valsartan	Pharma			38	biofiltration	Carpenter and Helbling (2017)		
Valsartan	Pharma	70	99	84.5	field	Di Marcantonio (2020)		
Valsartan	Pharma			100	field	Hrakl et al. (2023)		
Valsartan acid	Pharma	92	100	96	field	Hrakl et al. (2023)		
Venlafaxine	Pharma	0	2	1	biofiltration	Carpenter and Helbling (2017)		
Verapamil	Pharma			100	batch	Onesios et al. (2009)		
Warafarin	Pharma	39	68	53.5	column	Rattier et al. (2014)		
γ-Hexachlorcyclohexan	Herbicide			42	field	Schmidt (2006)	1,270	394
γ-Hexachlorcyclohexan	Herbicide			80	field	Schmidt (2006)	1,270	394
γ-Hexachlorcyclohexan	Herbicide	70	99	84.5	field	Schmidt (2006)	1,270	394
γ-Hexachlorcyclohexan	Herbicide			97	field	Schmidt (2006)	1,270	394
γ-Hexachlorcyclohexan	Herbicide			78	field	Schmidt (2006)	1,270	394

Compound	Class	Min. bank filtration rate [%]	Max bank filtration rate [%]	Arithmetic mean bank filtration rate [%]	Type of study	Reference	K_{oc} [mg/L]	$DT_{50,\ water-sediment}$ [d]
γ-Hexachlorcyclohexan	Herbicide			32	pilot	Schmidt (2006)	1,270	394
γ-Hexachlorcyclohexan	Herbicide			90	pilot	Schmidt (2006)	1,270	394
γ-Hexachlorcyclohexan	Herbicide	3	29	16	pilot	Schmidt (2006)	1,270	394
γ-Hexachlorcyclohexan	Herbicide	50	53	51.5	pilot	Schmidt (2006)	1,270	394
γ-Hexachlorcyclohexan	Herbicide			0	column	Schmidt (2006)	1,270	394
γ-Hexachlorcyclohexan	Herbicide			99	column	Schmidt (2006)	1,270	394

A.3 Summary of investigated factors in field studies

Reference	DOI	Subsurface properties	Subsurface retention time & flow distance	Hydrometeorology & climate change	Reduction of concentrations	Influence of temperature	Influence of redox conditions	Influence of microbial activity	Influence of compound properties
Abdelrady et al. (2020)	10.3390/w12061816		x						
Abogabal et al. (2020)	10.21608/EJCHEM.2020.17965.2093	x				x		x	

Reference	DOI	Subsurface properties	Subsurface retention time & flow distance	Hydrometeorology & climate change	Reduction of concentrations	Influence of temperature	Influence of redox conditions	Influence of microbial activity	Influence of compound properties
Ahmed and Marhaba (2017)	10.1007/s10098-016-1266-0		x			x			
Bertelkamp et al. (2016)	10.1016/j.scitotenv.2015.11.035				x			x	
Bertrand et al. (2022)	10.1007/s13762-021-03558-x	x				x			
Bradley et al. (2014)	10.1016/j.envpol.2014.06.028	x			x				
Carpenter and Helbling (2017)	10.1016/j.watres.2017.04.071		x					x	
De Carvalho et al. (2022)	10.1016/j.envpol.2022.118916	x							
Díaz-Cruz and Barceló (2008)	10.1016/j.chemosphere.2008.02.031					x	x		
Dragon et al. (2019)	10.1007/s12665-019-8598-0		x		x				

Reference	DOI	Subsurface properties	Subsurface retention time & flow distance	Hydrometeorology & climate change	Reduction of concentrations	Influence of temperature	Influence of redox conditions	Influence of microbial activity	Influence of compound properties
D'Alessio et al. (2015)	10.1016/j.scitotenv.2014.10.032	x				x	x	x	
Epting et al. (2018)	10.1016/j.scitotenv.2017.09.219	x		x			x	x	
Essl et al. (2014)	10.2166/ws.2014.026			x					
Filter et al. (2017)	10.3390/w9050349	x			x		x		x
Filter et al. (2021)	10.1016/j.chemosphere.2021.129774		x						
Gillefalk et al. (2021)	10.3390/w10091240					x		x	
Glorian et al. (2018)	10.3390/w10121804		x						
González et al. (2006)	10.1016/j.envpol.2006.02.021							x	
Górski (2011)	10.1007/978-94-007-0026-0_16		x						

Reference	DOI	Subsurface properties	Subsurface retention time & flow distance	Hydrometeorology & climate change	Reduction of concentrations	Influence of temperature	Influence of redox conditions	Influence of microbial activity	Influence of compound properties
Greskowiak et al. (2017)	10.1016/j.watres.2017.09.017	x					x		
Gross-Wittke et al. (2010)	10.2166/wcc.2010.005					x	x	x	
Hamann et al. (2016)	10.1016/j.scitotenv.2015.12.057								x
Handl et al. (2020)	https://doi.org/10.1007/s00506-020-00714-4	x		x		x	x		
Handl et al. (2023)	10.1016/j.chemosphere.2023.137852		x						
Heberer et al. (2002)	10.1016/S0378-4274(02)00041-3				x				x
Heberer et al. (2008)	10.1016/j.chemosphere.2008.06.056				x		x		
Henzler et al. (2016)	10.1016/j.jhydrol.2016.01.044					x	x		x

Reference	DOI	Subsurface properties	Subsurface retention time & flow distance	Hydrometeorology & climate change	Reduction of concentrations	Influence of temperature	Influence of redox conditions	Influence of microbial activity	Influence of compound properties
Hiemstra et al. (2003)	10.2166/aqua.2003.0004				x				
Hiscock and Grischek (2002)	10.1016/s0022-1694(02)00158-0								x
Hrkal et al. (2023)	10.1007/s12665-023-10785-7	x			x				
Hu et al. (2016)	10.1016/j.jhydrol.2016.08.004			x		x	x	x	
Huntscha et al. (2013)	https://doi.org/10.1021/es401802z						x		x
Im et al. (2016)	10.1016/j.chemosphere.2015.10.104								x
Jaramillo et al. (2019)	10.1007/s10098-018-1627-y				x				x
Jüttner (1999)	10.2166/wst.1999.0278		x					x	

Reference	DOI	Subsurface properties	Subsurface retention time & flow distance	Hydrometeorology & climate change	Reduction of concentrations	Influence of temperature	Influence of redox conditions	Influence of microbial activity	Influence of compound properties
Kahle et al. (2008)	10.1021/es8009309				x				
Kolpin et al. (1998)	10.1021/es970412g				x				x
Kondor et al. (2020)	10.1016/j.envpol.2020.114893		x		x			x	
Kodešová et al. (2011)	10.1016/j.jhazmat.2010.11.040	x					x		x
Kovačević et al. (2017)	10.1007/s11356-016-7959-4		x		x		x		
Kruć et al. (2019)	10.3390/w11112238		x		x				
Kruć-Fijałkowska et al. (2022)	10.1038/s41598-022-07385-z				x				
Labad et al. (2002)	10.1016/j.envpol.2022.120504				x				
Linde (1994)		x						x	

Reference	DOI	Subsurface properties	Subsurface retention time & flow distance	Hydrometeorology & climate change	Reduction of concentrations	Influence of temperature	Influence of redox conditions	Influence of microbial activity	Influence of compound properties
Maeng et al. (2010)	10.1016/j.watres.2010.03.035		x			x	x	x	x
Maeng et al. (2011)	10.1016/j.watres.2011.02.017						x		x
Malaguerra et al. (2013)	10.1016/j.jhydrol.2012.11.010	x	x		x				x
Massmann et al. (2007)	10.1007/s00767-007-0036-7		x						
Massmann et al. (2008b)	10.1007/s00254-007-0792-9					x	x	x	
Mathys (1994)					x				
Munz et al. (2019)	10.1016/j.watres.2019.06.041					x		x	x
Nagy-Kovács et al. (2018)	10.3390/w10121861	x	x		x				x
Obeid et al. (2023)	10.1007/s00506-023-00974-w		x						

Reference	DOI	Subsurface properties	Subsurface retention time & flow distance	Hydrometeorology & climate change	Reduction of concentrations	Influence of temperature	Influence of redox conditions	Influence of microbial activity	Influence of compound properties
Oberleitner et al. (2020)	10.1016/j.chemosphere.2020.126255	x	x				x		
Pan et al. (2018)	10.3390/w10040491		x			x			
Petrovic et al. (2009)	10.1098/rsta.2009.0105					x	x		
Postigo et al. (2010)	10.1016/j.jhydrol.2009.07.036				x				
Postigo and Barcelo (2015)	10.1016/j.scitotenv.2014.06.019								x
Rauch-Williams et al. (2009)	10.1016/j.watres.2009.08.027		x				x		
Ray et al. (2002)	10.1002/j.1551-8833.2002.tb09459.x	x	x						
Regnery et al. (2015)	10.1016/j.chemosphere.2014.12.076				x				

Reference	DOI	Subsurface properties	Subsurface retention time & flow distance	Hydrometeorology & climate change	Reduction of concentrations	Influence of temperature	Influence of redox conditions	Influence of microbial activity	Influence of compound properties
Schmidt et al. (2007)	10.2166/ws.2007.060	x					x		
Schmidt et al. (2004)			x		x		x		
Sharma et al. (2012b)	10.2166/aqua.2012.013	x	x	x		x	x		
Sprenger et al. (2011)	10.1016/j.scitotenv.2010.11.002			x	x		x		
Storck et al. (2012)	10.2166/wst.2012.150	x	x			x	x	x	
Stuyfzand et al. (2007)					x				
Trinh et al. (2012)	10.1016/j.envpol.2012.05.026				x			x	
Verstraeten (2002)	10.1016/s0022-1694(02)00163-4	x			x				
Wang and Squillace (1994)	10.1021/es00062a018	x	x						

Reference	DOI	Subsurface properties	Subsurface retention time & flow distance	Hydrometeorology & climate change	Reduction of concentrations	Influence of temperature	Influence of redox conditions	Influence of microbial activity	Influence of compound properties
Weiss et al. (2003a)	10.1002/j.1551-8833.2003.tb10512.x				x				
Weiss et al. (2003b)	10.1002/j.1551-8833.2003.tb10475.x				x				
Yang et al. (2017)	10.1007/s11356-017-8999-0	x							
Ziegler (2001)			x		x				

A.4 Summary of investigated factors in laboratory studies

Reference	DOI	Investigated factor	Column length [cm]	Column material	Flow velocity [m/d]	Residence time [d]	Redox conditions	Temperature [°C]	Microbiology	pH [-]	DOC [mg/L]
Abdelrady et al. (2019)	10.1016/j.jece.2019.102904	temperature, compound properties, DOC, microbiology	batch	silica sand		30	oxic	20, 25, 30	with microorganisms/ without microorganisms	7.4-8.3	4.05; 10.62; 10.31; 9.41

Reference	DOI	Investigated factor	Column length [cm]	Column material	Flow velocity [m/d]	Residence time [d]	Redox conditions	Temperature [°C]	Microbiology	pH [-]	DOC [mg/L]
Abogabal et al. (2020)	10.21608/EJCHEM.2020.17965.2093	temperature, redox, microbiology	batch	dry silica sand		7	aerobic/ anoxic	15, 25, 30		8.1	
Bai et al. (2019)	10.1016/j.chemosphere.2018.12.167	redox, microbiology	100	sand	6.3936	5; 11	oxic/sub oxic	11.5			
Bajeer et al. (2012)	10.4236/ajac.2012.38079	subsurface properties	30	sandy loam	100 mL/h					8.5	
Banzhaf et al. (2012)	10.1016/j.scitotenv.2012.08.041	redox	35.1	organic rich sediment	0.19872		oxic/ nitrate reducing redox conditions			6.9	
Baumgarten et al. (2011)	10.1016/j.watres.2010.08.034	inflow concentration, redox, C_{org}	200	quartz sand		14	oxic	11		8.1	7.8
Benotti et al. (2012)	10.2166/ws.2011.068	compound properties	59	sand		36	oxic			7.9	
Bertelkamp et al. (2014)	10.1016/j.watres.2013.10.068	compound properties	100	sand	1.0368		oxic	20			
Bertelkamp et al. (2015)	10.1016/j.scitotenv.2015.07.056	subsurface properties, microbiology	100	oxic sandy soils	0.50112			12		7.9	

Reference	DOI	Investigated factor	Column length [cm]	Column material	Flow velocity [m/d]	Residence time [d]	Redox conditions	Temperature [°C]	Microbiology	pH [-]	DOC [mg/L]
Bertelkamp et al. (2016a)	10.1016/j.chemosphere.2015.09.017	inflow concentration, C fractions of inflow	100	sand	0.5184	5	oxic	20			4; 8
Bertelkamp et al. (2016b)	10.1016/j.scitotenv.2015.11.035	inflow concentration, redox, compound properties	2x100; 10x100; 22x100	sand	0.5184		oxic/suboxic/anoxic	12		8	3.71
Boivin et al. (2005)	10.1016/j.chemosphere.2005.03.024	subsurface properties	batch								
Burke et al. (2014)	10.1016/j.scitotenv.2014.02.098	temperature, redox	120	medium sized sand	1.3824		oxic/suboxic/penoxic	6.5; 19.7			
Burke et al. (2018)	10.3390/w10121736	redox	105	fine to coarse sand	1.0368	19 h; 22 h	oxic/suboxic/anoxic	21			> 1
Carpenter and Helbling (2017)	10.1016/j.watres.2017.04.071	flow velocity, microbiology	5	fine sand	2.4192; 9.504		oxic	22			
D'Alessio et al. (2015)	10.1016/j.scitotenv.2014.10.032 0048-9697	temperature, redox	14.5	sand			<2; 8 mg O_2/L	6; 21			

Reference	DOI	Investigated factor	Column length [cm]	Column material	Flow velocity [m/d]	Residence time [d]	Redox conditions	Temperature [°C]	Microbiology	pH [-]	DOC [mg/L]
Filter et al. (2017)	10.3390/w9050349	subsurface properties	18	sand	0.0864	0.58	oxic	23			7
Gonzalez et al. (2006)	10.1016/j.envpol.2006.02.021	microbiology		no sand, membranes			oxic	21			
Grünheid et al. (2008)	10.2166/wst.2008.207	temperature	50	technical sand, coarser gravel on top (3 cm)	880 mL/m/d 904 mL/m/d		11.2 mg O_2/L	5; 15; 25		7.9	7.32
Hoppe-Jones et al. (2012)	10.1016/j.scitotenv.2012.08.009	microbio-logy, DOC	100	alluvial sand		7; 28	oxic/ anoxic	20		7.4	<0.5; 1.7-3.9
Im et al. (2015)	10.1016/j.chemosphere.2015.10.104	microbio-logy, compound properties	30	sand		0.46	oxic	17	yes/no	7.03	2.95
Jaramillo et al. (2019)	10.1007/s10098-018-1627-y	flow velocity	50	coarse sand	0.4406; 0.9504			20			
Litz et al. (2011)	10.1016/j.watres.2011.02.015	distance, inflow concentra-tion	100	sandy substrate, traces of organic matter	0.05011			8		7.7	3-4
Maćerak et al. (2018)	10.1007/s11368-018-2084-2	compound properties	20	sediment	1.2 mL/min						

Reference	DOI	Investigated factor	Column length [cm]	Column material	Flow velocity [m/d]	Residence time [d]	Redox conditions	Temperature [°C]	Microbiology	pH [-]	DOC [mg/L]
Massmann et al. (2008a)	10.1016/j.chemosphere.2007.12.017	redox	100	Sediment	0.1728		oxic/ anoxic	21			
Sanchez-Perez et al. (2013)	10.1051/limn/2013041	microbiology	20	sand/ gravel	1.4688		oxic	15	yes/no		
Trussel et al. (2018)	10.1016/j.watres.2018.07.012	no focus	366	sand/ gravel		150; 180	oxic				5.57 (TOC)
Tuxen et al. (2002)	10.1016/S0045-6535(99)00533-0	subsurface properties	105	97% sand, 2.1% gravel; 86% sand, 13% gravel	0.05616	140	11.5 mg O_2/L			6.4	2.1 (TOC)
von Rohr et al. (2014)	10.1016/j.watres.2014.05.018	temperature, flow rate, DOC	30	sand	0.01642	0.14; 1.67	oxic	30			yes/no
Ziegler (2001)		distance, inflow concentra-tion	2x100; 1x100+200	sand	0.35424; 0.80352	5; 9.3					6.7