TEXTE
133/2025

Final report

Groundwater discharges of biocides from façades in urban regions

GRUBURG

by:
MichaelBurkhardt, Mirko Rohr, Michael Patrick, Olaf Tietje
Institute for Environment and Process Engineering (UMTEC), OST- Eastern Switzerland University of Applied Sciences, Rapperswil, Switzerland

Jens Lange, Felicia Linke
Hydrology, Faculty of Environment and Natural Resources, University of Freiburg (UNI), Freiburg im Breisgau, Germany

Dimitrios Skodras, Michael Klein, Judith Klein
Fraunhofer Institute for Molecular Biology and Applied Ecology (IME), Schmallenberg, Germany

publisher:
German Environmental Agency

German Environment Agency

TEXTE 133/2025

Ressortforschungsplan of the Federal Ministry for the Environment, Nature Conservation, Nuclear Safety and Consumer Protection

Project No. (FKZ) 3721 67 401 0
FB001701/ENG

Final report

Groundwater discharges of biocides from façades in urban regions

GRUBURG

by

Michael Burkhardt, Mirko Rohr, Michael Patrick, Olaf Tietje
Institute for Environment and Process Engineering (UMTEC),
OST- Eastern Switzerland University of Applied Sciences,
Rapperswil, Switzerland

Jens Lange, Felicia Linke
Hydrology, Faculty of Environment and Natural Resources,
University of Freiburg (UNI),
Freiburg im Breisgau, Germany

Dimitrios Skodras, Michael Klein, Judith Klein
Fraunhofer Institute for Molecular Biology and Applied Ecology (IME),
Schmallenberg, Germany

On behalf of the German Federal Environment Agency

Imprint

Publisher
Umweltbundesamt
Wörlitzer Platz 1
06844 Dessau-Roßlau
Tel: +49 340-2103-0
Fax: +49 340-2103-2285
buergerservice@uba.de
Internet: www.umweltbundesamt.de

Report performed by:
OST- Eastern Switzerland University of Applied Sciences (UMTEC)
Oberseestrasse 10
8640 Rapperswil
Schweiz

Hydrology, Faculty of Environment and Natural Resources, University of Freiburg
Friedrichstraße 39
79098 Freiburg im Breisgau

Fraunhofer Institute for Molecular Biology and Applied Ecology (IME)
Auf dem Aberg 1
57392 Schmallenberg

Report completed in:
November 2024

Edited by:
Section IV 1.2 Biocides
Schwander, Maura; Meier, Christiane

DOI:
https://doi.org/10.60810/openumwelt-7661

ISSN 1862-4804

Dessau-Roßlau, October 2025

Abstract: Groundwater discharges of biocides from façades in urban regions

This study addresses the emissions of biocides from construction materials, specifically focusing on their leaching to groundwater. Biocides, commonly used in building materials, are released through precipitation and can contaminate the groundwater. Despite the well-documented risks, current risk assessment models do not adequately reflect these emissions. To close this gap, this project develops realistic worst-case emission scenarios based on a holistic source-path-target framework, considering building geometry, weather conditions, and urban soil properties. The study evaluates the transport of biocides through urban pathways—vegetated soils, permeable pavements, and infiltration systems—by applying the dynamic leaching model COMLEAM and the soil transport models PEARL and PELMO. A representative building geometry was derived, refining standard regulatory geometries, to better model biocide emissions of façades. Furthermore, the research integrates data on urban soils and weather conditions in urban areas to enhance the modeling of biocide transport to groundwater. The project underscores the importance of considering multiple emission pathways in urban areas and biocide load emissions to better describe biocide emissions to groundwater and preserve groundwater resources. Recommendations for refining the European Emission Scenario Documents (ESD) for biocides are presented, suggesting improvements in the characterization of building geometries and the inclusion of diverse urban emission pathways. The study's findings culminate in the development of a guideline for architects, engineers, and municipalities, promoting sustainable construction practices to reduce biocide emissions. These measures aim to enhance groundwater protection in urban areas, advocating for the use of biocide-free materials and sustainable rainwater management as part of broader blue-green infrastructure strategies.

Kurzbeschreibung: Grundwassereinträge von Bioziden aus Fassaden in urbanen Gebieten

Diese Studie befasst sich mit den Emissionen von Bioziden aus Baumaterialien, insbesondere mit deren Auswaschung ins Grundwasser. Biozide, die üblicherweise in Baumaterialien verwendet werden, werden durch Niederschläge freigesetzt und können das Grundwasser kontaminieren. Trotz der gut dokumentierten Risiken spiegeln die derzeitigen Risikobewertungsmodelle diese Emissionen nicht angemessen wider. Um diese Lücke zu schließen, entwickelt das Projekt realistische Worst-Case-Emissionsszenarien auf der Grundlage eines ganzheitlichen Quelle-Pfad-Ziel-Ansatzes, der die Gebäudegeometrie, die Wetterbedingungen und die städtischen Bodeneigenschaften berücksichtigt. Die Studie evaluiert den Transport von Bioziden durch städtische Pfade - begrünte Böden, durchlässige Beläge und Versickerungsanlagen - unter Anwendung des dynamischen Auswaschungsmodells COMLEAM und der Bodentransportmodelle PEARL und PELMO. Zur besseren Modellierung der Biozidemissionen aus Fassaden wurde eine repräsentative Gebäudegeometrie abgeleitet, die die standardmäßigen regulatorischen Geometrien verfeinert. Darüber hinaus werden Daten über städtische Böden und Wetterbedingungen in städtischen Gebieten einbezogen, um die Modellierung des Biozidtransports ins Grundwasser zu verbessern. Das Projekt unterstreicht, dass die Berücksichtigung mehrerer Emissionspfade in städtischen Gebieten und von Biozidbelastungen wichtig ist, um die Emissionen in das Grundwasser besser zu beschreiben und die Grundwasserressourcen zu schützen. Es werden Empfehlungen zur Verfeinerung der europäischen Emissions-Szenarien-Dokumente (ESD) für Biozide vorgelegt, die Verbesserungen bei der Charakterisierung von Gebäudegeometrien und die Einbeziehung verschiedener städtischer Emissionspfade vorschlagen. Die Ergebnisse der Studie münden in die Entwicklung einer Planungshilfe für Architekten, Ingenieure und Kommunen, um nachhaltige Baupraktiken zur Reduzierung von Biozidemissionen zu fördern. Diese Maßnahmen zielen darauf ab, den Grundwasserschutz in städtischen Gebieten zu verbessern, indem die Verwendung biozidfreier Materialien und eine nachhaltige Regenwasserbewirtschaftung als Teil umfassenderer Strategien für eine blau-grüne Infrastruktur gefördert werden.

Table of Contents

List of figures

List of tables

List of abbreviations

BAC	Benzalkonium chloride
BIT	Benzisothiazolinone
BPR	Biocidal product regulation
CHC	Chlorinated hydrocarbons
COMLEAM	Construction material leaching model
DCOIT	Dichlorooctylisothiazolinone
DDAC	Didecyldimethylammonium chloride
DIBt	Deutsches Institut für Bautechnik
DWA	Deutsche Vereinigung für Wasserwirtschaft, Abwasser und Abfall
ECA	Evaluating Competent Authority
ECHA	European Chemical Agency
EQS	Environmental quality standard
ESD	Emission scenario document
FOCUS models	Forum for co-ordination of pesticide fate models and their use
GIS	Geoinformation systems
GRUBURG	Groundwater discharges of biocides from façades in urban regions
GrwV	Groundwater ordinance – „Grundwasserverordnung“
IME	Institut für Molekularbologie und angewandte Ökologie
IPBC	3-iodo-2-propynyl butylcarbamate
LOD2	Level of Detail 2
MACRO	Model of water flow and solute transport in macroporous soil
MIT	Methylchloroisothiazolinone
MS	Member states
OECD	Organisation for economic co-operation and development
OIT	Octylisothiazolinone
OST	Swiss Easter University of Applied Sciences
PEARL	Pesticide emission assessment at regional and local scales
PELMO	Pesticide leaching model
PNEC	Predicted no effect concentration
PRZM	Pesticide Root Zone Model
PT	Product type
PTF	Pedotransfer function
QAC	Quaternary ammonium compound
TP	Transformation product
UNI	University of Freiburg
WFD	Water framework directive
WHG	German Water Resources, Wasserhaushaltsgesetz

Summary

The leaching of biocides from roofs and façades coatings due to precipitation can lead to pollution of stormwater runoff in urban regions and to transfer of active substances into soil, groundwater and surface water. Various studies have shown that the emission of biocides and the occurrence of their transformation products are influenced by different factors at the building, the transfer pathway and in soil and groundwater. Although these emissions are well-documented, they are not yet adequately represented in current risk assessments due to a lack of suitable models. This project aims to address this gap.

The present project develops urban emission scenarios for the worst-case assessment of biocide leaching from roofs and façades into groundwater and develops a practice-oriented, policy-based guideline to avoid or reduce unintended substance emissions into groundwater. A literature survey first collects existing knowledge on biocides in groundwater in Germany and various European countries. For example, different active substances, entry routes (e.g. point and diffuse source emissions) and endpoints of contamination are distinguished.

In the pursuit of establishing scenarios for the release of biocides from buildings into groundwater, a holistic source-path-target framework is adopted. This approach encompasses an examination of biocide emissions from buildings (façades as the source), the pathways through which these emissions travel (the urban surface types and soils), and the emission target, i.e. groundwater.

In assessing building-related biocide emissions, factors such as the presence of biocide-containing products, building geometry, exposure area, and site-specific meteorological conditions are scrutinized. A comprehensive review of pertinent soil properties in urban locales is undertaken to delineate the emission pathways. This entails compiling information on representative surface types through which substances infiltrate the soil, ultimately reaching groundwater reservoirs. Special emphasis is placed on vegetated soils, partially sealed surfaces, and urban stormwater infiltration structures. National technical guidelines governing the design of swales and permeable pavements in Europe are analyzed to identify key parameters pertinent to the emission scenario definition.

Furthermore, the depth to groundwater and dilution factors in several German cities are investigated to ascertain realistic conditions for entries into the groundwater. This multifaceted approach ensures a thorough understanding of the complex interplay between sources, pathways, and targets of biocide emissions.

Following the comprehensive characterization of source, path, and target components, several models were evaluated for their efficacy in delineating biocide groundwater emissions. To model the leaching of biocides from construction materials, the dynamic construction material leaching model COMLEAM was juxtaposed with the established Emission Scenario Documents (ESD) provided by the European Chemicals Agency (ECHA) for the emission patterns of biocidal products. Concurrently, two FOCUS models (PEARL, PELMO) were compared for their suitability in simulating the transport of biocides through soil.

Benchmark simulations were conducted to assess the performance of these models against each other and against groundwater simulations and existing field data. This comparative analysis facilitated the selection of the most suitable models for the simulation of the defined worst-case biocide scenarios to groundwater in urban areas.

Furthermore, the relevance of different emission pathways and the applicability of the defined scenarios were evaluated. This process involved large-scale simulations in the urban district

Vauban (Freiburg im Breisgau), supplemented by a comparison with measured biocide groundwater concentrations on site.

The project findings lead to two main conclusions. Firstly, based on the research conducted and the modeling results obtained, recommendations for refinements in the Emission Scenario Documents (ESD) for the biocide authorization procedure under the Biocidal Products Regulation 528/2012/EU are formulated. These recommendations aim to characterize the emissions of biocides more realistically to groundwater, thereby enhancing the protection of this vital resource. By providing insights into potential improvements in regulatory frameworks, this aspect of the project contributes to advancing policies geared towards safeguarding groundwater quality. Secondly, a practice-oriented, policy-based guideline is developed for architects, engineers, and municipalities. This guideline suggests refined and target-oriented measures at both the source (source-control) and end-of-pipe solutions.

Zusammenfassung

Die Auswaschung von Bioziden aus Dach- und Fassadenbeschichtungen durch Niederschläge kann in urbanen Regionen zur Verschmutzung von Regenwasserabflüssen und zum Eintrag von Wirkstoffen in Boden, Grundwasser und Oberflächengewässer führen. Studien haben gezeigt, dass die Emission von Bioziden und das Auftreten ihrer Transformationsprodukte durch verschiedene Faktoren am Gebäude, auf dem Transportweg sowie in Boden und Grundwasser beeinflusst werden. Obwohl die Faktoren gut dokumentiert sind, werden sie in der gängigen Risikobewertung aufgrund fehlender geeigneter Modelle noch nicht ausreichend berücksichtigt. Das vorliegende Projekt zielt darauf ab, die Lücke zu schließen und die Risikobewertung zu verbessern.

Daher sollten urbane Emissionsszenarien für eine Worst-Case-Betrachtung der Biozidauswaschung von Dächern und Fassaden ins Grundwasser entwickelt und eine Planungshilfe zur Vermeidung solcher Stoffeinträge ins Grundwasser erarbeitet werden. Im Rahmen eine Literaturrecherche ist zunächst der Wissensstand zu Biozideinträgen im Grundwasser zusammengetragen worden. Beispielsweise wurden unterschiedliche Wirkstoffe, Eintragswege (z. B. punktuelle und diffuse Quelleneinträge) und Endpunkte der Belastung recherchiert.

Um die vorgesehenen Worst-Case-Szenarien für die Freisetzung von Bioziden aus Gebäuden in das Grundwasser zu erstellen, wurde ein Quelle-Pfad-Zielkompartiment-Ansatz verfolgt. Diese Vorgehensweise umfasst die Biozidemissionen aus Gebäuden (Quelle), die Differenzierung sowie Charakterisierung der Transportpfade, über die die Substanzen verlagert werden (z. B. städtische Oberflächen und Böden) und die Beschreibung des zu schützenden Grundwassers.

Für die Bewertung der gebäudebezogenen Emissionen wurden Faktoren wie die Verbreitung der biozidhaltigen Produkte, die Gebäudegeometrie, die Expositionsfläche und die standortspezifischen meteorologischen Bedingungen analysiert. Die Transportwege und Bodeneigenschaften in urbanen Gebieten wurden bewertet, um die relevanten Pfade zu identifizieren. Dazu wurden Informationen über repräsentative, abflussrelevante Flächen gesammelt, über die Stoffe in den Boden und in das Grundwasser gelangen. Besonderes Augenmerk lag auf bewachsenen Böden, teilversiegelten Flächen und Versickerungsanlagen für Regenwasser in Städten. Um Schlüsselfaktoren der Eintragswege zu identifizieren und festzulegen, die für die Emissionsszenarien relevant sind, wurden nationale technische Richtlinien und Empfehlungen für die Gestaltung von Versickerungsanlagen und wasserdurchlässigen Belägen in Europa beigezogen.

Darüber hinaus wurden die Grundwasserflurabstände und Verdünnungsfaktoren in deutschen Städten untersucht. Diese beeinflussen die Wahrscheinlichkeit eines Eintrags in das Grundwasser. Damit wurde sichergestellt, dass die komplexen Wechselwirkungen zwischen Stofffreisetzung, -verlagerung und -eintrag in Boden und Grundwasser ganzheitlich abgebildet und die verschiedenen Aspekte des Grundwasserschutzes in den Szenarien berücksichtigt werden.

Nach der umfassenden Charakterisierung des Wirkungsgefüges wurden verschiedene Modelle auf ihre Eignung zur Darstellung der Biozideinträge in das Grundwasser bewertet. Zur Modellierung der Auswaschung von Bioziden aus Baumaterialien (Fassaden) wurde das dynamische Auswaschmodell COMLEAM mit den etablierten Emissionsszenarien (ESD) der

Europäischen Chemikalienagentur (ECHA) hinsichtlich des Emissionsverhaltens von Biozidprodukten verglichen. Darüber hinaus wurden die FOCUS-Modelle PEARL und PELMO auf ihre Eignung zur Simulation des Transports von Bioziden im Boden überprüft.

Zahlreiche Simulationen wurden durchgeführt, um die Aussagekraft der Modelle unter Berücksichtigung von Felddaten zu bewerten. Die vergleichende Analyse ermöglichte die Auswahl der geeigneten Konzepte für die Simulation von Biozidemissionen ins Grundwasser von städtischen Gebieten.

Weiterhin wurde die Relevanz der Emissionspfade und die Plausibilität der ausgewählten Szenarien bewertet. In diesem Schritt wurden großräumige Simulationen für den Stadtteil Vauban in Freiburg im Breisgau durchgeführt und die Resultate mit mit gemessenen Biozidkonzentrationen im Grundwasser verglichen.

Auf Basis der durchgeführten Untersuchungen und der erarbeiteten Ergebnisse können klare Empfehlungen zur Verfeinerung der Emissionsszenarien für das Biozid-Zulassungsverfahren gemäß der Biozidprodukte-Verordnung 528/2012/EU formuliert werden. Diese Empfehlungen zielen darauf ab, die Einträge von Bioziden ins Grundwasser realistischer abzuschätzen und damit den Schutz dieser wichtigen Ressource zu verbessern. Durch Hinweise auf Verbesserungsmöglichkeiten im bestehenden Regulierungsrahmen tragen die Erkenntnisse zur Weiterentwicklung von Maßnahmen zum Schutz des Grundwassers bei.

Die entwickelte praxisorientierte Planungshilfe für Architekten, Ingenieure und Kommunen bietet verfeinerte und zielgerichtete Maßnahmen sowohl an der Quelle (Emissionsminderung) als auch nachgeschaltete Lösungen an. Damit können Biozideinträge in das abfließende Regenwasser sowie in das Grundwasser vermieden bzw. deutlich reduziert werden. Bei Umsetzung der Lösungen ist der Grundwasserschutz bei Schwammstadtkonzepten gewährleistet.

1 Introduction

The leaching of biocides from coatings for roofs and façades (plasters, paints), containing material preservatives due to precipitation can result in contaminated runoff in urban areas, with the active substances being introduced into soil, groundwater, and surface waters (Burkhardt et al., 2012; Jungnickel et al., 2008; Kahle and Nöh, 2009; Paijens et al., 2020a). This has been documented at numerous European urban sites. Among the nearly ten available biocides for paints/plasters, the long-lasting ones such as terbutryn, isoproturon, diuron, and carbendazim are particularly prominent in monitoring (Bollmann et al., 2014; Burkhardt et al., 2007; Paijens et al., 2020b; Wicke et al., 2021; Wittmer et al., 2011). Their transformation products (TP), especially those formed through photodegradation, are also regularly detected (Bollmann et al., 2016). However, current risk assessments for these biocides and their TPs are still insufficient. It is important to explicitly consider TPs in future evaluations to better understand the environmental impact of biocide products.

The European Chemicals Agency (ECHA) oversees the approval of biocidal active substances and the authorization process of biocidal products containing approved active substances in the European Union. The Working Group Environment under the Biocidal Products Committee of ECHA employs scenarios to evaluate potential risks associated with their use. Upon application submission, the evaluating Competent Authority (eCA) of Member State (MS) meticulously assesses data concerning the biocide's properties, intended applications, and potential impacts on human health and the environment. Scenarios are then selected to simulate typical usage conditions, aiding in comprehensive risk assessments. Based on these assessments, tailored risk management measures are devised to mitigate if unacceptable risks are identified, often involving usage restrictions, protective measures, or labeling requirements. Ultimately, this procedure aims to ensure the safe and effective use of biocides while safeguarding human health and the environment.

The Emission Scenario Documents (ESDs) are an integral part of the authorization process for biocidal products in the European Union. These documents provide crucial guidance for estimating and assessing the potential emissions and exposure of substances from biocides throughout their lifecycle, enhancing the effectiveness of the authorization process and the protection of human health and the environment (Article 1 of the Biocidal Products Regulation (EU) No 528/2012).

In the context of the authorization of such biocidal products, environmental risks are assessed simulating emissions into the soil from a model house. However, numerical models with scenarios for estimating possible groundwater contamination, like those available for years in plant protection products approval with models like PEARL, MACRO, or PELMO linked to scenarios (specific soils, weather, etc.), are lacking for façade biocides in urban areas. This relatively rudimentary assessment may also be attributed to the fact that, while the relevance of entries into groundwater compared to other transfer pathways is generally recognized, the underlying processes are still not sufficiently understood. This may be due to a lack of comprehensive evaluation of monitoring data for such biocides in urban groundwater, especially considering catchment areas, or because such empirical data is scarce.

This project aims to assess the release of biocides in urban soils using computer models to generate representative and relevant scenarios for the authorization process of biocides. This necessitates a comprehensive characterization of input parameters, which is more extensive in scope compared to the established ESDs of ECHA. To achieve this, a holistic source-path-target concept was employed, which encompasses the description of the source (façade), the path (soils and substrates), and the target (groundwater). Several representative urban soils are identified, and realistic urban site scenarios are developed, simulated using soil transport models (software tools), with particular consideration given to FOCUS PEARL and PELMO. Groundwater simulations are conducted, including parameter variation. The approach is iterative. Despite various questions about deriving worst-case parameters, such as the relevance of building and soil parameters, the scenarios are preferably presented simply and comprehensibly with few parameters to maximize acceptance.

The Groundwater Ordinance regulates the admissible pesticide concentrations in groundwater indicating a maximum concentration of 0.1 µg/L per individual substance, including relevant degradation products, and of 0.5 µg/L for the sum of all individual substances (GrwV, 2017). These requirements address the protection of the groundwater i.a. as an important drinking water resource. Accordingly, stormwater quality is of particular importance during infiltration. However, the significance of infiltrations on the input of biocides into urban groundwater is still unclear.

It should be noted that in many European countries, decentralized or semi-centralized facilities for rainwater infiltration are increasingly being constructed, driven in Germany, for example, by the infiltration requirement in the Water Resources Act. Additionally, façade runoff infiltrates along building perimeters through backfills, gravel fillings, etc., diffusely into the subsurface or remains in the unsaturated zone. Questions remain regarding the relevance of infiltrations for groundwater contamination, especially in comparison to other pathways into the environment.

Potential contamination of rainwater runoff should already be considered in the planning of drainage systems. For instance, if infiltration through basins or trench systems is planned, insufficient retention of the soil could lead to groundwater contamination (Lange et al., 2017). Often, runoff rainwater also diffusely enters the environment, such as water dripping in the base area of façades, and infiltrates uncontrollably.

Infiltrations such as soil filters, basins, basin-trench systems, or adsorber systems must be planned and operated according to the state of the art. With proper execution, their hydraulic capabilities remain intact for 10 to 20 years of operation (Kluge et al., 2016). Since organic pollutants such as biocides are often not the focus of the regulations, their retention efficiency is uncertain or not guaranteed (Bork et al., 2021; Burkhardt and Hodel, 2019). Infiltration measures lacking barrier effects thus serve as entry points for biocides into groundwater.

Experience from relevant studies (Burkhardt et al., 2017) and soil physics/chemistry indicate that the retention of substances in soils or substrates of infiltration systems and surfaces along buildings particularly with high hydraulic conductivities, is primarily determined by the quantity and quality of the organic fraction (organic content (OC), clay fraction). Typically, substance properties such as partitioning coefficient of octanol and water (P_{OW}) and water solubility, as well as adsorption isotherms (K_d, K_{oc}), describe the binding capacity or mobility. However, information regarding the corresponding adsorption behavior of biocides in urban soils and substrates is generally not readily available in the literature or existing maps. This study aims at providing such parameters for representative standardized scenarios.

As urban water resources are to be protected by the EU Water Framework Directive (WFD) and the Surface Water and Groundwater Regulations (with the aim of preventing exceedance of environmental quality standards), measures (at the source and end-of-pipe) against relevant biocide entries into soil and water are to be established, considering monitoring data and process knowledge.

Therefore, this project also aims to investigate the significance of biocide entries from façades and roofs into groundwater during infiltration. This approach delineates the entire pathway from emission source to the receiving environmental compartment, thereby addressing an existing gap in assessing environmental exposure to biocidal substances.

Building upon this research, a practical, action-oriented guideline for municipalities to minimize and prevent biocide entries into groundwater is provided. This guideline summarizes effective measures at the source to avoid and minimize biocide emission to groundwater as well as end of pipe solutions, complementing already existing recommendations. Construction and product-specific risk mitigation measures, along with sustainable rainwater management concepts are presented in a user-friendly format within the practical guideline.

2 Biocide emissions to groundwater: Overview and literature review

2.1 Importance of biocides in groundwater

2.1.1 Groundwater as a vulnerable resource to biocides

Groundwater is an important resource for drinking water, industry and agriculture, and is essential for ecosystems. In Germany, 70 % of drinking water is groundwater (DSTATIS, 2019). It is therefore very important to prevent groundwater pollution.

One potential source of pollutants arises from biocides employed in film preservatives (Product Type 7 according to Annex V of the BPR). These substances, utilized in paints and plasters, prevent the growth of algae and fungi at façades. However, the leaching of biocides used in film preservatives poses a potential environmental threat to groundwater. Chapter 3.2.1 provides a detailed overview of the biocides used in façades, with the herbicide diuron, the fungicide octylisothiazolinone (OIT) and the algaecide terbutryn being used most frequently in Germany. All three substances and various transformation products (TPs) have been found in urban groundwater (Hensen et al., 2018).

2.1.2 Biocide emissions from façades

Biocides are washed off during rain events and represent a quasi-continuous leaching into the environment with possible negative environmental impacts (Bollmann et al., 2017). Biocide emissions depend on initial biocide concentrations, paint and plaster composition, runoff, irradiation, temperature, length of dry periods and other factors (Paijens et al., 2020a). The main factors influencing the leaching of the biocide terbutryn were found to be wind driven rain, runoff, irradiation and dry periods (Wicke et al., 2021; Junginger et al., 2023). A larger fraction of biocides is leached from façades facing the prevailing wind direction (Vega-Garcia et al., 2020). Most biocides are emitted in the first year after biocide application (Bollmann et al., 2016), although biocides can leach more than 15 years after the last application (Hensen et al., 2018). Biocide concentrations are highest at the source and decrease as they spread in the environment due to dispersion, dilution, adsorption and degradation.

In order to determine biocide emissions for individual paints and plasters, laboratory tests investigate factors that influence leaching (e.g. Schoknecht et al., 2009; Urbanczyk et al., 2019; Wangler et al., 2012). However, they tend to overestimate biocide emissions and thus represent a worst-case scenario (Junginger et al., 2023; Schoknecht et al., 2016). Under natural weather conditions, experiments with artificial walls (e.g. Bollmann et al., 2016; Burkhardt et al., 2012) can help to understand field conditions. However, these experiments typically do not run for more than 2-5 years, while buildings are usually repainted at longer intervals. Therefore, both laboratory tests and artificial wall experiments do not necessarily represent field conditions for buildings in urban districts.

2.1.3 Biocide degradation

Biocides form TPs as a result of photolysis, hydrolysis and biodegradation. The transformation can occur on the façade, in runoff water, and within soil and the resulting TPS can be more toxic than their parent compounds (Hensen et al., 2020).

Terbutryn and diuron have both been used as pesticides in agriculture, and numerous studies have investigated their degradation in soil (Attaway et al., 1982; Avidov et al., 1985; Daho, 1994). Both substances are quite persistent, as indicated by long half-lives (DT50) in water and soil. For terbutryn, a DT50 of 354 day in water was found (Paijens et al., 2020a). In soil, half-lives range from 10 to 202 hours under laboratory conditions to 231 days under field conditions (Bollmann et al., 2016; Bollmann et al., 2017; Junginger et al., 2022). For diuron, the DT50 in water is 113 to 2190 days and more than 2500 days in soil (Bollmann et al., 2017; Paijens et al., 2020a). OIT degrades more rapidly with a DT50 of 2 to 15 days in water and about 9 days in soil (Bollmann et al., 2017, ECHA, 2017). Degradation depends on the environmental conditions such as temperature, moisture, irradiation, and redox potential.

TPs of biocides can be quantified if analytical standards are available. Diuron-desmethyl, the main degradation product of diuron, and various TPs of terbutryn have been measured in façades and stormwater runoff and in groundwater (Burkhardt et al., 2011; Hensen et al., 2018; Linke et al., 2021). The amounts of TPs leached can be greater than the amount of biocide. This was shown for terbutryn in a field experiment, where a transformation product of terbutryn, terbutryn-sulfoxide, leached more than terbutryn (Junginger et al., 2023). This shows the importance of TPsts when considering the leaching of biocides and assessing the environmental impact.

2.1.4 Environmental effects of biocides

Biocides can have adverse effects on ecosystems and organisms. Ecotoxicity tests are conducted to evaluate these effects on various species in both aquatic and terrestrial environments. The results of these tests are used to establish Predicted No Effect Concentrations (PNECs), which are concentrations below which no harmful effects on organisms are expected. Environmental Quality Standards (EQS), on the other hand, are set according to the EQS Directive and represent legally binding limits for concentrations of substances in different environmental compartments, such as surface water, sediment, and biota.

Currently, no EQS have been established for soil in the case of most biocides, as indicated by Silva et al. (2019). Nevertheless, a number of studies have investigated the toxicity of terbutryn and OIT, with findings suggesting that OIT is the more toxic compound of the two (Bollmann et al., 2017). This observation aligns with the PNEC values of the two substances. Another study found that long-term exposure of soil microorganisms to terbutryn for up to 40 days had more severe effects on bacterial and fungal proliferation than short-term exposure for up to 7 days (Fernández-Calviño et al., 2021). A recent study showed that biocides reduce the total soil microbiome, affecting bacteria richness more significantly than that of fungi (Reiß et al., 2024). In addition, in-can preservatives used in façade paint and plasters, such as benzisothiazolinone (BIT) and methylchloroisothiazolinone (MIT), can stress sediment and aquatic organisms (Kiefer et al., 2024).

For most substances, there are no substance-specific Environmental Quality Standards (EQS) defined in groundwater. However, according to the German Groundwater Ordinance (GrwV) the same quality standards apply to groundwater as for drinking water with 0.1 µg/L for a single pesticide and 0.5 µg/L for the mixture (Council Directive 98/83/EC, 1998).

The pathways through which biocides reach urban groundwater are uncertain owing to the scarcity of monitoring data and limited modeling approaches.

The following subchapters summarize the current knowledge on possible pathways to groundwater (2.2), available monitoring data (2.3) and national guidelines for the protection of groundwater from biocides (2.4). This knowledge forms the basis for the emission scenarios defined in chapter 3.

2.2 Pathways of biocide emissions through soil to urban groundwater

2.2.1 Characteristics of urban soils

Biocides infiltrate to groundwater via urban soils. Urban soils have characteristics that are different from their natural counterparts (Craul, 1985). Due to intense anthropogenic influence, they are generally characterised by

- modified, often compacted soil structure,
- ubiquitous sealing,
- restricted aeration and water drainage,
- interrupted nutrient cycling and modified, often hampered activity of soil organisms,
- presence of anthropogenic materials and other contaminants, and
- more extreme soil temperature regimes.

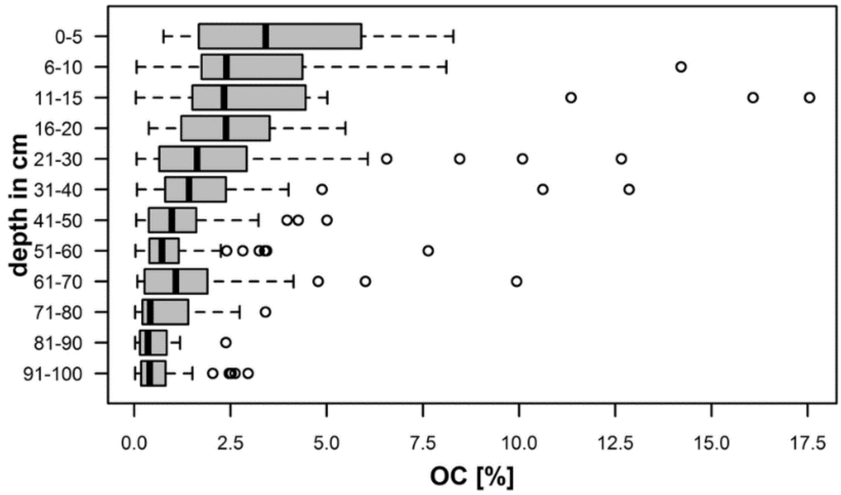
These characteristics interact, cause great vertical and spatial variability, and pose problems to define typical urban soil types and profiles.

In urban areas, natural soils are generally refilled or redeposited. In addition, urban soils contain anthropogenic components e.g. brick debris, garbage, mine deposits or organic residues. As a result of the destruction of World War II in the city of Berlin, for example, the fine earth soil fractions contain 3–5 % bricks, while the coarse fractions contain up to 50 % (Nehls et al., 2013). At other locations, soil compaction prevails, which occurs deliberately during construction activities or unintentionally by traffic. In principle, soil compaction increases surface runoff and at the same time reduces water infiltration and pollutant transport to groundwater. On top of that, sealing by impervious surfaces such as asphalt and concrete is common.

Natural soils generally show a gradual decrease of OC with depth, while in urban soils OC-enriched layers may be stripped or buried. Thus, unexpectedly high contents of OC be found in deeper soil horizons. However, most urban soil profiles have low OC (1–2 %), because of the parent material (Puskás and Farsang, 2009).

Recently, Makki et al. (2021) analysed OC in the area of Berlin (Figure 1). They found that urban green spaces exhibited higher OC stocks in the topsoil than forested areas on the north-western and south-eastern outskirts. Soil carbon storage in the subsoil varied even more and depended on the substrate available for soil formation. However, in deeper soil layers the measured OC was not exclusively attributable to natural origin, but also originated from a wide variety of technogenic materials.

Figure 1: Depth profiles of organic carbon contents (OC) of different soil types in the area of Berlin (N = 441)

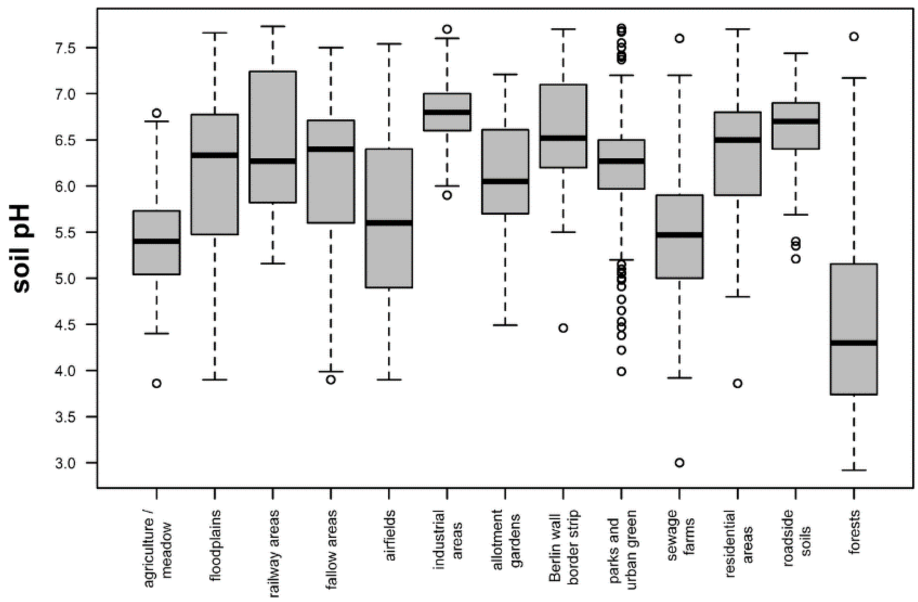


Source: Makki et al. (2021)

With only few exceptions, urban soil pH is more alkaline compared to e.g. forest soils, which can be attributed to filling materials contaminated with building wastes, such as concrete and cement. Examples of measured urban soil range from 7.4 to 8.6 in Siena, Italy (Nannoni et al., 2014), from 7.6 to 9.1 in Szeged, Hungary (Puskás and Farsang, 2009), or from 7.2 to 8.2 in Murcia, Spain (Acosta et al., 2014).

Again, the study of Makki et al. (2021) in Berlin provided the most extensive overview of urban pH-values and also facilitated a relation to structure types and a comparison to natural forests surrounding the urban area (Figure 2).

Figure 2: pH values of soils in Berlin grouped by the urban structure (N = 1'794)



Source: Makki et al. (2021)

2.2.2 Biocide pathways to groundwater

Directly around buildings, at the bottom of the façades, surfaces can be distinguished according to four characteristics (Figure 3).

Gravel beds are designed to prevent splashing during rainfall, but they do not provide retention for biocides. If they are not sealed at the base and connected to the underground, they must be considered as a hotspot for biocide leaching to groundwater. These hotspots are not typically for urban areas and should be avoided where possible. Therefore, they are not considered in the representative scenarios presented in this study. However, the transport of biocides in gravel beds is not controlled by the properties of the substances, and the most hazardous substances would only be defined by their toxicity and persistence.

Figure 3: Typical surfaces at the bottom of building façades that accept façade runoff

Source: Own photos, UNI Freiburg. Taken by M. Bork

In contrast, asphalt surfaces can be considered as sealings without infiltration and without groundwater contamination risk. However, façade runoff to asphalt enters the stormwater drainage system and finally reaches infiltration facilities, i.e. swales of swale-trench systems, in districts with separate sewer systems.

Urban soils are characterized by an organic topsoil and are comparable to topsoil of infiltration facilities. Façade runoff on permeable pavements can partly infiltrate. Here, the amount of infiltration (described by the runoff coefficient) mainly depends on joint size and material.

In summary, biocides enter urban groundwater through the following three main pathways:

(1) in vegetated soils at the bottom of façades (S1),

(2) via infiltration through permeable pavements (S2), and

(3) via urban stormwater infiltration facilities, i.e. swales or swale-trench systems (S3).

These pathways form the baseline for an estimation of biocide emission to groundwater. Existing field information for each pathway is summarized in the following chapter, while their individual characteristics for the GRUBURG-scenarios are deduced in chapter 3.3.

2.3 Monitoring data of biocides in urban pathways

Biocides may reach groundwater via the three main pathways S1-3 outlined above. However, an accurate assessment of the extent to which biocides reach groundwater through various pathways is challenging if not impossible. The mere presence of biocides along a pathway does not directly correspond to groundwater concentrations or loads, adding complexity to the measurement and assessment process. This is where modeling approaches, presented in chapter 4, come into play. Nevertheless, experimental data and field measurements of biocide concentrations can help to assess the relevance of each pathway and provide the basis for a reality check of the scenarios outlined in following chapters. Only the three most used biocides in façade coatings in Germany, i.e. diuron, OIT and terbutryn, are included in this overview.

2.3.1 Vegetated soil (S1)

In a study in Denmark, 17 soil samples were taken below façades that had been painted within the last five years (Bollmann et al., 2017). Biocide concentrations ranged from low ng/g concentrations up to 100 ng/g with terbutryn measured in 2 samples, diuron in 1 and OIT in 3. Several TPs of terbutryn were also quantified in the low ng/g range (Bollmann et al., 2017). In another study, soil samples were taken in a stormwater retention swale (Linke et al., 2022). Terbutryn was detected in 73 % of the samples taken across the pond with most samples showing concentrations below 1 ng/g. Again, TPs of terbutryn were detected (Linke et al., 2022). Highest biocide concentrations (max. 26 ng/g) were found below the inlet. In Sweden, terbutryn was detected at one site out of 17 stormwater ponds(100 ng/g) (Flanagan et al., 2021). A recent study sampling soils in infiltration systems in Germany and France indicted that recently painted buildings may lead to higher concentrations in sediments (Linke et al., 2023).

In a field experiment, biocides were applied to lysimeters (0.8 m^2x 0.4 m) with typical urban materials (Junginger, 2022). After addition, the lysimeters were exposed to natural weather conditions and biocides concentrations measured in the leachate. The vegetated soil consisted of 10 cm soil with grass on 17 cm sand, geotextile and 2 cm gravel. In this lysimeter, biocide percolation was found to be negligible. However, 7.2 % of the applied terbutryn was found in the uppermost soil and sand layers with highest OC. The presence of TPs may describe degradation within the soil (Junginger, 2022).

These studies illustrate that biocides can be expected in vegetated soils below façades. Concentrations are usually below or close to the detection limit of a few ng/g, rarely up to 100 ng/g. Terbutryn is most commonly detected as it is quite stable (DT50: 231 days) and adsorbs readily to soil (K_{oc}: 663 mL/g) (Mensink and Linders, 1991; Bollmann et al., 2017). TPs of terbutryn are often quantified, although low concentrations indicate further degradation in soil. In contrast, OIT degrades rapidly (DT50: 0.9 days) and diuron is more mobile (ECHA, 2017.

2.3.2 Permeable pavements (P2)

Permeable pavements must be regarded as potential entry pathways of biocides to groundwater, although direct field measurements in leachate or groundwater beneath permeable pavements are lacking. However, also here the field lysimeter experiments by Junginger (2022) may serve as a guideline to estimate how much biocide may theoretically pass a permeable pavement. His pavement lysimeter was covered with pavement stones (20 × 9.5 × 8 cm) with joints filled with sand, followed by a sand layer (20 cm), a layer of geotextile and 2 cm of filter gravel. Almost 17 % of the applied terbutryn leached through the lysimeter, another 13 % in the shape of terbutryn TPs. After dismantling, most biocides were found in deeper sand layers but none in the joint material. Overall, biocide retention was by far lower compared to the vegetated soil lysimeter.

Recent soil samples from permeable pavement joints in pedestrian areas in Freiburg, Germany (Figure 4), showed low concentrations of terbutryn in one sample (0.4 ng/g), while other samples were below the limit of quantification (3 samples) or below the limit of detection (7 samples). These low concentrations of terbutryn in joints may indicate either limited OC and hence limited sorption capacity, or low overall concentrations in urban stormwater. Overall, more research is needed to fully clarify the entry of biocides into groundwater via permeable pavements.

Figure 4: Sampling of joint material on pavements

Source: Own photos, UNI Freiburg. Taken by F. Linke

2.3.3 Swales and infiltration to groundwater (S3)

There is incontrovertible evidence that biocides can reach groundwater via stormwater infiltration facilities. This was demonstrated by comparing biocide concentrations in groundwater upgradient and downgradient of a stormwater infiltration system. Biocide concentrations were higher downgradient of the system, suggesting biocide infiltration (Hensen et al., 2018). For example, Diuron concentrations ranged from less than 10 ng/L upgradient to 25 ng/L downgradient and terbutryn concentrations were less than 5 ng/L upgradient and up to 10 ng/L downgradient. Also, TPs of terbutryn and diuron showed higher concentrations downgradient than upgradient of the swale-trench system. Notably, these concentrations were generally lower than those observed for the biocide. Similar results for diuron were obtained by another study with a similar setup of wells up- and downgradient of stormwater infiltration facilities (Pinasseau et al., 2020). OIT was only detected in single monitoring wells, underlying fast degradation in soil (Hensen et al., 2018).

There is a high inter-event variation of biocides measured in standing water in swales (Hensen et al., 2018, Linke et al., 2021). Preferential flow paths may accelerate biocide breakthroughs when swales age (Bork et al., 2021). This means that young swales resemble the characteristics of vegetated soils (S1 above), while in older swales biocide retention is more limited, see also 3.3.4. As outlined above, recent measurements in soils of swales in the cities of Freiburg and Strasbourg showed higher concentrations of terbutryn in the soils of recently constructed swales (Linke et al., 2023).

2.4 National guidelines for swales and permeable pavements

2.4.1 EU level legislation

Urban stormwater infiltration prevents flooding and sewage overflows, helps to prevent water pollution, increases biodiversity and improves the microclimate (Fletcher et al., 2015). These objectives form part of various EU Directives that European member states are required to implement in order to:

- assess and manage the flood risk (EU Floods Directive, 2007/60/EC),
- achieve good qualitative and quantitative status of all water bodies (EU Water Framework Directive, 2000/60/EC) (this does not include a requirement for separated sewer systems),

- protect the environment from the adverse effects of urban wastewater discharges (Urban Waste Water Treatment Directive, 91/271/EEC). This directive specifically addresses the treatment of wastewater from urban areas before discharge but does not cover stormwater management,
- comply with environmental quality standards for surface water (2008/105/EC), and
- protect groundwater (2006/118/EC).

National legislation implements EU legislation. Thereby, technical guidelines and standards provide details on the planning and design of stormwater infrastructure. These are presented below. As outlined above, the focus of this report is on relevant pathways of biocides to urban groundwater (2.3), i.e. surface infiltration through vegetated soils or permeable pavements and stormwater infiltration systems with a vegetated surface (swales).

2.4.2 German technical guidelines for stormwater infiltration

According to §55 of the German Water Resources Act (Wasserhaushaltsgesetz, WHG), stormwater should be infiltrated or discharged into water bodies. Decentralized methods are preferred for stormwater management. In addition, §47 of the WHG requires to preserve groundwater, both in terms of chemical composition and water quantity.

The guideline DWA-A 138-1 (DWA, 2024) describes the planning, construction and operation of stormwater infiltration systems in Germany. In stormwater infiltration systems with a vegetated surface, runoff is stored for a short time and then infiltrated through an extensive vegetated soil zone. Thereby, the standing water level should not exceed 30 cm. For large systems and swales with slopes, cascades or multiple swales are required. The required area and storage volume of an individual swale depends on the extent of connected area types multiplied by their runoff coefficients, the area of the swale that receives rainfall, the amount of the design rainfall and the infiltration rate (DWA, 2024).

Surface infiltration takes place on flat surfaces without intermediate storage. This can be on vegetated soils or via permeable pavements. In Germany, permeable pavements must be approved by a technical authority, by the Deutsches Institut für Bautechnik (DIBt). A continuous infiltration rate of 270 L/s*ha is required, as well as a possible cleaning if the infiltration rate is reduced. The required area of a permeable pavement depends on the design rainfall (usually 10 minutes, for larger areas 15 min), the runoff coefficient of the connected catchment area and the infiltration rate. European standards for permeable pavement, particularly for concrete elements, specify dimensions, weathering resistance, abrasion resistance, slip/slide resistance, and the components of a test report (EN 1338 and EN 13369). All requirements are tested according to a standardized procedure and a certificate is issued for each type of surface material. DIN 18318 gives further information about requirements for permeable pavements, such as a minimum slope of 1.5 % for pedestrian areas and 2 % for traffic areas. Further information on particle retention capacity and cleaning requirements can be found in (FGSV, 2016).

The water quality requirements for stormwater infiltration systems with a vegetated soil layer are based on the thickness and the composition of the soil layer. The requirements depend on stormwater pollutants (type, amount and properties) and are divided into three classes depending on characteristics of the connected catchment area, such as traffic volume and surface area (DWA, 2024; FGSV, 2016). These requirements ensure groundwater protection, with the unsaturated soil and underground acting as an additional buffer. Normally, the quality limits are met after soil passage of a stormwater infiltration system and dilution within the groundwater. However, certain contaminants, such as chloride and biocides, are not sufficiently retained and require the implementation of additional measures (Helmreich et al., 2022). So far, biocides are not clearly considered in the technical guidelines (e.g. DWA, 2024). Rather, recommendations are made to avoid biocides at the source by using materials, construction products or operating methods that produce less harmful emissions (Helmreich et al., 2022).

2.4.3 European technical guidelines for stormwater infiltration

In **Belgium**, the technical guideline contains similar recommendations for stormwater infiltration as the German guideline DWA-A 138-1 (Bouteligier et al., 2005). Infiltration on vegetated grass or permeable pavement is possible; design parameters are traffic and other loads and infiltration rates. For stormwater infiltration, the dimensions are similar, e.g. with a maximum level of standing water of 30 cm, a top layer of 0.3-0.5 m and 5-10 m^2 of swale per 100 m^2 of sealed area (Table 1). The swale must be emptied within 24 h. For permeable pavements, an infiltration rate of 270 L/(s*ha) is required (Table 2).

In the **Netherlands,** a technical guideline provides information on the planning, design and maintenance of stormwater infiltration systems (Boogaard and Rombout, 2008). The infiltration capacity must be 0.2 m per day. Thereby, 1 m^2 of swale collects the runoff from 10-12 m^2 of sealed surface. Swales can be slightly deeper than in Germany and Belgium, up to 0.5 m. The required volume of a swale is calculated using a design rainfall, the connected catchment area and a runoff coefficient. For permeable pavements, again a minimum infiltration rate of 270 L/s*ha is required. Overall, requirements are similar to Germany and Belgium (Table 1 and Table 2).

In **Denmark**, a design guide for stormwater retention and infiltration provides details on different types of systems including swales with a vegetated soil surface (DANVA, 2018). For dimensioning, it is important to consider the overflow return period, the infiltration rate and the acceptable water retention time of the system (max. 24 h, similar to other guidelines). Biocides are not mentioned, but chloride from road de-icing is described as a possible impact to shallow groundwater. Hence, a modest leaching risk of pollutants from stormwater remains (DANVA, 2018).

In **Austria**, recommendations for the type of infiltration system depend on the pollution expected from the drained catchment area, similar to the guidelines described above (ÖWAV, 2015). For stormwater infiltration systems, the drained catchments must be marginally polluted such as footpaths, roof areas, parking lots or areas with low traffic. More polluted areas require additional soil filters. Infiltration via permeable pavements is approved for slightly contaminated surfaces, similar to regulations for stormwater infiltration systems. Permeable pavements are acceptable for parking lots that use grass pavers and soil filter material, or where groundwater contamination is not expected due to subsurface conditions. For surface infiltration, the k_f value must be greater than 10^{-5} m/s. In Austria, values from DWA-A 138-1 from Germany are often used (Aschauer et al., 2021). A recent guideline explicitly mentions biocides when stormwater is used for irrigation (Kleidorfer et al., 2019).

In **France**, there are no national regulations or technical guidelines for stormwater infiltration. Based on the Water Framework Directive, which has been incorporated into French law (Loi sur l'eau 2006), soil sealing should be limited. Municipal regulations tend to promote infiltration. A report links stormwater infiltration with water quality and gives recommendations on how to avoid contamination (Tedoldi et al., 2020). These include soil characteristics (e.g. 5-6 % OC) and a minimum soil thickness of 20 cm. The size of stormwater infiltration facilities is based on a design rainfall event (NF EN 752-2) and a minimum depth to groundwater of 1 m is required (Goutaland et al., 2015). For surface infiltration and permeable pavements, similar regulations apply.

In **Finland,** there is a stormwater guide “Hulevesiopas” as well as a national standard file including regulations and product files (Kuntaliitto, 2012; Vilminko et al., 2021). Design rainfall events and runoff coefficients of the connected catchment area are the basis for swale volume calculations, similar to other EU countries (Kuntaliitto, 2012).

In **Spain**, new urban development areas are required to use sustainable drainage systems (Royal Decree 638/2016). This is similar to countries such as Germany or Denmark. The guideline “La Gestión Integral del Agua de Lluvia en Entornos Edificados” provides detailed recommendations for different sustainable stormwater management elements, including swales and permeable pavements (TRAGSA, 2015). The capacity of swales needs to be calculated depending on the connected catchment area and a design rainfall.

Several countries in the EU do not have specific national guidelines or legislation to promote stormwater infiltration, such as **Poland** (Kordana and Slyś, 2020). Other countries, such as **Estonia** and **Latvia,** lack manuals of stormwater management and use wastewater regulations to manage stormwater (Vilminko et al., 2021).

Outside the EU, **Switzerland** prioritizes stormwater infiltration over surface water discharge. The VSA guideline “Abwasserbewirtschaftung bei Regenwetter” (Oppliger and Hasler, 2019) provides details on the design of a stormwater infiltration system, such as a clay content between 10-20 % and a humus content of at least 3 % in the topsoil of at least 20 cm thickness. A minimum depth of 1 m to groundwater from the infiltration system is required. To improve the quality of the infiltrating water, different pollution classes are defined, depending on the type of infiltration, i.e. through the soil layer. In general, more polluted stormwater can be infiltrated through soil layers. Technical adsorption systems are required where soil filters are not feasible (BAFU/ARE, 2022).

A similar technical guideline, CIRIA, exists in the **UK** (Cooper and Cooke, 2016). Swales should be at least 10 cm deep, with a drainage time of at least 10 min.

Outside Europe, **Australia** has been promoting water-sensitive urban design since the 1990s with the aim of managing the water balance, improving water quality, encouraging water conservation and maintaining water-related environmental and recreational opportunities (Fletcher et al., 2015). The Clean Water Act regulates urban stormwater management in the **United States**, focusing initially on water quantity and subsequently on water quality. Here, swales and permeable pavements are called low impact development or green infrastructure (Novaes and Marques, 2022). In **China**, the Sponge Cities Initiative aims to reduce flood risk and pollution from runoff while increasing water supply (Novaes and Marques, 2022). These examples show that sustainable urban stormwater management is globally in the ascendant.

2.4.4 Design parameters for swales and permeable pavements

Table 1 shows selected design parameters for stormwater infiltration facilities. The parameters in Germany are largely within the range of Belgium and The Netherlands.

Table 1: Design parameters for swales in selected EU countries

Design parameter	Unit	Germany DWA (2005)	The Netherlands Boogaard and Rombout, (2008)	Belgium Bouteligier et al. (2005)
Swale area/ drained area	m^2/m^2	> 7	5 - 10	5 - 10
Distance to houses	m	1.5	> 1	-
Swale water depth till overflow	m	< 0.3	< 0.3	< 0.3
Width of bottom	m	0.6	> 0.5	0.5 - 1
Longitudinal slope	V:H	< 1:4	<1:3	< 1:3
Thickness of filter soil	m	> 0.1	0.3 - 0.5	0.3 - 0.5
Humus in top layer	%	3-5	3-5	-
Infiltration capacity Kd	m / day	0.86 < Kd < 86.4	> 0.5	> 0.086
Overflowing frequency	1 /year	0.2	1 to 2	0.2 – 0.5
Water retention time (to empty)	hour	< 24	< 24	< 24

The main design parameters for permeable pavements are in Germany like those of other countries (Table 2). The infiltration rate in Germany is based on a defined stormwater event (10 min duration, 5 years return period).

Table 2: Design parameters for permeable pavements in selected EU countries

Design parameter	Unit	Germany DWA (2024), FGSV (2016)	The Netherlands Boogaard and Rombout, (2008)	Belgium VLARIO (2005)	Denmark (Støvring et al., 2018)
Infiltration capacity	L/(s*ha)	270	270	270	190 to 230
Percentage of joints	%	3-25 %	-	-	-
Minimum distance to groundwater	m	1	0.5 to 0.7	-	-

2.4.5 Implementation of stormwater infiltration in the EU

Based on the legislation and technical guidelines presented, urban stormwater infiltration practices are increasing worldwide and are common in the **EU**. There is currently no specific information on the number of swales or permeable pavements that have been constructed at national or EU level. However, data from case studies and the growing number of guidelines suggest that swales and permeable pavements are being constructed with increasing frequency.

In **Germany**, a stormwater management survey of 5,079 professionals from architecture and engineering firms, construction companies, government agencies, universities, and building material distributors found that 84 % of these professionals were involved in stormwater infiltration. This represents a slight increase of 3 percentage points from a previous survey conducted in 2020 (Mall, 2023). There has been an increase in stormwater infiltration systems over the past 35 years due to climate adaptation strategies (Helmreich et al., 2022). Stormwater infiltration facilities are known as best management practices and can often be constructed without further approval from stormwater management authorities (Dierkes et al., 2015). Swales are more common than swale-trench systems. The implementation of the stormwater fee in many communities has led to an increase in the number of stormwater infiltration facilities. This is attributed to the fact that the fee is levied based on the size of sealed area, prompting the application of measures to enhance stormwater management (Dierkes et al., 2015).

European countries report about the implementation of swales and permeable pavements, often in new development areas (IAHS, 2006). In Scandinavia, infiltration basins are widely used as they can additionally store snow. In contrast, in Southern Europe (Greece, Italy, Spain and Portugal), the use of infiltration basins is sometimes limited due to “high peak intensity flow conditions”.

For the **Netherlands**, the interactive website climatescan.org lists more than 800 swales, 250 grass filled pavers and 350 mostly impermeable concrete interlocking pavers. These numbers are not representative but show the ubiquitous use of swales and permeable pavements. Swales have been used in the Netherlands since 1998 (Boogaard, 2015).

In **Denmark**, 64 % of urban catchments have separated sewer systems (Jensen et al., 2020). Trench systems and permeable pavements are commonly used (Kai Bester, personal communication).

In **Switzerland,** permeable pavements are commonly used with both small (< 3 %) and large (> 6 to 12 %) joint proportions, as well as grid systems and grass pavers (Thomas Rohr, personal communication). Permeable pavements are mainly built in private areas. Porous concrete or asphalt are rarely used, also because of clogging and low resistances by freeze-thaw cycles in winter.

A study in **Spain** found that out of 21 investigated sustainable urban drainage projects studied, only 5 included bioretention, vegetated swales or infiltration systems (Andrés-Doménech et al., 2021). However, swales and permeable pavements were already used for the Barcelona 1992 Olympic Village (IAHS, 2006).

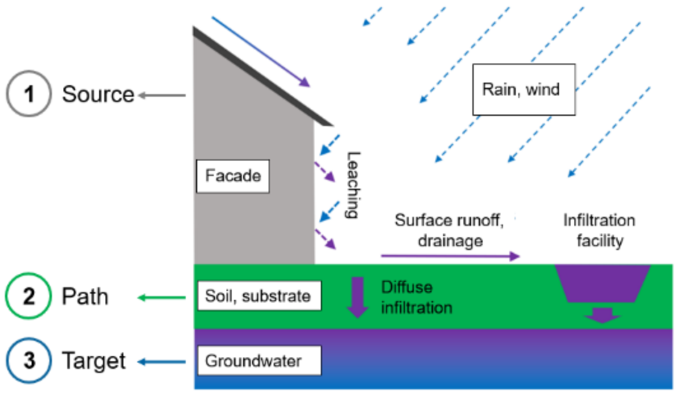
3 Emission scenarios definition

3.1 A holistic source – path – target concept

This project aims to assess the release of biocides in urban soils using computer models to generate representative and relevant scenarios for the biocide authorization process. This necessitates a comprehensive characterization of input parameters, which is more extensive in scope compared to the established Emission Scenario Documents (ESD) of the European Chemicals Agency (ECHA). To achieve this, a holistic **source-path-target** concept was employed (Figure 5), which encompasses the description of the source (façade), the pathway (soils and substrates), and the target (groundwater).

Firstly, it is essential to characterize the **source** to accurately estimate the type and quantity of emitted biocides. The prevalence of biocides in Germany was ascertained through a comprehensive survey of manufacturers. Furthermore, to establish typical building geometries in urban areas, extensive GIS data sets were analyzed and statistically evaluated.

Figure 5: The source – path – target concept



A representation of the holistic source – path – target approach to biocide emissions from façades to groundwater.
Source: Own illustration, OST

Secondly, it is necessary to determine and parameterize the physicochemical properties of substrates near buildings and infiltration facilities (**path**). For this purpose, characteristics of surfaces near buildings and dominant pathways of urban stormflow were identified. As a result, a classification between permeable pavements and infiltration systems is proposed for the emission of biocides into urban soils. An overview of urban soils in several German residential areas is provided in the following chapter. This information was obtained by evaluating urban soil maps provided by state agencies (state geological offices, state soil research offices, environmental offices, etc.) as well as data from literature and unpublished studies.

Finally, the investigation extends to representative attributes of the **target** component, i.e., groundwater. Parameters such as the depth to groundwater and the dilution effects are scrutinized. Despite the complexity of biocide emissions from buildings in urban regions, this study aims to define simple but realistic scenarios characterized by the key parameters influencing the emission process. Effort is placed on optimizing the level of detail of the scenarios to maximize simplicity and acceptability while ensuring representativeness.

In the following chapters, the various scenario parameters and their derivation are described in detail.

3.2 Source term

3.2.1 Biocide Products

To realistically estimate the relevant biocides as well as their embedding form (free vs. encapsulated) and the quantities used in Germany, stakeholders (manufacturers, associations) were surveyed. The questionnaires sent covered various aspects, including the quantity, concentration and relevance of the biocides used. Substances of the product type 7 “film preservatives” (PT 7) for paints and plasters of exterior façades, disinfectants and algaecides for façade cleaning (PT 2) and construction material preservatives (PT 10) were considered. A total of 7 questionnaires were dispatched, in which the most important manufacturers of biocides were addressed. As a result, the findings should provide a comprehensive representation of the biocide market share in Germany. The feedback from the manufacturers reflects the situation until the end of 2021 (Figure 6).

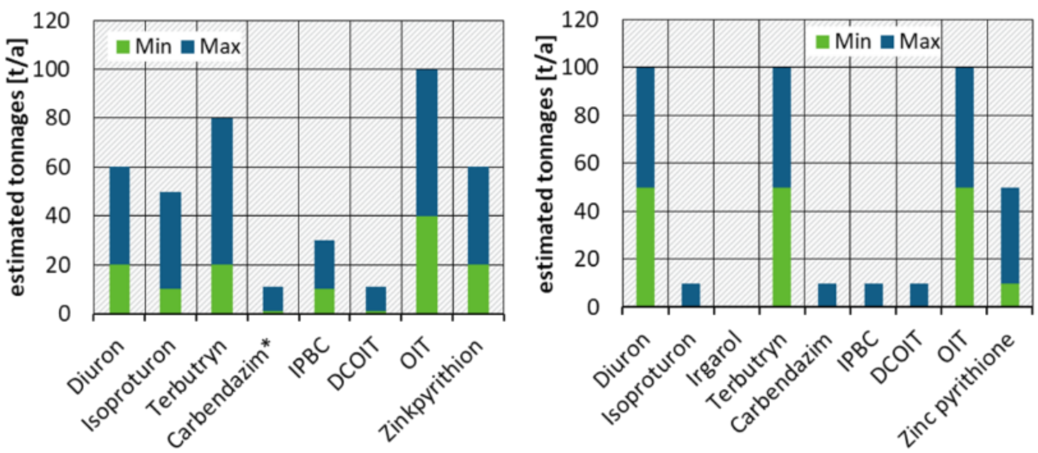
Results for PT7

According to the manufacturer's response to the survey related to PT7, several substances including DCOIT, diuron, IPBC, isoproturon, OIT, terbutryn and pyrithione zinc are used for applications on façades. No other substances were identified for this specific application. Furthermore, the survey revealed that Carbendazim will be discontinued from the year 2022 on.

Regarding the embedding form of the substances, manufacturer's information differed greatly based on the substance. For instance, IBPC is available in both encapsulated and non-encapsulated form, depending on the manufacturer. Although variable embedding forms were reported for most of the above-mentioned substances, a general tendency towards increased encapsulation was observed. Manufacturers expressed the view that, in the future, all biocidal active ingredients from PT7 will be encapsulated.

The concentrations recommended by biocide manufacturers for use in plasters ranged from 100 to 1000 ppm, depending on the substance. For paints, the recommended amount is usually higher, falling in the range of 100 – 1500 ppm depending on the substance. This coincides with the findings from a previous survey (Burkhardt and Dietschweiler, 2015).

Figure 6: Annual usage tonnages of various biocides estimated by manufacturers



Left: Survey within this project with data of 2021; Right: Earlier survey (Burkhardt and Dietschweiler, 2015).
Source: Own illustrations, OST

According to manufacturer estimates, the consumption of diuron, isoproturon, terbutryn, OIT, and carbendazim as film preservatives (PT7) constitutes a significant portion, ranging from

80 % to 100 % of the total consumption volume across all product types (PT1-PT22). However, for IPBC, the amount consumed as PT7 is comparatively lower, estimated to be only 10 % - 20 % of the total consumption across all product types (PT1-PT22). In the case of DCOIT and zink pyrithione, the manufacturers did not agree on how large the amount used as PT7 is compared to other applications. For DCOIT, the figures varied between 40 – 100 % and for zinc pyrithione between 10 - 80 %, as DCOIT is also increasingly used for applications in PT21 (antifouling) and zinc pyrithione is also widely used in PT6 as a in-can preservative for interior paints.

Manufacturers were also queried about the use of biocides in roof paints. The estimated market share of biocides in roof paints is minor, accounting for less than 5 % of the total usage of substances falling under PT7. According to information provided by manufacturers, the annual consumption volume of biocides in roof paints typically falls within the range of 1 to 10 tons per annum. Itis worth noting that for the application of biocides in roof paints, the substances are reported to be exclusively utilized in encapsulated form.

Results for PT2

The survey findings indicate that only quaternary ammonium compounds (QACs), specifically BAC (benzalkonium chloride) and DDAC (didecyldimethylammonium chloride), are used in product type PT 2 (disinfectants and algaecides for outdoor surfaces, for façade cleaning and green pavement removal). These substances are applied at concentrations ranging from 0.1 % to 1 %. Other substances such as nonanoic acid, lactic acid and chlorocresol were not mentioned by any manufacturer. However, UBA has information that both nonanoic acid and lactic acid are listed in PT2 registrations.

At 20 – 30 t/a, the consumption of substances falling under PT2 are significantly lower compared to the substances of PT7 (120–280 t/a). The market share of QACs in PT2, when compared to all product types (PT 1-22), is estimated to be less than 5 %, or < 1 % for applications on roof areas. This indicates that the applications within PT2, which exclusively involve quaternary ammonium compounds (QACs) based on the survey results, have a relatively minor significance in the broader context of the product types relevant to this project.

Results for PT10

In the field of construction material preservatives (PT10), BAC is the most commonly used biocide, with a consumption of 20-30 t/a. OIT also finds application in PT10, but its consumption volume of < 1 t/a is significantly lower than that of BAC.

The market share for PT10, in the case of BAC, falls within the range of 5 % to 10 % when compared to all product types (PT1-PT22). For OIT it is estimated to be < 5 %. Due to the effort and costs involved in substance registration, manufacturers anticipate that the use of active ingredient in PT10 (as well as PT2) will remain stable or slightly decrease over time. The comparison survey's results with a previous study confirms this assumption (Burkhardt and Dietschweiler, 2015). In fact, 10–50 t/a QACs and 1-10 t/a OIT were used as PT10 in 2015, a decrease of nearly 50 % compared to this study's survey.

3.2.2 Building geometry

To estimate the release of biocides from façades, the building geometry must be described, as it influences the total façade area available for leaching. Multiple standard building geometries are documented in literature for research and regulatory purposes (e.g. BPR/OECD house, DIBt house), which are rarely confirmed by a true empirical basis. This section aims to establish a representative building geometry for the emission of biocides in urban areas using satellite data, as well as to verify the suitability of already existing standard geometries.

Three-dimensional building models with a Level of Detail 2 (LOD2) were collected for entire Switzerland and for several cities in Germany (Berlin, Braunschweig, Dresden, Freiburg, Göttingen, Hannover, Leipzig, Osnabrück). The data was analysed using the geographic information system software ArcGIS Pro to derive the average width, length and height of residential buildings in urban regions. A detailed description of the methodology used can be found in the Appendix (Section A.1).

In total, the datasets characterize over 5.5 million buildings. Of these, only buildings with a length, width, and height greater than 2 m were selected for further analysis, resulting in of approximately 3.3 million buildings. An example of this selection is shown in Figure 7 for an area of Braunschweig that includes both residential and industrial buildings. Having this said, even if all buildings were to be included the average width, length and height would have deviated by less than 15 %.

Figure 7: Selection of residential buildings

The two images illustrate an area of Braunschweig containing both residential and industrial buildings. Only the former, shown in yellow, were selected for deriving a reference building geometry, while the latter, shown in white, were excluded (left). The satellite image (right) is provided for reference.
Source left: Own illustration, OST. Data taken by the Office for Geoinformation and Land Surveying of Lower Saxony
Source right: Google Maps, 2022

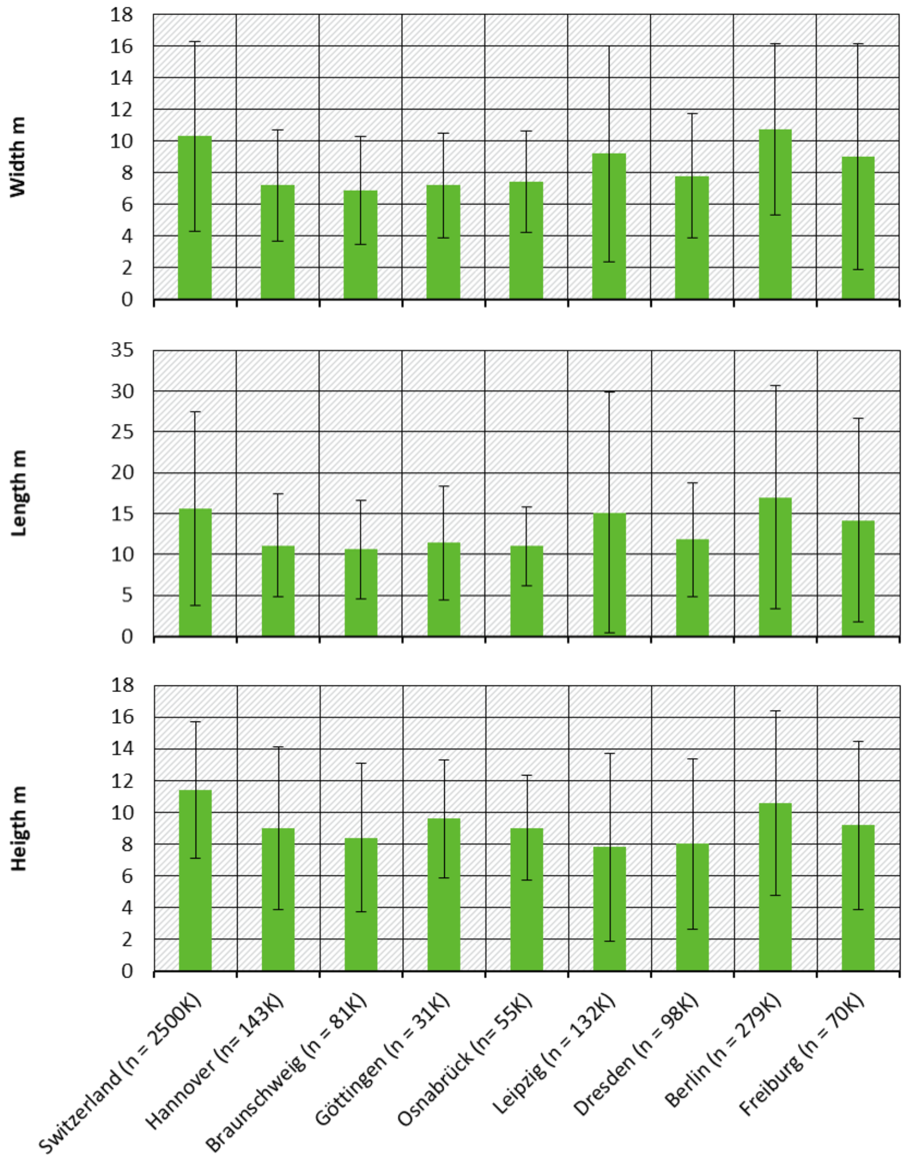
In order to assign a single width, length and height to each building, complex building geometries had to be simplified and each building was represented by the smallest possible rectangle containing the entirety of the building. For this purpose, the ArcGIS Pro processing tool "Minimal Bounding Geometry" was used, as shown in Figure 8.

Figure 8: Simplification of building geometries

Simplified representation of building geometries as rectangles (right) based on LOD2 building models (left).
Source: Own illustrations, OST. Data taken by swissBUILDING3D 2.0, Swisstopo.

Figure 9 shows the average width, length and height of residential buildings in urban areas of Switzerland as well as in several German cities, with a total of over 3.3 million buildings. No statistically significant differences in the width, length, and height of residential buildings were found for the different regions examined, with the mean width, length, and height being approximately 8.5 m, 13 m, and 9 m, respectively.

Figure 9: Average width, length and height of residential buildings in Switzerland and German cities



Average width, length and height of residential buildings in urban regions of Switzerland and in selected German cities based on analyses of building models (LOD2) in ArcGIS Pro. The black bars indicate the standard deviation.
Source: Own illustrations, OST

Table 3 provides an overview of the most used reference geometries for research and regulation related to biocide leaching from façades. The average width and length determined from empirical building models (Figure 9) fit quite well with the already existing reference building geometries. The same cannot be said for the building height, which is especially underestimated by the BPR/OECD house.

Table 3: Building geometries used for regulation and in research

Parameter	BPR/OECD house	DIBt house	Multi-storey house	EmbaPro house
Defined in	ECHA ESD	Hochstrasser et al., 2016	Tietje et al., 2018	Burkhardt et al., 2021a
Length (m)	17.5	17.5	17.5	17.5
Width (m)	7.5	7.5	7.5	7.5
Height (m)	2.5	7	21	10
Plaster façade (%)	100	100	80	100
Orientation	n/d	n/d	Longer sides E/W	Longer sides E/W
Roof area (m^2)	145	n/d	n/d	145
Roof form	Pitched 25°	n/d	n/d	Flat roof
Roof material	n/d	n/d	n/d	100 % bitumen

n/d = not defined.

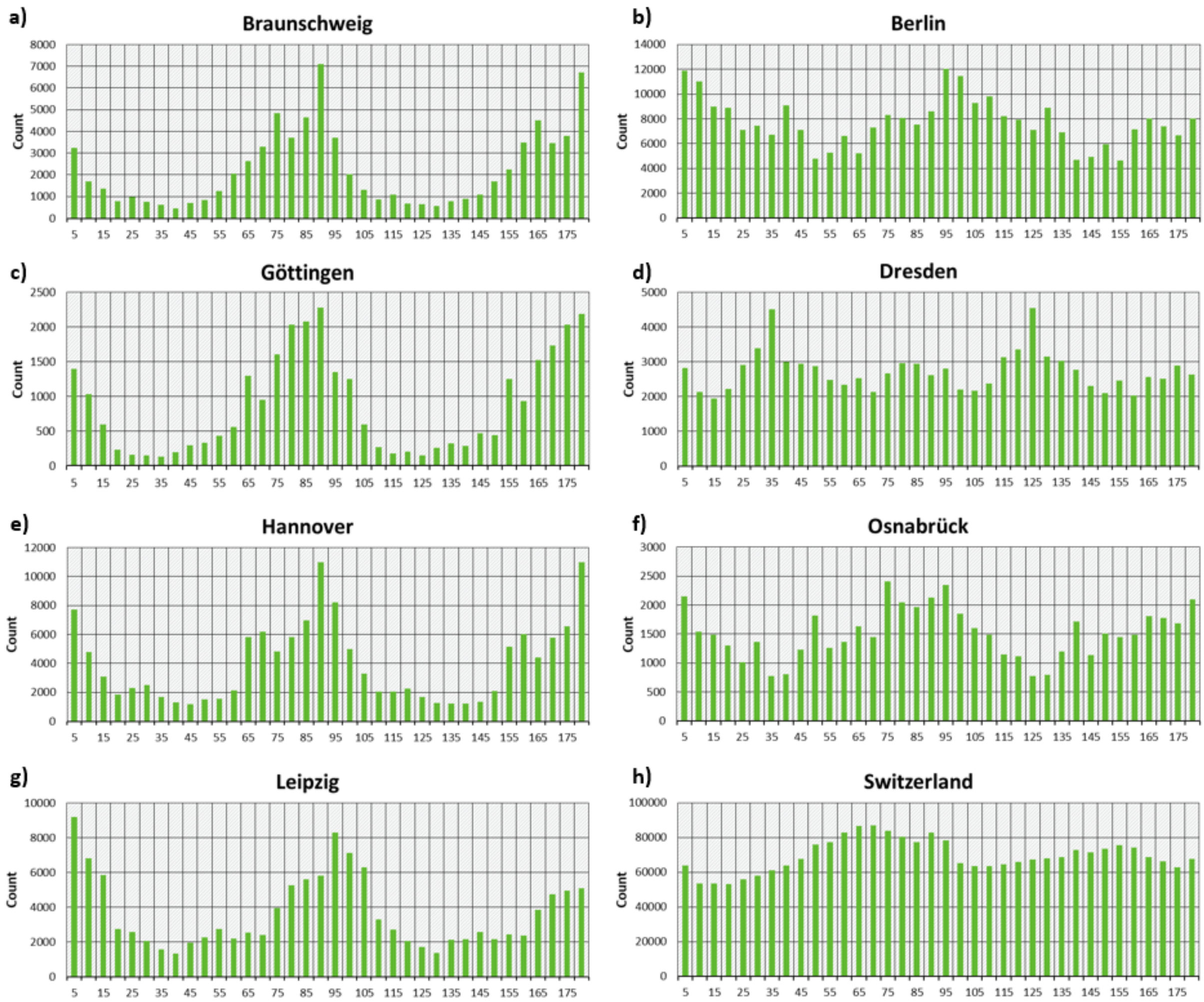
To estimate the release of biocides from façades, not only the total area of the façade but also its orientation should be considered. This since a façade perpendicular to the prevailing wind direction of a given region leads to greater exposure to wind-driven rain and thus to higher emission of biocides. Broadly speaking, the prevailing wind direction in Central Europe is west, which means that buildings whose longest façades face west tend to experience greater biocide leaching than buildings whose longest façades face other cardinal directions.

Figure 10 illustrates the orientation of residential buildings in urban areas of Switzerland and several German cities, with respect to the longest façade of the building. In general, the longest façades of most buildings in the German cities investigated are preferably facing north (resp. south) and west (resp. east), with fewer façades facing northwest (resp. southeast) or northeast (resp. southeast). This observation is particularly pronounced for Braunschweig, Göttingen, Hannover and Leipzig, while this is less evident for Berlin and Osnabrück. Both in Dresden and in urban regions of Switzerland, the orientation of buildings seems to be more evenly distributed across all cardinal directions. The differences may be due to the different topology of each region. This could explain why the distribution of building orientations is most homogeneous in Switzerland, which has the greatest topological diversity of the examined datasets.

The worst-case scenario for Europe would be to assume that all buildings are oriented so that the longest façades face west, since the prevailing wind direction in Central Europe is west. In reality, the portion of buildings whose longest façade faces west is unlikely to exceed 50 % at a regional or city scale, while higher portion are possible at a district or neighborhood level.

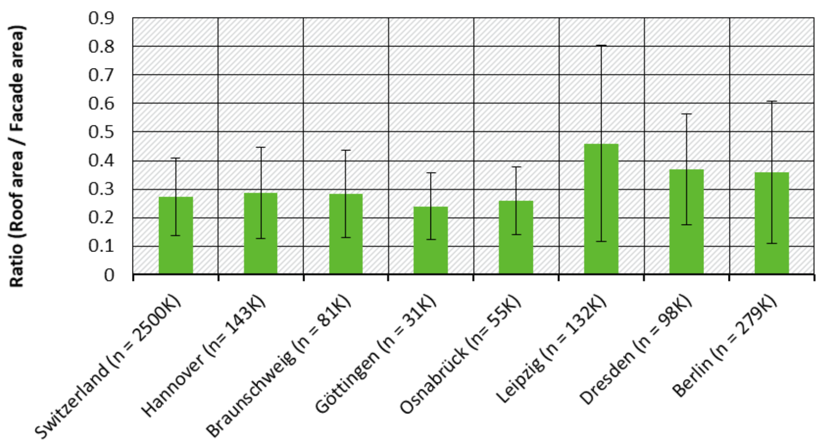
Biocide concentrations in stormwater are influenced by runoff from surfaces that contribute to dilution. Therefore, when characterizing the building geometry, it is necessary to consider roofs as well. Figure 11 provides information about the ratio between the projected roof area and the façade area of the analyzed locations. On average, a ratio of 0.3 was observed (SD = 0.2). This indicates that a standardized building will have about three square meters of façade area for every square meter of roof area. This observation closely aligns with the data presented in Table 3 for the EmbaPro and DIBt standard houses, which have a roof-to-façade area ratio of 0.29 and 0.38, respectively. The roof-to-façade ratio is approximately 1.1 for the BPR/OECD building and approximately 0.13 for the multi-storey building, due to the difference in building height.

Figure 10: Orientation of residential buildings in German cities and in urban areas of Switzerland



Orientation of residential buildings in Switzerland and German cities based on the longest façade. 0° and 180° indicate that the façade is directed to the north (resp. south) and thus faces west (resp. east) and 90° indicates that the façade is directed to the east (resp. west) and thus faces north (resp. south).
Source: Own illustrations, OST

Figure 11: Roof to façade surface ratio



Ratio between projected roof area and façade for residential buildings in urban regions of Switzerland and in selected German cities based on analyses of building models (LOD2) in ArcGIS Pro. The black bars indicate the standard deviation.
Source: Own illustration, OST

3.2.3 Building materials

The GIS assessment of building geometry (see 3.2.2), does not include information regarding the typical material composition of an average building. To address this gap, a review of various studies was conducted to empirically derive a representative material composition. The following sections outline these studies and provide a comparative analysis of their findings.

Project "BaSaR"

In a study conducted by Wicke et al. (2021), two distinct residential areas, referred to as area A and B, within the city of Berlin were investigated. The research involved a comprehensive approach that included field investigations, product testing, and model simulations. The study aimed to provide insights into the release of biocidal substances from building components and their subsequent impact on stormwater quality. To achieve this goal, samples of roof and façade runoff were collected and analyzed in the two newly developed residential areas in Berlin over a span of 1.5 years. Moreover, the buildings' orientation and material composition (material type and occurrence) were recorded.

Each of the two residential areas included around 120 apartments. For each building, the areas of all façades and roofs were calculated. The façades were divided into façade (plaster), glass (windows) and balconies. The detailed outcomes for area A and B are shown in the Annex Section A.2 (Table 17, Table 18). Area A comprised about 10'000 m^2 of façade area, of which 70 % was plaster, 10 % glass and about 20 % balconies. The composition of the individual buildings did not vary significantly.

The composition of area B resembled that of area A. With a mean value of 65 %, the fraction of plaster in area B represented the largest share of the façade area. Glass accounted for 17 %, which was slightly higher than the corresponding figure in area A. Conversely, the proportion of balconies in area B was lower at 18 %. Figure 12 offers a representative view of the two areas to illustrate the examined buildings, which are typical modern multi-story buildings.

Figure 12: Buildings of area A (left) and area B (right)

Source: Wicke et al. (2021)

Building survey in Zürich by OST

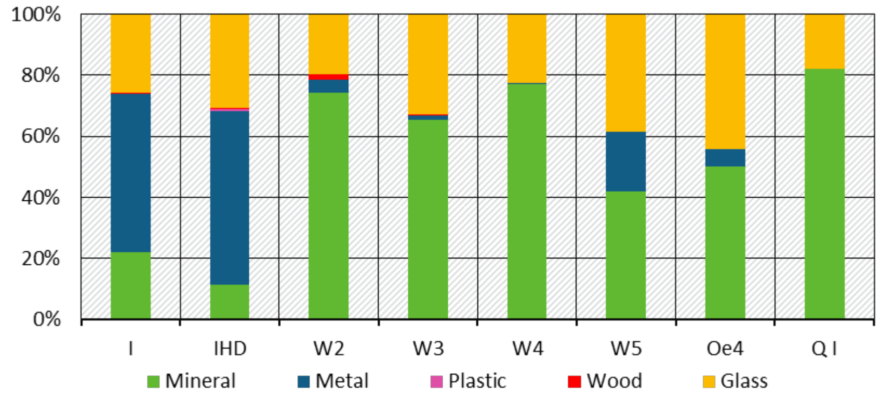
As part of a student project at OST, surveys were conducted in 2015 in Zürich (Switzerland) on approximately 200 buildings in four different districts. For each district, 8 different area zones were further distinguished according to the building and zoning regulations of the city of Zürich: industrial zones (I), industrial zones with trade and service enterprises (IHD), zones for public buildings (Oe4), neighborhood preservation zones (Q), and 2-5-storey residential zones (W2-

W5). The residential zones (W2-W5) comprised most of the buildings surveyed, with 142 buildings. (Annex Section A.2, Figure 42).

The material proportions of the individual façades were determined with a resolution of 10 %. The materials were divided into the categories glass, wood, plastics, metals and mineral materials (which also included plastered façades), with various subcategories being defined for each category. For example, a mineral surface could stand for a façade made of exposed concrete, as well as for a plastered façade. The age of the examined buildings was obtained from the building plan of the city of Zürich.

Figure 13 displays the resulting proportions of the different material categories for the various zones. Notably, metal is mainly used in the industrial zone (I) and in the industrial zone with trade and service companies (IHD), where it constitutes more than 50 % of the total façade area. In the remaining zones, metal in façades is of lesser significance. Only in the 5-storey residential zone (W5) does metal occur with a share of about 20 %. This observation suggests that buildings exceeding a certain height are less likely to have plastered façades, and instead, metal cladding of the building envelope is more prevalent.

Figure 13: Mean façade material proportions [m^2] of the different zones from the survey in Zürich. Shown are the results of all surveyed districts



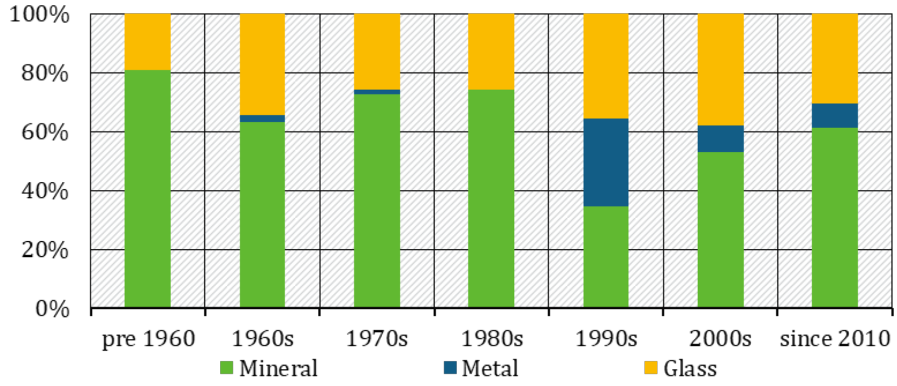
Industrial zones (I), industrial zones with trade and service enterprises (IHD), zones for public buildings (Oe4), neighborhood preservation zones (Q), and two- to five-story residential zones (W2 - W5)
Source: Own illustration, OST

In the zones pertinent to this study (W2-W5), it's evident that mineral materials are the primary choice for façades. On average, in categories W2 to W5, mineral materials make up 58 % of the total façade area. Within this mineral fraction, nearly half (48 %) is attributed to plastered façades, while the rest predominantly consists of concrete façades. Consequently, it can be concluded that approximately every other residential building featured plastered façades, accounting for 28 % of the total façade areas under consideration.

The average proportion of glass in relation to the total façade area was 32 % when considering all types of zones. Within residential areas, the average contribution of glass was nearly identical, standing at 33 %, with variations ranging from 22-44 %. It's noteworthy that the material categories of plastics and wood had a negligible presence in all zones.

To assess the influence of the building age, the material composition of the buildings was compared by year of construction, as depicted in Figure 14. Specifically, this analysis focused on buildings within the residential areas W2 to W5, excluding considerations of wood and plastics. The comparison of material composition across different decades reveals that the material composition of residential buildings has remained relatively consistent over the last few decades. The most noticeable change was a temporary increase in the use of metal in the 1990s, which has since decreased. Consequently, mineral materials remain the prevailing choice for the composition of residential building façades.

Figure 14: Material proportions of residential buildings (W2-W5) with different years of construction



Source: Own illustration, OST

Building survey in Freiburg by UNI

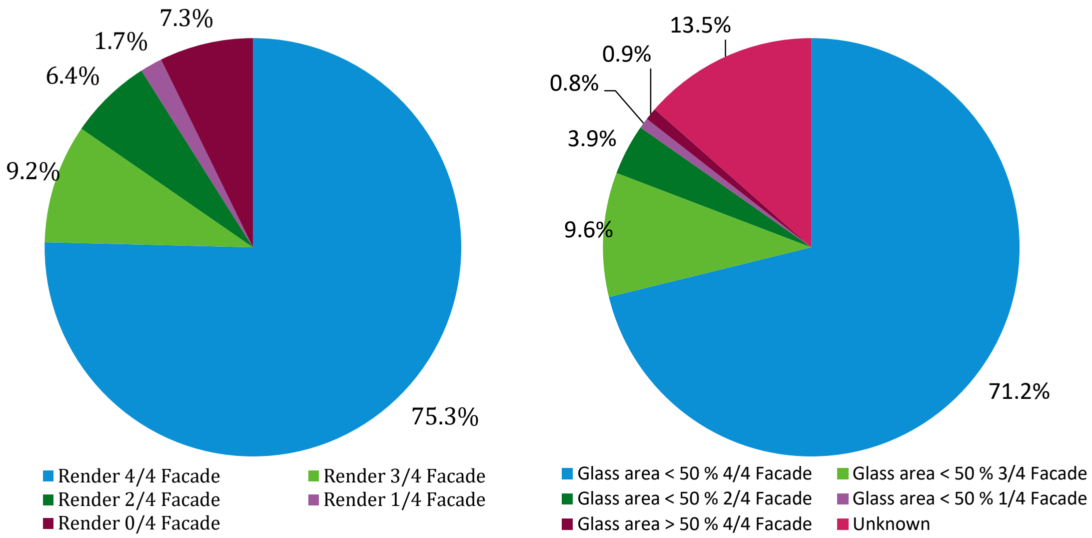
Between 2019 to 2021, several building surveys were conducted by students of the University of Freiburg (NAVEBGO, 2023). In total, the surveys included approximately 2200 buildings in 15 different neighborhoods. For each façade, it was recorded, among other things, whether the proportion of glass was less than 50 % (=1) or more than 50 % (=0) of the total façade area. Additionally, the surveys documented whether each façade was plastered (1) or not plastered (0).

The study did not measure the precise areas covered by glass, plaster, or other materials on façades. Instead, when the glass area on a façade (considering both glass and plaster) was less than 50 %, the plaster percentage was recorded as greater than 50 %. Numerical values for "glass fraction" and "plaster fraction" were then calculated for each façade and averaged for the entire building. Consequently, the binary values assigned to individual façades led to whole-building values of 0, 0.25, 0.5, 0.75, and 1.

Figure 15 presents the survey results, indicating that a majority of the buildings featured some level of plastering. Specifically, 75 % of all buildings had plaster on all four of their façades, while an additional 10 % were plastered on three out of four façades. The average area of the façades could not be estimated from the data. However, since 75 % of the buildings included in the study were plastered on all façades (4/4) and 71 % of the buildings had less than 50 % glass on all façades, it can be assumed that the total plastered façade area is on average greater than 50 %. For example, the study demonstrates that 56 % of the buildings surveyed are plastered on all four façades and contain less than 50 % glass.

The examination of the glass fractions reveals that approximately 70 % of the buildings had less than 50 % glass on all façades (Figure 15, right). About 10 % of the buildings showed a glass percentage of < 50 % for three of the four façades. For 13 % of the buildings the glass fraction was not recorded. Across all buildings surveyed, 93 % of the façades consists of less than 50 % glass.

Figure 15: Results of building surveys in Freiburg



Left: Occurrence of plaster on façades, right: Occurrence of glass surfaces on façades
Source: Own illustration, UNI Freiburg

Summary of the studies on building materials

A comparison of the results is provided in Table 4. It should be noted that in the Berlin and Zürich studies, the material composition and fractions were based on the total façade area examined, while in the Freiburg study, they were related to the number of buildings surveyed.

Regarding the distribution of plastered buildings, the studies show fractions ranging from 50-100 %. However, it's worth highlighting that the study in Berlin (BaSaR) specifically focused on plastered buildings, so it's not representative in this regard as it intentionally targeted such structures.

Table 4: Comparison of the building materials from three different studies

	Berlin (BaSaR)	Zürich (OST)	Freiburg (UNI)
Buildings considered	12	200	2200
Districts considered	2	4	15
Proportions based on	Area (m^2)	Area (m^2)	Buildings (-)
Plastered buildings	100 %	-	86 %
Proportion mineral	68 %	65 %	-
Proportion plaster	68 %	28 %	> 50 % (valid for at least 56 % of total façade area
Proportion glass	11 %	33 %	< 50 % (valid for 93 % of total façade area)
Proportion balconies	21 %	-	-

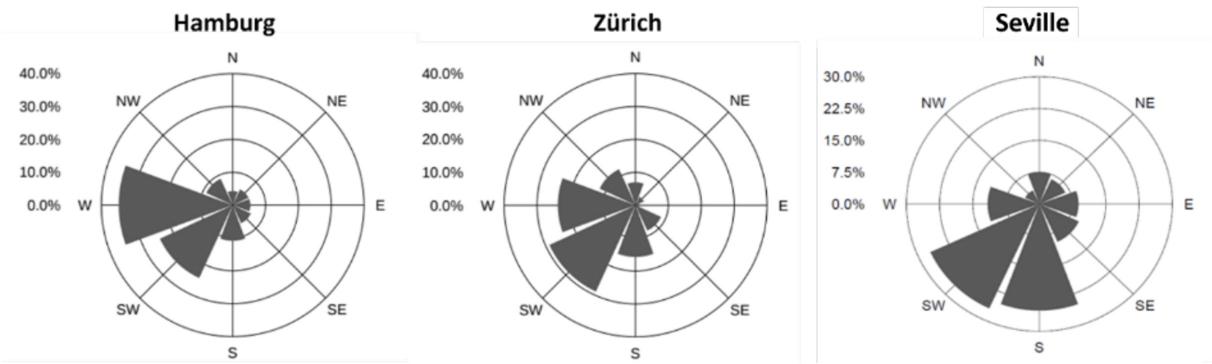
3.2.4 Weather conditions

Precipitation, wind speed, and wind direction are key factors influencing biocide emissions from façades. In this project, three distinct locations (Hamburg, Zürich and Seville) were selected to represent different climatic zones across Europe. Hamburg is situated in a temperate region with a strong maritime influence, characterized by high and frequent precipitation along with windy conditions. Zürich, on the other hand, is in a pre-alpine region with an annual precipitation exceeding 1000 mm per year. Meanwhile, Seville is positioned in a Mediterranean climate zone, where total precipitation is relatively low, but occasional intense precipitation events occur. Hamburg and Seville, with average yearly precipitation of about 770 mm and 540 mm respectively, are among the selected locations included in the FOCUS models for the regulation of plant protection products.

Climate data series with hourly resolution spanning the period from 2005 to 2015 were chosen for the modelled scenarios. The essential parameters necessary for the modeling included precipitation, wind direction, wind speed, temperature, relative humidity, global radiation, and potential evapotranspiration.

Wind-driven rain drives biocide emissions from façades and is strongly influenced by wind distribution. Figure 16 shows the relative wind distribution for the three locations throughout the specified time period. Hamburg is notably influenced by westerly winds, whereas in Zürich, the wind distribution leans somewhat more toward the west-southwest. In Seville, the prevailing wind direction tends to be southwest to south. Additionally, it is evident that in Hamburg and Zürich, the wind predominantly flows in one primary direction, whereas in Seville, the wind exhibits a more even distribution across multiple directions.

Figure 16: Relative wind distribution at the Hamburg, Zürich and Seville sites for the years 2005 to 2015



Source: Own illustrations, OST

3.2.5 Dynamic vs. static emission modelling

Biocide release from building façades is not linear but decreases with time (Burkhardt et al., 2012). Consequently, in addition to the dynamic release due to wind-driven rain, the nonlinear progression of the emission from the building products should also be considered for a realistic characterization of biocide emissions from façades. The COMLEAM model (COnstruction Material LEAching Model) can be used to simulate such dynamic biocide emissions.

COMLEAM uses precipitation, wind distribution and wind speed with an hourly temporal resolution as well as material properties to estimate the biocide leaching from building materials. Detailed documentation about the model and the calculation methodology can be found online at www.comleam.ch. To assess the relevance of biocide emission to groundwater for different scenarios, several calculations were performed using the COMLEAM model. These calculations were then compared to the established static emission models provided by ECHA in the form of the ESDs, see chapter 5.1.

3.3 Emission pathways

3.3.1 Relevant soil profiles for biocide infiltration to groundwater

To establish representative soil profiles for the emission pathway of biocides to groundwater, three different experimental setups, each with two soil horizons, are proposed in accordance with the literature review in chapter 2.2

(1) **Urban soil (S1)** consists of vegetated soils with an organic top layer (ca. 10 cm), underlain by urban subsoil**.**

(2) **Permeable pavements (S2)** are characterized by different types of paving stones embedded into sandy or gravelly seam material underlain by urban subsoil.

(3) **Infiltration facilities (S3)** are represented by an organic top layer (5 – 30 cm depth) underlain by urban subsoil, or in the case of swale-trench-systems by sand with direct contact to groundwater.

For these three setups relevant soil parameters are required. These are defined in following chapters.

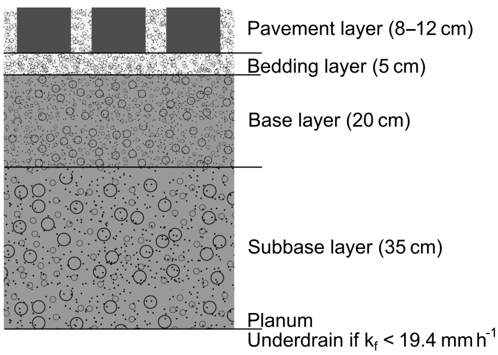
3.3.2 Urban soil

There is no systematic evaluation of urban soils, particularly at direct contact to building façades. On the one hand, OC in topsoil of urban spaces can exceed those of forested areas (Makki et al., 2021). On the other hand, loose soil material in the immediate vicinity of buildings can be expected to also consist of remnants from building activities, which are often in the sandy fraction.

3.3.3 Permeable pavements

According to German regulations, permeable pavements must be designed to fully infiltrate a 10 min rainfall with a return period of 5 years. This results in a surficial infiltration capacity of at least 97 mm h^{-1} and in a saturated hydraulic conductivity of underlying soils of at least 19 mm h^{-1} (Borgwardt, 1998). Figure 17 shows the typical layers and extent of a permeable pavement that has been built in accordance with German national regulations (Schaffitel et al., 2020).

Figure 17: Layers of a typical permeable pavement built in accordance to national regulations



Source: Schaffitel et al. (2020)

Schaffitel et al. (2020) determined the dimensions and dominating grain sizes of 18 permeable pavements in the city of Freiburg (Table 5). With a few exceptions, the pavement layer had a thickness of 8 cm. Mixtures of sand and gravel dominated base and subbase layers, only rarely finer grain sizes were found. The average degree of sealing of the permeable pavements was about 83 % (54-97 %). Infiltration rates determined with a double ring infiltrometer test are used as an estimate of the saturated hydraulic conductivity (k_f). For the study and scenarios, k_f values of 15 permeable pavements were averaged (0.000034 m/s).

Table 5: Vertical dimensions and the grain sizes in different depths of 18 permeable pavements in the city of Freiburg

No.	Depth [cm]					
	paving stones	silt	clay	sand	gravel	mortar
1	0-8	/	/	8-45	8-45	/
2	0-8	/	/	8-45	8-45	/
3	0-8	/	/	8-45	8-45	/
4	0-8	/	/	8-45	8-45	/
5	0-8	/	/	8-28	11-45	28-45
6	0-7	/	16-45	7-16	7-45	/
7	0-13	/	27-45	13-27	13-45	/
8	0-9	20-45	/	8-10, 20-45	10-20	/
9	0-8	13-45	/	8-13	8-45	/
10	0-8	/	/	14-40	8-45	/
11	0-9	/	/	/	8-45	/
12	0-8	13-21	/	9-13	8-45	21-45
13	0-8	/	/	8-23	8-45	22-45
14	0-12	/	/	12-20	12-45	20-45
15	0-8	29-45	/	8-29	8-45	/
16	0-8	29-45	/	16-29	0-45	8-16
17	0-8	/	/	35-45	8-45	8-35
18	0-8	/	/	8-13, 23-45	8-45	13-23

Source: (Schaffitel et al., 2020)

Seams in the pavement layer are decisive for water infiltration and biocide retention. With increasing age, the original seam filling (usually coarse sand) becomes less conductive (Borgwardt, 1998; Wessolek and Facklam, 1997) due to accumulations of e.g. foliage, soot, oil, etc. Whether these accumulations can act as a pollutant filter, is still largely unknown. Nehls (2007) sampled seam material of permeable pavements in the cities of Berlin and Warsaw. A dark layer at 0–1 cm depth was always distinguishable from a much brighter 1–5 cm layer. Texture of the uppermost dark layer was as follows:

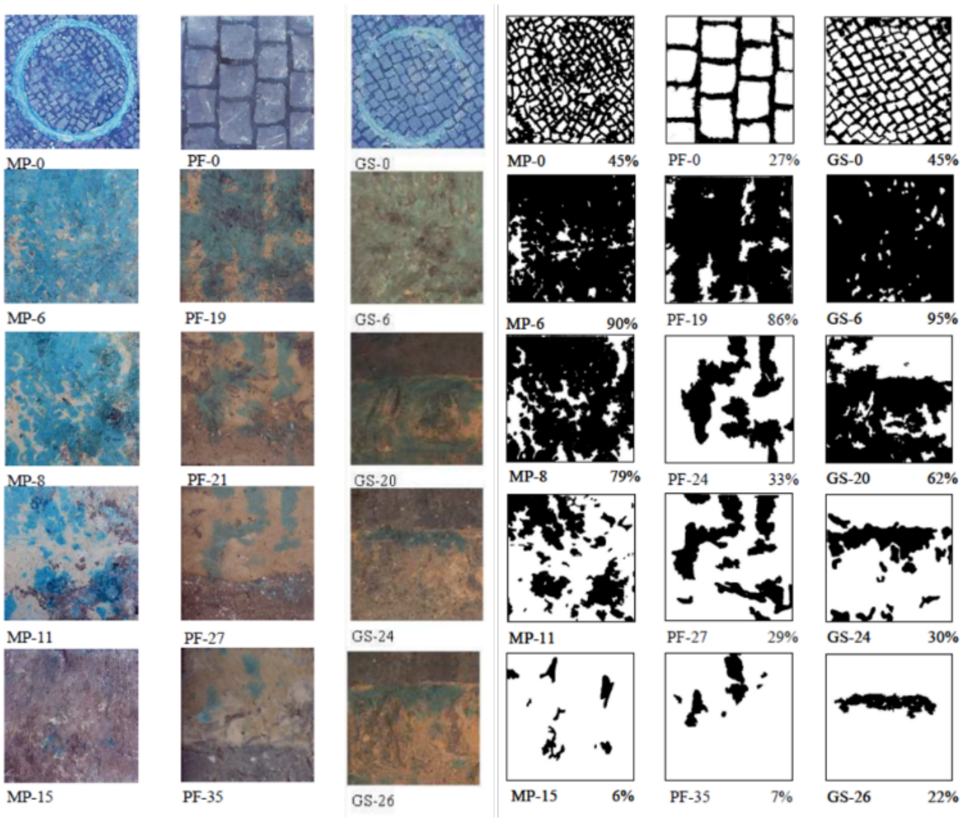
- Sand (63 – 2000 µm): 85.5 % (59.4 - 100 %)
- Silt (2 – 63 µm): 11.9 % (4.6 - 19.1 %)
- Clay (<2 µm): 2.6 % (1.7 - 3.7 %)

The texture of the brighter 1-5 cm layer was as follows:

- Sand (63 – 2000 µm): 95.8 % (78.9 - 100 %)
- Silt (2 – 63 µm): 3.3 % (2.4 - 4.2 %)
- Clay (<2 µm): 1.0 % (0.4 - 1.6 %)

The two layers also had different bulk densities, while the dark layer had a value of 1.48 g cm^{-3} (1.15 – 1.67 g cm^{-3}), whereas the bright layer was denser (1.61 g cm^{-3}; 1.57– 1.65 g cm^{-3}). The biggest difference, however, occurred in the OC. The dark uppermost 1 cm layer with OC of about 22 % (12.0 - 48.2 %), while the bright deeper layer had only 2.2 % (0.2 - 3.8 %). Tracer experiments with Brilliant Blue revealed the importance of preferential flow in the soil beneath the plasters (Figure 18).

Figure 18: Photos and binary images of the flow paths of the dye tracer solution in paved urban soils at three sites in Berlin



Numbers following the site label indicate depth in cm, the flow path cross-sectional area is given in percent.
Source: Nehls (2007)

3.3.4 Infiltration facilities

In a study by Claußner (2013), stormwater infiltration facilities on private properties were investigated. For this purpose, development plans from municipalities and selected suitable facilities for further examination were reviewed. The study particularly focused on older swale systems, of which 19 were chosen, nine of which receiving stormwater from commercial buildings.

The systems were tested by double ring infiltrometer measurements and soil samples were collected from three different soil profiles. Subsequently, the soil parameters including grain size distribution, pH value, carbonate, OC, and bulk density were determined. For the scenario definitions, an average pH of 7.2 (6.8–7.5), OC of 1.7 % (0.58-5.28 %) and bulk density of the topsoil of 1.40 g cm^{-3} (1.11 - 1.57 g cm^{-3}) and k_f (0.0000030–0.0010 m s^{-1}) of 0.00016 m s^{-1} was derived. The mean depth of the top layer (19 swales) was 23 cm (4 - 30 cm). Texture of 17 swales resulting in the followings (min, max ranges):

- Coarse, Skeleton (> 2000 µm): 25.2 % (5.5 - 61.1 %)
- Sand (63 – 2000 µm): 59.0 % (34.6 - 94.7 %)
- Silt (2 – 63 µm): 29.8 % (3.2 - 49.2 %)
- Clay (<2 µm): 11.2 % (2.2 - 17.9 %)

More recently, Bork et al. (2021) carried out column experiments with undisturbed sediment cores extracted from the top layer of three swale systems of different age. Interestingly, the typical depth gradients of pH, OC and bulk density were absent in the youngest swale, while existing in the older systems (Table 6).

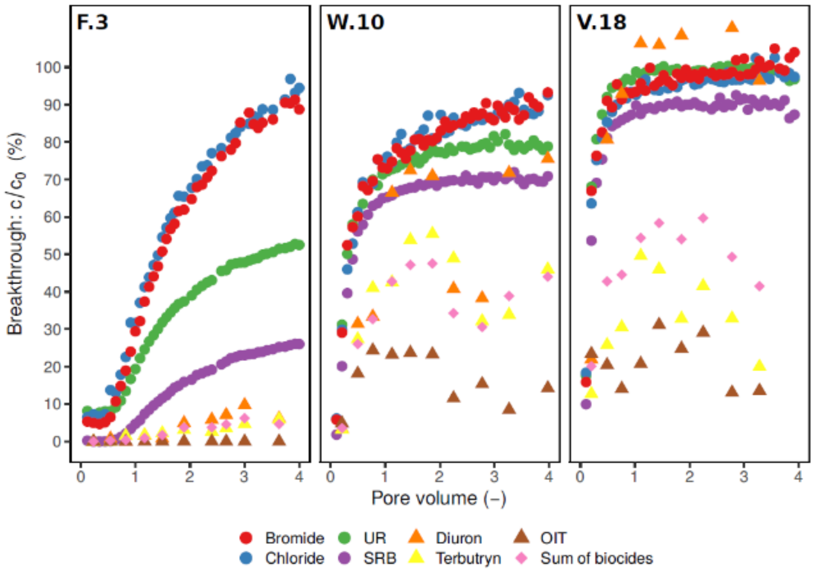
Table 6: Depth profiles of relevant soil parameters measured at three different swales in the city of Freiburg

Site	Age	Depth	pH	OC	Bulk density	Skeleton	Sand	Silt	Clay
	yrs.		-	%	g/cm-3	%	%	%	%
F.3	3	0-5	7.4	1.43	1.54	35.9	79	16	5
		5-10	7.5	1.07	1.51	42.6	-	-	-
		10-15	7.6	0.95	1.58	42.6	81	14	5
		15-20	7.5	0.99	1.56	60.9	-	-	-
		20-25	7.5	1.17	1.60	43.4	-	-	-
W.10	10	0-5	7.1	2.9	1.32	16.9	69	23	8
		5-10	7.2	-	1.52	41.2	75	18	7
		10-15	7.2	1.33	1.48	36.	73	20	6
		15-20	7.3	1.15	1.39	40.6	75	18	7
		20-25	7.4	0.98	1.48	37.3	77	16	7
V.18	18	0-5	7.0	3.65	1.02	2.9	53	35	12
		5-10	7.0	3.01	1.12	7.3	54	35	11
		10-15	7.1	1.88	1.31	18.7	54	37	9
		15-20	7.2	1.23	1.50	21.4	69	25	7
		20-25	7.2	0.85	1.50	19.6	63	31	7
		25-30	7.3	0.76	1.50	22.5	-	-	-

Source: Bork et al. (2021)

The breakthrough curves of tracers and biocides in the saturated column experiments can be used to illustrate the effect of preferential flow paths (Figure 19). These had become progressively more important with increasing age of the swale system. While preferential flow paths were absent in the 3-year swale (F.3), they caused quick breakthroughs in the 18-year swale system (V.18).

Figure 19: Breakthrough curves of tracers and biocides in soil column experiments of swale soils



The tracers used are bromide, chloride, uranine (UR), sulforhodamine B (SRB), diuron, terbutryn and OIT. F3: 3 year swale system, W.10: 10 year swale system, V.18: 18 year swale system.
Source: Bork et al. (2021)

3.4 Target

3.4.1 Depth to groundwater

The depth to groundwater defines the depth of the unsaturated zone and thus the depth of a representative soil profile for the scenarios in this study. Depth to groundwater beneath cities is highly variable and depends on the local geology (Table 7). Appendix A.4 provides a detailed analysis of six German cities, while data for Berlin is presented in detail below. A representative minimum depth to urban groundwater in Germany typically stands at 1 m, with the lowest values occurring in proximity to the rivers or within floodplains.

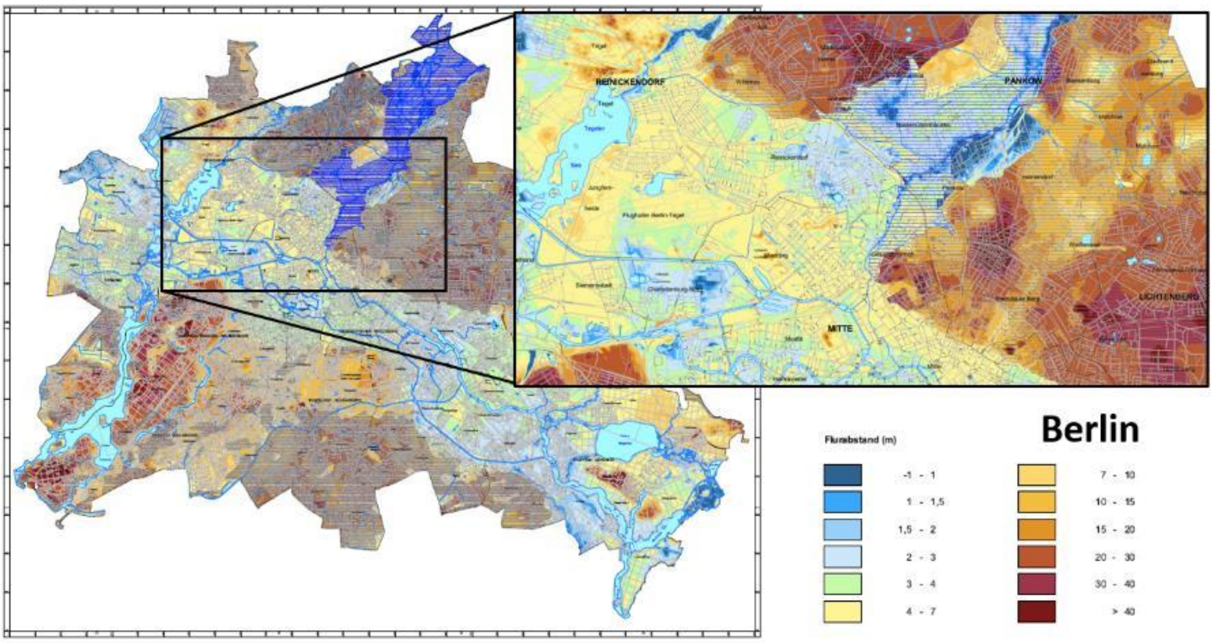
Table 7: Depth to groundwater and local geology of six German cities

City	Minimum depth to groundwater [m]	Range of depth to groundwater [m]	Geology
Berlin	1	<2 to 40	Glacial valley
Hamburg	1	<2.5 to 90	North German lowland, glacially shaped
Dresden	2	<2 to 60	Elbe floodplain
Munich	2	<2 to 18	Munich gravel plain
Mannheim	2	<2 to 20	Upper Rhine Valley
Ingolstadt	1	1 to 8	Donau Floodplains

Berlin

Within the central glacial valley, the depths to groundwater in the city of Berlin are in the range of 2-4 m below ground (Figure 20). Distances of less than 2 m are generally found in the vicinity of surface waters, in districts of Pankow, or in the Spandau Forest. In the plateau areas, the depth to groundwater generally increases, often exceeding 10 m. Collectively, the categories of 2–4 m, 4-10 m, 10–20 m and 20–40 m each account for approximately 20 % of Berlin's city area. Areas with groundwater distances of less than 2 m still constitute around 12 % of the city area. Very high distances to groundwater exceeding 40 m only occur at morphological high altitudes in 1 % of the city area. For this study, a realistic scenario for the minimum depth to groundwater is 1 m.

Figure 20: Depth to groundwater in the city of Berlin



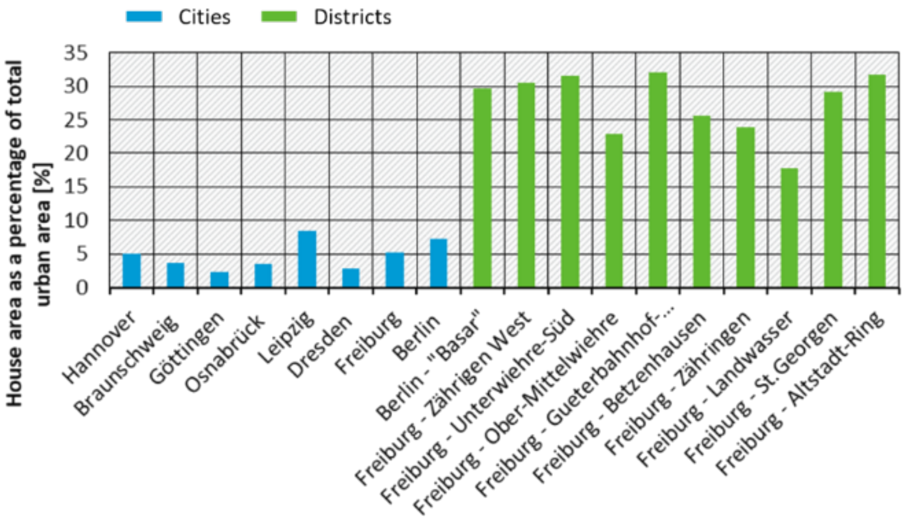
Source: www.berlin.de/umweltatlas/wasser/flurabstand/2006/karten/artikel.998083.php

3.4.2 Transfer-factor to groundwater

The groundwater concentration of biocides emitted from façades is affected by the building density in a given urban area. Figure 21 presents the projected surface of residential buildings as a percentage of total urban area for several German cities and urban districts. A distinct difference can be noted between the city and district level, signifying a lower potential for groundwater dilution and, conversely, a higher building density at the district level. On average, the total projected surface of residential buildings in cities accounts for approximately 5 % of the total urban area, and up to 30 % in urban districts. This implies that each building can be assigned a groundwater area equal to about 20 times its projected surface in cities and about four times its area in urban districts.

This suggests that, when defining a worst-case scenario for modeling groundwater biocide concentrations, it may be more appropriate to establish boundaries at a representative urban district scale rather than at the broader city scale.

Figure 21: Projected area of residential buildings as a percentage of total urban area

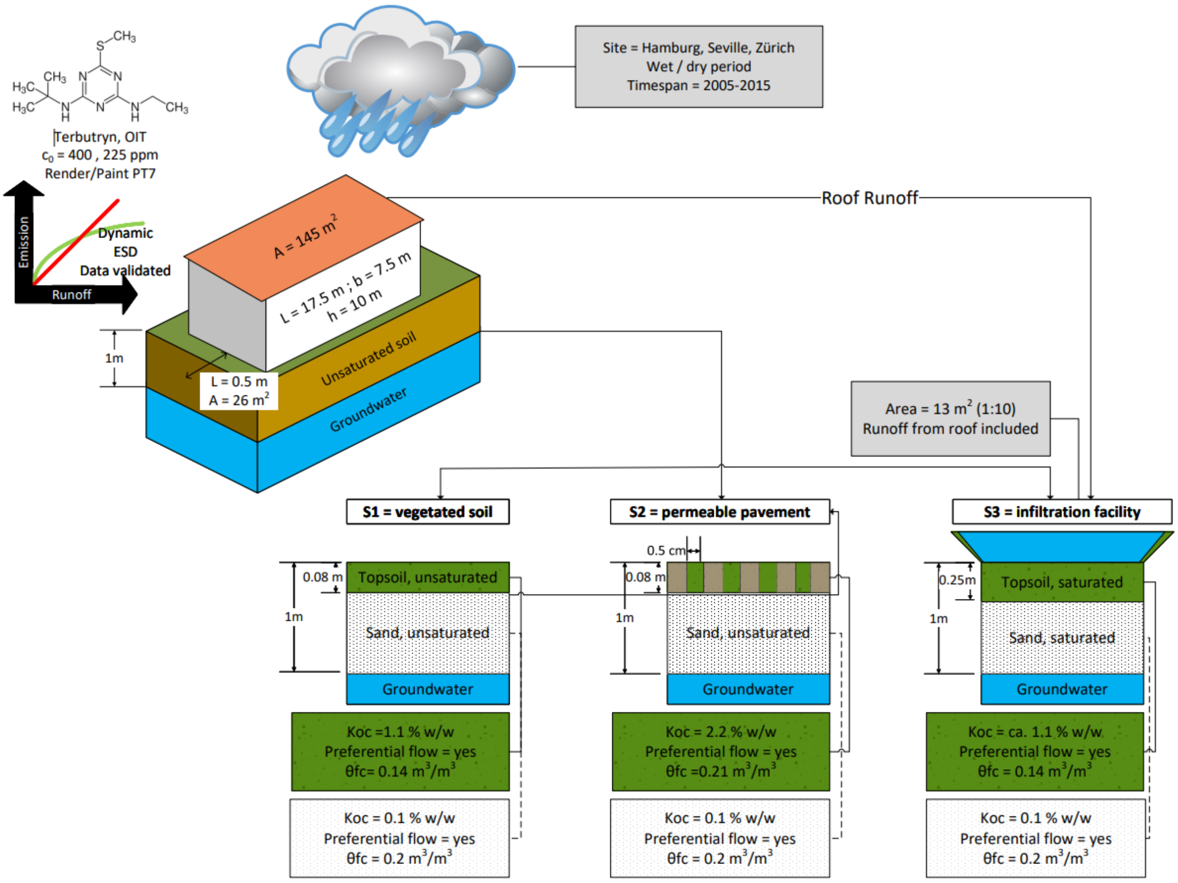


Projected area of residential buildings as a percentage of total urban area for several German cities in blue and for districts in Berlin (project "Basar" - Wicke et al., 2021) and Freiburg im Breisgau in green (see 2.1.3- building survey in Freiburg) based on analyses of building models (LOD2) in ArcGIS Pro.
Source: Own illustration, OST

3.5 Scenario definition

Realistic worst-case scenarios describing the emission of biocides from facades to groundwater need to take into account site-specific characteristics (3.2), emission pathways (3.3), and groundwater (3.4). Figure 22 provides an overview of the defined scenarios.

Figure 22: Scenarios overview



Schematic overview of the defined scenarios

Source: Own illustration, OST

Geometry

The source of biocide emissions is represented by a standardized geometry very similar to the BPR/OECD house, with a revised height of 10 meters and a flat roof. This geometry is consistent with building geometries currently used for regulatory purposes and observations from LOD2 data. Table 8 summarizes the selected geometry parameters based on the review in chapter 3.2. The standardized building is oriented with the longest façade facing west and has a fully plastered façades with a runoff coefficient of 0.9.

The choice was made to focus on a single building as a representative unit, to which a specific infiltration surface can be allocated. By establishing the ratio between the biocide emitting surface (façade), infiltration area (pathways) and equivalent groundwater surface, the outcomes can be scaled. This approach provides a simplified but representative characterization of emissions for urban regions.

Table 8: Geometry properties of the defined house

Modified BPR House	
Length [m]	17.5 (=BPR)
Width [m]	7.5 (=BPR)
Height façade [m]	10
Plaster façade [%]	100
Runoff coefficient façade	0.9
Runoff coefficient roof	1.0
Orientation	W and E = longer façades

Weather data

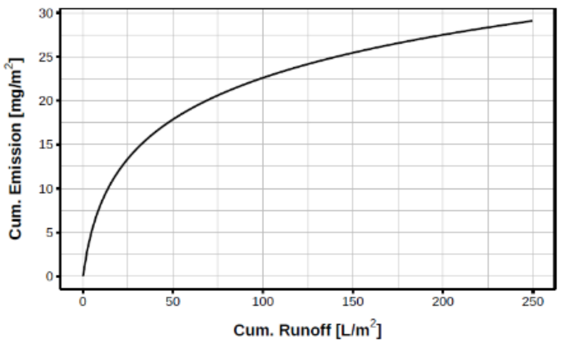
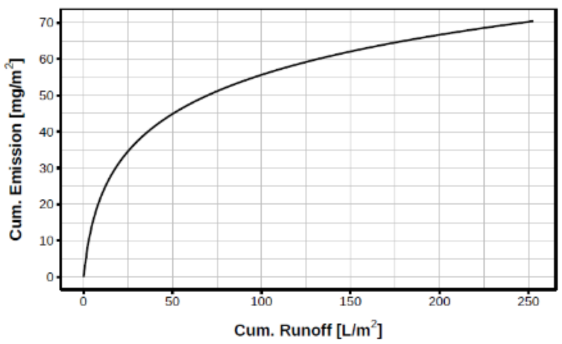
To account for the different climatic conditions, weather data from three different locations, Hamburg, Seville, and Zürich, were used to simulate building runoff and biocide emissions, as described in section 3.2.4.

Substances

According to the survey of biocidal product manufacturers, the most widely used substances relevant for biocide emissions to groundwater from buildings belong to group PT7, with terbutryn and OIT being the most extensively used substances. Consequently, these two biocides were chosen due to their high prevalence in façades coatings and their representation of substances with low and high degradability.

For the simulations, leaching data from Tietje et al. (2018) were parameterized into logarithmic emission functions as suggested. The leaching curves and the corresponding function parameters are provided in Table 9.

Table 9: Emission functions for terbutryn and OIT derived from leaching data of Tietje et al. (2018)

Terbutryn	OIT
	
Initial concentration: 1400 mg/m^2	Initial concentration: 800 mg/m^2
Parameter a: 7.30073 [mg/m^2]	Parameter a: 16.293 [mg/m^2]
Parameter b: 0.21099 [m^2/L]	Parameter b: 0.294342 [m^2/L]

This dataset is particularly valuable as it offers emission data derived from a field experiment conducted under real weather conditions over a two-year period for both substances. The data describes the emission from a plaster and paint system containing encapsulated terbutryn and OIT at an initial concentration of 1400 mg/m² (400 ppm) and 800 mg/m² (225 ppm), respectively. This choice reflects the use of an optimized product in terms of its initial concentration and embedding (encapsulation), which should be considered when evaluating the scenario results. The leaching data were parameterized into logarithmic emission functions as suggested by (Tietje et al., 2018). An illustration of the leaching curves and the corresponding function parameters are provided in Table 9.

Soils

Three different emissions pathways (Figure 23) can be distinguished according to the information provided in chapter 3.3

Figure 23: Images of the different emission pathways

Vegetated soil S1 | Permeable pavement S2 | Infiltration facility S3

Source: Own photos. Taken by UNI Freiburg

- Vegetated soils (S1)

Scenario S1 "vegetated soils" describes infiltration into a vegetated soil located directly at a building façade (Figure 23, S1). The infiltration area consists of a surface of 26 m² resulting from a 0.5 m wide belt surrounding the building, in accordance with the ESD for PT10 (ECHA). The ratio between the projected building surface and the infiltration area is 1:5. The soil structure in S1 consists of an 8 cm unsaturated topsoil layer, followed by a 92 cm unsaturated sand layer extending to the groundwater (Table 10). In this scenario, only façade runoff and direct precipitation are considered to infiltrate into the ground and roof runoff is excluded. The topsoil has an identical composition to infiltration facilities (S3), with an average OC of 1.1 % and a field capacity of 2.2 m³/m³. However, the topsoil layer is limited to 8 cm for a reasonable comparison. The remaining 92 cm consist of a sandy sublayer, similar to the parameters for permeable pavements (S2).

- Permeable pavements (S2)

Scenario S2 "permeable pavements" represents the infiltration of the façade runoff over permeable pavements (Figure 23, S2). The partially sealed area is directly adjacent to the façade as in the previous scenario for vegetated soils, so that the total infiltration area amounts to 26 m². The ratio between the projected building area and the infiltration area is again 1:5. The soil structure consists of an 8 cm thick layer of modular interlocking concrete paving system with 6 % joint area followed by an unsaturated sand layer (92 cm, Table 11). Relevant parameters are adopted from Nehls (2007) for the pavement seam material and from Schaffitel et al. (2020) for the stone content. The spacing of the joints was set to 0.5 cm (Junginger, 2022). The material between the joints is filling material in which OC is accumulated. The K_{oc} of the joint material with OC of 2.2 % is higher than of the topsoil's K_{oc} with OC of 1.1 % in the S1 scenario. Similar S1, only façade runoff and direct precipitation is drained into the soil. For the sandy subsoil, the same parameters as for the first setup are proposed. The average value of the experiments of Schaffitel et al. (2020) is used for k_f 0.000034 m s^{-1}.

- Infiltration facilities (S3)

The third scenario "infiltration facilities" reflects the infiltration of runoff into an infiltration swale (Figure 23, S3). In contrast to scenarios S1 and S2, the infiltration area per building is 13 m^2. This value is calculated based on the typical ratio of swale areas to drained building areas, which is commonly provided in various national guidelines (Table 1) and often ranges between 1:5 to 1:10. To account for a worst-case scenario, the ratio of 1:10 is used. Given the projected area of the standard building considered here (ca. 132 m^2), the infiltration area corresponds to about 13 m^2 per building. In addition, the building's roof runoff is also discharged to the infiltration system which is consistent with common engineering practice. The proposed infiltration facility consists of a 25 cm saturated topsoil layer (due to frequent waterlogging) of a three-year old urban swale following Bork et al. (2021) with OC of 1.1 % situated on top of a 75 cm sand layer (Table 12). A mean value of k_f 0.00016 m/s is assigned.

Groundwater

A conservative depth to groundwater of 1 m was established for all scenarios based on the information provided in chapter 3.4.1.

Table 10: Parameters for vegetated soils (S1)

Depth	pH	OC	Stones (> 2 mm)	Bulk density	Sand (0.063–2 mm)	Silt (0.002–0.063 mm)	Clay (< 0.002 mm)
	-	% w/w	% w/w	g cm^{-3}	% w/w	% w/w	% w/w
0-8	7.52	1.12	45.1	1.6	80	15	5
8-100	7.50	0.10	0	1.6	100	0	0

Topsoil parameters taken as arithmetic means of Table 12

Table 11: Parameters for permeable pavements (S2)

Depth	pH	OC	Stones (sealing %)	Bulk density	Sand (0.063 – 2 mm)	Silt (0.002 – 0.063 mm)	Clay (< 0.002 mm)
	-	% w/w	% w/w	g cm^{-3}	% w/w	% w/w	% w/w
0-8	7.1	2.2	94 %	1.6	95.7	3.3	1.0
8-100	7.50	0.1	0	1.6	100	0	0

Sealing from Schaffitel et al. (2020), seam parameters from Nehls (2007)

Table 12: Parameters for infiltration facilities (S3)

Depth	pH	OC	Stones (> 2 mm)	Bulk density	Sand (0.063 – 2 mm)	Silt (0.002 – 0.063 mm)	Clay (< 0.002 mm)
	-	% w/w	% w/w	g cm^{-3}	% w/w	% w/w	% w/w
0-5	7.42	1.43	35.9	1.54	79	16	5
5-10	7.51	1.07	42.6	1.51	80	15	5
10-15	7.56	0.95	42.6	1.58	81	14	5
15-20	7.54	0.99	60.9	1.56	81	14	5
20-25	7.55	1.17	43.4	1.6	81	14	5
25-100	7.50	0.1	0	1.6	100	0	0

Topsoil parameters from Bork et al. (2021)

4 Modelling leaching of biocide to groundwater

4.1 Biocide transport in soil

4.1.1 Selection of a suitable 1-D Model

There are four standard FOCUS (FOrum for Co-ordination of pesticide fate models and their USe) models originally developed for the risk assessment of plant protection products simulating the leaching pesticides to groundwater.

- FOCUS PEARL (Pesticide Emission Assessment at Regional and Local scales),
- FOCUS PELMO (PEsticide Leaching MOdel),
- FOCUS PRZM (Pesticide Root Zone Model),
- FOCUS MACRO (model of water flow and solute transport in MACROporous soil)

These substance soil transfer models are freely accessible on the European Commission's Ground Water - ESDAC website (europa.eu). FOCUS developed higher tier numerical models with detailed environmental scenarios for major agricultural areas across Europe (FOCUS, 2000). The FOCUS groundwater scenarios consist of a set of nine standard combinations of weather, soil and cropping data. As surrogate for groundwater concentrations, FOCUS uses percolate concentrations at a depth of 1 m.

At present, PEARL serves as the standard model for the risk assessment of biocides leaching to groundwater. It has been developed by three Dutch institutes (ALTERRA/WENR, PBL and RIVM).

PELMO is currently the most important model used for regulation of plant protection products and the only model used for product registration in Germany. The first version of PELMO was released in 1991 (Klein, 1991).

PRZM was released by the US Environmental Protection Agency in 1984. The program simulates the vertical movement of pesticides in the unsaturated soil. The PRZM model has been chosen by the FOCUS group for surface water as the preferred calculation tool for determining runoff input.

MACRO was developed at the Swedish University of Agricultural Sciences, Uppsala. In this model the process of macro-pore flow is included. Macro-pore flow is just one form of preferential flow, but it is the only form of preferential flow considered in FOCUS 2009.

In general, the four FOCUS models describe processes similarly (Table 13). For example, biodegradation is modelled as a function of soil temperature, moisture and depth. In PELMO, photodegradation at topsoil layer can additionally be integrated using a photolysis rate together with the reference radiation.

All FOCUS models are used and widely accepted by European member states and thus also seem to be promising to predict leaching of organic pollutants in urban areas. However, PELMO and PEARL are preferred for the calculation of groundwater biocide concentrations.

Since the properties of urban soil scenarios are very different from agricultural soils for which the models were initially developed, this serves as a test for the compatibility of their calculations. Especially the high input of water and a quasi-permanent emission of substances into the soil surface conceptually differ from agricultural applications.

Table 13: Comparison of selected properties of the four FOCUS groundwater models

Property	PEARL	PELMO	PRZM	MACRO
Soil hydrology	Richards' equation	capacitance models	capacitance models	Richards' equation
Chromatographic transport in soil	Yes	Yes	Yes	Yes
Macro-pore flow	Only in special version	Yes	No	Yes
Surface runoff	Infiltration capacity	Runoff curve number (RCN)	RCN	No
Sorption	Freundlich	Freundlich	Freundlich	Freundlich
Time dependent sorption	Yes	Yes	Yes	Yes
Moisture dependent sorption	Yes	Yes	No	No
pH-dependent sorption	Yes	Yes	No	No
Temperature dependent biodegradation	Yes	Yes	Yes	Yes
Moisture dependent biodegradation	Yes	Yes	Yes	Yes
Depth dependent biodegradation	Yes	Yes	Yes	Yes
Photolytic degradation at topsoil layer	No	Yes	No	No

4.1.2 Two 1-D Models in comparison

PEARL and PELMO are chosen to calculate the transport of biocides in soil. The primary interests are the percolate concentrations, biocide contents in soil and leached mass which might enter groundwater.

The soil transport models in principle need four types of input:

1. Climate data: This encompasses precipitation, potential evapotranspiration and temperature (maximum, average). The weather data utilized are outlined in 3.2.4.
2. Soil data: Parameters include bulk density, soil texture, OC and pH-value for each soil layer. These are determined in 3.5 (Table 10, Table 11 and Table 12).
3. Substance data: Those are determined by the biocides of interest (Table 14) and the emission scenarios (Section 5.1):
    a) Properties such as adsorption constant, half-life in soil, water solubility, vapor pressure, molar mass, Freundlich exponent.
    b) Date and amount of mass per area emitted to the soil surface.
4. Crop data: In urban scenarios, a bare soil is assumed.

Substance properties

For this study two substances are tested in the different urban scenarios, terbutryn and OIT. The relevant substance properties are outlined in Table 14. Although both substances are only slightly mobile, OIT is non-persistent with a very short half-life, while terbutryn is considered persistent. Due to the absence of experimental values for the Freundlich exponent, a worst-case assumption of 1.0 is applied.

Both models allow for further adjustment of substance parameters. Nevertheless, considering the dominating influence of the parameters specified in Table 14 and the scarcity of experimental data, any supplementary values are set to default.

Table 14: Properties of the two biocides used in the simulations

Quantity\Substance	Terbutryn	OIT
DT50 in d	231 (Bollmann et al., 2017)	0.9 (ECHA, 2017)
K_{OC} in mL/g	663 (Mensink and Linders, 1991)	982 (ECHA, 2017)
Freundlich exponent	1.0 (worst-case)	1.0 (worst-case)
Water solubility in mg/L	25 (IVA, 1990)	406 (ECHA, 2017)
Vapor Pressure in Pa	1.3E-04 (Mensink and Linders, 1991)	3.1E-03 (ECHA, 2017)
Molar mass in g/mol	241.36	213.34

Substance output to soil

In contrast to agricultural scenarios where a substance is applied to the soil at single dates, biocides are continuously leached from façades during rain events in the urban scenarios. Two approaches are considered here to calculate the leaching of biocides from façades. The first is COMLEAM, which provides dynamic results depending on daily weather conditions as described in Sections 3.2.5 and 5.1. The second is based on ECHA's ESD for PT10 (construction material preservatives), also applicable for PT7.

Soil parameters

To assess the movement of a compound within the soil matrix, it is essential to analyze the flow of water through the soil, as it plays a crucial role in transporting a compound to deeper soil layers. Here, PEARL and PELMO employ different approaches. PELMO utilizes a tipping bucket model, where one soil layer fills with water, and upon reaching capacity, it empties into the underlying layer. Conversely, PEARL calculates water flux using the partial differential Richards' equation, incorporating the Mualem-van Genuchten relationships for water retention and hydraulic conductivity.

For both models, crucial model parameters for individual layers of the specified soil pathways are missing and have to be deduced from available soil characteristics which include:

- Depth of the layer,
- Bulk density,
- Soil texture (percentages of sand, silt, and clay),
- Organic carbon content (OC),
- pH value.

In PELMO, both field capacity and wilting point are linearly dependent on the soil texture percentages, as specified in the corresponding manual. For PEARL, more information is needed including e.g. saturated hydraulic conductivity and total porosity of each individual soil layer. The Mualem-van Genuchten approximations do not follow linear functions why pedotransfer functions (PTFs) are needed to estimate the required model parameters from the available soil characteristics. An appropriate set of PTFs is euptfv2 (Szabó et al., 2020). These PTFs were used to derive the necessary soil parameters for PEARL, which are provided in the Appendix A.5 (Table 19, Table 20 and Table 21) for the three urban soil scenarios, respectively.

5 Emission Scenarios: A Case Study of OIT and terbutryn

5.1 Emission of biocides from façades

To meet regulatory requirements, the emission of biocides from façades is generally estimated using standardized leaching tests, the results of which are included in ECHA's ESDs. For biocides employed in applications such as masonry preservation (PT10), the emissions during their service life are evaluated across three distinct assessment periods: 30 days, 1 year, and 5 years. However, this approach does not account for site-specific weather conditions that affect façades emissions and biocides transport through soil. For this reason, the established ESD approach is herein compared to a dynamic emission model using COMLEAM (chapter 3.2.5).

The two biocides terbutryn and OIT are used as model substances for the comparison. These two substances were selected because they are most frequently used in façades (3.2.1) and are representative of a substance with low and high degradability. The emission functions used in the model were parameterized using nonlinear regression from the leaching data as described in 3.5.

Biocide leaching with COMLEAM

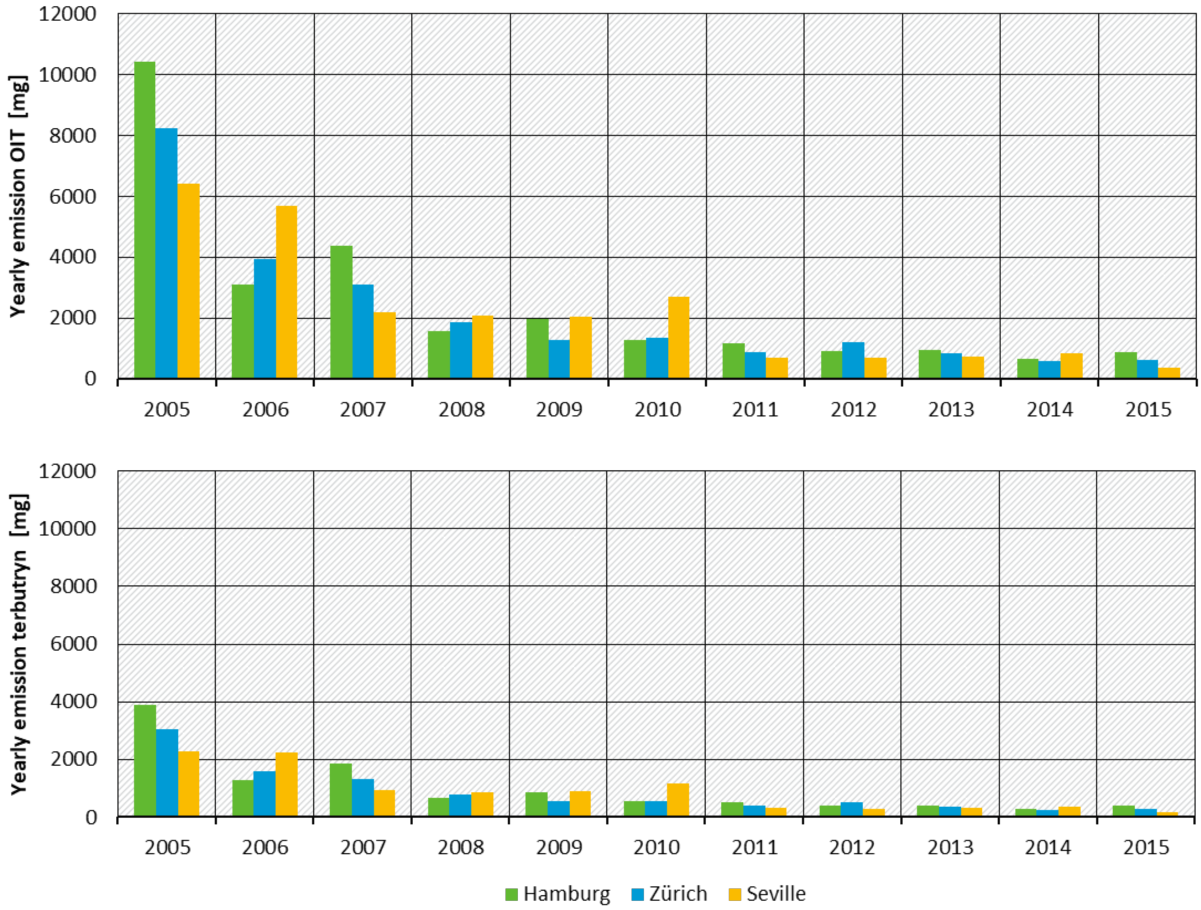
The yearly cumulative façade emission of the two model substances OIT and terbutryn resulting from the dynamic simulation in COMLEAM is shown in Figure 24, based on the simulation parameters described in chapter 3.5. The same results normalized per m^2 façade and expressed as a percentage of the total biocide present in the model building façade, can be found in the Appendix (Figure 43). For the COMLEAM simulations weather data from Hamburg, Zürich and Seville from 2005 to 2015 were used (3.2.4) as well as a standardized house geometry with a façade area of 500 m^2 (3.2.2). The resulting façade runoff for the different locations calculated according to ISO-15927-3 is shown in the Appendix, Figure 44.

On average, higher biocide emissions are observed in Hamburg, followed by Seville and finally Zürich with total OIT emissions of about 27 g, 25 g and 24 g and terbutryn emissions of about 11.0 g, 9.9 g and 9.6 g, respectively, from 2005 to 2015. Although biocide façade emissions are generally driven by higher precipitation amounts, it is noted that higher cumulative emissions are observed in Seville with an average annual precipitation amount about half that of Zürich (about 500 mm vs. 1000 mm between 2005 and 2015). The reason for this apparent discrepancy is that the amount of precipitation by wind direction is more evenly distributed across all four house façades in Seville than in Zürich. This means that although more precipitation is observed in Zürich, not all façades contribute as much to emissions as in Seville, as shown in Figure 44 in the Appendix. This example illustrates how dynamic modeling can be helpful in more accurately describing biocide façade emissions by taking into consideration wind driven rain.

Comparing the emissions of terbutryn and OIT, it is apparent that the load of OIT emitted is about twice as much as that of terbutryn, despite the fact that the initial concentration in the façades was 1400 mg/m^2 for terbutryn and 800 mg/m^2 for OIT, both of which encapsulated. This result arises directly from the different leaching behavior of the two substances, which is enhanced in the case of OIT due to its higher water solubility. Also noteworthy is the fact that about 75 % of emissions from both OIT and terbutryn occur in the first five years, suggesting that the five-year assessment period used in the ESD is a reasonable assumption.

The emission data with daily temporal resolution resulting from the dynamic simulation with COMLEAM were used as input to the soil modeling in Section 5.2.

Figure 24: Dynamic emission of OIT and terbutryn using COMLEAM



Yearly cumulative façade emission of the two model substances OIT and terbutryn resulting from the dynamic simulation in COMLEAM for a standardized house with a façade area of 500 m^2 using weather data from Hamburg, Zürich and Seville from 2005 to 2015.
Source: Own illustrations, OST

Biocide leaching in comparison of COMLEAM and ESD

The question arises as to whether dynamic simulation in COMLEAM is necessary for accurate simulation of biocide transport in soil, or whether a simpler method for determining the biocide emission from the source term would produce similar results. To address this, the façade emissions estimated using COMLEAM are compared to those obtained through the established ESD approach.

The ESD for PT10 (ESD PT 10, Table 18, p.41) for calculating the release of biocides during the service life of a house derives the biocide emission from leaching tests. Here, the same field leaching tests from Zürich included in the dynamic simulation in COMLEAM were used for this purpose (3.5). This approach to determining biocide emission from façades is referred to as the "strict ESD method" in this study.

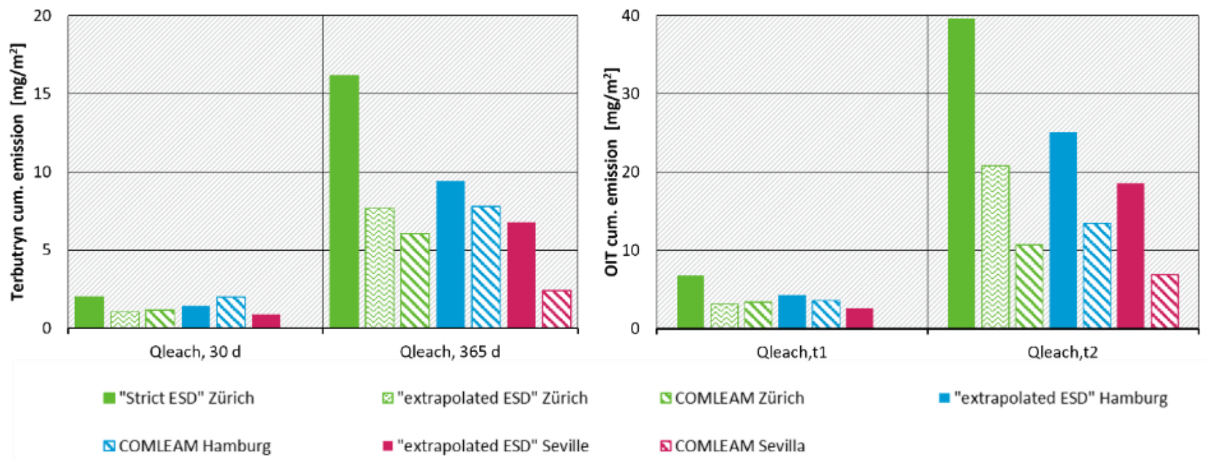
Field leaching tests, and to a greater extent, laboratory leaching tests, have a drawback in that they primarily represent the site and conditions under which they were conducted, which may not necessarily align with the site and conditions of the commercial product's usage. To calculate cumulative leaching loads for ESD that are specific to different locations, a decision was made to extrapolate these values from the leaching curves associated with the various assessment periods defined in the ESD for PT10 (pertaining to the service life of the product). This extrapolation is done using the yearly average façade runoff data simulated in COMLEAM for Hamburg, Zürich, and Seville, spanning from 2005 to 2015. The outcome is an extrapolation of cumulative leached loads for a standardized ESD, which, nonetheless, remains site-specific. This data can be compared to the dynamic simulations performed using COMLEAM. A schematic illustration of this approach, here referred to as the "extrapolated ESD method" is shown in the Appendix, Figure 46.

Figure 25 compares the cumulative leached biocide loads for the assessment period of 30 days and 1 year resulting from the three different mentioned approaches:

- dynamic simulation with hourly resolution using COMLEAM
- strict ESD method
- extrapolated ESD method

It can be observed that the highest cumulative load results from the "strict ESD method", followed by the "extrapolated ESD method", with the lower emissions for each location resulting generally from the dynamic simulation in COMLEAM. The observation that the ESD approach tends to result in higher emissions compared to dynamic simulations in COMLEAM is consistent with a previous investigation (Burkhardt et al., 2021b).

Figure 25: Cumulative biocide loads leached from façades calculated by ESD and COMLEAM



Cumulative terbutryn and OIT loads leached per m² façade according to leaching tests (strict ESD) and dynamic modelling using COMLEAM (S1-3 Hamburg, Zürich, Seville). The assessment period of 5 years is not given since the field leaching test (Strict ESD) was limited to a period of just over 2 years and is only available for Zürich.
Source: Own illustrations, OST

5.2 Emissions to groundwater

This section presents and discusses the results of the soil transport of the two model substances terbutyn and OIT for the defined urban scenarios in 3.5. Initially, simulations are performed for two biocide leaching models (see 5.1), three climate regions (see 3.2.4), three emission pathways (see 3.3) and two soil transport models (see 4.1.2), resulting in 36 simulations per substance.

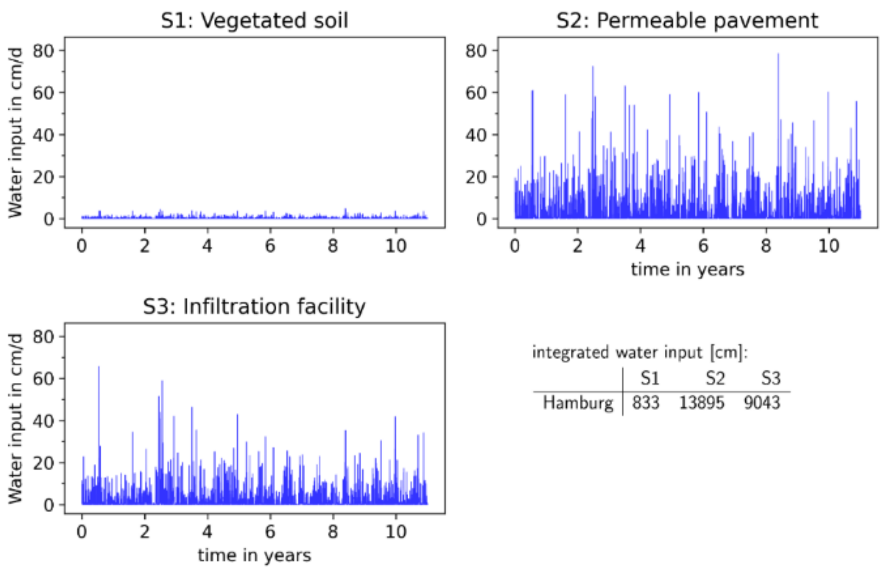
For each simulation, results are compared to identify driving factors for biocide emission to groundwater and redundant variations. Based on the results the urban scenarios are consolidated to one leaching model (ESD123), two climate regions (Hamburg, Seville), three emission pathways (S1, S2, S3), and one soil transport model (PEARL), thereby reducing the number of simulations to 6 per substance (5.2.9). The chapter predominantly focuses on terbutryn, with corresponding results for OIT available in the Appendix.

5.2.1 Runoff and infiltration amounts

A driving factor influencing the transport of biocides through soil is water. The water inflow for the different urban scenarios does not only include precipitation on the infiltrating soil surface but also façade runoff (calculated with COMLEAM) in the case of vegetated soils (S1) and permeable pavements (S2) along with roof runoff for infiltration facilities (S3). Figure 26 illustrates the water input per infiltration area for each emission pathway (S1, S2, S3), using Hamburg weather as an example (2005-2015).

In infiltration facilities (S3), higher quantities of infiltrating water per area are observed, compared to vegetated soils. The highest values are observed for the permeable pavements (S2). This is a direct consequence of the assumption that the entire volume of water percolates through the joints of the paving. With a joint ratio of 6 %, the water input is therefore about 17-times higher compared to S1.

Figure 26: Water infiltration for the three different emission pathways in Hamburg



Infiltrating water amount per area for the different emission pathways using weather data from Hamburg (2005-2015).
Source: Own illustrations, IME. Plotted using the Python Package Matplotlib (Hunter, 2007).

5.2.2 COMLEAM and ESD

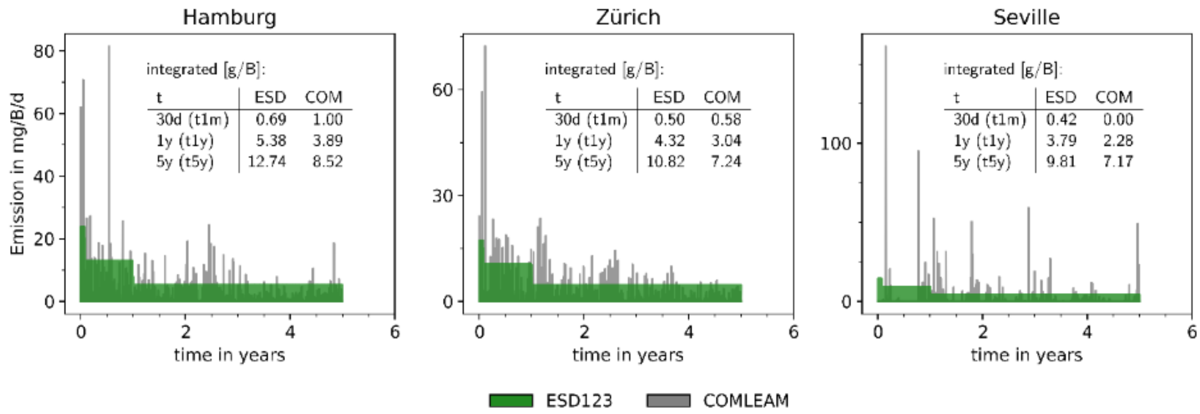
The amount of the biocide emitted from the standardized building serves as input for the soil transport models PEARL and PELMO. The leached amount in the different climatic regions (Hamburg, Zürich and Seville) is estimated using the dynamic model COMLEAM over a simulation period of 5 years. As a comparison, the leached biocide load is also estimated using the ESD for PT10 (see 5.1, extrapolated ESD method) for the assessment periods of 30 days (t_1), 1 year (t_2) and 5 years (t_3). The three ESD assessment periods are then combined to create a single emission timeseries (ESD t_{123}) of 5 years.

Figure 27 illustrates the emitted load of terbutryn from the whole building geometry according to both COMLEAM and ESD. Notably, COMLEAM reveals emission peaks aligned with intense precipitation events, a characteristic not captured by the ESD method. The emission patterns in Zürich and Hamburg appear to be similar, whereas Seville, characterized by infrequent but high-volume precipitation events, exhibits a corresponding emission pattern with fewer but more prominent peaks compared to Zürich or Hamburg. Almost identical patterns emerge for OIT (Figure 53).

In this chapter, results for OIT are generally summarized and compared to those for terbutryn. Supporting information for OIT can be found in the Appendix A.7. Generally, the short half-life of 0.9 days for OIT impedes its accumulation in soil. Consequently, this results to isolated emission peaks into groundwater.

The integrated emitted load over the various assessment periods (1 month, 1 year, 5 years) indicates that, with two exceptions (Hamburg, Zürich, t_{1m}), the ESD method consistently estimated higher biocide emissions, making it a more conservative approach.

Figure 27: Terbutryn building emission according to COMLEAM and ESD



Daily emission of terbutryn from COMLEAM and the combined ESD123 for three locations and per building B.
Source: Own illustrations, IME. Plotted using the Python Package Matplotlib (Hunter, 2007)

To evaluate whether the notable emission peaks identified in COMLEAM could potentially lead to accelerated biocide transport in the soil, especially in the context of preferential flow during heavy rainfall events, percolate concentrations were calculated using PEARL and PELMO. Figure 28 presents the simulation results for PELMO with variations in emission schemes, climate regions, and soil scenarios for terbutryn. Each subplot displays the calculated percolate concentrations at a depth of 1 meter. No significant differences were observed using the soil transport model PEARL. It is crucial to highlight that while the biocide emission from the building was simulated over a 5-year period, the soil transport model considers a 10-year timespan to accommodate the buffering effect of the soil, resulting in delayed emissions to groundwater.

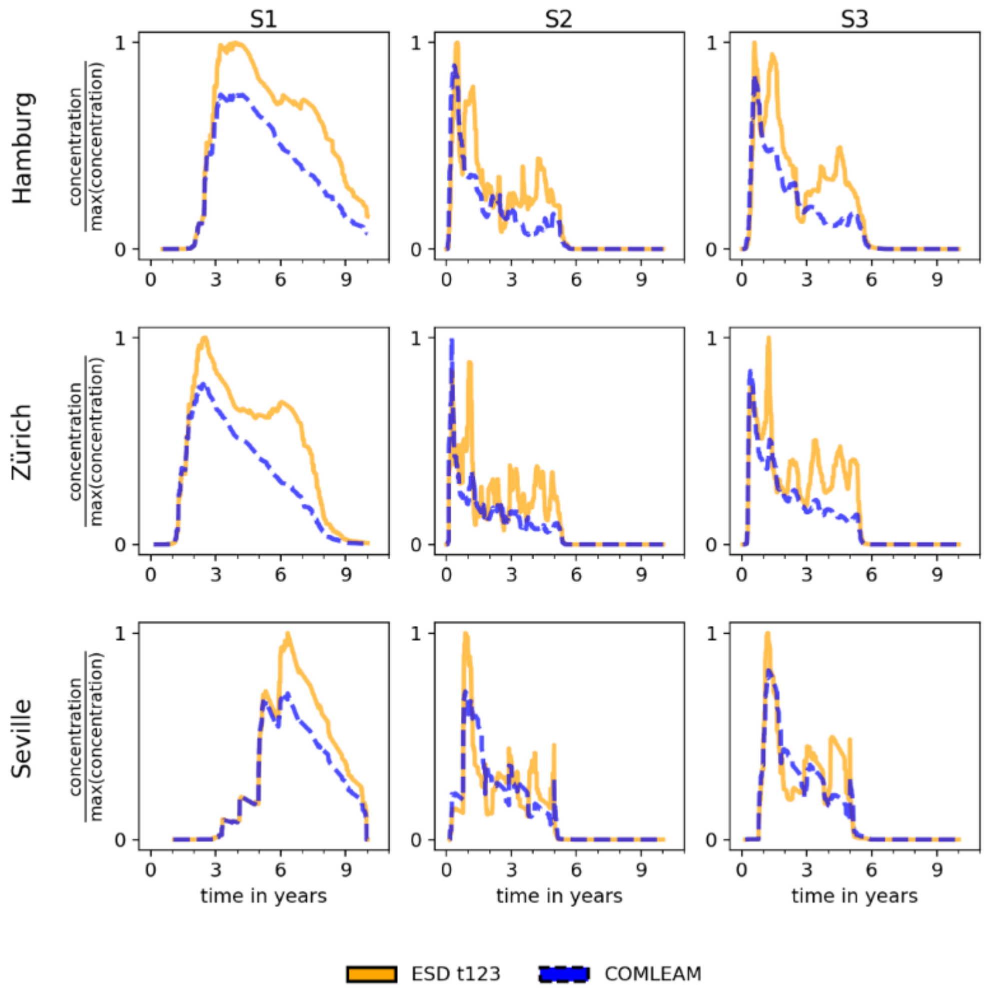
For terbutryn, the ESD emission consistently yields to higher percolate concentrations than COMLEAM for most of the simulation period. This aligns with expectations, given COMLEAM's tendency to predict lower emissions over time. Nevertheless, there are time spans, especially for permeable pavements and infiltration facilities in Seville, where the opposite occurs. This is likely attributed to the interplay between infrequent but intense emission peaks and significant water input, both correlated with rare but high-volume precipitation events in this climate region. This effect can be seen even more clearly in case of OIT (Figure 54), where the pattern consists mostly of individual emission peaks rather than a curve. For OIT, neither the ESD nor the COMLEAM emission schemes yield consistently higher percolate concentrations.

In general, COMLEAM predicts lower percolate concentrations of terbutryn than ESD. Moreover, the concentration peaks do not significantly differ in amplitude or temporal occurrence. This cannot be said for OIT in general where the pattern depends more on the location.

Therefore, the ESD method is retained as the preferred emission scheme. It is worth noting, however, that COMLEAM may be implemented in a tiered approach.

- In summary, the ESD offers a more conservative approach, whereas COMLEAM excels in describing biocide emission peaks from buildings. However, these peaks do not appear to substantially translate into elevated soil percolate concentrations, thanks to the buffering function of the soil. A special exception is OIT in the Seville scenario with COMLEAM yielding higher concentrations than ESD.

Figure 28: Comparison of terbutryn percolate concentrations for COMLEAM and ESD



Percolate concentrations at 1 m depth resulting from the terbutryn building emission (source-term) estimated with COMLEAM and ESD. The results are presented in rows for each location (Hamburg, Zürich, Seville) and in columns for each emission pathway (vegetated soil – S1, permeable pavements – S2, infiltration facilities – S3). The terbutryn percolate concentration was calculated using PELMO.

Source: Own illustrations, IME. Plotted using the Python Package Matplotlib (Hunter, 2007).

5.2.3 Comparison of the soil transport models PEARL and PELMO

The transport of terbutryn and OIT to groundwater is compared in this section using the model PEARL and PELMO. Details on the soil transport models can be found in Section 4.1.

Figure 29 displays the percolate concentration of terbutryn at a depth of 1 meter in Hamburg and Seville for various emission pathways calculated using the PEARL and PELMO. Both models simulate very similar percolate concentrations, with PELMO generally estimating slightly lower values, especially in Seville.

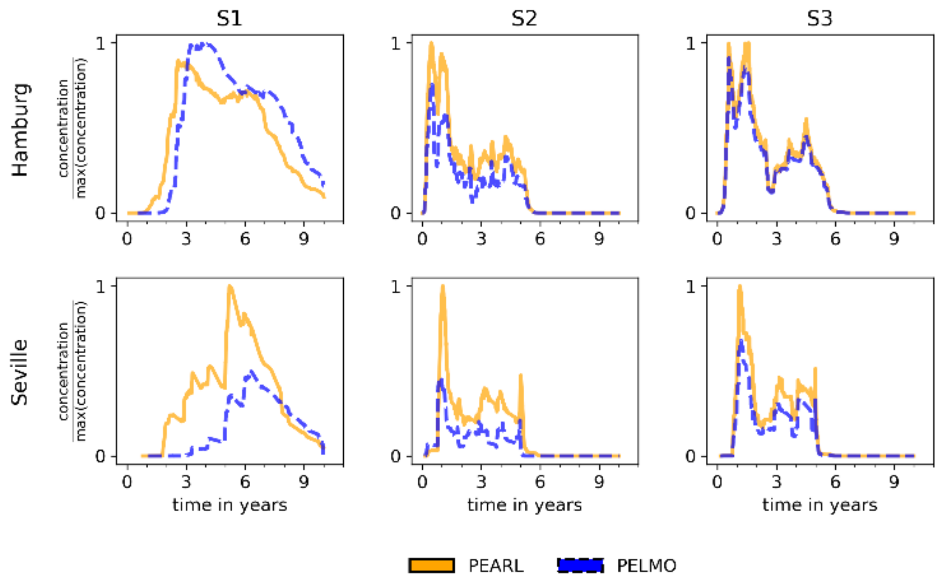
The terbutryn percolate concentrations calculated for the permeable pavement (S2) and the infiltration facility (S3) show an almost identical temporal pattern with both models. For vegetated soil (S1), the concentrations calculated with PELMO lag behind those of PEARL by approximately one year.

Due to the short half-life and resulting peak emission pattern of OIT, no clear conclusion can be drawn for the comparison between PEARL and PELMO for this substance (Figure 55). In most cases PEARL predicts higher percolate concentrations than PELMO, making it the more conservative option.

PELMO and PEARL employ distinct approaches for calculating water flow in soil, with PELMO utilizing a simple tipping bucket model and PEARL employing the differential Richard's equation. The remarkable similarity in terbutryn percolate concentrations obtained for the permeable pavement (S2) and infiltration facility (S3) with Hamburg climatological input suggests a convergence of the models, particularly under conditions of substantial water input. However, proof of this claim is beyond the scope of this study. For smaller water inputs, as seen in Seville and for vegetated soil (S1), the variations in approaches likely contribute to the differences in percolate concentration.

► PEARL consistently calculates percolate concentrations that are generally higher but very similar to those calculated by PELMO. Both PELMO and PEARL are well established for pesticide risk assessment. However, for biocides, PEARL is the preferred model and is therefore selected here as the primary soil transport model for biocide transport to groundwater in urban areas due to its tendency to yield more conservative results and its superior accuracy in hydraulic modeling. Having this said, in the following sections, PEARL and PELMO are used interchangeably due to their similar outcomes. Only explicit discrepancies between the results of the two models will be further discussed.

Figure 29: Comparison of terbutryn percolate concentrations using PELMO and PEARL



Terbutryn percolate concentrations at 1 m depth in Hamburg and Seville for the three emission pathways calculated using PELMO and PEARL (vegetated soil – S1, permeable pavements – S2, infiltration facilities – S3).
Source: Own illustrations, IME. Plotted using the Python Package Matplotlib (Hunter, 2007)

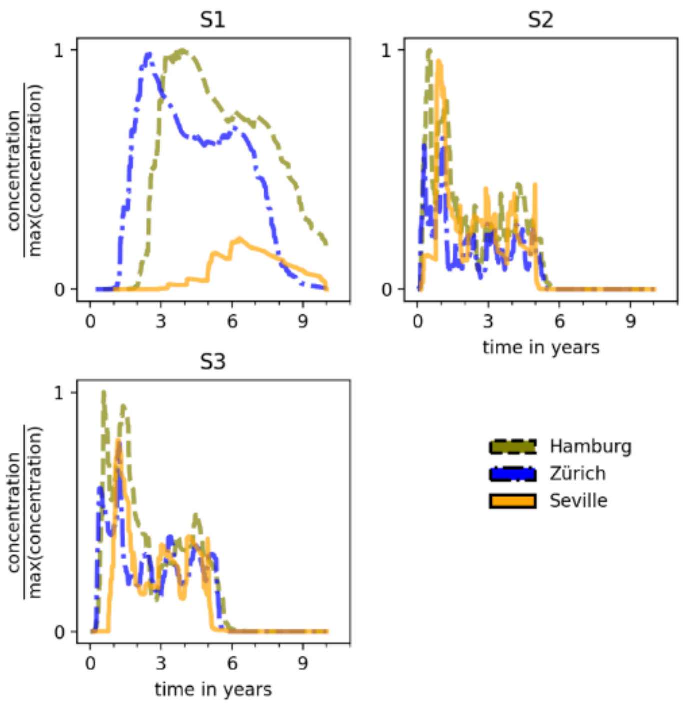
5.2.4 Biocide emissions to groundwater by location

This section compares the influence of weather conditions on biocide transport to groundwater in three distinct climate regions: Hamburg, Zürich, and Seville, representing Northern, Central, and Southern European regions, respectively, as detailed in Section 3.2.4.

Figure 30 shows the percolate terbutryn concentration at 1 meter depth for the different locations and emission pathway calculated with PELMO. Results in the same order of magnitude were observed using the soil transport model PEARL. For vegetated soils (S1), substantially lower terbutryn percolate concentrations are observed in Seville compared to Zürich and Hamburg. This discrepancy is likely attributed to lower precipitation in Seville in comparison to the other two locations. Lower precipitation in Seville also contributes to an increase in terbutryn percolate concentrations occurring years later than in Hamburg and Zürich.

However, it is noteworthy that for permeable pavements (S2) and infiltration facilities (S3), the differences among locations are significantly less pronounced. This phenomenon may be attributed to the concentration of more water on a smaller infiltrating surface in the joints of permeable pavements and in infiltration facilities (Figure 26). In these emission pathways, smaller precipitation events lead to a more rapid transport of substances to deeper soil layers. Consequently, the steep increase in percolate concentration occurs shortly after the simulation begins for permeable pavements and infiltration facilities, while it is delayed in vegetated soils. This phenomenon appears to mitigate differences between locations in permeable pavements and infiltration facilities, as water flow becomes less limiting for soil transport compared to vegetated soils.

Figure 30: Comparison of terbutryn percolate concentrations for three climate regions



Terbutryn percolate concentrations at 1 m depth in Hamburg, Zürich and Seville for the three emission pathways calculated using PELMO (vegetated soil – S1, permeable pavements – S2, infiltration facilities – S3).
Source: Own illustrations, IME. Plotted using the Python Package Matplotlib (Hunter, 2007)

For OIT, no clear pattern is evident (Figure 56). The Zürich climate exhibits the peak with the highest magnitude for all emission pathways. This likely follows from a strong precipitation event transporting the substance quickly through the soil. Due to the short half-life of OIT, percolate concentrations at 1 m depth mostly occur as peaks following heavy rainfall events. In contrast, due to its persistence, terbutryn tends to accumulate in the soil and is emitted to groundwater even after smaller rain events. Moreover, terbutryn results in percolate concentrations generally above those of OIT, despite the load of OIT leached from the façade being around three times higher than that of terbutryn.

These observations suggest that local climatic conditions strongly influence biocide transport to groundwater in emission pathways with a low building surface to infiltration area. Conversely, this influence becomes less significant for emission pathways with high building surface to infiltration area.

- Results for Zürich and Hamburg are comparable across all emission pathways. Since only Hamburg and Seville are included in the FOCUS scenarios, Zürich is excluded.
- The impact of climatic conditions on biocide transport in groundwater varies with the specific emission pathway. Distinctions in climatic conditions become less prominent when runoff from extensive building surfaces is directed towards concentrated infiltration areas.

5.2.5 Biocide emissions to groundwater related to emission pathways

This section compares the influence of the three emission pathways on biocide transport to groundwater. The investigated emission pathways are vegetated soil (S1), permeable pavement (S2) and infiltration facility (S3), as defined in Sections 3.3.2, 3.3.3 and 3.3.4, respectively.

Figure 31 illustrates terbutryn percolate concentrations at a depth of 1 meter for different emission pathways calculated with PELMO. No significant differences were observed using the soil transport model PEARL. Similarities are observed between the percolate concentration curves for the permeable pavement (S2) and infiltration facility (S3). In both cases, there is a pronounced increase in percolate concentration shortly after the simulation begins. In contrast, the vegetated soil (S1) displays a slower terbutryn transport, attributed to a reduced water inflow.

The quantity of infiltrating water not only influences the rate of biocide transport in soil but also directly impacts percolate concentration. Elevated water flow leads to increased percolate volumes without a corresponding rise in the transported biocide load. This phenomenon is evident in the permeable pavement, consistently displaying smaller percolate concentrations compared to the infiltration facility. This difference can be attributed to the directed flow of water through the joints, which induces heightened dilution of the biocide in the permeable pavement.

As discussed in Section 5.2.4, climatic conditions play a pivotal role in influencing the transport of biocides through vegetated soils. Hamburg's vegetated soil (S1) exhibits the highest terbutryn percolate concentrations, despite transporting a comparable terbutryn load with relatively lower amounts of infiltrating water per area compared to permeable pavements and infiltration facilities. In contrast, in Seville, where precipitation events are infrequent, terbutryn persists in the soil matrix for an extended period, allowing for degradation and adsorption. This climatic condition results in lower percolate terbutryn concentrations.

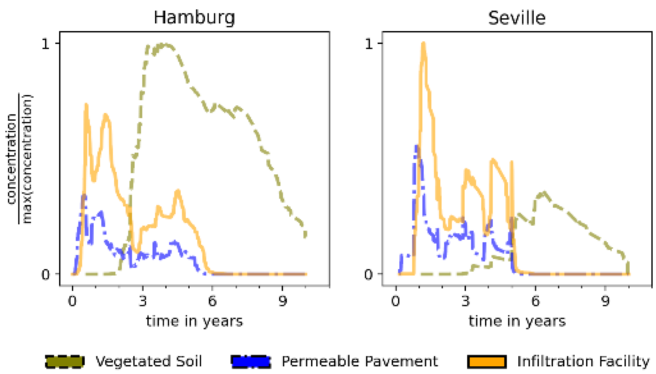
Results for OIT show a different pattern (Figure 57). Percolate concentrations at 1 m depth are negligible for vegetated soil (S1) in both locations, as the infiltrating water volume water is insufficient for transporting the compounds before degradation occurs. However, this is not the case for the high percolate volume in the permeable pavement scenario (S2) and for infiltration facilities (S3), which results in some peak emissions. In the case of OIT, the amount of infiltrating water appears to be the driving factor for emissions reaching the groundwater. The estimated

OIT percolate concentrations at 1 m depth, however, are approximately one order of magnitude below those of terbutryn.

In conclusion, permeable pavements and infiltration facilities exhibit a similar pattern, with slightly lower (higher) percolate concentrations for permeable pavements when considering terbutryn. This observation is contingent upon the pavement's joint percentage and may not be universally applicable. Given that results for S1 differ significantly from S2 and S3 in all climatic regions, all three emission pathways are retained for the urban scenarios.

- The simulations highlight the importance of considering the various emission pathways in urban settings when evaluating the transport of biocides to groundwater. The distinct soil structures and hydraulic conditions result in significantly different dynamics in the transport of biocides to groundwater.

Figure 31: Comparison of terbutryn percolate concentrations for the three emission pathways



Percolate concentrations at 1 m depth are displayed for Hamburg and Seville calculated using PELMO. The three emission pathways are shown together for comparison.
Source: Own illustrations, IME. Plotted using the Python Package Matplotlib (Hunter, 2007)

5.2.6 Groundwater concentrations by percolation in soil

In the previous section, it was shown that terbutryn percolate concentrations at a depth of 1 meter for vegetated soils can exceed those observed in permeable pavements and infiltration facilities. While elevated biocide percolate concentrations might imply a worst-case scenario, relying solely on percolate concentrations to assess the risk of biocide emissions in urban areas could lead to misleading interpretations.

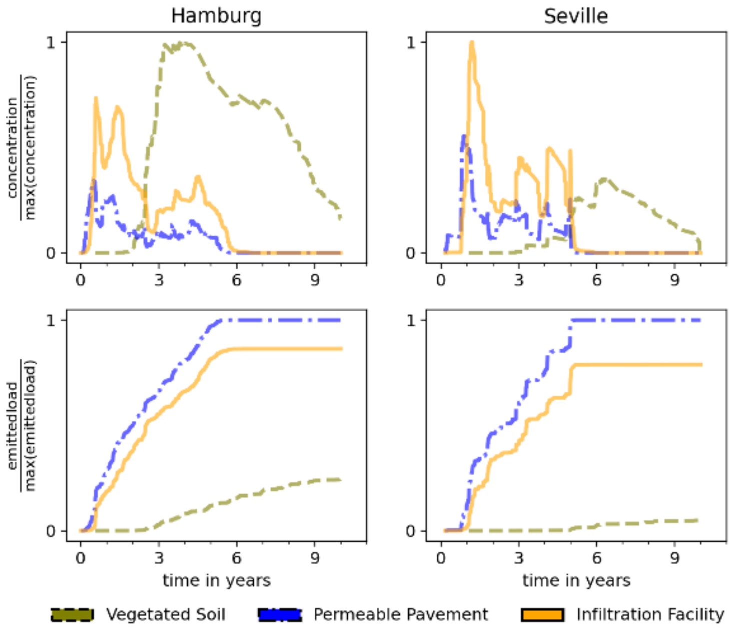
On a first glance, higher biocide percolate concentrations suggest an increased risk for groundwater contamination. However, when only small volumes of water reach groundwater, the percolated biocide mass may be relatively small. In contrast, a dilution effect occurs when large amounts of water infiltrate. The rapid movement of water through the soil column provides limited time for biocides to degrade and sorb which may result in a higher biocide mobility and a higher biocide mass finally leached to groundwater, despite a lower percolate concentration. When evaluating the risk of biocides in urban scenarios, it is therefore meaningful to consider not only the percolate concentration but also the leached mass which dictates biocide concentrations in groundwater. Due to its short half-life, this consideration is not as relevant for OIT as it is for terbutryn (Figure 58).

This phenomenon can be observed, for example, in Figure 32 for the permeable pavement (S2) and infiltration facility (S3) in Hamburg. Despite the lower percolate concentrations estimated for S2 and S3 compared to the vegetated soil (S1), larger terbutryn loads reach the groundwater in S2 and S3 compared to S1 at a depth of 1 meter. However, this pattern is not observed in

Seville, indicating no clear correlation between percolate concentration and transported biocide load.

- The terbutryn case study underscores the importance of evaluating both percolate concentration and leached mass to assess the risk of biocide emission to groundwater from façades, given the significant variation in hydraulic conditions among emission pathways. Estimating the actual groundwater biocide concentration could be achieved using a dilution factor (3.4.2).

Figure 32: Terbutryn percolate concentrations and emitted loads to groundwater



Terbutryn percolate concentrations and emitted load at 1 m depth in Hamburg and Seville calculated using PELMO. The three emission pathways are shown together for comparison.

Source: Own illustrations, IME. Plotted using the Python Package Matplotlib (Hunter, 2007)

5.2.7 Groundwater concentration (point of interest)

In order to preserve groundwater resources, it is important to focus on the groundwater concentrations resulting from biocide emission in urban areas. As highlighted in the previous section (5.2.6), relying solely on percolate concentrations at 1 meter depth from different urban emission pathways can lead to misleading assessments. This is predominantly due to the significantly different hydraulic conditions present in the diverse urban emission pathways (S1 - vegetated soils, S2 - permeable pavements, and S3 - infiltration systems). In fact, unlike the areal infiltration observed in agriculture, urban infiltration tends to be spatially heterogeneous.

To provide a more accurate depiction of the risk to groundwater resources, it is recommended to prioritize the assessment of groundwater concentrations as the point of interest. A simplified mass balance approach, using the different emission scenarios developed in this study, is proposed below. The PEARL and PELMO soil transport models have a significant advantage in that they enable a realistic determination of the emitted load during different assessment periods. This information can be used to estimate the resulting groundwater concentration.

The approach involves aggregating the cumulative loads from all three pathways, determining a representative concentration of urban percolate using the cumulative percolate volumes from each pathway, and calculating their mean for an assessment period of 5 years. While the precise relevance of the different emission pathways for a specific region often remains unclear, chapter 6 (3D Modelling in Vauban) illustrates the significant contribution of all three emission pathways for a realistic characterization. This mean percolate concentration is subsequently multiplied by a transfer factor (3.4.2) to conservatively assess the groundwater concentration in the urban area. Although further dilution occurs within the groundwater, this process is subject to considerable variability and is influenced by numerous unaccounted factors. Considering regional disparities, a pragmatic approach is adopted by utilizing average values.

- Table 15

Table 15 provides the estimated groundwater concentration using this approach for Seville and Hamburg, utilizing PEARL and PELMO and a transfer factor of 10. It can be observed that PELMO and PEARL again provide very similar results (5.2.3). Furthermore, the differences between the locations of Seville and Hamburg are minor.,

- Significant differences in groundwater concentrations occur for the two biocides, OIT and terbutryn, due to the differences in their biodegradability. The groundwater concentrations of terbutryn are higher compared to the measured concentrations in the large-scale modeling in Vauban (Table 15) (see 6.2). It is likely due to the simplified approach used, which accounts for a transfer factor of 10, whereas the 3D model in Vauban is based on a dynamic simulation that considers groundwater transport and recharge. Furthermore, this approach considers newly constructed buildings, whereas the Vauban catchment includes buildings of different ages.
- A simplified approach to mass balancing is proposed to assess the groundwater concentrations resulting from the different emission pathways. This approach has the advantage of placing groundwater at the point of interest to better protect this resource and take into account the heterogeneity of urban emission pathways.

Table 15: Estimated groundwater concentration of terbutryn and OIT for Seville and Hamburg resulting from the different emission pathways (S1, S2, S3) using a simplified mass balance approach

Location	Estimated groundwater concentration [ug/L]			
	PEARL		PELMO	
	Terbutryn	OIT	Terbutryn	OIT
Hamburg	3.4	0.003	3.1	0.001
Seville	3.0	0.001	2.4	0.003

5.2.8 Biocide content in soils

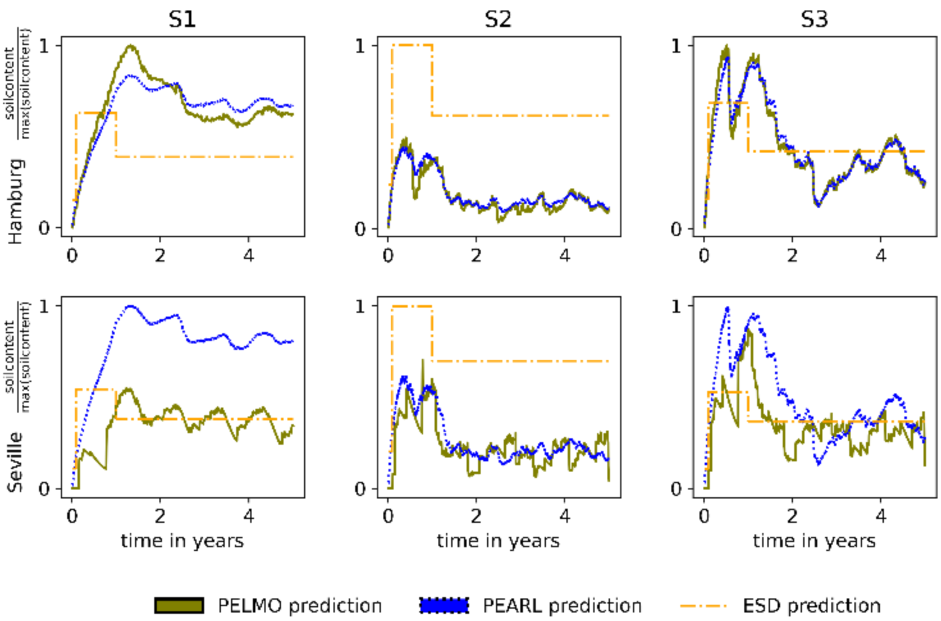
The biocide contents in the soils were calculated using PEARL, PELMO, and ESD PT 8 for wood preservatives (treated wood in service). PT8 was selected due to the absence of alternative scenarios for calculating soil biocide content, specifically for PT10 or PT7, which include degradation. The soil volume is defined by 50 cm distance from the façades and a depth of 50 cm, according to ESD PT8, resulting in a 13 m^3 soil volume. ESD PT8 provides the soil content as a time-weighted average or at the end of the assessment period. Here, the biocide content at the end of the assessment period is considered.

Figure 33 illustrates the soil terbutryn concentration under varying climate region and emission pathways. While ESD provides constant predictions for the entire volume for each assessment period (1 month, 1 year, 5 years), PEARL and PELMO calculate time-resolved values over multiple soil layers. Therefore, for comparison, the arithmetic average of the soil layers to a depth of 50 cm is presented.

PELMO and PEARL consistently yield very similar estimates for soil biocide content, with notable differences observed in Seville for vegetated soils. This further suggests that, in general, PEARL and PELMO can be used interchangeably. The biocide content estimated using ESD PT8 at the end of the assessment periods (30 d, 1 y, 5 y) falls within the same order of magnitude compared to the simulations in PEARL and PELMO. Only in the case of permeable pavements (S2), the soil biocide content derived from the ESD consistently exceeds the values from the soil transport models.

When considering OIT, similar conclusions can be drawn regarding the comparison between PELMO/PEARL, as they yield comparable results (Figure 59). However, the soil OIT content estimated with ESD PT8 is lower compared to the values calculated with PELMO/PEARL. This difference arises because ESD PT8 (treated wood in service) estimates the biocide content at the end of the three assessment periods, while PELMO/PEARL simulations provide the biocide content across the entirety of the simulation period. Consequently, the first-order degradation applied over the entire assessment period in ESD for PT8 results in lower biocide contents in comparison to the more dynamic emission pattern simulated with PEARL and PELMO. The disparity between these two approaches is particularly pronounced for substances such as OIT with short half-lives, and is less prominent for substances with long half-lives like terbutryn.

Figure 33: Terbutryn contents in soil according to ESD, PELMO, and PEARL

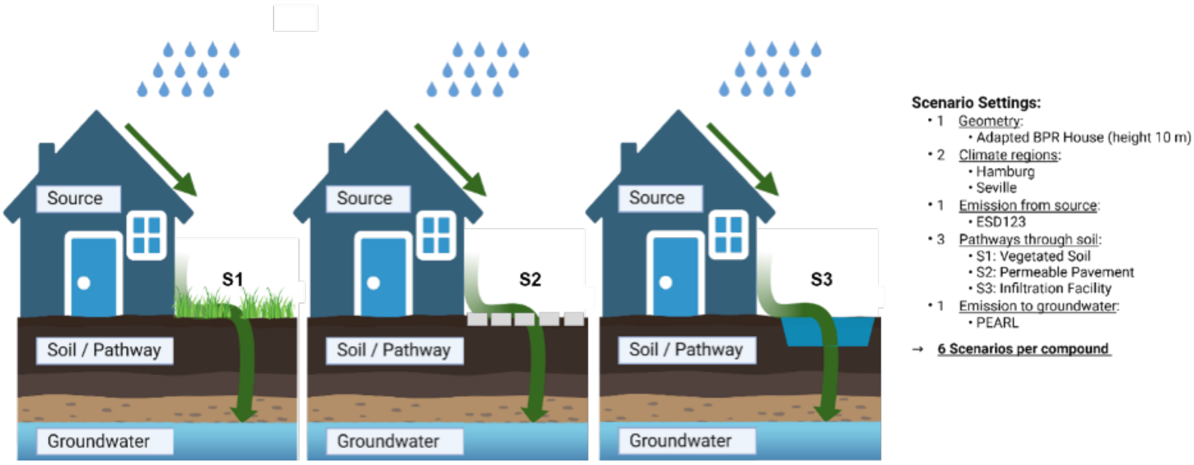


Average soil terbutryn content to a depth of 50 cm (V = 13 m³) in Hamburg and Seville for the three emission pathways (vegetated soil – S1, permeable pavements – S2, infiltration facilities – S3). The results from the two soil transport models PELMO and PEARL are presented alongside predictions from ESD for comparison.
Source: Own illustrations, IME. Plotted using the Python Package Matplotlib (Hunter, 2007)

5.2.9 Consolidated scenarios

Starting with 36 scenarios, this chapter culminates in the reduction to 6 scenarios for assessing potential groundwater risks associated with biocide usage in urban areas. Biocide leaching assessed through ESD and the soil transport model PEARL are favored over their alternatives, COMLEAM and PELMO, due to similar outcomes and wider acceptance in biocide regulation. Zürich is excluded from the climate locations, given its comparable results to Hamburg, an established FOCUS scenario. The consolidated scenario settings are illustrated in Figure 34.

Figure 34: Depiction of consolidated scenario settings



Source: Own illustration, IME. Created with BioRender.com

6 Relevance assessment of the different scenarios

6.1 Large-Scale extrapolation: 3D modelling in Vauban

The objective of this chapter is to comprehensively assess the significance of different pathways of biocides to urban groundwater. To reach this aim, a 3D model is set up to prove the relevance of the GRUBURG scenarios S1, S2, and S3 in a real-world case study. The district of Freiburg-Vauban offers the exceptionality to validate model results against measured field data. Here, biocides and TPs were found in the groundwater by entering via the swale-trench system (Hensen et al., 2018).

6.1.1 Study area and available data

The district of Freiburg-Vauban is located in the south-west of Germany. Former military barracks were transformed into a modern urban district between 1998 and 2009. The district has approximately 5300 inhabitants (City of Freiburg, 2021).

The sustainable stormwater management of the district includes green roofs, permeable pavements and swale-trench systems (Jackisch et al., 2013). Two main swale-trench systems, designed as two linear cascades, collect and retain stormwater. Here, the stormwater slowly infiltrates to the groundwater through 0.5 m of soil. A layer of gravel or plastic blocks (Rigofill inspect) is installed beneath to increase porosity and available water storage (Hensen et al., 2018). Geology mainly consists of flood sediments down to a maximum depth of 0.8 to 3.1 m with a sandy clay layer and gravel below (Wagenmann-Gaiser, 2004). Groundwater flows from Southeast to Northwest.

The former military site includes a contamination site with chlorinated hydrocarbons (CHC). The main TPs and contaminants are vinyl chloride, 1,2-dichloroethene, trichloroethene and tetrachloroethylene, which spread with the groundwater. Groundwater monitoring is carried out twice a year and documents a quasi-stationary plume due to remediation measures. Groundwater level was measured at 15 monitoring wells in 10-20 min steps (2014-2020). The biocides terbutryn, diuron and OIT were quantified in groundwater, in standing water in the swales and during a façade sprinkling experiment (Hensen et al., 2018).

The GRUBURG 3D model is based on a groundwater flow and transport model developed by Zimmermann, 2021. The input data and certain settings were updated for the GRUBURG model and are described below. The entire urban district covers an area of 41 ha, of which 38 ha is the model area. Approximately 19 ha are connected to the swale-trench system (Figure 35). Twelve individual swale catchment areas drain to corresponding swale fractions. In these catchments, infiltration takes place either within the swales or diffusely in the swale catchment areas. The remaining area is connected to a combined sewer system (grey area in Figure 35) and therefore excluded from calculating biocide emissions to groundwater. In the model, geology consists of two layers: an upper layer has a lower permeability due to deposited floodplain sediments while a lower layer has a higher permeability and represents the main aquifer. Groundwater levels and monitoring data for CHC contaminants were used to calibrate the groundwater model of (Zimmermann, 2021).

Figure 35: Study area with monitoring wells, swale-trench systems and 12 swale catchments

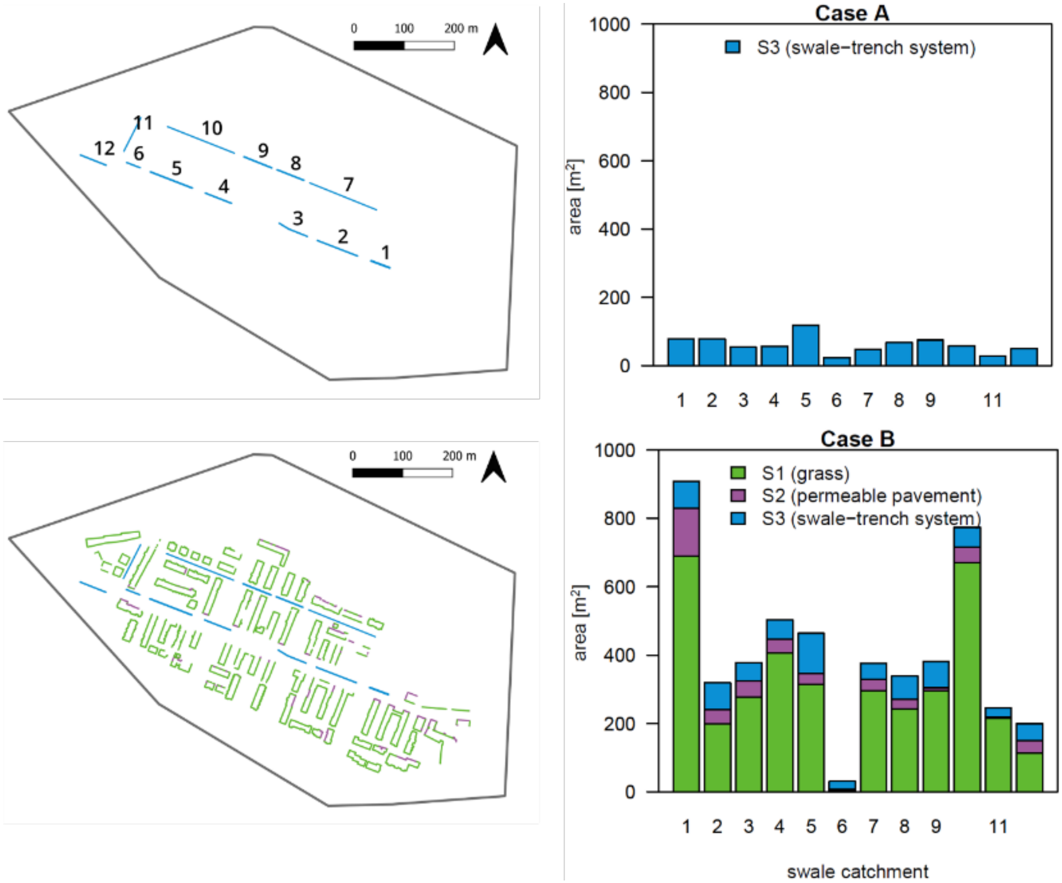
Source: Own illustration, UNI Freiburg

6.1.2 Modelling biocide entry to groundwater

There are two ways in which biocides enter the groundwater in the GRUBURG 3D model: via swales (S3) or diffusely in the swale catchments (S1, S2). This helps to assess the importance of the pathway scenarios as described in Section 3. Figure 36 shows the distribution of areas where biocides may leach to groundwater within each swale catchment.

In case A, biocides can only reach the groundwater by the swale-trench systems (S3) while in case B all pathways are represented. Here, the emitted biocides are uniformly distributed in a 0.5 m buffer around the façades to vegetated soils (S1, 68 % of total leaching area) and permeable pavements (S2, 10 %) and enter groundwater via the swale-trench systems (S3, 22 %).

Figure 36: Areas where biocides may leach to the groundwater. The maps show the areas distributed in the district and the numbers refer to swale catchments. The figures on the right show the corresponding areas



The top row shows case A where biocides can only enter the groundwater via the swale-trench system. The lower row shows case B, where biocides can enter diffusely next to buildings or in the swale-trench systems.
Source: Own illustrations, UNI Freiburg

6.1.3 Model structure and input data

Terbutryn was chosen as the model biocide for its common usage (3.2.1), environmental relevance, frequent measurement in the catchment (Hensen et al., 2018) and availability of leaching data (Burkhardt et al., 2012). The GRUBURG 3D model has a daily temporal resolution and simulates terbutryn concentrations in groundwater during the period from 9 April 2015 to 31 December 2017. As described above, the model covers the Freiburg-Vauban urban district and focusses on the 12 swale catchments connected to the swale-trench systems (Figure 35).

The GRUBURG 3D model combines four individual models into a **model chain**: for the water balance, the biocide emission, the transport in soil and in groundwater. First, the water balance model and the biocide emission model are run individually. The results from these two models are combined and used as input for the soil transport model. All three models run from the beginning of urban development in Freiburg Vauban (2000) until the end of the groundwater simulation period. In a final step, the groundwater model uses the results of the water balance model and the soil transport model to calculate biocide concentrations in groundwater. Figure 37 and Figure 38 show the model structures for cases A and B.

The **water balance model** RoGeR_WB_Urban was previously developed to establish the water balance in the Vauban district (Steinbrich et al., 2021). Input data was taken from the weather station DWD Freiburg, located approximately 5.3 km north of the urban district (DWD, 2023).

GIS data was provided by the city of Freiburg. The water balance model provides daily percolation data [L] to the groundwater within the individual swales, in the buffer area of 0.5m adjacent to the façades and in the remaining area of the swale catchments.

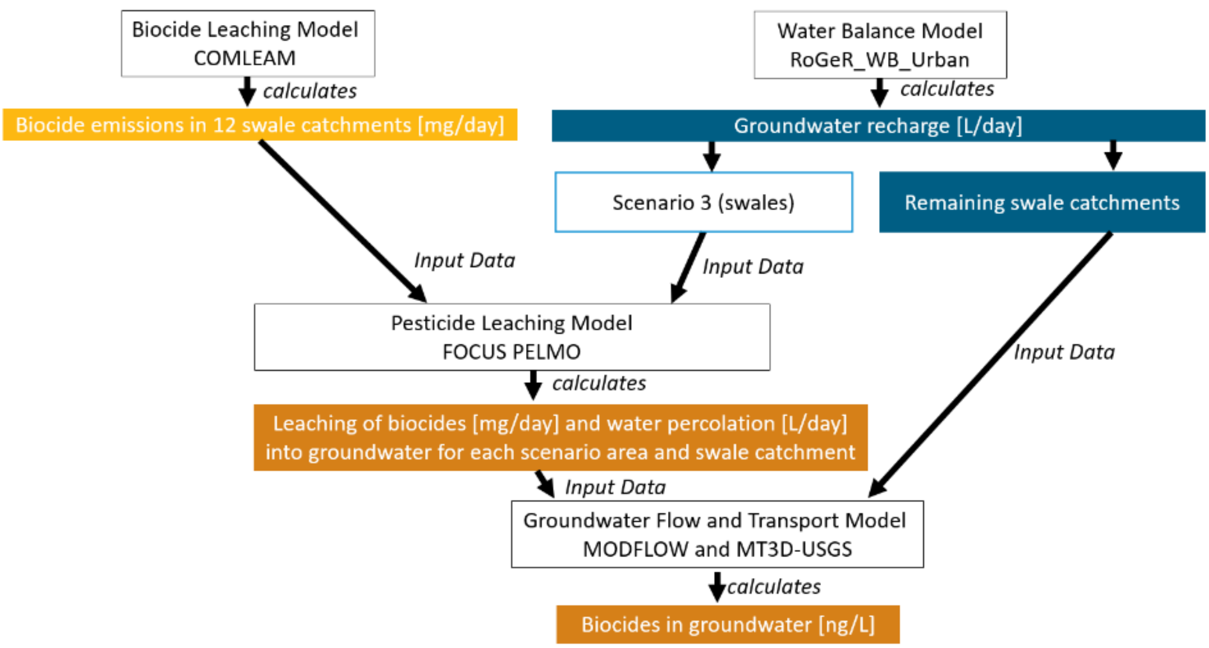
The **biocide emission model** COMLEAM dynamically calculates the biocide emissions from the façades (Burkhardt et al., 2021b). The input data for the façade geometry are based on available GIS data, field observations and data from Google Maps. Buildings were assumed to have been painted at the time of construction without renovation. The buildings are of different ages due to several construction phases. Emissions were calculated based on results from field experiments and an estimated initial terbutryn concentration of 2250 mg/m² (Burkhardt et al., 2012). The model output data were summarized as daily biocide emissions [mg] per swale catchment.

The **soil transport models** PELMO (chapter 5) calculates the transport of biocides through the soil. It combines the daily percolation and the biocide emissions from the two previous models. In case A, all biocides enter exclusively through swales and in case B, biocides were distributed to swales (S3) and to the 0.5 m soil around the façades (S1 and S2). For both cases, PELMO provides daily terbutryn emission [kg/ha] and percolation water [cm] to groundwater (1 m depth after soil passage).

The **groundwater flow model** MODFLOW 6 Version 6.4.2 in the Vauban district was developed and initially calibrated by (Zimmermann, 2021; Langevin et al., 2023). The model was updated with the described water balance model and biocide emissions. The groundwater model first calculates the groundwater flow and then biocide transport in the saturated zone using MT3D-USGS (Bedekar et al., 2016). The output of daily groundwater levels and groundwater biocide concentrations can be compared with observed data.

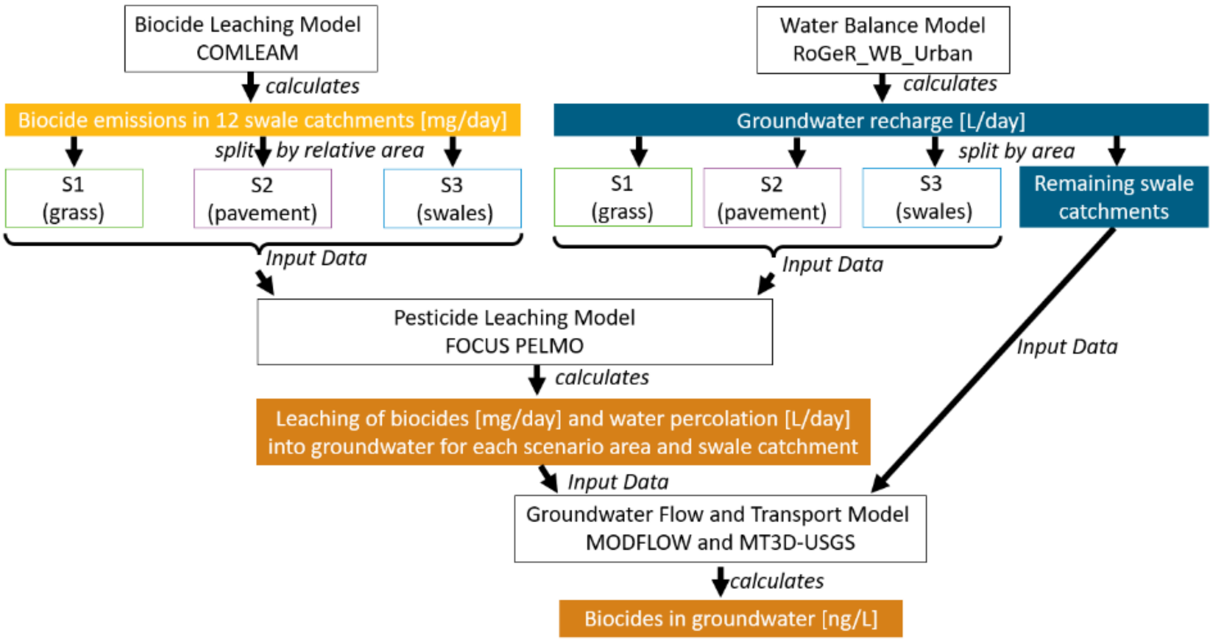
The GRUBURG 3D model does not consider terbutryn degradation in groundwater or at façades, only within soil by PELMO. This represents a conservative worst-case scenario, because terbutryn degradation is partly neglected. In contrast, the model does not include renovation or repainting of buildings, which could increase biocide emissions from façades.

Figure 37: Model chain with biocide leaching only in swale-trench systems (case A)



Source: Own illustration, UNI Freiburg

Figure 38: Model chain with biocide leaching via all three scenarios (case B)



Source: Own illustration, UNI Freiburg

6.1.4 Validation for biocide emissions and water balance

To internally validate the GRUBURG 3D model chain, simulated biocide emissions were compared with available measurement data obtained from a sprinkling experiment on a façade within the district, as well as from sampling of standing water in two swales during three separate rain events (data published in Hensen et al., 2018).

The sprinkling experiment, carried out in 2017, involved the application of an estimated 5 to 10m^3 of water onto a 36 m^2 façade. This volume significantly exceeds that of an average storm event, where only a small fraction contributes to façade runoff. Collection of water occurred at the base of the façade. Biocide concentrations were measured for terbutryn, diuron and OIT and selected TPs. Concentrations were low with a range of 0.2 - 1.9 ng/L for terbutry, 3.6 – 18 ng/L for diuron and 0.3 - 2.2 ng/L for OIT. A TP of diuron was found at even higher concentrations of up to 690 ng/L (TP-219). These findings indicate both the application of biocides at the façade and a continuous leaching even after 14 years of exposure (Hensen et al., 2018).

The model check of this individual façade used the same emission assumptions as the input for the 3D model (6.1.3). The total area of the façade was 36 m^2, facing north. It was last painted in 2003. The model results for biocide emissions were averaged over a period of 30 days before and after the sprinkling experiment. The emitted biocide masses were then included into 5 – 10 m^3 of applied sprinkling water during the experiment and yielded terbutryn concentrations of 1.2 - 2.5 ng/L. Those were in very good agreement with the measured concentrations of 0.2 - 1.9 ng/L. COMLEAM biocide emissions can thus be regarded as a realistic estimate for the whole district, despite inherent uncertainties such as initial biocide concentrations or biocide loss from the façade prior to the sprinkling experiment.

In a second model check, measured biocide concentrations in standing swale water were compared to a combination of COMLEAM biocide emissions to the swales and the amount of water in the swales calculated by ROGER_WB_Urban. Terbutryn concentrations in the standing water in the swales during three events ranged from 15 – 137 ng/L for swale 1. In a second swale, terbutryn concentrations ranged from 1–6 ng/L (Table 16). These differences are due to various factors, including differences in buildings, orientations, paints used and connectivity to the swale.

Table 16: Measured and modelled biocide concentrations in stormwater of two swales

Event	Swale	Measured [ng/L]	case A [ng/L]	case B [ng/L]
1	1	137	373	32
2	1	22	406	35
3	1	15	1658	143
1	2	6.3	22	5.6
2	2	1.0	19	4.5
3	2	4.3	56	14

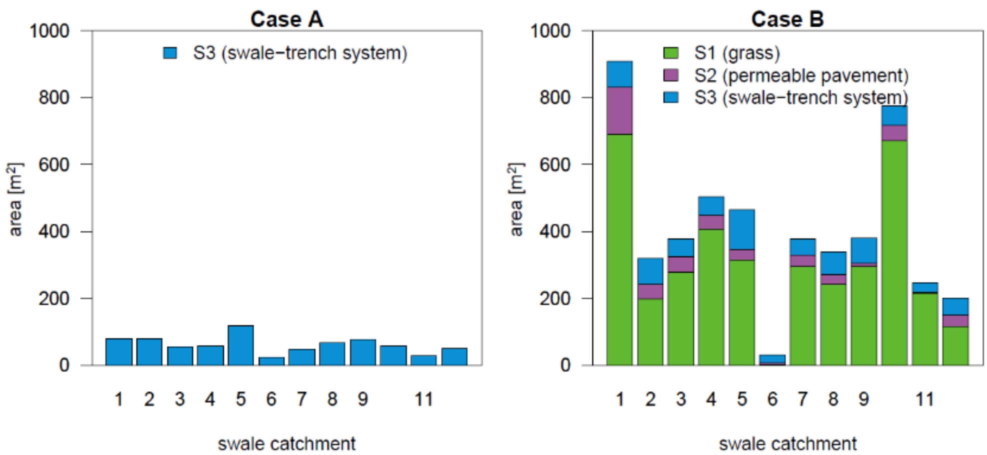
Modelling was carried out as described in 6.1.3 using COMLEAM and ROGER_WB_Urban for cases A and B. The biocide emissions [mg] for swale 1 and swale 2 were divided by the ponded water volume [L] and compared to measured data (Table 16). The modelled concentrations for case A were too high since no diffuse infiltration of biocides was considered. case B provided biocide concentrations that were in better agreement with the measurements yet did not reproduce the variability during single events. This points to uncertainties in both the measured and modelled data. On the one hand, the collected point samples were not flow proportional and therefore not representative for an event. On the other hand, the modelled data is based on various assumptions including estimates of biocide emissions or façade geometry, among others. Nevertheless, the 3D model could reproduce realistic order of magnitudes.

6.2 Relevance of the different emission pathways (model results)

6.2.1 Biocide emissions to groundwater

The biocide emissions to groundwater are based on the calculations in the PELMO model. They are slightly different for case A and B. Figure 39 shows the input to groundwater after modelling the leaching through the soil passage with PELMO.

Figure 39: Biocide input to groundwater after soil passage for case A and B per swale catchment



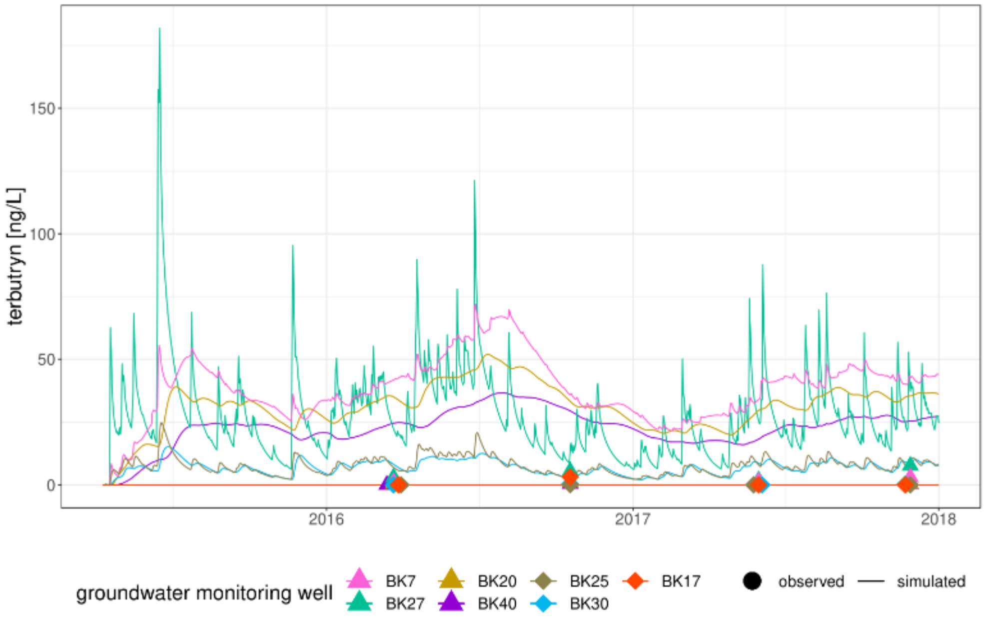
Source: Own illustrations, UNI Freiburg

For case A, 94-99.8 % of the biocide input reaches the groundwater via S3 (swale-trench system) and case B 71-96 % for S1 (grass), 96-99 % for S2 (permeable pavement) and 43-99 % for S3 (swale-trench system). Despite to the variability in the catchments, the 3D model results that the main amount of the biocide passing the soil will enter the groundwater.

6.2.2 Biocide concentrations in groundwater

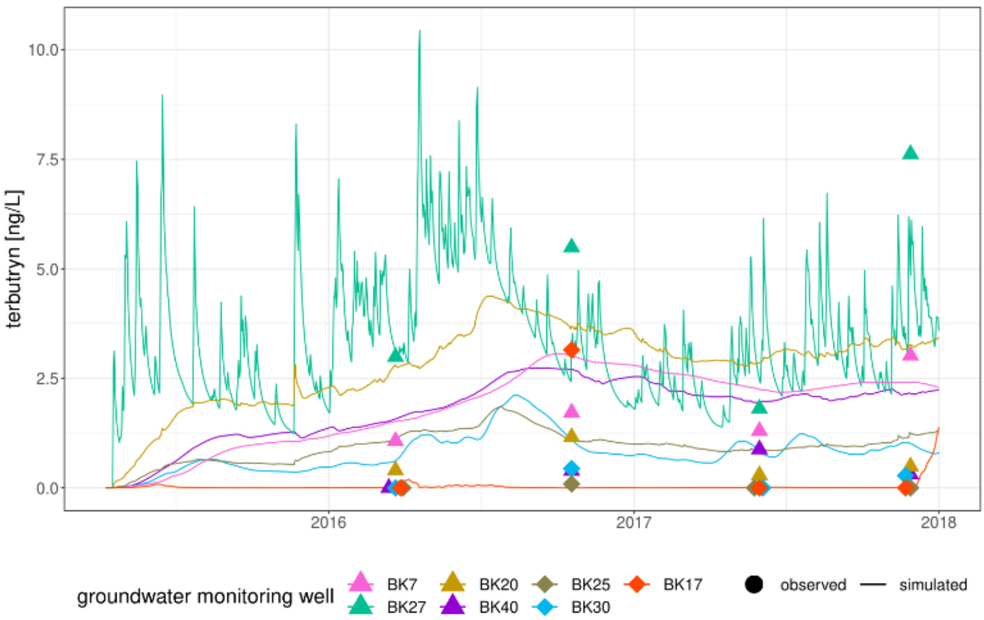
Simulated biocide concentrations in groundwater were compared with concentrations for cases A and B (Figure 40 and Figure 41). Case A overestimates biocide concentrations by a factor of 15, while concentrations of case B more accurately represent measured biocide concentrations.

Figure 40: Modelled and observed terbutryn concentrations in groundwater for case A



Source: Own illustration, UNI Freiburg

Figure 41: Modelled and observed terbutryn concentrations in groundwater for case B



Source: Own illustration, UNI Freiburg

The modelled spatial terbutryn distribution are presented in Figure 60 and Figure 61 in the Appendix A.8. In case A, terbutryn plumes originating from the swale-trench system are prominently visible. Conversely, in case B, the highest concentrations are situated alongside façades (Figure 61). Notably, the terbutryn plumes from the swale-trench system exhibit considerably lower concentrations.

6.2.3 Relevance of different emission pathways

The outcomes of the GRUBURG 3D model exercise conducted in urban district of Freiburg Vauban indicate that vegetated soils and permeable pavements must be regarded as crucial pathways for biocide emissions from urban façades into groundwater. Notably, when incorporating transport through permeable pavements and vegetated soils (case B), the modeled results closely aligned with measured terbutryn concentrations in swales and groundwater. In contrast, directing all biocide emissions through swales (case A) resulted in significant overestimations of measured biocide concentrations. Suggestion of the substantial relevance of diffuse emissions of biocides to groundwater in urban areas are also reported in scientific literature (Junginger, 2022). Other studies reported diffuse losses of terbutryn and of diuron within urban catchments before runoff reached the connected stormwater sewer system (Burkhardt et al., 2021c; Linke et al., 2022). These losses may contribute towards diffuse emissions of biocides to groundwater.

It is important to acknowledge numerous uncertainties in the GRUBURG 3D model chain stemming from various assumptions including building geometry, biocide emissions, and the distribution of scenario areas within the district. Nevertheless, the model results, when compared with measured data available, suggest that a comprehensive assessment of the realistic potential impacts of biocide input to groundwater should encompass all three emission pathways. However, considering transport solely through infiltration facilities can be a viable option as a conservative worst-case scenario.

7 Conclusions

Groundwater plays a vital role as a resource for drinking water, industrial and agricultural purposes, and is indispensable for ecosystems. This study aims to safeguard urban groundwater from biocide emissions originating from buildings by developing convincing groundwater protection scenarios for biocide authorization. To formulate these scenarios, an overview of pertinent soil properties in urban areas is compiled. Additionally, emissions are assessed in connection with factors such as building geometry, weathering surfaces, and site-specific weather conditions. The suitability of the scenarios is then scrutinized through simulations using FOCUS models (PELMO, PEARL), and a three-dimensional chain of four models in an urban catchment.

To estimate the most relevant biocides and their usage, stakeholders such as manufacturers and associations were surveyed. Based on the feedback from biocidal product manufacturers, substances belonging to group PT7 were identified as the most commonly used and relevant for biocide emissions into groundwater from buildings, with terbutryn and OIT being the most extensively employed. As a result, this study selected terbutryn and OIT as model substances. These two biocides were chosen due to their widespread use on façades and their representation of substances with varying degradability, spanning from low to high.

To assess the release of biocides from façades in urban areas, a representative building geometry was derived utilizing 3D building models and satellite data, and existing regulatory standard geometries were verified for suitability. The source of biocide emissions is depicted by a standardized geometry closely resembling the BPR/OECD house, but with a revised height of 10 meters and a flat roof. This geometry aligns with building geometries commonly employed for regulatory purposes and is supported by observations from LOD2 data in Germany.

Biocides reach groundwater by percolation through urban soils. To establish representative soil profiles for the emission pathway of biocides to groundwater, three different emission pathways—vegetated soils, permeable pavements, and infiltration facilities—were incorporated into the scenarios based on a literature review. Relevant soil parameters were deduced from literature and of field measurements in mainly two German cities, Berlin and Freiburg. In a research endeavor, existing national guidelines for swales and permeable pavements in Europe were compared. A conservative depth to groundwater of 1 meter was established for all scenarios based on groundwater maps of several German cities.

To fulfill regulatory requirements, the estimation of biocide emissions from façades typically relies on standardized leaching tests, the outcomes of which are integrated into ECHA's Emission scenario documents (ESDs). However, this method overlooks site-specific weather conditions that influence façade emissions and the transport of biocides through soil. Consequently, the established ESD approach was compared with the dynamic emission model COMLEAM. The observation indicated that the ESD approach generally offers a valid conservative option for describing source emissions and that COMLEAM could be implemented in a tiered approach for the biocide authorization procedure.

In describing biocide transfer in soil, the two FOCUS models (PEARL, PELMO) were compared, and pertinent aspects like preferential flow and the model's hydraulic setup were discussed. Both PEARL and PELMO were deemed suitable for modelling biocide transfer in urban areas, but PEARL was chosen for applying the emission scenarios outlined in this project due to its established use in the field of biocide authorisation procedure and accurate hydraulic modelling. Simulations showed that local weather conditions strongly influence the transport of biocides through the soil to groundwater, especially for emission pathways with a high ratio of infiltration to leaching area (façade). In addition, soil modelling showed clear differences between the different emission pathways, indicating that vegetated soils lead to higher leachate concentrations but lower load emissions compared to permeable pavements and infiltration systems.

The developed scenarios, grounded in empirical data, underscore the significance of considering biocide loads emitted to groundwater and groundwater concentrations alongside soil leachate alone. To aggregate results from various emission scenarios and assess resulting groundwater concentrations while still accounting for the heterogeneity of urban soils, a simplified and conservative mass balance approach is proposed (5.2.7).

To better assess the relative significance of various pathways contributing to the emissions of biocides into groundwater, a 3D model chain was established for the district of Freiburg-Vauban. Various emission pathways were compared by applying the scenarios outlined in this project, thereby illuminating biocide emission dynamics in urban areas. The results of the 3D modelling in the Vauban catchment suggest that for the model substance terbutryn retention in the unsaturated zone is limited and that vegetated soils and permeable pavements play crucial roles as pathways for diffuse biocide emissions from urban façades into groundwater.

The findings of this study are utilized to formulate measures for architects, engineers, and municipalities aimed at preventing and reducing the emission of biocides into groundwater in urban areas. Additionally, recommendations for the biocide authorization procedure are presented below.

7.1 Measures for architects, engineers and municipalities

In order to address and control the release of environmentally relevant substances from construction products into the groundwater, a comprehensive guideline with an additional information sheet was developed. The guideline targets architectures, experts in urban planning, practitioners, housing construction companies, as well as municipalities, associations and manufacturers. It has two main objectives. On the one hand, causes and effects of pollutants released into the urban water cycle by construction activities are demonstrated to stakeholders. The main focus here is on the effects of biocides from building façades. On the other hand, the guideline addresses the handling of rainwater for a sustainable blue-green infrastructure, summarized in the term sponge city.

In the context of the sponge city, decentralized rainwater management is encouraged through unsealing of surfaces, promotion of green roofs and expansion of green spaces. In order to prepare urban areas for the effects of climate change, it is necessary to close urban water cycles and keep rainwater in place instead of draining. This can be accomplished through infiltration, retention, evaporation or irrigation. However, if rainwater is contaminated, it must first be cleaned to prevent pollution hazards, primarily for groundwater.

The proposed guidelines therefore aim at holistic solutions that do not require the use of biocides and in this way sustainably protect groundwater resources. In the case of algae and fungi on façades, those might be handled as living parts of future urban ecosystems. In the second part of the guide, approaches and solutions are presented on how the goals of the sponge city can be achieved through sustainable construction.

In addition to source control measures, the guide and information sheets also summarize possible end-of-pipe measures. The information and recommendations draw upon various studies, with a particular emphasis on the insights derived from the BaSaR project (Wicke et al., 2021). The findings of this project supplement and refine the guidelines, with a specific focus on groundwater protection and retention of biocides.

In conclusion, the recommended measures can be summarized as follows:

- First and foremost, sustainable urban development and construction should focus on measures at the source in order to avoid contamination of urban runoff.
- The use of materials free of biocides or other emerging pollutants such as clinker, natural stone, glass or biocide-free plasters and paints is possible and a promising strategy to avoid pollution.
- Furthermore, structural weather protection or green façades are options for sustainable construction.
- If biocides cannot be avoided, it is important to ensure that they are used according to best practice and that stormwater infiltration facilities are designed and operated properly. A large amount of information is already available in this respect, which is referred to by the guide.

7.2 Recommendations for the biocide authorization procedure

This study provides a realistic set of worst-case scenarios for the modelling of biocide emissions into groundwater in urban areas. These are based on a holistic source-path-target concept. The parameters describing the building geometry, biocide leaching, weather conditions, urban soil properties and biocide soil transport are based on scientific observations and consolidated into the different emission scenarios. Building upon the formulation and application of scenario models, the following paragraphs focus on specific aspects of the biocide authorization procedure, proposing refinements to the ESD for PT7.

To assess the release of biocides from façades, it is crucial to select a representative building geometry. While various standard building geometries, such as the BPR/OECD house and DIBT house, are documented in literature for research and regulatory purposes, they are often not empirically derived. Considering the analysis of 3D building models (LOD2), it is suggested to refine the height of the BPR/OECD house to 10 meters for a more representative building geometry.

Biocide emissions into urban groundwater occur through multiple pathways, and the resulting concentrations in groundwater are significantly influenced by the physicochemical properties of the soil and biocides. The scenarios outlined in this project integrate biocide leaching dynamics, following the established ESD, with the soil transport model PEARL and PELMO. This combined approach enables a worst-case, yet realistic characterization of biocide emissions to groundwater, considering climatic conditions, adsorptive soil processes, and degradation. Consequently, it provides a more detailed estimate of biocide emissions in groundwater compared to the ESD approach alone. Furthermore, the inclusion of the biocide leaching model COMLEAM in a tiered approach can enhance the level of detail, offering a comprehensive description of biocide leaching from façades.

The established Emission Scenario Document (ESD) for biocides of PT 7 does not account for various emissions pathways to groundwater. This project identified, characterized, and consolidated the most relevant emission pathways in defined scenarios. Comparing modelled biocide concentrations using these scenarios with actual biocide occurrences in a 38 ha urban catchment underscores the importance of incorporating different emission pathways (vegetated soils, permeable pavements, infiltration facilities) for a representative characterization of biocide emissions from urban areas into groundwater. Notably, the results emphasize the significance of diffuse emissions through vegetated soils and permeable pavements. Solely considering infiltration facilities would result in an overestimation of biocide emissions to groundwater, making it a conservative approach if necessary.

The consideration of various emission pathways underscores the importance of assessing not only the percolate biocide concentration, as currently done in the established ESD for PT7, but also the emitted load and resultant groundwater biocide concentration. This becomes particularly relevant in urban areas where biocide emission is continuous, but infiltration occurs in spatially concentrated form around buildings, through joints in permeable pavements or in infiltration facilities. Relying exclusively on percolate concentration, as is the current practice for pesticides in agriculture (FOCUS), may lead to misleading interpretations in such a setting. Therefore, this study recommends incorporating assessments of emitted loads to groundwater and groundwater concentrations to ensure effective groundwater protection in urban areas.

The recommendations for refining the ESD for PT7 are summarized as follows:

- Refinement of the building geometry to better characterize biocide emissions.
- Inclusions of multiple emission pathways, namely vegetated soil, permeable pavements and infiltration facilities to account for the spatial heterogeneity of urban areas and rainwater infiltration.
- Combination of ESD with soil transport model PEARL into simplified scenarios to improve the characterization of biocides emission to groundwater in urban areas.
- Assessment of emitted biocide loads to groundwater as well as groundwater biocide concentrations alongside percolate concentration to better protect urban groundwater resources.

As a methodology for risk assessment during biocide authorization, the following procedure is proposed. The approach involves aggregating the cumulative loads from all three identified urban pathways using the soil transport model PEARL, determining a representative concentration of urban percolate using the cumulative percolate volumes from each pathway, and calculating their mean for an assessment period of 5 years. This combined mean percolate concentration is subsequently multiplied by a transfer factor to estimate an average representative groundwater concentration in the urban area. This groundwater concentration is then evaluated for the risk assessment.

This methodology builds upon the framework of established ESDs for PT7 and offers a data-driven concept that could be employed as a tiered approach or as an alternative to characterize and assess biocide emissions to groundwater, while still using standardized scenarios more realistically. Although the additional modeling steps introduce added complexity, the scenarios remain strongly standardized and can be easily accessed by users through a simplified interface (Appendix, Figure 62), where only selected input parameters need to be provided. This approach mirrors the simplicity of the current ESDs, ensuring a user-friendly experience.

8 List of references

Acosta, J.A., Faz, A., Martínez-Martínez, S., Arocena, J.M. (2014). Grass-induced changes in properties of soils in urban green areas with emphasis on mobility of metals. Journal of Soils and Sediments, 14, 819–828. DOI: 10.1007/s11368-013-0830-z

Andrés-Doménech, I., Anta, J., Perales-Momparler, S., Rodriguez-Hernandez, J. (2021). Sustainable Urban Drainage Systems in Spain: A Diagnosis. Sustainability, 13, 2791. DOI: 10.3390/su13052791

Aschauer, J., Kolmer, C., Laimer, W., Mühleder, W., Schützeneder, G. (2021). Leitfaden Verbringung von Niederschlagswässern von Dachflächen und befestigten Flächen. Amt der Oö. Landesregierung, Direktion Umwelt und Wasserwirtschaft, Linz, p. 20. www.land-oberoesterreich.gv.at/files/publikationen/ww_lf_verbringung_von_niederschlagswaessern.pdf (viewed: 6.12.2024)

Attaway, H.H., Camper, N.D., Paynter, M.J.B. (1982). Anaerobic Microbial Degradation of Diuron by Pond Sediment. Pesticide Biochemistry and Physiology, 17, 96–101. DOI: 10.1016/0048-3575(82)90130-4

Avidov, E., Aharonson, N., Katan, J., Rubin, B., Yarden, O. (1985). Persistence of terbutryn and atrazine in soil as affected by soil disinfestation and fungicides. Weed Science, 33, 457–461. DOI: 10.1017/S0043174500082655

BAFU/ARE (2022). Regenwasser im Siedlungsraum: Starkniederschlag und Regenwasserbewirtschaftung in der klimaangepassten Siedlungsentwicklung. Federal Office for the Environment (BAFU) and Federal Office for Spatial Development (ARE). Umwelt-Wissen, No 2201, p. 115, Bern. www.bafu.admin.ch/bafu/de/home/themen/klima/publikationen-studien/publikationen/regenwasser-im-siedlungsraum.html (viewed: 6.12.2024)

Bedekar, V., Morway, E.D., Langevin, C.D., Tonkin, M.J. (2016). MT3D-USGS version 1: A U.S. Geological Survey release of MT3DMS updated with new and expanded transport capabilities for use with MODFLOW. U.S. Geological Survey Techniques and Methods 6-A53, p. 69. DOI: 10.3133/tm6A53

Bollmann, U.E., Vollertsen, J., Carmeliet, J., Bester, K. (2014). Dynamics of biocide emissions from buildings in a suburban stormwater catchment - Concentrations, mass loads and emission processes. Water Research, 56, 66-76. DOI: 10.1016/j.watres.2014.02.033

Bollmann, U.E., Minelgaite, G., Schlüsener, M., Ternes, T., Vollertsen, J., Bester, K. (2016). Leaching of Terbutryn and Its Photodegradation Products from Artificial Walls under Natural Weather Conditions. Environmental Science and Technology, 50, 4289–4295. DOI: 10.1021/acs.est.5b05825

Bollmann, U.E., Fernández-Calviño, D., Brandt, K.K., Storgaard, M.S., Sanderson, H., Bester, K. (2017). Biocide Runoff from Building Façades: Degradation Kinetics in Soil. Environmental Science and Technology, 51, 3694–3702. DOI: 10.1021/acs.est.6b05512

Boogaard, F. (2015). Stormwater characteristics and new testing methods for certain sustainable urban drainage systems in The Netherlands. Doctoral thesis, Technische Universiteit Delft, p. 147. DOI: 10.4233/uuid:d4cd80a8-41e2-49a5-8f41-f1efc1a0ef5d

Boogaard, F., Rombout, J. (2008). Ondergrondse infiltratie van regenwater: Een literatuur- en praktijkonderzoek naar milieurisico's. Stichting RIONED, 12.

Borgwardt, S. (1998). Merkblatt für wasserdurchlässige Befestigungen von Verkehrsflächen. FGSV Forschungsgesellschaft für Straßen- und Verkehrswesen, Köln.

Bork, M., Lange, J., Graf-Rosenfellner, M., Hensen, B., Olsson, O., Hartung, T., Fernández-Pascual, E., Lang, F. (2021). Urban storm water infiltration systems are not reliable sinks for biocides: evidence from column experiments. Scientific Reports, 11, 7242. DOI: 10.1038/s41598-021-86387-9

Bouteligier, R., Vaes, G., Berlamont, J., Beeldens, A., Blomme, P., Michielsen, K., T'Joen, C., Van Belle, L., van Gucht, G., Vennekens, D., Verhoeven, H., Augustyns, J., Monnaers, A. (2005). Katern afkoppelen, bufferen en infiltreren. VLARIO vzw, Hoboken, Belgium, p. 93. https://www.vlario.be/files/katernafkoppelen1.pdf (viewed: 6.12.2024)

Burkhardt, M., Kupper, T., Hean, S., Haag, R., Schmid, P., Kohler, M., Boller, M. (2007). Biocides used in Building Materials and their Leaching Behavior to Sewer Systems. Water Science and Technology, 56, 63-67. DOI: 10.2166/wst.2007.807

Burkhardt, M., Zuleeg, S., Vonbank, R., Schmid, P., Hean, S., Lamani, X., Bester, K., Boller, M. (2011). Leaching of additives from construction materials to urban storm water runoff. Water Science and Technology, 63, 74–82. DOI: 10.2166/wst.2011.128

Burkhardt, M., Zuleeg, S., Vonbank, R., Bester, K., Carmelit, J., Boller, M., Wangler, T. (2012). Leaching of Biocides from Façades under Natural Weather Conditions. Environ. Sci. Technol. 46, 5497–5503. DOI: 10.1021/es2040009

Burkhardt, M., Dietschweiler, C. (2015). Reduction of environmental risks from the use of biocides: Environmental sound use of disinfectants, masonry preservatives and rodenticides - Annex IV: Case study on PT 7/10: Masonry preservatives and facade paints and plaster. UBA-Texte 36, Federal Environment Agency, Dessau-Roßlau, p. 31. https://www.umweltbundesamt.de/sites/default/files/medien/378/publikationen/texte_53_2015_annex_iv_0.pdf (viewed: 6.12.2024)

Burkhardt, M., Schmidt, S., Gohl, M., Zenker, A., Schmocker, M., Zbinden, D., Loretz, A., Bigler, R., Boller, M. (2017). Behandlung von Regenwasser - Grosstechnische Erfahrung mit unterirdischer Retention und nachgeschaltetem Adsorberfilter. Aqua und Gas, 4, 78-85. vsa.ch/wp-content/uploads/2020/04/Behandlung_von_Regenabwasser.pdf (viewed: 6.12.2024)

Burkhardt, M., Hodel, P. (2019). Abschwemmung von Metallflächen und Eintrag ins Grundwasser - Literaturrecherche und Messungen unter Berücksichtigung von drei urbanen Pestiziden. Report, contracted by Federal Office for the Environment (BAFU), OST, Rapperswil, p. 41. https://www.comleam.ch/user/pages/01.home/07._projekte/Projekt_05_190520_MEDAUG_Schlussbericht.pdf (viewed: 6.12.2024)

Burkhardt, M., Klingler, M., Savi, D., Rohr, M., Tietje, O., Junghans, M. (2021a). Entwicklung einer emissionsbasierten Bauproduktebewertung – Anwendung des Konzepts für Dachbahnen und Fassadenputze. Federal Office for the Environment (BAFU), Bern, and Amt für Hochbauten der Stadt Zürich (AHB), Zürich, p. 115. https://www.bafu.admin.ch/dam/bafu/de/dokumente/wirtschaft-konsum/externe-studien-berichte/entwicklung-einer-emissionsbasierten-bauproduktebewertung.pdf.download.pdf/Emissionsbasierte%20Produktbewertung_Schlussbericht_2021.pdf (viewed: 6.12.2024)

Burkhardt, M., Gehrig, S., Rohr, M., Tietje, O. (2021b). Auswaschung von Bioziden aus Bauprodukten und Exposition in der Umwelt - Berechnung von ESD-Szenarien und Modellierung mit der Software COMLEAM. Report, contracted by Federal Office for the Environment (BAFU), OST, Rapperswil, p. 75. https://www.bafu.admin.ch/dam/bafu/de/dokumente/wirtschaft-konsum/externe-studien-berichte/entwicklung-einer-emissionsbasierten-bauproduktebewertung.pdf.download.pdf/Emissionsbasierte%20Produktbewertung_Schlussbericht_2021.pdf (viewed: 6.12.2024)

Burkhardt, M., Rohr, M., Wicke, D., Tatis-Muvdi, R., Rouault, P., Zerball-Van Baar, P., Dünnbier, U. (2021c). Urbanes Niederschlagsabwasser: Emissionen, Belastungen und wirksame Massnahmen. Aqua und Gas, 10, 34–41.

City of Freiburg (2021). Stadtbezirksatlas Freiburg. Amt für Bürgerservice und Informationsmanagement, Freiburg im Breisgau, p. 274. www.freiburg.de/pb/site/Freiburg/get/params_E886714817/1828649/Stadtbezirksatlas_2021_komprimiert.pdf (viewed: 6.12.2024)

Claußner, C. (2013). Anwendung der allgemein anerkannten Regeln der Technik bei dezentralen Anlagen zur Regenwasserversickerung. Master thesis, University of Freiburg, p. 64. https://www.hydrology.uni-freiburg.de/abschluss/Claussner_C_2013_MA.pdf (viewed: 6.12.2024)

Cooper, N., Cooke, S. (2016). Assessment and management of unexploded ordnance (UXO) risk in the marine environment. CIRIA, London UK, p. 180.

Council Directive 98/83/EC (1998). Council Directive of 3 November 1998 on the quality of water intended for human consumption. L 330, Official Journal of the European Communities, 41, 32-54. https://eur-lex.europa.eu/legal-content/EN/TXT/PDF/?uri=CELEX:31998L0083 (viewed: 6.12.2024)

Craul, P.J. (1985). A description of urban soils and their desired characteristics. Journal of Arboric, 11, 330–339. DOI: 10.48044/jauf.1985.071

Daho, M.B. (1994). Ecotoxicological evaluation of the herbicide terbutryn. Projektrapport från utbildningen i Ekotoxikologi, Ekotoxikologiska avdelningen, Uppsala, No 107, p. 59.

DANVA (2018). DESIGNGUIDE FOR REGNVANDSBASSINER. DANVA vejledning nr. 102, DANVA, Skanderborg, p. 45. https://www.danva.dk/media/4817/danva_regnvandsbassiner_designguide_2018_final.pdf (viewed: 6.12.2024)

Dierkes, C., Lucke, T., Helmreich, B. (2015). General Technical Approvals for Decentralised Sustainable Urban Drainage Systems (SUDS)—The Current Situation in Germany. Sustainability, 7, 3031–3051. DOI: 10.3390/su7033031

DSTATIS (2019). Öffentliche Wasserversorgung und öffentliche Abwasserbeseitigung. Fachserie 19, Reihe 2.1.1, Statistisches Bundesamt, Wiesbaden. https://www.destatis.de/DE/Themen/Gesellschaft-Umwelt/Umwelt/Wasserwirtschaft/Publikationen/Downloads-Wasserwirtschaft/wasser-oeffentlich-2190211199005.html?nn=211848 (viewed: 6.12.2024)

DWA (2024). Arbeitsblatt DWA-A 138-1: Anlagen zur Versickerung von Niederschlagswasser – Teil 1: Planung, Bau, Betrieb. DWA Deutsche Vereinigung für Wasserwirtschaft, Abwasser und Abfall e. V., Hennef, p. 98.

DWD (2023). Precipitation Data: Station 1443 - Freiburg. DWD Deutscher Wetterdienst. https://cdc.dwd.de/rest/metadata/station/html/812300590823 (viewed: 6.12.2024)

ECHA (2017). Evaluation of active substances: OIT, Product-type 08. Assessment Report Regulation (EU) No 528/2012, United Kingdom.

Fernández-Calviño, D., Rousk, J., Bååth, E., Bollmann, U.E., Bester, K., Brandt, K.K. (2021). Short-term toxicity assessment of a triazine herbicide (terbutryn) underestimates the sensitivity of soil microorganisms. Soil Biology and Biochemistry, 154, 108130. DOI: 10.1016/j.soilbio.2021.108130

FGSV (2016). Merkblatt für Versickerungsfähige Verkehrsflächen. FGSV Forschungsgesellschaft für Straßen- und Verkehrswesen, Köln, p. 56.

Flanagan, K., Blecken, G.-T., Österlund, H., Nordqvist, K., Viklander, M. (2021). Contamination of urban stormwater pond sediments: a study of 259 legacy and contemporary organic substances. Environmental Science and Technology, 55, 3009–3020. DOI: 10.1021/acs.est.0c07782

Fletcher, T.D., Shuster, W., Hunt, W.F., Ashley, R., Butler, D., Arthur, S., Trowsdale, S., Barraud, S., Semadeni-Davies, A., Bertrand-Krajewski, J.-L., Mikkelsen, P.S., Rivard, G., Uhl, M., Dagenais, D., Viklander, M. (2015). SUDS, LID, BMPs, WSUD and more – The evolution and application of terminology surrounding urban drainage. Urban Water Journal, 12, 525–542. DOI: 10.1080/1573062X.2014.916314

FOCUS (2000). FOCUS groundwater scenarios in the EU review of active substances. Report of the FOCUS Groundwater Scenarios Workgroup, EC Document Reference Sanco/321/2000 rev.2, p. 202. www.ime.fraunhofer.de/content/dam/ime/de/documents/AE/FOCUS_2000_GW_Report_Main.pdf (viewed: 6.12.2024)

Goutaland, D., Roux, G., Winiarski, T. (2015). Les ouvrages d'infiltration la fonction filtration: recommandations à l'usage des gestionnaires. GRAIE, Villeurbanne Cedex, p. 33. www.graie.org/othu/pdfothu/Gessol-ouvrages-infiltration-web.pdf (viewed: 6.12.2024)

GrwV (2017): Grundwasserverordnung - V Grundwasserverordnung vom 9. November 2010 (BGBl. I S. 1513), die zuletzt durch Artikel 1 der Verordnung vom 12. Oktober 2022 (BGBl. I S. 1802) geändert worden ist. www.gesetze-im-internet.de/grwv_2010/BJNR151300010.html (viewed: 6.12.2024)

Helmreich, B., Schneider, F., Grotehusmann, D., Hüpperling, R., Kaiser, M., Kasting, U., Kirsten, T., Nickel, D., Pfeifer, R., Anselm, J., Borchert, G., Benecke, H., Bürger, M., Kocher, B. Kolks, I., Maurer, W., Müller, M. Roth, J., Tatzber, J. (2022): Diskussion qualitativer Anforderungen für die Versickerung von Niederschlagswasser. Korrespondenz Abwasser Abfall, 69, 22-27.

Hensen, B., Lange, J., Jackisch, N., Zieger, F., Olsson, O., Kümmerer, K. (2018). Entry of biocides and their transformation products into groundwater via urban stormwater infiltration systems. Water Research, 144, 413–423. DOI: 10.1016/j.watres.2018.07.046

Hensen, B., Olsson, O., Kümmerer, K. (2020). A strategy for an initial assessment of the ecotoxicological effects of transformation products of pesticides in aquatic systems following a tiered approach. Environment International, 137, 105533. DOI: 10.1016/j.envint.2020.105533

Hochstrasser, F., Burkhardt, M., Tietje, O. (2016). Schlagregenberechnung für Gebäudefassaden Exemplarische Anwendung der Simulationssoftware COMLEAM. T 3340, Fraunhofer IRB Verlag, Stuttgart, p. 24. https://www.irbnet.de/daten/rswb/16089001501.pdf (viewed: 6.12.2024)

Hunter, J.D. (2007). Matplotlib: A 2D Graphics Environment. Computing in Science & Engineering, 9, 90–95. DOI: 10.1109/MCSE.2007.55

IAHS (2006). Proceedings of the IAH (IRISH GROUP) - 26th Annual Groundwater Conference. International Association of Hydrogeologists (Irish Group), Tullamore Court Hotel, Dublin. www.iah-ireland.org/conference-proceedings/2006.pdf (viewed: 6.12.2024)

IVA (1990). Wirkstoffe in Pflanzenschutz- und Schädlingsbekämpfungsmitteln - Physikalisch-chemische und toxikologische Daten. Industrieverband Agrar e.V., BLV Verlagsgesellschaft, München, Germany.

Jackisch, N., Brendt, T., Weiler, M., Lange, J. (2013). Evaluierung der Regenwasser bewirtschaftung im Vauban gelände, Freiburg i.Br. - unter besonderer Berücksichtigung von Gründächern und Vegetation. Final report, University of Freiburg, p. 96. www.hydrology.uni-freiburg.de/forsch/regenwasservauban/Regenwasserprojekt_Vauban_Endbericht_Final.pdf (viewed: 6.12.2024)

Jensen, D.M.R., Thomsen, A.T.H., Larsen, T., Egemose, S., Mikkelsen, P.S. (2020). From EU Directives to Local Stormwater Discharge Permits: A Study of Regulatory Uncertainty and Practice Gaps in Denmark. Sustainability 12, 6317. DOI: 10.3390/su12166317

Junginger, T. (2022). Transport and degradation of urban biocides from façades to groundwater. Doctoral thesis, Earth Sciences, Université de Strasbourg, Strasbourg, p. 283. https://theses.hal.science/tel-04226095v1 (viewed: 6.12.2024)

Junginger, T., Payraudeau, S., Imfeld, G. (2022). Transformation and stable isotope fractionation of the urban biocide terbutryn during biodegradation, photodegradation and abiotic hydrolysis. Chemosphere, 305, 135329. DOI: 10.1016/j.chemosphere.2022.135329

Junginger, T., Payraudeau, S., Imfeld, G. (2023). Emissions of the Urban Biocide Terbutryn from Façades: The Contribution of Transformation Products. Environmental Science and Technology, 57, 14319–14329. DOI: 10.1021/acs.est.2c08192

Jungnickel, C., Stock, F., Brandsch, T., Ranke, J. (2008). Risk assessment of biocides in roof paint - Part 1: Experimental determination and modelling of biocide leaching from roof pain. Environmental Science Pollution Research, 15, 258-265. DOI: 10.1065/espr2007.12.465

Kahle, M., Nöh, I. (2009). Biozide in Gewässern: Eintragspfade und Informationen zur Belastungssituation und deren Auswirkungen. UBA-Texte 09, Federal Environment Agency, Dessau-Roßlau, p. 52. https://www.umweltbundesamt.de/sites/default/files/medien/publikation/long/3811.pdf (viewed: 6.12.2024)

Kiefer, N., Nichterlein, M., Reiß, F., Runge, M., Biermann, U., Wieland, T., Noll, M., Kalkhof, S. (2024). Eluates from façades at the beginning of their service time affect aquatic and sediment organisms. Science of the Total Environment, 906, 167531. DOI: 10.1016/j.scitotenv.2023.167531

Kleidorfer, M., Zeisl, P., Ertl, T., Simperler, L., Kretschmer, F., Stöglehner, G., Himmelbauer, P., Muschalla, D., Krebs, G., Leimgruber, J. (2019). Leitfaden Regenwasserbewirtschaftung: Entwicklung flexibler Adaptierungskonzepte für die Siedlungsentwässerung der Zukunft – Praxisleitfaden aus dem Projekt Flexadapt. Federal Ministry of Agriculture, Forestry, Regions and Water Management, Wien, p. 107. www.umweltfoerderung.at/fileadmin/user_upload/umweltfoerderung/betriebe/Wasser_Betriebe/Studien_Wasserwirtschaft/20190618_Flexadapt_Leitfaden_final.pdf (viewed: 6.12.2024)

Klein, M. (1991). PELMO: Pesticide Leaching Model - User manual version 2.01. IME Fraunhofer-Institut für Umweltchemie und Ökotoxikologie, Schmallenberg.

Kluge, B., Kaiser, M., Sommer, H., Markert, A., Pallsch, M., Facklam, M. (2016). Leistungsfähigkeit und Zustand betriebener dezentraler Regenwasserversickerungsanlagen. Gwf Wasser|Abwasser, 157, 628-636. DOI: 10.17560/gwfwa.v157i06.1837

Kordana, S., Słyś, D. (2020). An analysis of important issues impacting the development of stormwater management systems in Poland. Science of the Total Environment, 727, 138711. DOI: 10.1016/j.scitotenv.2020.138711

Kuntaliitto (2012). Hulevesiopas. Suomen Kuntaliitto - Association of Finnish Local and Regional Authorities, Helsinki, Finnland, p. 298. www.kuntaliitto.fi/julkaisut/2012/1481-hulevesiopas (viewed: 6.12.2024)

Lange, J., Olsson, O., Jackisch, N., Weber, T., Hensen, B., Zieger, F., Schütz, T., Kümmerer, K. (2017). Urbane Regenwasserversickerung als Eintragspfad für biozide Wirkstoffe in das Grundwasser? Korrespondenz Wasserwirtschaft, 10(4), 198-202. DOI: 10.3243/kwe2017.04.001

Langevin, C.D., Hughes, J.D., Provost, A.M., Russcher, M.J., Panday, S. (2023). MODFLOW as a Configurable Multi-Model Hydrologic Simulator. Groundwater, 62, 111-123. DOI: 10.1111/gwat.13351

Linke, F., Edun, O., Junginger, T., Payraudeau, S., Preusser, F., Imfeld, G., Lange, J. (2023). Biocides in Soils of Urban Stormwater Infiltration Systems—Indications of Inputs from Point and Non-point Sources. Water, Air & Soil Pollution, 234(586). DOI: 10.1007/s11270-023-06613-0

Linke, F., Olsson, O., Preusser, F., Kümmerer, K., Schnarr, L., Bork, M., Lange, J. (2021). Sources and pathways of biocides and their transformation products in urban storm water infrastructure of a 2 ha urban district. Hydrology Earth and System Sciences, 25, 4495–4512. DOI: 10.5194/hess-25-4495-2021

Linke, F., Olsson, O., Schnarr, L., Kümmerer, K., Preusser, F., Bork, M., Leistert, H., Lange, J. (2022). Discharge and fate of biocide residuals to ephemeral stormwater retention pond sediments. Hydrology Research, 53(11), 1441. DOI: 10.2166/nh.2022.075

Makki, M., Thestorf, K., Hilbert, S., Thelemann, M., Makowsky, L. (2021). Guideline for the description of soils in the Berlin metropolitan area: an extension for surveying and mapping anthropogenic and natural soils in urban environments within the German soil classification system. Journal of Soils and Sediments, 21, 1998–2012. DOI: 10.1007/s11368-020-02832-8

Mall (2023). Marktbefragung 2023 "Umgang mit Regenwasser". Mall AG, Donaueschingen, p. 7. https://www.mall.ch/fileadmin/user_upload/produkte/regenwasserbewirtschaftung/prospekte/bundesweite-marktbefragung-umgang-mit-regenwasser-2023.pdf (viewed: 6.12.2024)

Mensink, H., Linders, J. (1991). Terbutryn EQS dossier 2011 - Adviesrapport 88/678801/171. National Institute of Public Health and Environmental Protection, Bilthoven, The Netherlands, p. 30. https://circabc.europa.eu/sd/a/6a543374-01c4-4002-a7b5-f6fbd2794c41/Terbutryn%20EQS%20dossier%202011.pdf (viewed: 6.12.2024)

Nannoni, F., Protano, G., Rossi, S. (2014). Soil properties and metal accumulation by earthworms in the Siena urban area (Italy). Applied Soil Ecology, 77, 9–17. DOI: 10.1016/j.apsoil.2014.01.004

NAVEBGO (2023). Risikofaktoren Biozidauswaschung — Nachhaltige Verringerung des Biozideintrags in Grundwasser am Oberrhein. University of Freiburg. www.navebgo.uni-freiburg.de/de/risikofaktoren-biozidauswaschung (viewed: 6.12.2024)

Nehls, T. (2007). Water and Heavy Metal Fluxes in Paved Urban Soils. Doctoral thesis, Technische Universität Berlin, Berlin, p. 128. DOI: 10.14279/depositonce-1657

Nehls, T., Rokia, S., Mekiffer, B., Schwartz, C., Wessolek, G. (2013). Contribution of bricks to urban soil properties. Journal o Soils and Sediments, 13, 575–584. DOI: 10.1007/s11368-012-0559-0

Novaes, C.A., Marques, R.C. (2022). Institutional paradigm shift: transitions in stormwater management principles. Environmental Science and Pollution Research International, 30, 17179–17192. DOI: 10.1007/s11356-022-23325-w

Oppliger, S., Hasler, S. (2019). Abwasserbewirtschaftung bei Regenwetter - Eine neue Richtlinie des VSA. Aqua und Gas, 4, 62–66. www.aquaetgas.ch/wasser/abwasser/20190328_ag4_abwasserbewirtschaftung-bei-regenwetter (viewed: 6.12.2024)

ÖWAV (2015). Oberflächenentwässerung durch Versickerung in den Untergrund. ÖWAV-Regelblatt 45, Österreichischer Wasser- und Abfallwirtschaftsverband, Wien, p. 45. https://www.oewav.at/Publikationen?current=293666&mode=form (viewed: 6.12.2024)

Paijens, C., Bressy, A., Frère, B., Moilleron, R. (2020a). Biocide emissions from building materials during wet weather: identification of substances, mechanism of release and transfer to the aquatic environment. Environmental Science and Pollution Research International, 27, 3768–3791. DOI: 10.1007/s11356-019-06608-7

Paijens, C., Bressy, A., Frère, B., Tedoldi, D., Mailler, R., Rocher, V., Neveu, P., Moilleron, R. (2020b). Urban pathways of biocides towards surface waters during dry and wet weathers: Assessment at the Paris conurbation scale. Journal of Hazardous Materials, 402, 123765. DOI: 10.1016/j.jhazmat.2020.123765

Pinasseau, L., Wiest, L., Volatier, L., Mermillod-Blondin, F., Vulliet, E. (2020). Emerging polar pollutants in groundwater: Potential impact of urban stormwater infiltration practices. Environmental Pollution, 266, Part 2, 115387. DOI: 10.1016/j.envpol.2020.115387

Puskás, I., Farsang, A. (2009). Diagnostic indicators for characterizing urban soils of Szeged, Hungary. Geoderma, 148, 267–287. DOI: 10.1016/j.geoderma.2008.10.014

Reiß, F., Kiefer, N., Purahong, W., Borken, W., Kalkhof, S., Noll, M. (2024). Active soil microbial composition and proliferation are directly affected by the presence of biocides from building materials. Science of the Total Environment, 912, 168689. DOI: 10.1016/j.scitotenv.2023.168689

Schaffitel, A., Schuetz, T., Weiler, M. (2020). A distributed soil moisture, temperature and infiltrometer dataset for permeable pavements and green spaces. Earth Systems Science Data, 12, 501–517. DOI: 10.5194/essd-12-501-2020

Schoknecht, U., Gruycheva, J., Mathies, H., Bergmann, H., Burkhardt, M. (2009). Leaching of Biocides Used in Façade Coatings under Laboratory Test Conditions. Environmental Science Technology, 43, 9321–9328. DOI: 10.1021/es9019832

Schoknecht, U., Mathies, H., Wegner, R. (2016). Biocide leaching during field experiments on treated articles. Environmental Sciences Europe, 28, 6. DOI: 10.1186/s12302-016-0074-9

Silva, V., Mol, H.G.J., Zomer, P., Tienstra, M., Ritsema, C.J., Geissen, V. (2019). Pesticide residues in European agricultural soils – A hidden reality unfolded. Science of the Total Environment, 653, 1532–1545. DOI: 10.1016/j.scitotenv.2018.10.441

Steinbrich, A., Leistert, H., Weiler, M. (2021). RoGeR – ein bodenhydrologisches Modell für die Beantwortung einer Vielzahl hydrologischer Fragen. Korrespondenz Wasserwirtschaft, 14, 94–101. www.hydro.uni-freiburg.de/publ/pubpics/roger21 (viewed: 6.12.2024)

Støvring, J., Dam, T., Bergen Jensen, M. (2018). Surface sedimentation at permeable pavement systems: implications for planning and design. Urban Water Journal, 15, 124–131. DOI: 10.1080/1573062X.2017.1414273

Szabó, B., Weynants, M., Weber, T.K.D.W. (2020). Updated European hydraulic pedotransfer functions with communicated uncertainties in the predicted variables (euptfv2). Geoscientific Model Development, 14, 151–175. DOI: 10.5194/gmd-14-151-2021

Tedoldi, D., Gromaire, M.-C., Chebbo, G. (2020). Infiltrer les eaux pluviales c'est aussimaîtriser les flux polluants. OPUR, État des connaissances et recommandations techniques pour la diffusion de solutions fondées sur la nature, p 75. https://enpc.hal.science/hal-03118775/file/Guide%20infiltration%20D.%20Tedoldi.pdf (viewed: 6.12.2024)

Tietje, O., Burkhardt, M., Rohr, M., Borho, N., Schoknecht, U. (2018). Emissions- und Übertragungsfunktionen für die Modellierung der Auslaugung von Bauprodukten. UBA-Texte 28, Federal Environment Agency, Dessau-Roßlau, p. 58. www.umweltbundesamt.de/publikationen/emissions-uebertragungsfunktionen-fuer-die (viewed: 6.12.2024)

TRAGSA (2015). La Gestión Integral del Agua de Lluvia en Entornos Edificados. TRAGSA Empresa de Transformación Agraria, S.A., Madrid, p. 175. https://www.tragsa.es/es/Documents/Publicaciones/GIAECuadernoTecnologicoActualizado.pdf (viewed: 6.12.2024)

Urbanczyk, M.M., Bester, K., Borho, N., Schoknecht, U., Bollmann, U.E. (2019). Influence of pigments on phototransformation of biocides in paints. Journal of Hazardous Materials, 364, 125–133. DOI: 10.1016/j.jhazmat.2018.10.018

Vega-Garcia, P., Schwerd, R., Scherer, C., Schwitalla, C., Johann, S., Rommel, S.H., Helmreich, B. (2020). Influence of façade orientation on the leaching of biocides from building façades covered with mortars and plasters. Science of the Total Environment, 734, 139465. DOI: 10.1016/j.scitotenv.2020.139465

Vilminko, H., Leskinen, P., Kaseva, A., Auranen, J. (2021). Current status of management of stormwater systems and solutions in four Baltic Sea countries. Report 279, Turku University of Applied Sciences, p. 42. www.theseus.fi/bitstream/handle/10024/818376/isbn9789522167934.pdf?sequence=2&isAllowed=y (viewed: 6.12.2024)

Wagenmann-Gaiser, K. (2004). Geotechnische Untersuchung im Bereich des ehemaligen Militärgeländes “Vauban”, Stadt Freiburg i. Br. Diploma thesis, University of Freiburg, p. 118.

Wangler, T.P., Zuleeg, S., Vonbank, R., Bester, K., Boller, M., Carmeliet, J., Burkhardt, M. (2012). Laboratory scale studies of biocide leaching from façade coatings. Building and Environment, 54, 168–173. DOI: 10.1016/j.buildenv.2012.02.021

Wessolek, G., Facklam, M. (1997). Standorteigenschaften und Wasserhaushalt von versiegelten Flächen. Zeitschrift für Pflanzenernährung und Bodenkunde, 160, 41–46. DOI: 10.1002/jpln.19971600109

Wicke, D., Burkhardt, M., Rohr, M., Pascale, R., Tatis-Muvdi, R., Zerball-van Baar, P., Dünnbier, U. (2021). Bauen und Sanieren als Schadstoffquelle in der urbanen Umwelt. UBA-Texte 155, Federal Environment Agency, Dessau-Roßlau, p. 108. www.umweltbundesamt.de/sites/default/files/medien/1410/publikationen/2022-01-28_texte_155-2021_bauen_sanieren_schadstoffquelle.pdf (viewed: 6.12.2024)

Wittmer, I., Schneidegger, R., Bader, H.-P., Singer, H., Stamm, C. (2011). Loss rates of urban biocides can exceed those of agricultural pesticides. Science of the Total Environment, 409, 920–932. DOI: 10.1016/j.scitotenv.2010.11.031

Zimmermann, F. (2021). Grundwassermodellierung im Stadtteil Vauban unter Berücksichtigung des Biozideintrags. Master thesis, University of Freiburg, p. 75. www.hydrology.uni-freiburg.de/abschluss/Zimmermann_F_2021_MA.pdf (viewed: 6.12.2024)

A Appendix

A.1 Site specific properties

Determination of building geometry from three-dimensional building models (LOD2)

To determine the average building geometry (width, length and height) of residential buildings in urban regions three-dimensional building models with a Level of Detail 2 (LOD2) were collected for Switzerland as well as multiple German cities (Berlin, Braunschweig, Dresden, Freiburg, Göttingen, Hannover, Leipzig, and Osnabrück). The Level of Detail refers to the degree of abstraction of real-world buildings. LOD2 data describe buildings with an outer shell consisting of horizontal or vertical surfaces with simplified but differentiated roof structures. For Switzerland the swissBUILDING3D 2.0 dataset was used, which was obtained from the Federal office of Topography "Swisstopo". The LOD2 data of the German cities were collected from the State Office for Geoinformation and Land Surveying of Lower Saxony (Braunschweig, Göttingen, Hannover, Osnabruck), the Saxon State Office for Geographic Information and Surveying (Dresden, Leipzig), the Berlin Senate Department for Urban Development, Building and Housing (Berlin) and the Surveying Office of the City of Freiburg i. Br. (Freiburg). All data was processed using the geographic information system software ArcGIS Pro (Version 2.8.2).

A.2 Building Materials

Table 17: Façade area and fraction of materials in area A

Criteria	Building Number									Total
	1	2	3	4	5	6	7	8	9	N=9
Total Façade [m²]	987	996	982	1245	1244	1484	1050	1065	990	10043
Thereof plaster [%]	73	67	73	64	66	62	76	74	72	69
Thereof glass [%]	9	7	10	7	6	6	6	7	9	7
Thereof balconies [%]	18	25	17	29	28	32	18	19	19	24
Total roof [m²]	270	275	267	371	371	367	281	293	272	2766
Thereof metal [%] (covering)	26	26	26	25	25	25	27	26	26	26
Thereof bitumen [%]	74	74	74	75	75	75	73	74	74	74

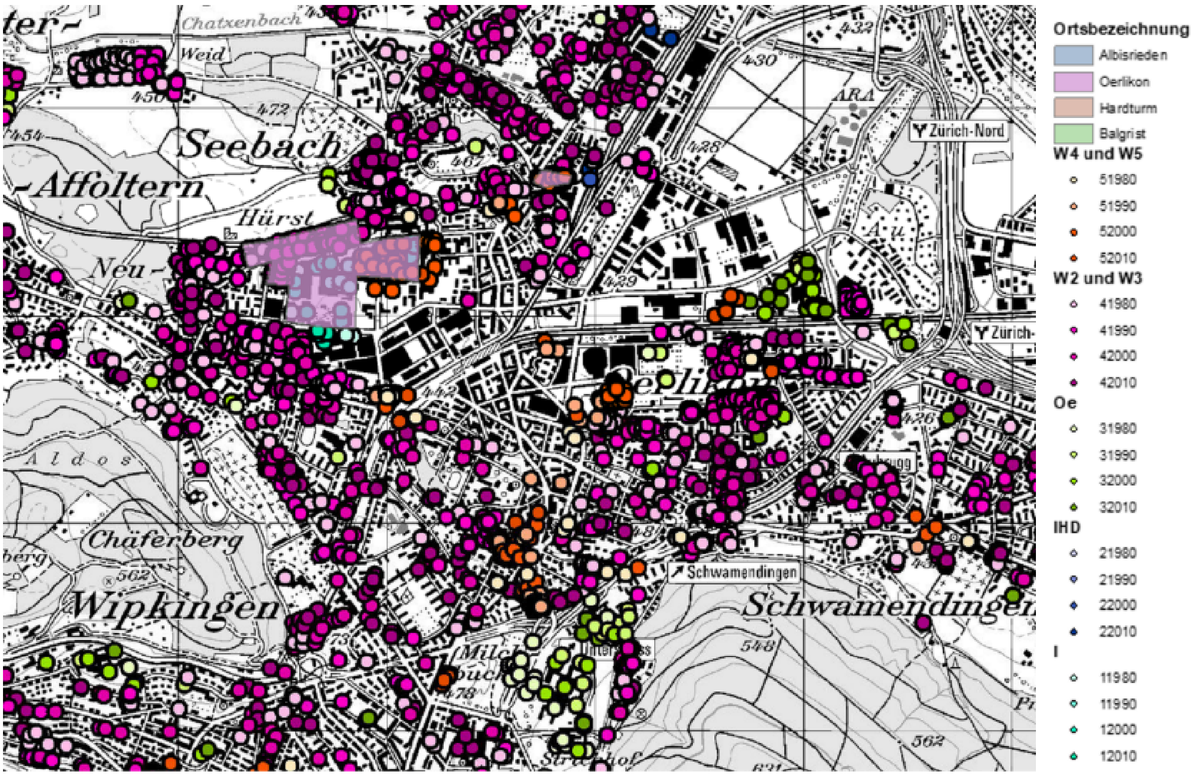
Conducted by (Wicke et al., 2021)

Table 18: Façade area and fractions of materials in area B

Criteria	Building Number			Total
	1	2	3	
Total Façade [m²]	4029	888	1244	6160
Thereof plaster [%]	62	76	67	65
Thereof glass [%]	18	14	15	17
Thereof balconies [%]	20	10	18	18
Total roof [m²]	1150	233	450	1833
Thereof metal [%] (covering)	11	14	10	11
Thereof bitumen [%]	89	86	90	89

Conducted by Wicke et al. (2021)

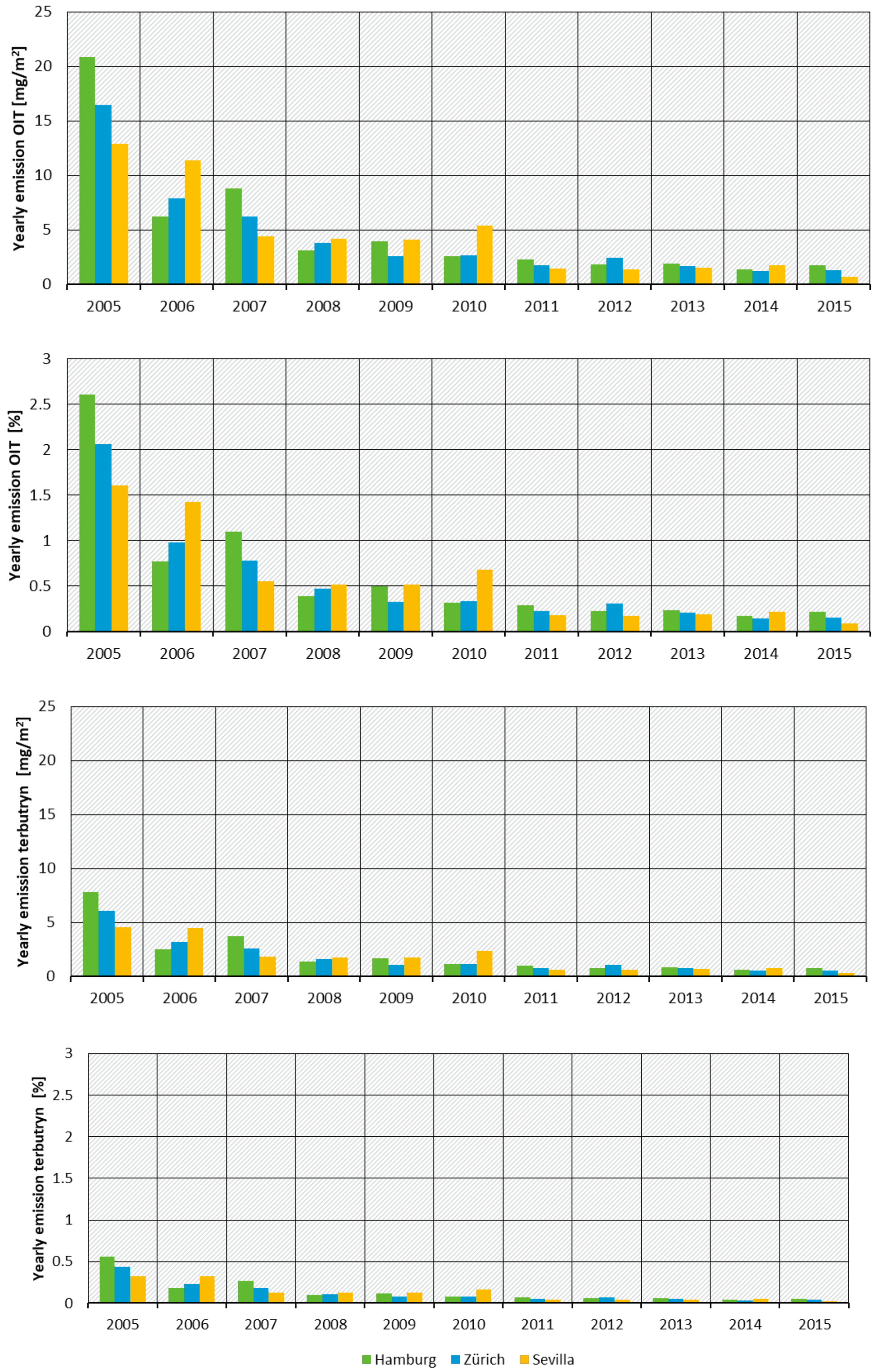
Figure 42: Survey in a district of Zürich. The colored dots indicate the surveyed buildings



Source: Own illustration, OST. Data taken from https://maps.zh.ch/

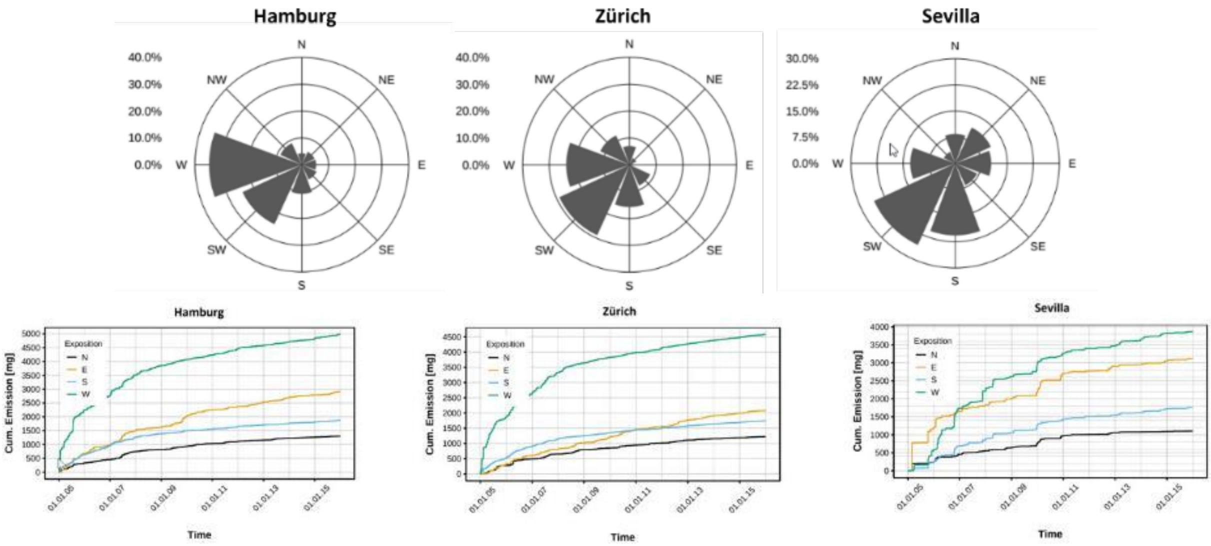
A.3 Emissions from façades (source term)

Figure 43: Emissions of OIT and terbutryn over time calculated by using COMLEAM



Yearly cumulative façade emission of OIT and terbutryn resulting from the dynamic simulation in COMLEAM for a standardized house with a façade area of 500 m^2 using weather data from Hamburg, Zürich and Seville from 2005 to 2015. The amount of biocide emitted is expressed as load per m^2 of façade and as a fraction of the total amount of biocide applied to the façade of the house.
Source: Own illustrations, OST

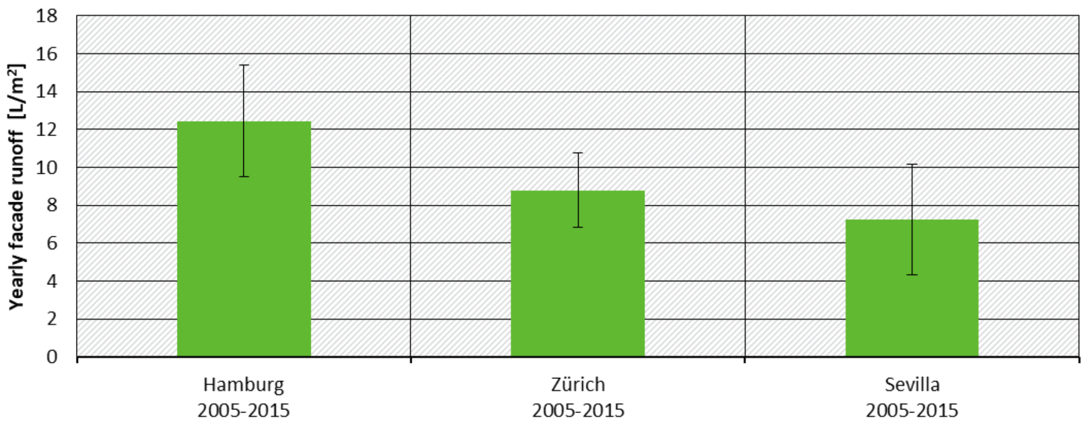
Figure 44: Amount of façade runoff in relation to wind heading and terbutryn emission per façade exposition



Amount of façade runoff in relation to wind heading (top row) and cumulative terbutryn emissions for individual façade expositions for Hamburg, Zürich and Seville from 2005 to 2015 based on a dynamic simulation for a standardized house with a façade area of 500 m^2 in COMLEAM (bottom).

Source: Own illustrations, OST

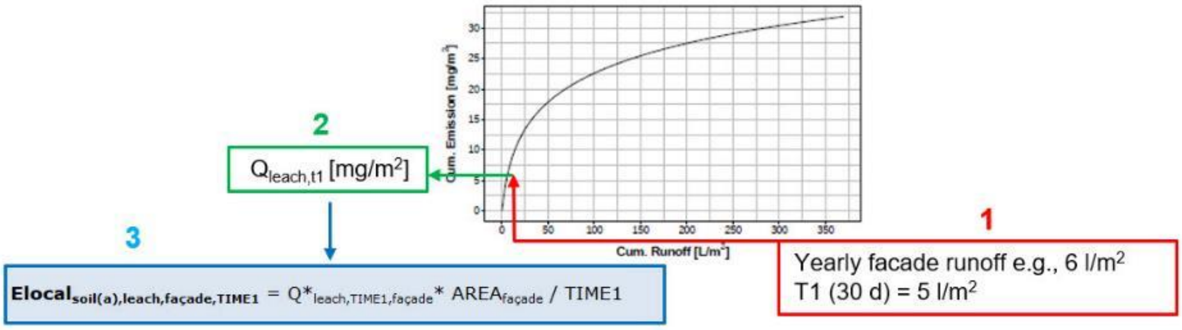
Figure 45: Simulated specific façade runoff for Hamburg, Zürich and Seville from 2005 to 2015 according to wind driven rain standard ISO-15927-3



Yearly average façade runoff and its standard distribution for all three locations based on hourly weather data.

Source: Own illustration, OST

Figure 46: Extrapolation of cumulative emission for ESD PT10 described as the extrapolated ESD method



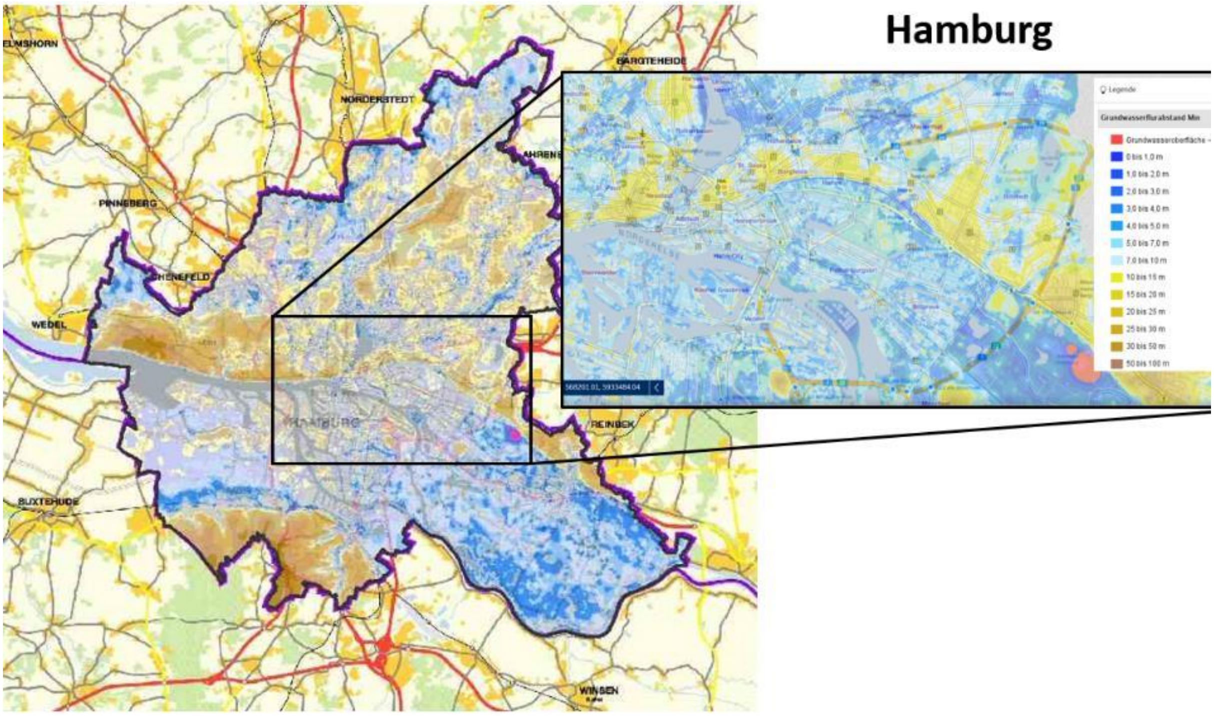
This illustration demonstrates how cumulative leached loads specific to different locations can be obtained using a leaching curve derived from a standardized leaching test and yearly façade runoff data for a specific location derived from COMLEAM. By determining the yearly façade runoff for a specific location, the cumulative leached loads for the ESD assessment periods can be read from the leaching curve.
Source: Own illustration, OST

A.4 Depth to groundwater

Hamburg

Morphologically significant are the Geest in the west (Falkenstein, Blankenese) and the Harburg mountains in the south of the City of Hamburg with groundwater levels up to 90 m below the surface (Figure 47). Further, in the area of the Harburger Vorgeest, groundwater levels are 5.0-7.5 m below ground, followed by the peripheral bog and seepage areas with very shallow groundwater (< 2.5 m). Also, in the Süderelbmarsch and Marschlanden (Bergedorf) the groundwater surface is shallow, approximately < 10 m below ground. In the port area, the groundwater levels are 10-15 m below ground level due to backfill areas for harbor structures. In the ground moraine areas north of the Elbe, the depth to groundwater is high and can reach 30 m or more. Due to extended areas with very shallow groundwater, we estimate 1 m as a realistic minimum depth to groundwater for the study's scenarios.

Figure 47: Depth to groundwater in Hamburg

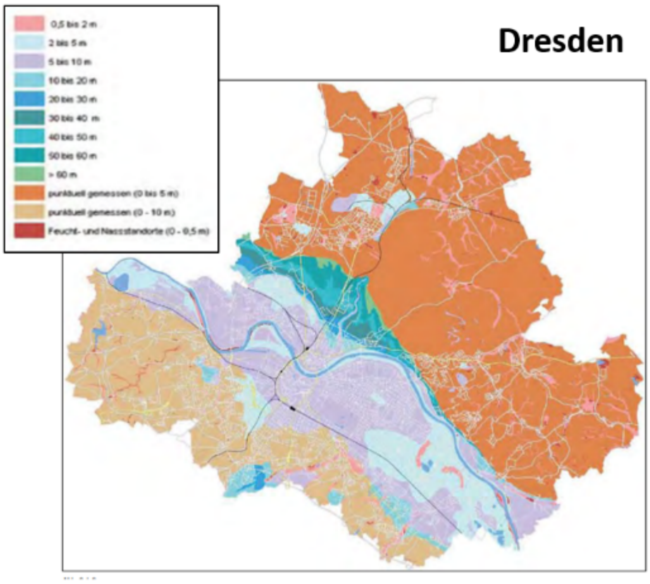


Source: Own illustration, OST. Data und maps taken from hwww.hamburg.de/planungskarten/2611068/flurabstandskarte/

Dresden

In the City of Dresden, the area around the Elbe floodplain is characterized almost everywhere by depths to groundwater of 2-5 m or 5-10 m (Figure 48). The only exceptions to this are small areas around old arms of the Elbe, the narrow Kaitzbach valley or immediate bank areas at the Elbe river, with depths to groundwater of less than 2 m. In the area of the glacial sands around the floodplain (also known as the "Hellerterrasse"), groundwater distances are much deeper and may reach 60 m or even more. For the scenarios in this study, this results in a realistic minimum depth to groundwater of 2 m.

Figure 48: Depth to groundwater in the City of Dresden

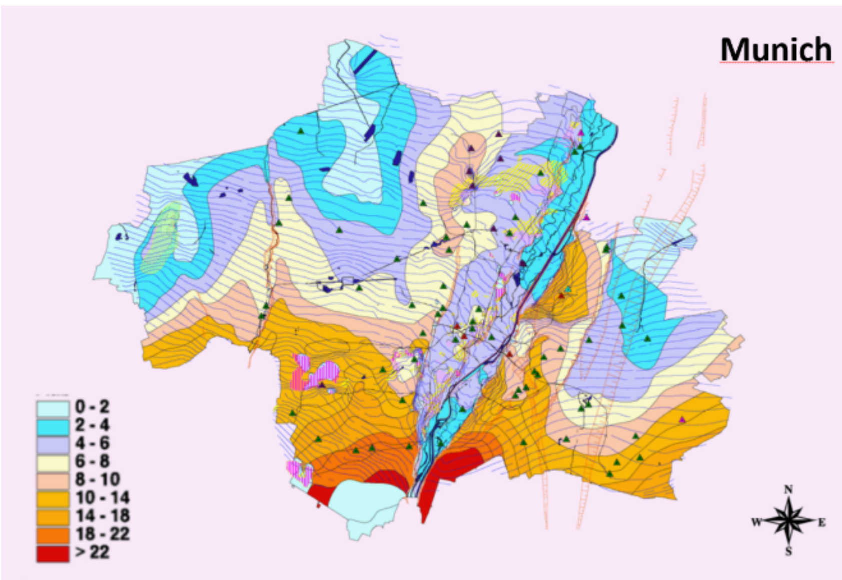


Source: Own illustration, OST. Data and mapy taken from www.dresden.de/media/pdf/umwelt/UB_Grundwasser.pdf

Munich

The gravel plain of the city of Munich has a south-north gradient of about 5 ‰ on average, while the groundwater gradient is about 2-3 ‰ on average. Therefore, groundwater distances decrease from south to north. Groundwater distances of more than 18 m can be found in the southern part of the city in the area of Fürstenried - Forstenried - Solln - Harlaching (Figure 49). Towards the north, groundwater distances generally decrease - especially in the area of the lower terraces - down to values of less than 2 m around the Aubinger Lohe, in the Ludwigsfeld - Feldmoching area and between Johanneskirchen/Englschalking and Ashheim. However, these outskirt areas are relatively small. The groundwater distances in the area of the incised old town step or the Isar alluvium are between 2 – 6 m. For the proposed scenarios, this results in a realistic minimum depth to groundwater of 2 m.

Figure 49: Depth to groundwater [m] in Munich

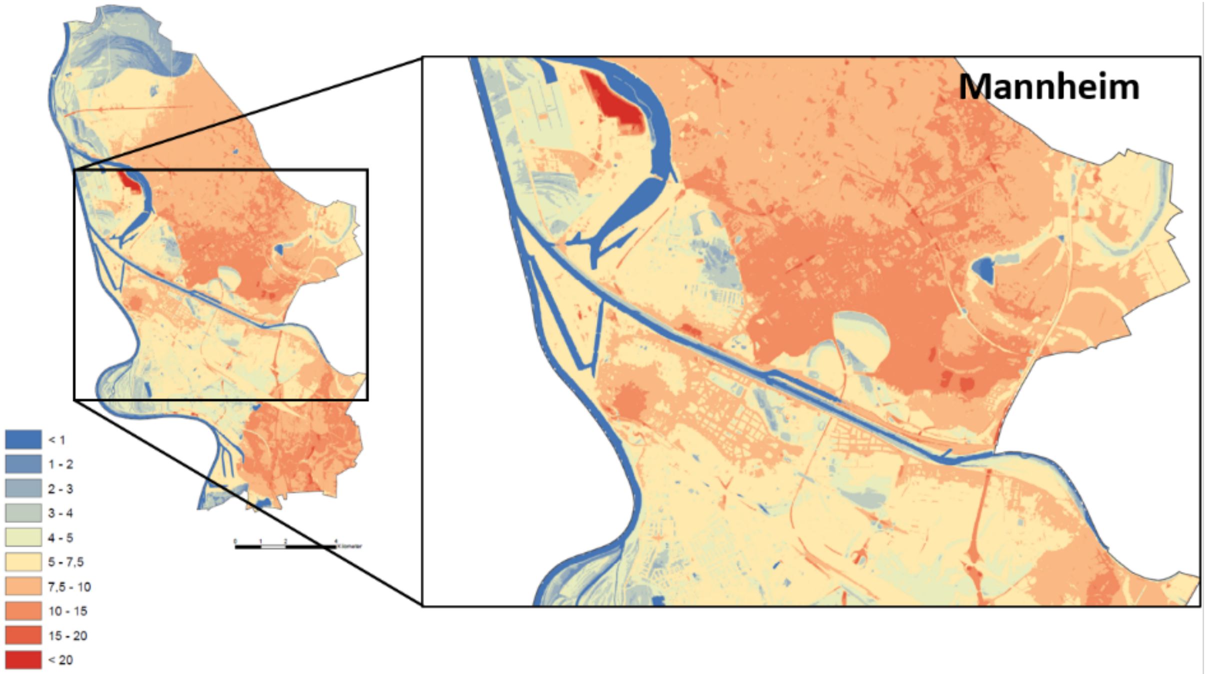


Source: Map taken from https://stadt.muenchen.de/infos/grundwasserdaten.html

Mannheim

In the majority of the city of Mannheim, depth to groundwater by far exceeds 2 m (Figure 50). Regions with shallower groundwater are only found close to rivers and old floodplain areas. These serve mainly as recreation areas and are not relevant for biocide infiltration. For the scenarios, this results in a realistic minimum depth to groundwater of 2 m (could even be 3 m).

Figure 50: Depth to groundwater [m] in Mannheim

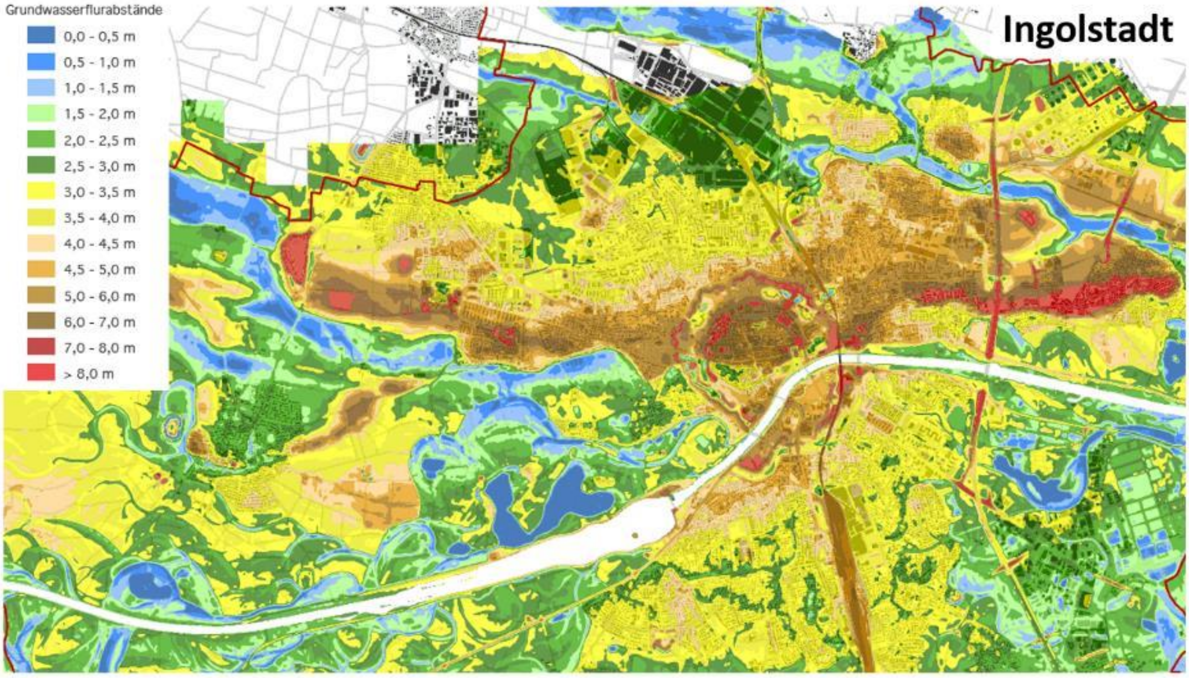


Source: Own illustration, OST. Data and map taken from www.mannheim.de/de/stadt-gestalten/planungskonzepte/oekologischer-planungsatlas/wasser/grundwasserflurabstand

Ingolstadt

The geological development of the Danube and its tributaries with the relocation of river bends and the formation of meanders is evident in the southern districts of the city of Ingoldstadt with average groundwater depths of 1-2 m (Figure 51). On the other hand, there are very large groundwater distances of up to 8 m along the southern margins of the Riss-Hochterrasse, where the groundwater flows relatively steeply southward into the Danube foothills. Near railway systems or fortifications (old town belt), larger groundwater table distances of 6 - 8 m are recorded due to artificial embankments. The seasonal range of fluctuation of the groundwater table is about 0.5 - 1.5 m in the city area. Values above this only occur occasionally, mainly caused by anthropogenic influences (construction water drainage) or extraordinary events such as floods. For the scenarios, this results in a realistic minimum depth to groundwater of 1 m.

Figure 51: Depth to groundwater in Ingolstadt



Source: Map taken from www.in-kb.de/Wasser/Grundwasser/Grundwasserflurabst %C3 %A4nde/

A.5 Modelling leaching of biocide to groundwater

Table 19: Soil parameters used in PEARL for the vegetated soil scenario (S1)

Depth	θsat (m3/m3)	θres (m3/m3)	αdry (1/cm)	αwet (1/cm)	n (-)	Ksat (m/d)	λ (-)
0-1	0.43	0.056	0.0288	0.078	1.8858	0.31151	4.3297
1-8	0.424	0.056	0.029	0.078	1.8815	0.27802	-0.1322
8-30	0.378	0.071	0.0182	0.133	3.0204	0.06265	-0.7669
30-60	0.366	0.072	0.0179	0.133	2.9707	0.051	-0.9863
60-100	0.375	0.073	0.0159	0.133	3.2759	0.04896	-0.9405

Table 20: Soil parameters used in PEARL for the permeable pavements scenario (S2)

Depth	θ_{sat} (m^3/m^3)	θ_{res} (m^3/m^3)	α_{dry} (1/cm)	α_{wet} (1/cm)	n (-)	Ksat (m/d)	λ (-)
0-1	0.436	0.061	0.0186	0.078	2.3577	0.18984	4.0611
1-8	0.437	0.061	0.0184	0.078	2.3527	0.18727	0.8847
8-30	0.378	0.071	0.0182	0.133	3.0204	0.06265	-0.7669
30-60	0.366	0.072	0.0179	0.133	2.9707	0.051	-0.9863
60-100	0.375	0.073	0.0159	0.133	3.2759	0.04896	-0.9405

Table 21: Soil parameters used in PEARL for the infiltration facilities scenario (S3)

Depth	θ_{sat} (m^3/m^3)	θ_{res} (m^3/m^3)	α_{dry} (1/cm)	α_{wet} (1/cm)	n (-)	Ksat (m/d)	λ (-)
0-1	0.396	0.038	0.0543	0.078	1.3868	0.6736	4.341
1-5	0.396	0.037	0.0567	0.078	1.3868	0.6807	-0.5049
5-10	0.396	0.044	0.0599	0.133	1.3595	0.6598	-0.6463
10-15	0.390	0.044	0.0530	0.120	1.3823	0.6378	-0.6043
15-20	0.392	0.046	0.0539	0.112	1.3836	0.6336	-0.5832
20-25	0.391	0.044	0.0562	0.112	1.4010	0.6436	-0.4492
25-100	0.381	0.031	0.0540	0.145	2.1699	0.7142	-0.8779

Table 22: Soil parameters used in PELMO for the vegetated soil scenario (S1)

Depth	ρ (kg/L)	Ldisp (cm)	FC (m3/m3)	WP (m3/m3)	OC (%)	pH-Value	BioDeg-factor (-)
0-8	1.56	5	0.137	0.027	1.122	7.52	1
8-30	1.6	5	0.2	0.03	0.1	7.5	1
30-60	1.6	5	0.2	0.03	0.1	7.5	0.5
60-100	1.6	5	0.2	0.03	0.1	7.5	0.3

Table 23: Soil parameters used in PELMO for the permeable pavements scenario (S2)

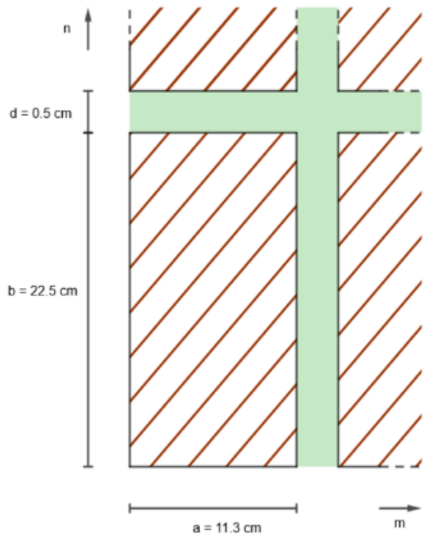
Depth	ρ (kg/L)	L_{disp} (cm)	FC (m^3/m^3)	WP (m^3/m^3)	OC (%)	pH-Value	BioDeg-factor (-)
0-8	1.61	5	0.211	0.034	2.2	7.1	1
8-30	1.6	5	0.2	0.03	0.1	7.5	1
30-60	1.6	5	0.2	0.03	0.1	7.5	0.5
60-100	1.6	5	0.2	0.03	0.1	7.5	0.3

Table 24: Soil parameters used in PELMO for the infiltration facilities scenario (S3)

Depth	ρ (kg/L)	L_{disp} (cm)	FC (m^3/m^3)	WP (m^3/m^3)	OC (%)	pH-Value	BioDeg-factor (-)
0-5	1.54	5	0.161	0.032	1.43	7.42	1
0-5	1.51	5	0.144	0.028	1.07	7.51	1
0-5	1.58	5	0.142	0.028	0.95	7.56	1
0-5	1.56	5	0.097	0.019	0.99	7.54	1
0-5	1.6	5	0.140	0.028	1.17	7.55	1
0-5	1.6	5	0.2	0.03	0.1	7.5	1
30-60	1.6	5	0.2	0.03	0.1	7.5	0.5
60-100	1.6	5	0.2	0.03	0.1	7.5	0.3

A.6 Calculation of joint area fraction

Figure 52: Permeable pavement dimensions

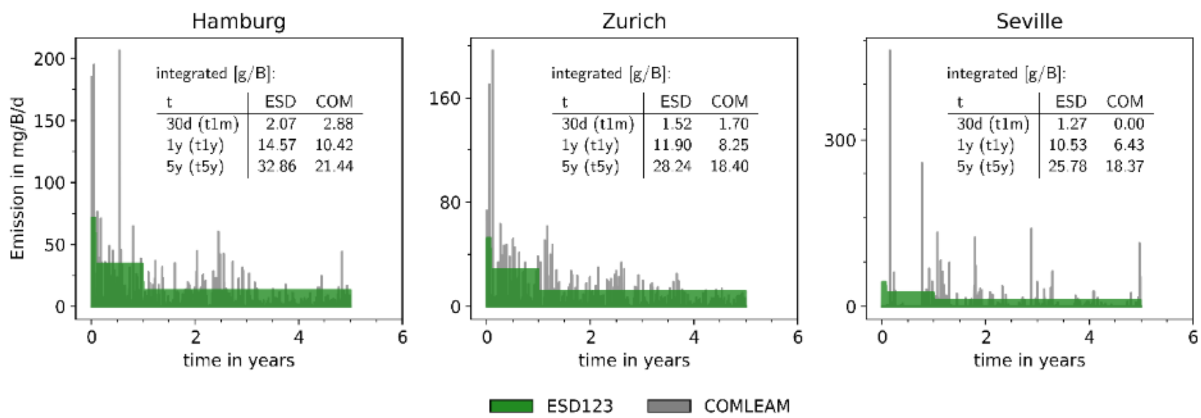


- $A_{block} = b * a$
- $A_{block+joint} = (b + d) * (a + d)$
- $A_{joint} = b * d + a * d + d^2$
- $A_{ges,block+joint} = (n * b + (n-1)d) * (m * a + (m-1)d)$
- $A_{ges,block} = n * b * m * a$
- $\lim_{n,m \to \infty} 1 - \frac{A_{ges,block}}{A_{ges,block+joint}} \approx 0.06$

Depiction of dimensions for the pavement blocks and the joints and computations of areas and joints.
Source: Own illustration, IME

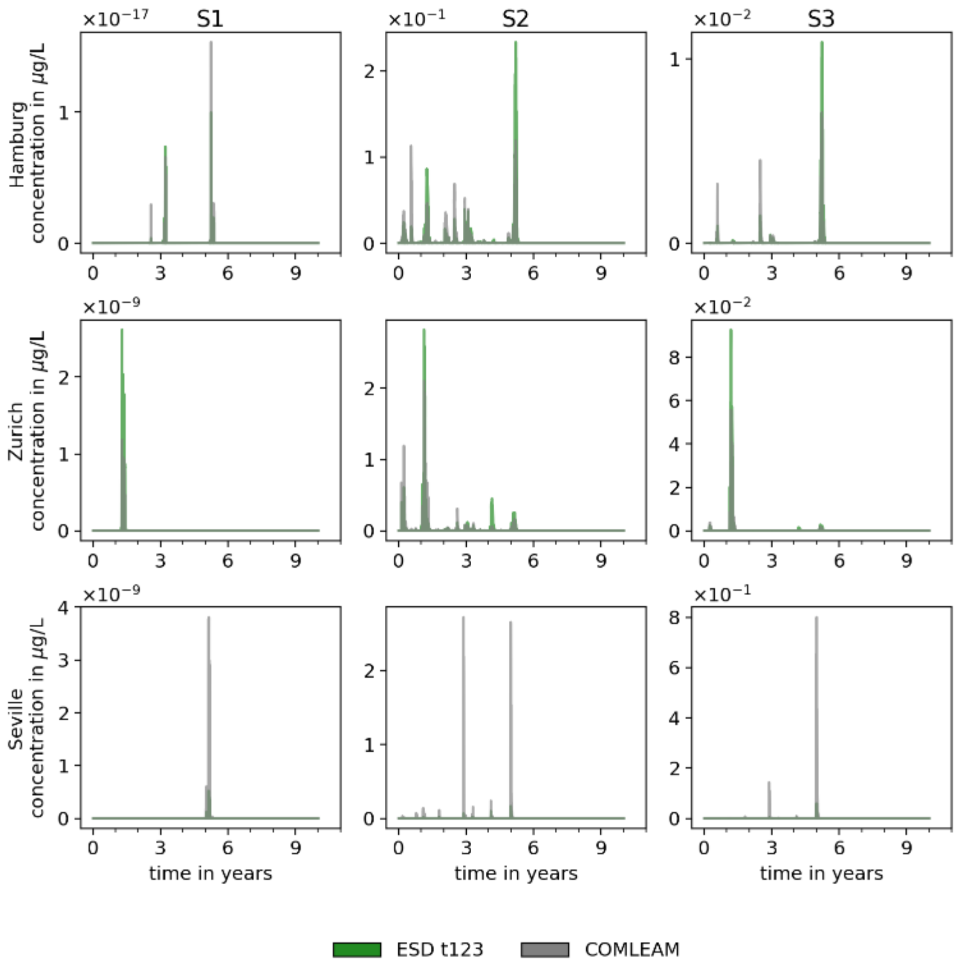
A.7 Emission Scenarios with OIT

Figure 53: OIT emissions of the defined building according to COMLEAM and ESD



Daily emission of OIT from COMLEAM and the combined ESD123 for three locations and per building B.
Source: Own illustrations, IME. Plotted using the Python Package Matplotlib (Hunter, 2007)

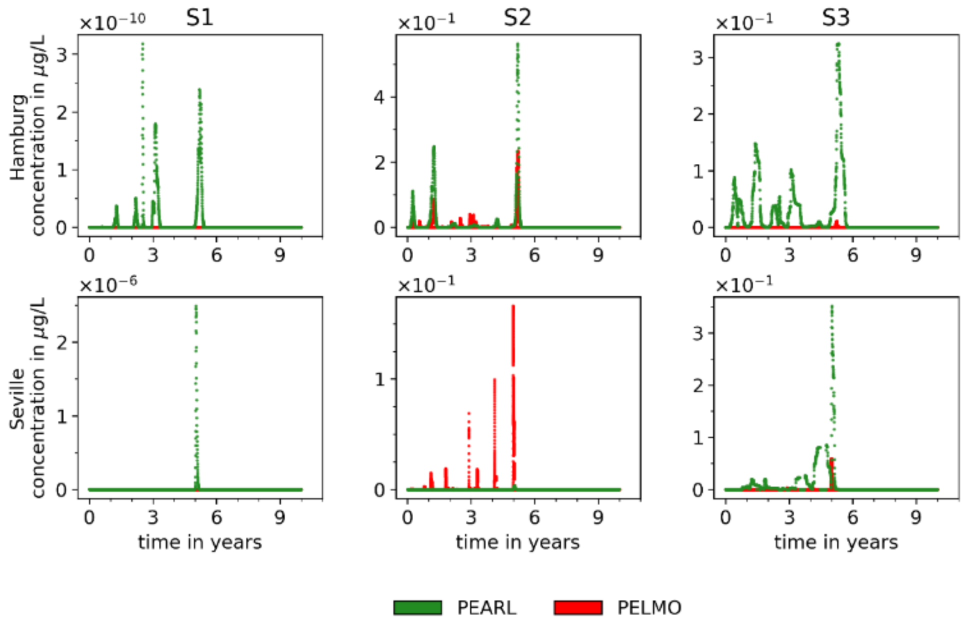
Figure 54: OIT percolate concentrations calculated by COMLEAM and ESD



Percolate concentrations at 1 m depth resulting from the OIT building emission (source-term) estimated with COMLEAM and ESD. The results are presented in rows for each location (Hamburg, Zürich, Seville) and in columns for each emission pathway (vegetated soil – S1, permeable pavements – S2, infiltration facilities – S3). The OIT percolate concentration was calculated using PELMO.

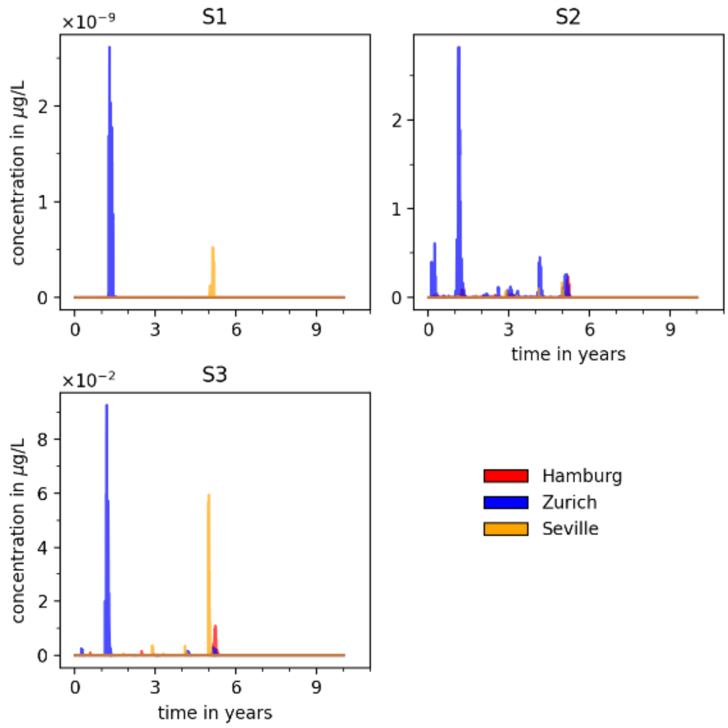
Source: Own illustrations, IME. Plotted using the Python Package Matplotlib (Hunter, 2007).

Figure 55: OIT percolate concentrations using PELMO and PEARL



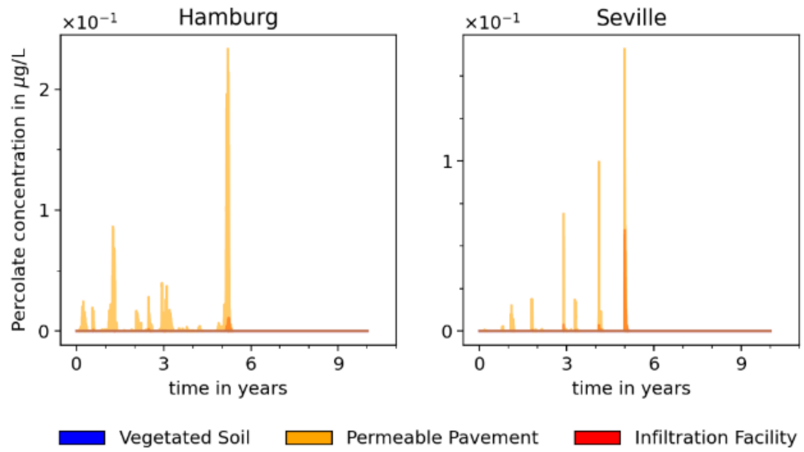
OIT percolate concentrations at 1 m depth in Hamburg, Zürich and Seville for the three emission pathways calculated using PELMO and PEARL (vegetated soil – S1, permeable pavements – S2, infiltration facilities – S3).
Source: Own illustrations, IME. Plotted using the Python Package Matplotlib (Hunter, 2007).

Figure 56: OIT percolate concentrations for the three climate regions



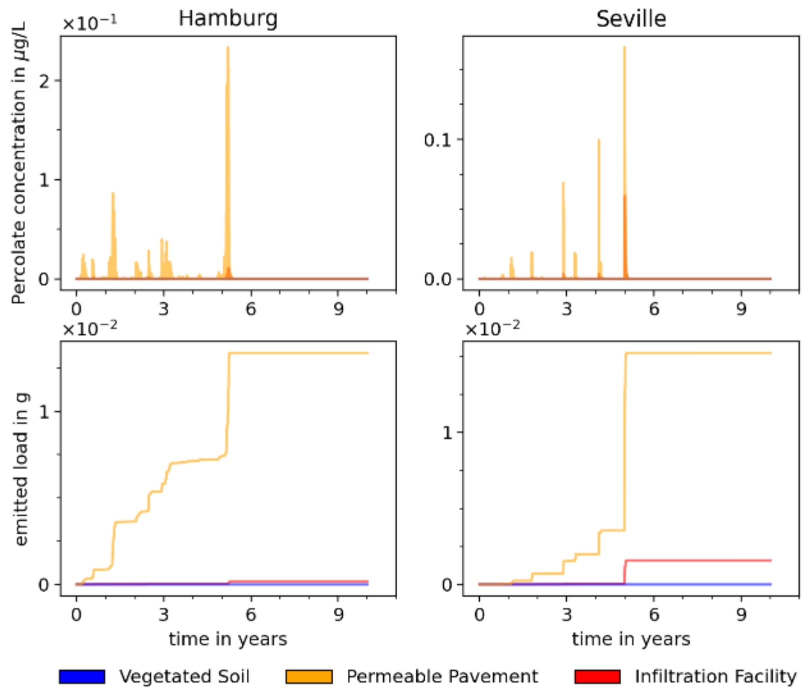
OIT percolate concentrations at 1 m depth in Hamburg, Zürich and Seville for the three emission pathways calculated using PELMO (vegetated soil – S1, permeable pavements – S2, infiltration facilities – S3).
Source: Own illustrations, IME. Plotted using the Python Package Matplotlib (Hunter, 2007).

Figure 57: OIT percolate concentrations for the three emission pathways



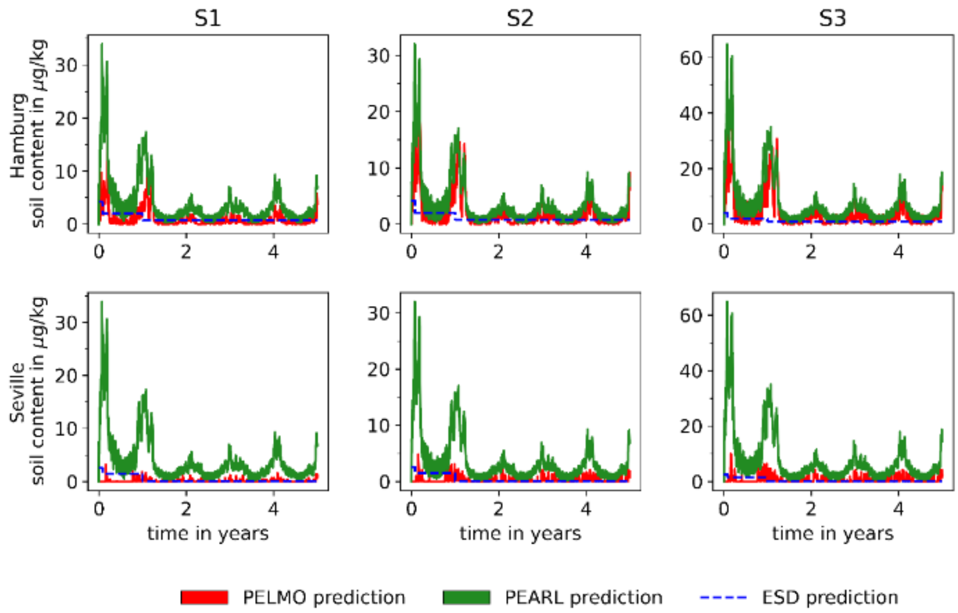
Percolate concentrations for OIT at 1 m depth are displayed for Hamburg and Seville calculated using PELMO. The three emission pathways are shown together for comparison.
Source: Own illustrations, IME. Plotted using the Python Package Matplotlib (Hunter, 2007).

Figure 58: OIT percolate concentrations and emitted load to groundwater



OIT percolate concentrations and emitted load at 1 m depth in Hamburg and Seville calculated using PELMO. The three emission pathways are shown together for comparison.
Source: Own illustrations, IME. Plotted using the Python Package Matplotlib (Hunter, 2007).

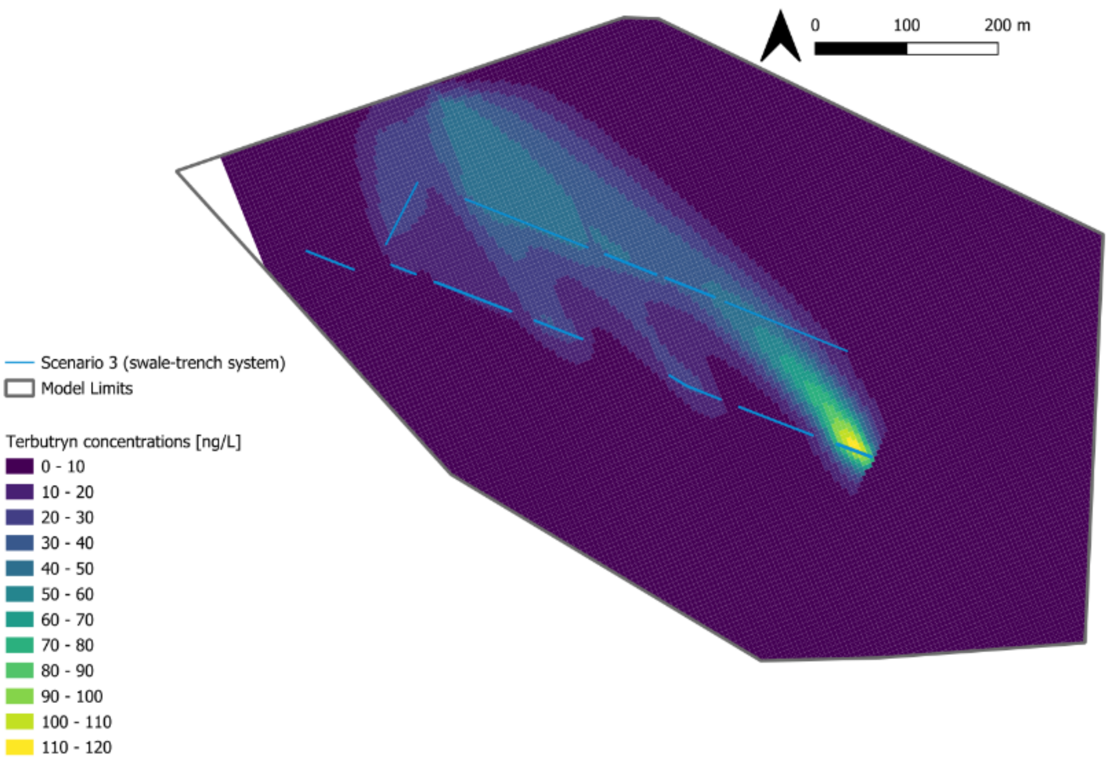
Figure 59: Average soil content of OIT according to the calculations by ESD and PELMO/PEARL



Average OIT soil content to a depth of 50 cm (V = 13 m³) in Hamburg and Seville for the three emission pathways (vegetated soil – S1, permeable pavements – S2, infiltration facilities – S3). The results from the two soil transport models PELMO and PEARL are presented alongside predictions from ESD for comparison.
Source: Own illustrations, IME. Plotted using the Python Package Matplotlib (Hunter, 2007).

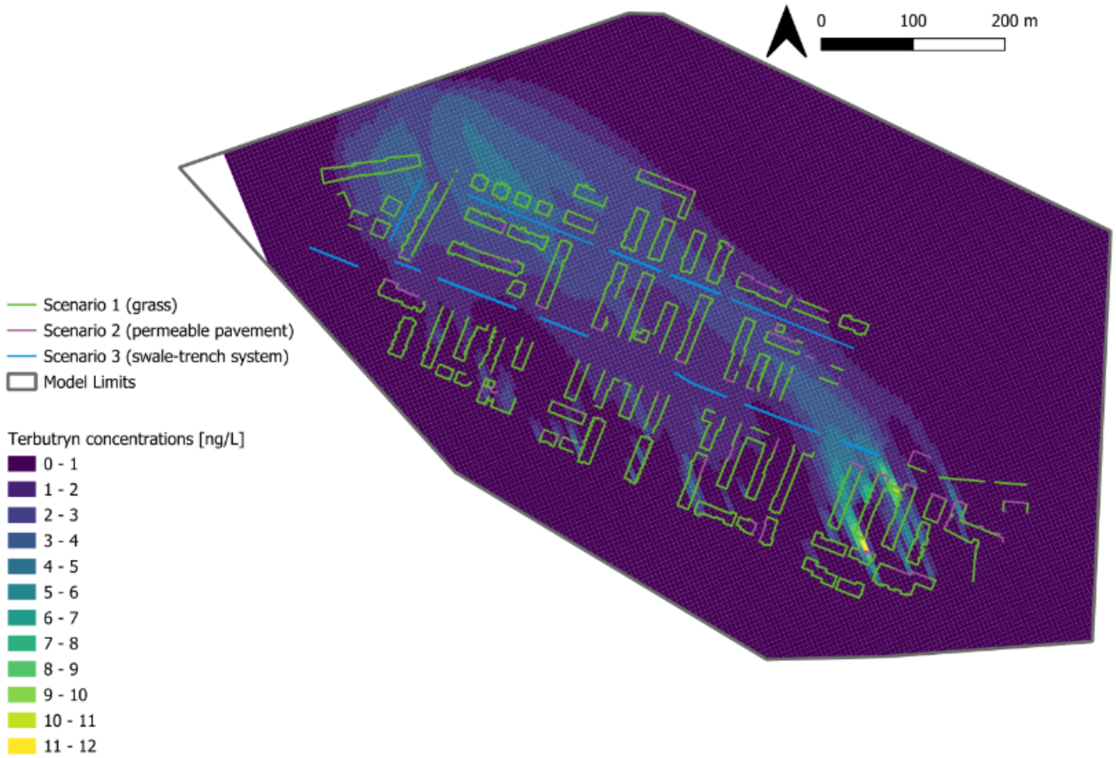
A.8 Groundwater model

Figure 60: Aerial view of simulated terbutryn concentrations at the end of the model period for case A



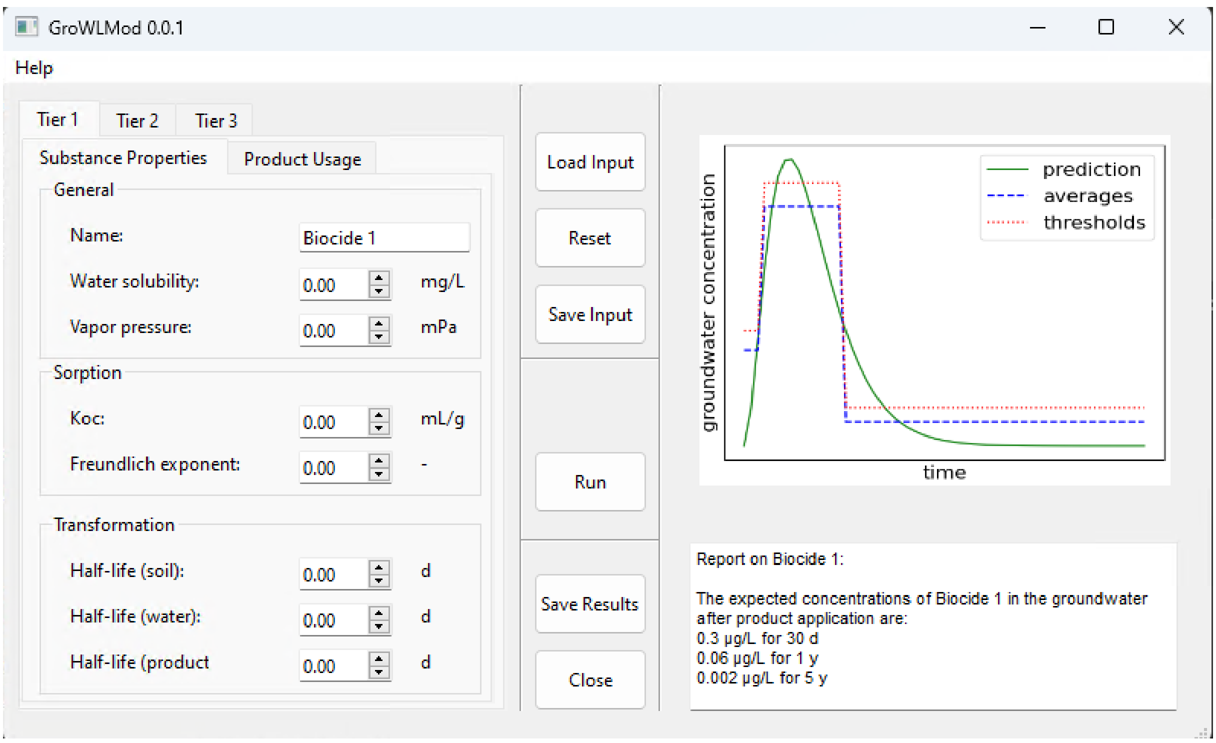
Source: Own illustration, UNI Freiburg

Figure 61: Aerial view of simulated terbutryn concentrations at the end of the model period for case B



Source: Own illustration, UNI Freiburg

Figure 62: Screenshot of the graphical user interface for a scenario calculation



Source: Own illustration, UNI Freiburg