National Institute for Public Health
and the Environment
Ministry of Health, Welfare and Sport

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A contribution to the knowledge base for environmental standards of building material standards

RIVM letter report 2022-0112
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Colophon

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Synopsis

Critical emission limit values for building materials: technical background, interpretation and reconstruction

A contribution to the knowledge base for environmental standards for building material

The Netherlands has the ambition to build a circular economy by 2050. This entails a decrease in the production of waste and an increase in the reuse of materials. Sustainable reuse of building materials is an aspect of a circular economy. However, building materials can contain contaminants such as heavy metals which can leach out over time. This can lead to the deterioration of soil and groundwater quality if building materials are applied on soils.

To prevent this, the RIVM and ECN derived critical emission limit values in 2007. These values specify the amount of a contaminant that can leach from a building material. The values formed the basis for the legal norms published in the Soil Quality Decree. The translation of critical emission limit values to legal norms was carried out by policymakers. During this process other aspects, such as the feasibility, were considered. For a building material to be applied on or in a soil, they need to meet these legal norms.

There are many new chemicals and building materials being produced and appearing on the market. This has led to an interest in the legal norms and how the critical emission limit values were derived. In order to offer meaningful advice to the ministry, the RIVM conducted this investigation into the technical background of the critical emission values and reconstructed the modelling approach used. Based on the reconstruction, it is evident that the technical background and modelling approach have been identified correctly as the critical emission limit values calculated during the reconstruction are comparable to those derived in 2007.

The critical emission limit values are based on a standard scenario for the use of building materials. If the use of building materials deviates from this standard scenario in practice, environmental impacts may be over or under estimated. The RIVM thus conducted a preliminary investigation into the influence that the building material use scenario has on the critical emission limit values. Based on this, suggestions for further investigations are presented. An example is investigating how specific characteristics of building materials and way in which building materials are used can be accounted for in critical emission limit values. Alternatively, critical emission limit values could be derived specifically for the most frequently used building materials. Finally, it may be meaningful to consider a longer time frame than the hundred years that current critical emission limit values are based on. This is because certain contaminants leach over longer periods of time.

Keywords: emission , building materials, soil, groundwater, modelling

Publiekssamenvatting

Kritische emissiewaarden voor bouwstoffen: technische achtergrond, duiding en reconstructie

Een bijdrage aan de kennisbasis voor milieunormen voor bouwstoffen

Nederland werkt aan een circulaire economie in 2050. Dat betekent dat er zo min mogelijk afvalstoffen zijn en zo veel mogelijk producten en materialen worden hergebruikt. Het hergebruik van bouwstoffen draagt bij aan de circulaire economie. Maar er kunnen verontreinigende stoffen, zoals metalen, in bouwstoffen zitten die er een lange tijd uit kunnen lekken. Als bouwstoffen op de bodem worden gebruikt, kan dat een negatief effect hebben op de kwaliteit van de bodem en het grondwater.

Om dit te voorkomen hebben het RIVM en ECN in 2007 ‘kritische emissiewaarden’ berekend. Deze waarden geven aan hoeveel van een verontreinigend metaal uit een bouwstof mag lekken. De kritische emissiewaarden zijn de basis voor de maximale emissiewaarden uit het Besluit Bodemkwaliteit. Beleidsmakers hebben de kritische emissiewaarden gebruikt om deze normen te bepalen. Ze hebben daarbij ook andere belangen, zoals haalbaarheid, meegenomen. Bouwstoffen moeten aan deze normen voldoen als ze op en in de bodem worden gebruikt en hergebruikt.

Er komen veel nieuwe chemische stoffen en bouwstoffen op de markt. Er is daardoor aandacht voor de emissiewaarden en hoe ze zijn bepaald. Om het ministerie goed over oude en nieuwe emissiewaarden te kunnen adviseren heeft het RIVM de technische achtergrond en modellering waarmee de emissiewaarden zijn afgeleid, gereconstrueerd. De werkwijze blijkt goed te zijn herleiden omdat de reconstrueerde waarden goed overeenkomen met uitkomsten van 2007.

De kritische emissiewaarden zijn gebaseerd op een standaard scenario voor het gebruik van bouwstoffen. Als het gebruik in de praktijk anders is dan het scenario, dan kunnen effecten op het milieu worden over- of onderschat. Daarom onderzocht het RIVM de invloed van verschillende scenario’s op kritische emissiewaarden en geeft het enkele suggesties voor verder onderzoek. Bijvoorbeeld om de kritische emissiewaarden per metaal te laten afhangen van de manier waarop het bouwmateriaal wordt gebruikt. Een ander idee is om aparte emissiewaarden te bepalen voor de meest gebruikte bouwstoffen. Verder kan het zinvol zijn het effect van een stof te onderzoeken over een langere periode dan de honderd jaar die nu gebruikelijk is. Sommige stoffen komen dan pas vrij.

Kernwoorden: emissie, bouwstoffen, bodem, grondwater, modellering

Contents

Summary

The re-use of old building materials and conversion of waste materials into building materials are aspects of the transition from a linear economy to circular economy. The use of such secondary building materials diminishes the demand for primary building materials but can lead to the deterioration of soil and groundwater quality due to leaching of contaminants. In recent years the RIVM has often been requested for advice relating to the leaching of contaminants from building materials. The requests touch upon multiple topics and range from the risks related to new contaminants, such as PFAS, to shortcomings of current emission limit values in relation to novel building materials, such as foam glass. These requests prompted this study which aims to reconstruct the methods used to derive critical emission limit values and understand the basis of the current legal norms reported in the Soil Quality Regulation. Additionally, a preliminary investigation into the avenues that could be explored to minimise the shortcomings of current legislation is presented. To achieve these goals the following were conducted:

1. The scientific and political choices used for the derivation of emission limit values in the Soil Quality Regulation were identified;
2. The modelling approach used by the RIVM to derive critical emission values was reconstructed and the critical emission values recalculated using HYDRUS-1D. This was done for a range of contaminants in granular building materials;
3. The critical emission limit values obtained in this study were compared with those derived by Verschoor et al. (2007) for the purpose of the Soil Quality Regulation;
4. An investigation was conducted into alternative scenarios and the sensitivity of soil and groundwater concentrations to variations in certain input parameters.

The scientific and political choices that were made to derive the critical emission limit values were identified. This includes the modelling approach used (i.e. the standard scenario as well as necessary modelling parameters) for the derivation of critical emission limit values. The critical emission limit values derived in this study are similar to those derived by Verschoor et al. (2007) for the Soil Quality Regulation. This indicates the that the scenario and modelling parameters used for the Soil Quality Regulation were identified correctly. While calculated soil and groundwater concentrations were similar, the time at which peak concentrations were modelled to occur in groundwater did show slight discrepancies. The discrepancies did not lead to differences in critical emission limit values for the majority of modelled contaminants.

The conducted sensitivity analysis offered insight into the importance of considering the specifications of the building material itself and the application. Generalizing such parameters can lead to overestimations or underestimations of the influence that building materials have on the quality of soil and groundwater. The sensitivity analysis also underscores the importance of using accurate adsorption coefficients. Based on the

analysis several potential avenues of investigation, which may lead to more robust and flexible critical emission limit values, are suggested:

1. The results of the sensitivity analysis can be used to generate a look-up table. Such a table contains the output for a multitude of scenario’s. A user could thus look-up the critical emission limit value associated with their custom scenario.
2. In practice certain granulated building materials are used much more frequently than other building materials. The rate at which specific contaminants leach from building materials vary strongly, which in turn leads to differences in the effects that a building material may have on soil or groundwater quality. Current critical emission limit values are based on an average leaching rate. It may thus be beneficial to determine critical emission limit values using building material specific leaching rates for the most used granulated building materials. This would offer a greater protection of soil and groundwater quality.
3. The critical emission limit values are based on a simulation period of a 100 years. There are however building materials from which contaminants leach slowly, or contaminants which readily adsorb to soil and thus do not enter the groundwater within the simulated period. This means that the critical emission limit values may not protect soil and groundwater quality in these cases. Increasing the simulation period may counteract this uncertainty and lead to more protective critical emission limit values.
4. For new contaminants, for which limited data are present, a tiered approach may be a cost-effective method by which soil and groundwater quality can be protected. Such an approach contains multiple levels complexity that can be implemented when more data are available or when an emission limit value derived using a simpler method is unworkable.

1 Introduction

Building materials are diverse and encompass primary materials, such as sandstone blocks, and secondary materials such as slag. The application and re-use of such materials is encouraged from the point of view of the circular use of raw materials. However this can have adverse effects on the quality of the underlying soil and groundwater due to the leaching of chemical constituents. Nonetheless the re-use of building materials remains necessary to limit the demand of primary materials. In addition to this, specifically secondary building materials offer an avenue for enhancing sustainable development as they can lead to a reduction in waste production and mining for primary building materials. In this study, the focus is placed on secondary building materials and the potential effects these have on soil and groundwater quality.

In recognition of the benefits but also side-effects related to using building materials the government of the Netherlands initiated the Building Materials Decree (1995; Eikelboom et al. 2001). The aim of the decree was to minimize the adverse impact that building materials have on the environment, specifically on the soil and groundwater quality. Within the decree a method to determine the permissible use of a building material was prescribed. The method used a combination of column tests and equations requiring location-specific data. However, the application of this method was complex and time consuming for contractors and licensing authorities. Moreover the generalized equations led to conservative limit values which hampered the re-use of some building materials. Therefore, for some contaminants, emission limits were set at a higher and thereby more feasible level. These limit values were laid down in a Temporary Exemption Regulation (2004). The Building Materials Decree and Temporary Exemption Regulation were replaced by the Soil Quality Decree and associated Soil Quality Regulation (2008).

In the Soil Quality Decree (2007), the screening of building materials was facilitated by offering a simple set of emission limit values that could be used to easily evaluate the permissible use of (secondary) building materials. The **emission limit values** (maximale emissiewaarden in Dutch) are legal values based on scientifically derived **critical emission values** (kritische emissiewaarden in Dutch). These critical emission values quantify the mass of a given contaminant that may leach from a mass unit of building material, that will not lead to the exceedance of soil and groundwater quality criteria. The critical emission values were scientifically derived by complex calculations of material leaching using realistic reactive-transport models for transport of substances in soil (Verschoor et al., 2007; Verschoor et al. 2008[1]). Policy choices of relevant scenarios, protection goals and acceptable consequences determined the final set of legal emission limit values in the Soil Quality Decree.

Critical emission value = scientifically derived value
Emission limit value = legal norm

The standards in the Soil Quality Decree include metals, metalloids and anions (bromide, chloride, fluoride and sulphate) and was based on leaching data representative of the building materials and applications used at that time. However, in the past decade concern has emerged for the environmental effects of new contaminants, new building materials and new applications. Concern for new contaminants is exemplified by the current concerns surrounding the environmental impacts of per- and polyfluoroalkyl substances (PFAS). There are currently no emission limit values for PFAS in building materials and consequently the environmental impact caused by the leaching of PFAS from building materials is unknown and unregulated. There are also examples of building materials, such as foam glass, for which current limit values do not accurately capture associated risks because their properties differ from traditional building materials. Furthermore, the government of the Netherlands has expressed their ambition of having a circular economy by 2050 (Ministry of Infrastructure and Water Management, 2016), which could stimulate the application of (new) secondary building materials in novel ways.

Due to the emergence of these new building materials, applications and a lack of relevant emission limit values for new substances, a readily applicable method for the derivation of critical emission values needs to be re-established. At the same time, modelling practices may be updated, and recommendations made in 2007 regarding the methodology underlying the Building Materials Decree could be considered.

1.1 Objective

Due to the emergence of new building materials and applications a readily applicable method for the derivation of critical emission values needs to be re-established. Initially, however, it is necessary to understand the considerations and methods used to derive the critical emission values on which current emission limit values are based. The objective of this study is not to evaluate current emission limit values or the methodology used to derive these values but to understand and reproduce the critical emission limit values. This study aims to:

1. Identify the scientific and political choices used for the derivation of emission limit values in the Soil Quality Regulation;
2. Reconstruct the modelling procedure used by the RIVM for the derivation of critical emission values and recalculate the critical emission values for a range of contaminants in granular building materials;
3. Compare the results of the “new” calculations with critical emission values derived for the Soil Quality Decree and clarify observed discrepancies if these are present;
4. Investigate alternative scenarios and conduct a sensitivity analysis for various parameters.

2 History of evaluation of building materials

In this chapter a brief overview is given of the evolution of the derivation of emission and leaching norms of contaminants from building materials from the Building Materials Decree in 1995 to the Soil Quality Regulation in 2008. The latter is still in place. Emphasis is given to sensitive parameters with relevance to policymakers.

2.1 Emission of contaminants from building materials

The leaching of contaminants from building materials and the subsequent transport through soil media are important processes to consider. These processes govern the extent to which soil and groundwater become contaminated.

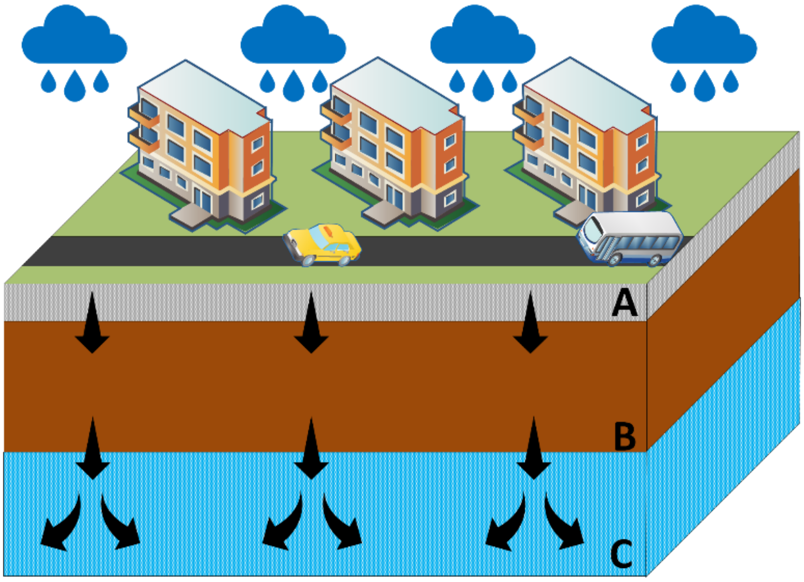


Figure 1 A schematic representation of contaminants leaching out of building materials (A) into the underlying soil (B) and ultimately the groundwater (C) where further transport may occur.

Due to the infiltration and percolation of rain water through the building material, contaminants may leach out of the building material and enter the underlying soil. Verschoor et al. (2007), have summarized the leaching characteristics of 35 different granulated stony building materials. The composition of the leachate and rate and total amount of a contaminant that leaches out varies between building materials. Besides this, the amount of rainfall and the amount of building material used also influence the emission of contaminants from building materials. Generally, the rate of emission of contaminants out of building materials decreases through time.

The type of experiments to be used to check of building materials comply with the emission limit values have been described in the Soil Quality Regulation article 3.3.1. The limit values are expressed in mg kg^{-1} (at liquid/solid ratio = 10; LS10) which means "mg contaminant leached from a kilogram of building material or soil after percolation of a volume of water that is 10x the mass of the building material or soil". Note that the value does not refer to the composition or total content of these contaminants in the building materials. In the case of granulated building materials the leaching behaviour of compounds is commonly determined by means of a column experiment (NEN7373 or NEN7383) or a batch test (NEN7371).

Once contaminants have entered the soil their downward transport may be retarded due to adsorption to soil constituents. The magnitude of retardation is dependent on soil characteristics such as pH, organic matter content and clay content. Many of these factor are variable in space and time. To circumvent the problem of variability standard scenarios were defined. Defining such scenarios gives an impression of the sensitivity of critical emission value for certain modelling choices.

2.2 Emission scenarios

For both the Building Material decree and the Soil Quality Regulation, critical emission values were derived for frequently occurring metals, metalloids and certain inorganic anions for a variety of stony material types, material application thicknesses, soil types and protections levels (see Table 1).

Table 1 Overview of scenarios used for derivation of critical emission values in. the Soil Quality Regulation.

Scenario specification	Calculation variants	Building Material Decree	Soil Quality Regulation
Material type	• granular • monolithic	both	both
Building layer thickness	• 0.2 m • 0.5 m • 0.7 m • 2 m	Case-by-case but at least 0.2 m	0.5 m
Leaching mitigation[1]	• none • isolation	both	both
Soil types[2]	• Sand • Peat • Clay	worst-case	worst-case
Protection level soil and groundwater[3]	• Negligible Risk • Maximum permissible risk • Serious risk	Negligible Risk	Maximum Permissible Risk

1. **none** refers to an open application, with an assumed effective infiltration of 300 mm rainwater/y; **isolation** refers to the so-called IBC measures (isolation, management and monitoring, in Dutch: Isoleren, Beheersen, Controleren) with an effective infiltration of 6 mm yr^{-1}.
2. The variety in soil types only reflect differences in adsorption. Hydrological properties were kept constant (as for sand).
3. **Negligible risk** corresponds to a concentration a 100 times lower than the maximum permissible risk. **Maximum permissible risk** for humans refers to a concentration where the risk of an extra tumour per year is smaller than 1 in 10^{-6} for carcinogenic contaminants and for non-carcinogenic compounds a concentration where no negative effects are expected given lifelong daily exposure. For ecosystems, the maximum permissible risk equates to a concentration where no effects are expected in 95% of exposed organisms. **Serious risk** is only applicable for ecosystems and refers to a concentration where negative effects are expected in 50% of exposed organisms or (microbial) processes.

The present report is focused on the impact of an open application of a 0.5 m thick layer of granulated building materials on soil and groundwater quality.

2.3 Calculation models

2.3.1 Modelling for Building Materials Decree

In the Building Materials Decree critical soil input values (in Dutch immissiewaarden) rather than critical emission values were derived. The calculation method supporting the derivation of critical soil input values in the Building Materials Decree is described by Aalbers et al. (1993). The Building Material Decree published critical soil input values for the evaluation of the environmental quality of building materials. The soil input value refers to the mass of contaminant leached from the construction and entering the soil (mg contaminant per m^2 soil per 100 years). During the period that the Building Materials Decree was in place, contractors and licensing authorities needed to convert leaching test results to soil input values, taking into account, amongst others, the amount of building material in the construction.

The critical soil input values were derived in a simplified way; that is by assuming that relatively mobile contaminants (e.g. chloride and sulphate salts) will leach entirely to the groundwater and that relatively immobile contaminants (e.g. metals) will accumulate entirely in the upper meter of the soil column (Aalbers et al., 1993). Values were derived in such a way that groundwater quality criteria were not exceeded for mobile contaminants and soil quality criteria were not exceeded for immobile contaminants.

2.3.2 Modelling for Soil Quality Decree

The calculation methods supporting the emission limit values in the Soil Quality Regulation have been described by Verschoor et al. (2007). Two reactive transport models were used to derive critical emission values. This was done to show the sensitivity of calculated critical emission values on the used model. The implemented models were PEARL version 2.2.2 (Leistra et al., 2000) and ORCHESTRA (Meeussen, 2003). Both models account for biochemical and hydrological processes that influence the transport of a compound. The models differ, amongst others, in how they deal with adsorption. PEARL is a model that describes chemical retardation using adsorption coefficients whilst ORCHESTRA is a more complex model that accounts for speciation and is able to distinguish adsorption of different chemical species of a metal to different soil constituents. Both approaches have been evaluated by the Technical Committee for Soil Protection (TCB), that judged that both models offer perspective for the derivation of critical emission values. The TCB (2006) emphasized that the quality of the critical emission value is determined more by the quality of the parameters than by the model choice. The following comments were made by the TCB regarding the two models:

- From a scientific point of view a chemical speciation model (e.g. ORCHESTRA) is preferable, because of its capability to deal with changing circumstances such as pH or soil type;

- However, it was found too early (in 2006) to adopt ORCHESTRA as a model for derivation of critical emission values because of the poor validation status of the model;
- The validation status of PEARL on the European level and the presence of consensus about scenarios and parameters is a strong feature of this model;
- Agreement of outcomes between PEARL and ORCHESTRA was satisfactory for relatively immobile elements (molybdenum, lead, arsenic, chromium, selenium, tin) and relatively mobile elements (antimony, bromide, chloride);
- It was recommended to widen the time window of the calculations to more than 100 years, because the cut-off time at 100 years led to disagreement in model outcomes for elements with intermediate mobility (zinc, nickel, cobalt, copper, cadmium and sulphate);
- The use on adsorption coefficients in PEARL requires sound information on the variation of this parameters. These data were not available for barium, mercury and vanadium.

2.4 Calculation endpoints

The models mentioned above calculate concentrations of substances in soil layers and in groundwater over time, caused by leaching from building materials. Transport of a substance through soil is a dynamic process, so choices needed to be made about the target depth and point in time evaluated. In order to remain in line with the previous Building Materials Decree, the following endpoints were chosen to derive critical emission values for the Soil Quality Decree:

- average concentrations over the upper meter soil 100 years post application;
- maximum concentration in the upper meter of groundwater within 100 years.

The lowest emission value derived from these two endpoints was proposed as the critical emission limit value as it would offer protection to both the soil and the groundwater (Figure 2.).

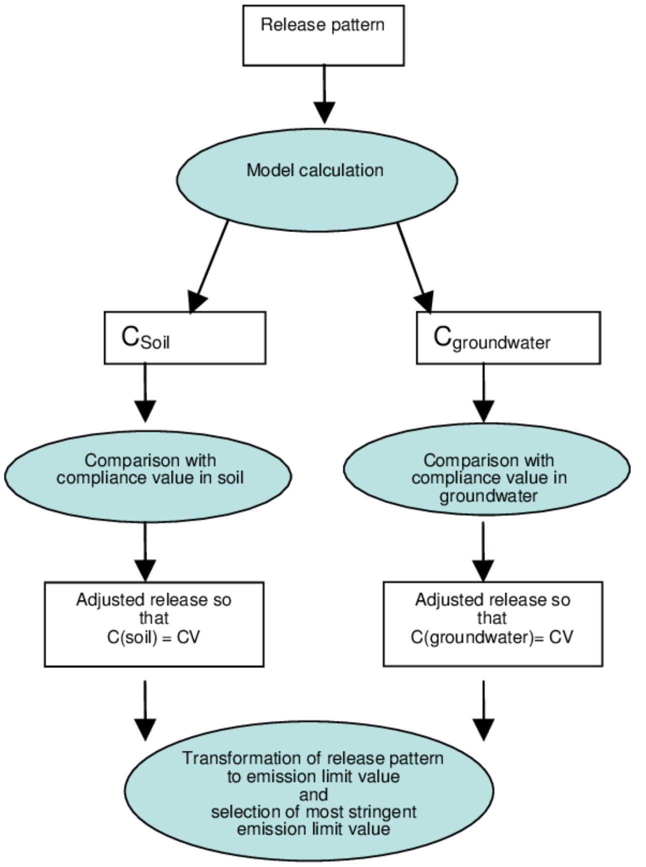


Figure 2 Overview of derivation process of critical emission value. C=concentration, CV= Critical value (e.g. Maximum Permissible Concentration).

These choices have the following implications:

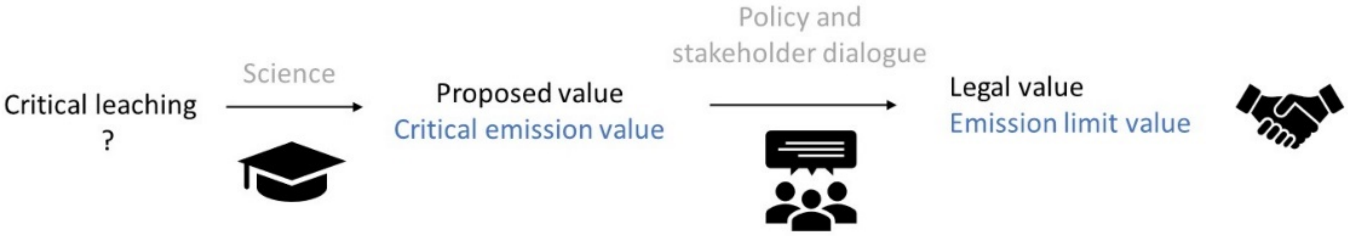
- The protection level for groundwater is higher than for soil because the criteria or groundwater is the maximum concentration during the simulated period and the criteria for soil is the average concentration at 100 years post application;
- In soil, temporary (earlier than 100 year) or spatial exceedances (in particular soil layers) of environmental quality standards are inevitable;
- In groundwater, concentrations still may increase after 100 years, especially for substances with moderate or low mobility.

The critical emission values derived on the basis of the two models did not vary drastically for relatively mobile and immobile contaminants (Verschoor et al., 2008). For certain metals with moderate mobility however, large differences in the derived critical emission values were observed. This was partially attributed to differences in calculated retardation but also in the chosen time frame, as peak concentrations for a given metal would occur within the set 100-year time frame for one model but not for the other.

Table 2 Comparison of critical emission values (mg kg^{-1} d.s.; LS10) derived with an adsorption model (PEARL) and a speciation model (ORCHESTRA) for a 0.5 meter application of granular building materials.

Contaminant	**Critical emission value (mg kg^{-1} d.s.)**		**Critical compartment**	
	PEARL	**ORCHESTRA**	**PEARL**	**ORCHESTRA**
Antimony	0.08	0.03	groundwater	groundwater
Arsenic	0.5	0.5	soil	soil
Barium	290	1.6	soil	groundwater
Cadmium	0.005	0.28	groundwater	groundwater
Chromium	0.7	0.6	soil	soil
Cobalt	0.06	0.5	groundwater	groundwater
Copper	0.03	3.4	groundwater	groundwater
Lead	91	77	soil	soil
Mercury	2.9	0.8	soil	groundwater
Molybdenum	75	64	soil	soil
Nickel	0.07	0.4	groundwater	soil
Selenium	0.2	0.2	soil	soil
Tin	44	39	soil	soil
Vanadium	0.7	0.8	groundwater	soil
Zinc	0.08	5.5	groundwater	groundwater

2.5 Summary of the decision-making process



2.5.1 *What’s at stake?*

The scientifically derived critical emission values are considered to protect both soil and water quality. Such values are important pillars for the decision making process. However, in a policy consideration process it is necessary to weigh the protection of soil and water against other societal and economic interests, such as the need to reduce the mining of raw materials and to re-use materials in a circular economy. Therefore, a variety of scenario’s reflecting different levels of protection were investigated by the RIVM (Verschoor et al. 2007). In both the Building Materials Decree and the Soils Quality Decree the proposed (i.e. calculated) values were not adopted directly as emission limit values.

2.5.2 *Uncertainties and variability*

Given the uncertainties in many modelling parameters the authors that derived the critical emission limit values considered differences of a factor 2 to be in rather good agreement. With that perspective in mind, in a policy consideration process there exist a large bandwidth to round suggested values or to keep current legal values unchanged, without a violation of the modelling outcomes. Given the model uncertainties and the variation in leaching of contaminants in column experiments, emission limit values with more than two significant numbers give a false impression of the accuracy that can be reached. Therefore outcomes were presented with no more than two significant numbers.

2.5.3 *Limit values in Building Materials Decree 1995 (BMD)*

For the Building Materials Decree almost all scientifically proposed values were initially adopted in the Regulation of 1995; only the values for molybdenum and barium were set to respectively 3 and 2.1 times higher than the calculated values (see Table 3). Between 2004 and 2006 legal exemptions were made for the critical soil input values of antimony, barium, molybdenum, selenium and vanadium as long as they did not exceed 3 times the critical soil input value. This was done because the generalized equations used in the derivation led to conservative limit values which hampered the re-use of some building materials

2.5.4 *Limit values in Temporary Exemption Regulation 2004 (TER)*

It was anticipated that the exemptions of 2004 – 2006 would no longer be needed if emission limit values were based on more sophisticated leaching models and maximum permissible risk levels. However, this did not appear to be the case. The metals and metalloids that were initially assumed to accumulate exclusively in the soil, using the simple models of the Building Materials Decree, appeared to be able to have the potential to exceed groundwater or surface water quality criteria, when numerical models were used for the Soil Quality Regulation.

2.5.5 *Limit values in Soil Quality Regulation 2007 (SQR)*

Three emission limit values from the Building Materials Decree and Temporary Exemption Regulation were replaced by values derived using the reactive transport models: PEARL or ORCHESTRA (see Table 3). These were the emission limit values for cobalt, chromium and nickel:

- Chromium was decreased from 1.7 (BMD value) to 0.63 mg kg^{-1};
- Vanadium was decreased from 1.3 (BMD value) to 0.44 mg kg^{-1}
- Cobalt was increased from 0.5 (BMD value) to 0.54 mg kg^{-1}.

In the research conducted by Verschoor et al. (2007), the consequence of the application of building materials to surface water bodies was also investigated. Based on these investigations it appeared that the critical emission values to surface water for mercury and lead were lower than those determined for soil and groundwater. Critical emission values for rivers, canals and ditches are respectively :

- Mercury: 3.2, 0.3 and 0.3 mg kg^{-1};
- Lead: 6.8, 0.7 and 0.6 mg kg^{-1}.

Because the critical emission limit values for surface water were approximately equal to the emission limit values that corresponded to the soil input values derived for the Building Materials Decree, it was decided to keep the emission limit values as they were; 0.02 mg kg^{-1} for mercury and 2.3 mg kg^{-1} for lead.

2.5.6 *A reconstruction of the policy considerations made*

Based on unofficial notes of the policy process the following rationale could be derived:

- If higher (less stringent) emission limit values were proposed based on the outcomes of both PEARL and ORCHESTRA, while a less stringent standard was not necessary, values were kept as they were in the BMD/TER. This was the case for **tin** and **molybdenum**.
- If higher (less stringent) emission limit values were proposed based on the outcomes of both PEARL and ORCHESTRA, while surface water modelling suggest lower values, the values of BMD/TER were kept, because they were in agreement with the surface water modelling. This was the case for **lead** and **mercury**.
- If lower (more stringent) values were proposed based on model outcomes, and this caused no obstacle for the recycling of building materials, the values specified in the BMD/TER were reduced. This was the case for **chromium, nickel** and **vanadium**. For chromium and vanadium the preferred values were derived with speciation modelling (ORCHESTRA).
- If lower values were proposed by both models, while this would lead to a problem in the application of building materials, values of the BMD/TER were not adjusted. This was the case for **arsenic**.
- If the two models suggested contradictory adjustments (i.e. one less stringent and the other more stringent), the values of the BMD/TER were not (significantly) changed. This was the case for **barium, cadmium, cobalt, copper** and **zinc.**
- A less stringent value has been set for **antimony**; the emission limit value has been set 2x higher than the value of the TER, which already was a factor 3 higher than the scientifically derived value of Aalbers et al. (1993) and is also 4-10 times higher than values proposed by PEARL and ORCHESTRA. Monitoring data of granulated asphalt, waste incineration ashes and thermally treated soil and sand indicate that such an increase would have been necessary in order to warrant the recyclability of these materials (Verschoor et al., 2007, Appendix B12.).

Table 3 Comparison of scientifically derived critical emission values and policy-based emission limit values. The columns under the Building Materials Decree (1995) show the scientifically derived critical input values and the critical input values that were decided upon. The columns under Temporary Exemption Regulation (2004) show the exemption values decided after broad and ample consideration. During this period the critical soil input values were also translated to emission limit values. The columns under the Soil Quality Regulation show the critical emission values derived using PEARL and ORCHESTRA, the emission limit values taken up in policy and the origin of the policy decision (BMD = Building Materials Decree; TER = Temporary Exemption Regulation).

Contaminant	**Building Materials Decree (1995)**		**Temporary Exemption Regulation (2004)**		**Soil Quality Regulation (2007)**				**Most vulnerable compartment**
	Scientific critical areal emission value (mg m^{-2}; Aalbers et al., 1993)	**Policy decided critical soil input value**	**Critical soil input value (mg m^{-2})**	**Equivalent emission value (mg kg^{-1} d.s.)**	**Scientific critical emission value (Verschoor et al., 2007)**		**Policy decided Emission limit value (mg kg^{-1} d.s.)**	**Background policy decision**	
				Considered for SQR (2007)	**PEARL**	**ORCHESTRA**			
Antimony	39	39	117	0.16	0.08	0.03	**0.32**	2x TER	groundwater
Cadmium	12	12		0.04	0.005	0.28	**0.04**	BMD	groundwater
Cobalt	300	300		0.5	0.1	0.5	**0.54**	ORCHESTRA≈BMD	groundwater
Copper	540	540		0.9	0.03	3.4	**0.9**	BMD	groundwater
Zinc	2100	2100		4.5	0.08	5.5	**4.5**	BMD	groundwater
Chromium	1500	1500		1.7	0.7	0.6	**0.63**	ORCHESTRA≈PEARL	soil
Arsenic	435	435		0.9	0.5	0.5	**0.9**	BMD	soil
Molybdenum	150	450	450	1	75	64	**1**	TER	soil
Selenium	15	15	45	0.15	0.2	0.2	**0.15**	TER	soil
Tin	300	300		0.4	44	39	**0.4**	BMD	soil
Lead	1275	1275		2.3	91	77	**2.3**	BMD	surface water
Mercury	4.5	4.5		0.02	2.9	0.8	**0.02**	BMD	surface water
Barium[a]	3000	6300	18900	22	290	1.6	**22**	TER	no consensus
Nickel[b]	525	525		1.3	0.07	0.4	**0.44**	ORCHESTRA	no consensus
Vanadium[b]	1020	2400	7200	5.5	0.7	0. 8	**1.8**	BMD	no consensus

a. Calculations made using PEARL indicate groundwater to be the critical compartment and calculations based on ORCHESTRA indicate soil to be the critical compartment.

b. Calculation made using PEARL indicate soil to be the critical compartment and calculations based on ORCHESTRA indicate groundwater to be the critical compartment.

3 Derivation of critical emission values

3.1 Model choice

In this study, HYDRUS-1D version 4 (Śimûnek et al. 2008) is used to recalculate the critical emission limit values. The calculated values are compared with those derived by Verschoor et al. (2007) to validate the derivation method used. The models used by Verschoor et al. (2007) are PEARL 2.2.2 and ORCHESTRA. HYDRUS-1D is similar to both models in that it simulates, water, heat and solute transport. The choice for HYDRUS-1D in this study has several reasons.

The first reason for choosing HYDRUS-1D is related to the current problems surrounding PFAS. Currently HYDRUS-1D is being modified to account for interfacial adsorption to the air-water interface (Silva et al., 2020). This process has been demonstrated to be an important mechanism for the retention of PFAS compounds in unsaturated soils under certain conditions (Brusseau, 2018). A version of the model that does not account for air-water interfacial adsorption has recently been used within the Netherlands to predict soil concentrations of PFOA and PFOS in sandy soils (Gerardu, 2021). Results of the study indicate the soil concentrations can be adequately predicted using HYDRUS-1D if K_d ranges are considered. In a study conducted to review models that could be used to adequately simulate the transport of PFAS in the unsaturated zone, HYDRUS-1D was marked as the most adequate model (Tabel 4; EGLE, 2020).

Table 4 Suitability of available models to describe PFAS transport in the unsaturated zone (taken from EGLE, 2020)

Vadose zone modelling code	Method of Solving Groundwater Flow	Non Equilibrium Sorption	Freundlich (non linear) Sorption	Partitioning to the Air Water Interface	Root Uptake Function	Dual Permea-bility	Advanced Geochemical Modeling Capabilities	1D, 2D or 3D	Surfactant Induced Flow	Availability
Hydrus	Richards Equation	Yes	Yes	Yes	Yes	Yes	PHREEQC Coupling, Colloid Transport	1D, 2D and 3D	Customized Code	Free (1D), Commercial (2D & 3D)
PEARL	Richards Equation	Yes	Yes	No	Yes	Yes	pH Dependence, User-Defined Functions	1D	No	Free (current)
RZWQM	Richards Equation	Yes (limited)	No	No	Nitrogen only	Yes	Limited Solute Transport, Cation Exchange, pH Considerations	1D	No	Free (current)
SVENVIRO	Richards Equation	No	Yes	No	Yes	No	No	2D and 3D	No	Commercial
CTRAN/W with SEEP/W	Darcy's Law	No	User-Defined Function	No	Yes	No	No	1D and 2D	No	Commercial
PELMO	Capacity-based Approach	No	Yes	No	Yes	No	2 Sorption Sites	1D	No	Free (current)
SESOIL	Infiltration-based Approach	No	Yes	No	No	No	No	1D	No	Commercial
PRZM	Darcy's Law	No	No (nitrogen only)	No	Solute only	No	No	1D	No	Free (not current)
VLEACH	Darcy's Law	No	No	No	No	No	No	1D	No	Free (not current)

Green = Ideal; Yellow = Less than ideal; Red = Least suitable / not recommended

HYDRUS-1D accounts for processes such as, equilibrium and kinetic adsorption, degradation and volatilization. It also contains a module, HP1, that allows for coupling with the geochemical model PHREEQC (Parkhurst and Appelo, 1999; Jacques and Šimůnek 2005). HYDRUS-1D can thus be used to approach reactive-transport problems mechanistically if desired. The model is used extensively within the scientific community to investigate waterflow and solute transport. Furthermore HYDRUS-1D is highly flexible and allows the user to define scenarios freely. This means that it can be used for generic as well as site-specific investigations.

In the context of the advice offered by the TCB (2006), HYDRUS-1D fulfils several, but not all, of the requirements. The TCB pointed out that models that consider speciation are preferable as they can account for geochemical changes in the soil environment. Furthermore, geochemical models can account for the competition that takes place between leached ions. The HP1 module of HYDRUS also has the capability to account for such changes. A further point of consideration is that complex speciation models are data intensive. Accurate parametrisation may be possible for well-studied metal cations, but is less likely to be the case for less intensively studied (organic) contaminants. For such contaminants (e.g. pesticides and PFAS) the use of a simple partitioning approach may be preferable.

The TCB also indicated that the validation status of PEARL and adoption of PEARL on a European level for pesticide regulation, and the scenarios and parameters contained within it, were strong features of the model. The flexibility of HYDRUS-1D allows for near identical adoption of scenarios and parameters used in PEARL. In this study, the scenarios and parameters that were used in PEARL were implemented in HYDRUS-1D (annex 2). HYDRUS-1D is also used within eLTER, a HORIZON 2020 funded project, which aims to facilitate research on, among others, the impacts soil degradation and pollution on European ecosystems. Finally, the results of this study show that the critical emission limit values derived using HYDRUS-1D are in most cases identical to those derived using PEARL (see chapter 4).

3.2 Simulation of PEARL runs with HYDRUS-1D

An important metric to determine whether the derivation method of the critical emission limit values have been implemented correctly is to compare the results yielded in this study with those derived by Verschoor et al. (2007). To test this, simulations were run using PEARL and HYDRUS-1D. To compare the results identical conditions (e.g. building material application, soil profile description and adsorption coefficients) were used in the two models. A more detailed overview of the used input parameters can be found in annex 2.

3.2.1 Building material application

The applied building material can vary in terms of density, leaching rate and thickness. Although there are other aspects in which building materials vary, these are the points which have been explicitly considered. The density of the building material is assumed to be 1,550 kg m^{-3}. This is based on the average density of the building materials considered in the past (Verschoor et al., 2007). Furthermore, the standard scenario is based on a granulated building material.

In this study standard leaching rate coefficients are used per contaminant, as was done by Verschoor et al. (2007). In actuality leaching rates vary per building material and per contaminant. The chosen coefficients are the average of coefficients derived for multiple building materials. Finally, the thickness of the applied building material in the calculated simulations is 0.5 m.

3.2.2 *Adsorption coefficients*

Adsorption coefficients are inherently variable, as a result of differences in soil properties. Because the derived emission limit values need to offer generic protection, simulations were conducted using a range of K_d values (as in Verschoor et al., 2007). In this study the emission limit value for the protection of groundwater is evaluated using a low K_d, as this makes groundwater more susceptible to contamination and thus adequately protects groundwater quality. The emission limit values for soil are based on simulations using high K_d, as this leads to accumulation in soils and thus yields conservative emission limit values for the protection of soil. An overview of the studies used to determine K_d values can be found in Verschoor et al. (2007).

3.2.3 *Hydrology*

In the presented simulations, the net yearly infiltration rate approximately amounts to 300 mm yr^{-1}. The daily precipitation and evaporation input used is based on an average of the precipitation records for the period 1981 – 2000.

In the simulations, the groundwater level is set to 1 m below the soil surface.

3.2.4 *Soil profile*

The parameters pertaining to the soil profile are acquired from PEARL. PEARL contains standard soil profiles, including hydraulic and chemical parameters, deemed representative for different European countries. The standard soils types are however relatively susceptible to leaching, as the model was developed to assess the risks associated with the leaching of pesticides. The standard soil type for the Netherlands is a sandy soil with a decreasing organic matter and clay content with depth. An overview of the soil profile and associated soil hydraulic parameters can be found in annex 2.

3.3 Sensitivity analysis

In addition to a comparison of model outcomes, a sensitivity analysis is also conducted in this study. The sensitivity analysis focused on two of processes that influence contaminant concentrations in soil and groundwater:

1. emission rate of contaminants from building materials
2. retardation of contaminants in soils.

Factors such as degradation or volatilization are not relevant for the metals and metalloids in this report, but may become important for organic contaminants.

The sensitivity analysis was conducted by investigating the influence that different combinations of leaching rates and adsorption coefficients have on soil and groundwater concentrations. Retardation was approximated using a range of adsorption coefficients (K_d). The other process, the leaching rate (LR), depends on the amount of building material on the soil, which is determined by the thickness (h) and density (ρ) of the applied building material, the leaching rate constant kappa (κ), and the effective infiltration (*F*) (Verschoor et al., 2007). The dependence of the leaching rate on these factors is presented in equation 1. The leaching rate of a contaminant increases as the density and thickness of the applied building material decrease, and as the contaminants leaching rate constant and effective infiltration increase. A high leaching rate implies a relatively rapid release of present contaminants.

$$LR = \frac{\kappa \cdot F}{h \cdot \rho} \qquad \text{Eq 1.}$$

For the sensitivity analysis, model simulations are run for 392 combinations of K_d (n = 14) and leaching rate (n = 28). K_d values range from (10 – 500 l kg^{-1}) and the leaching rates from (0.001 – 1 mm m^2 yr^{-1} kg^{-1}). Due to the time required to run this many simulations, a constant net infiltration input of 300 mm yr^{-1} is used. This is the equal to the average net infiltration reported by Verschoor et al. (2007).

4 Results

4.1 Comparison soil and groundwater concentrations

A comparison of the maximum concentrations in the upper meter of groundwater graphs and the associated average concentration in the upper meter of soil after 100 years are presented Table 5.

Metals that reach peak groundwater concentrations within the simulated period appear to be in agreement. For metals that reach peak concentrations later than 100 years (e.g. arsenic, barium) the concentration differences between PEARL and HYDRUS-1D are relatively larger.

The average concentrations in soil appear to agree as well. This is also reflected in the derived critical emission values (Table 6). For the metalloids (arsenic and antimony), lower concentrations are calculated in the soil column due to the contaminant not being fully leached within the simulated timeframe.

Table 5 The calculated maximum concentrations in the upper meter of groundwater within a 100 years and the average concentrations in the top meter of soil at 100 years. The presented concentrations are based on a standard emission of 100 mg m^{-2}.

Contaminant	**Max. concentration groundwater (µg l^{-1})**		**Average concentration soil (mg kg^{-1})**	
	PEARL 2.2.2	**HYDRUS-1D**	**PEARL 2.2.2**	**HYDRUS-1D**
Arsenic	8.3E-09	7E-09	18.3	21.1
Barium	3.7E-13	6E-19	64.3	67.5
Cadmium	9.13	7.36	64.5	67.7
Cobalt	4.34	3.53	63.7	67.0
Chromium	9.6E-22	<1E-20	64.5	67.7
Copper	5.18	4.07	64.5	67.7
Mercury	1.7E-09	4E-12	63.9	67.2
Molybdenum	0.003	0.003	64.5	67.7
Nickel	3.31	2.68	64.5	67.7
Lead	1.5E-10	5E-14	64.4	67.5
Antimony	3.45	3.17	47.5	52.5
Selenium	2.0E-05	5E-06	64.2	67.4
Tin	0.003	0.003	62.3	65.8
Vanadium	0.21	0.23	47.5	52.5
Zink	10.70	8.84	64.5	67.7

4.2 Comparison of scientifically derived critical emission values

The derived critical emission values for building materials using the model outputs of PEARL and HYDRUS-1D are presented in Table 6. The derived values generally appear to agree. The largest relative differences occurred for zinc and copper. This is presumably due to differences in peak concentrations calculated in this study and the study conducted by Verschoor et al. (2007).

Table 6 A comparison of the derived critical emission values (mg kg^{-1} d.w.) using HYDRUS-1D and the values derived by Verschoor et al. (2007) using PEARL.

Contaminant	PEARL	HYDRUS-1D	Ratio HYDRUS/PEARL
Critical compartment: Soil			
Arsenic	0.5	0.5	1.0
Barium	290	281	1.0
Chromium	0.7	0.7	1.0
Lead	91	88	1.0
Mercury	2.9	2.7	0.9
Molybdenum	75	73	1.0
Selenium	0.2	0.2	1.0
Tin	44	42	1.0
Contaminant	**PEARL**	**HYDRUS-1D**	**Ratio HYDRUS/PEARL**
Critical compartment: Groundwater			
Antimony	0.07	0.08	1.1
Cadmium	0.005	0.006	1.2
Cobalt	0.06	0.08	1.3
Copper	0.03	0.03	1.0
Nickel	0.07	0.08	1.1
Vanadium	0.7	0.64	0.9
Zink	0.08	0.1	1.3

4.3 Sensitivity analysis

The results of the sensitivity analysis are presented Figure 3. As described in paragraph 3.3, the sensitivity of soil and groundwater concentrations to the leaching rate and the adsorption coefficient are investigated with this analysis. The contour plots illustrate the relationship between leaching rate, adsorption and media concentrations. Note that the axes are scaled logarithmically. The first observation is that accumulation within groundwater occurs at lower K_d and larger leaching rates. For a given K_d, as the leaching rate decreases, less contaminant is expected in the groundwater as it is yet to be entirely leached from the building material or is still present in the soil profile. As K_d increases, accumulation tends to occur within the soil profile, which is to be expected with increased adsorption. The contour plots underscore the importance of using accurate K_d values for contaminants with values ranging from ~10 - ~50 l kg^{-1} as this determines which environmental compartment may be critical. It is important to note that the importance of this K_d range is specific to the studied scenario. Changes in either the simulated timescale or groundwater depth would lead to a shift in the K_d range above or below which accumulation occurs in soil or groundwater.

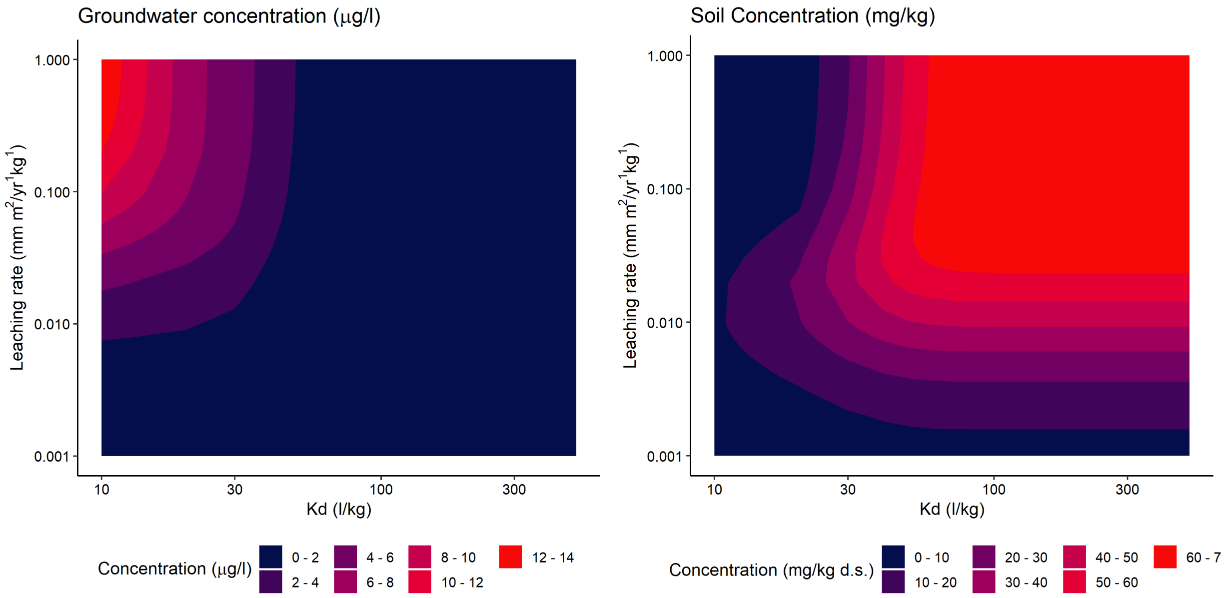


Figure 3 Contour plots for the maximum concentration simulated in groundwater (left) and the average concentration in soil after 100 years (right) as a function of K_d *and leaching rate .The colour gradients indicate the concentration in the media (see legends).*

The second relationship that the sensitivity analysis reveals, which is related to the cut-off of the simulated time, is that soil and groundwater concentrations are dependent on the leaching rate. This is because the leaching rate limits the amount of contaminant leached from the building material. At higher leaching rates most of the contaminant has time to distribute over soil or groundwater (depending on the K_d). At a lower leaching rate, a significant fraction of the contaminant has not or just shortly entered the soil and there is not enough time for the contaminant, even relatively "mobile" ones, to be entirely present in the soil or reach the groundwater. A contaminant for which this is the case is arsenic, the contaminant with the lowest leaching rate in this study (see Table 13 in annex 2). In the standard simulation arsenic is yet to fully leach from the building material, which can be deduced based on the mass balance information used to calculate soil concentrations (Table 5).

Like the K_d, an accurate estimate of the leaching rate constant (the most uncertain factor in the estimation of the leaching rate) is important in certain areas of the sensitivity plot. For the derivation of the critical emission value the lowest value derived from soil and groundwater concentrations is taken as this protects both media. Which compartment is decisive very much depends on the environmental quality standard that applies to that compartment.

5 Discussion

5.1 Model choice

The societal need for revision of emission limit values of the Building Materials Decree (including Temporary Exemption Regulation), and the wish to apply more realistic leaching models led to a time-consuming project in 2006 and 2007. The acceptance of the results was poor, though reasons for it could be justified. The different modelling approaches and differences model outcomes did not help in the acceptance of the proposed critical emission values. For 3 out of 15 metals and metalloids, the emission limit values were adjusted, whereas for remaining 12 the emission limit values remained unchanged.

These observations raise the question what an efficient approach is for new and emerging contaminants in building materials. Numerical models such as PEARL, ORCHESTRA and HYDRUS-1D, which account for physico-chemical and hydrological processes in varying degrees, require a large amount of input data regarding substance properties, building material properties, soil properties, groundwater and climate. This information is difficult to retrieve even for well-studied contaminants such as metals and metalloids. So for new and emerging substances the necessary information is likely to be not available in many cases. In such cases, with many unknowns, an approach "simple when possible, difficult when needed" may be a cost-effective way to respond when new critical emission values are requested. In Table 7, a possible approach is presented. In this approach successively more complex methods are applied depending on the amount of information available and workability of the derived environmental norm.

Table 7 Possible consecutive steps a cost-effective derivation of critical emission values for new and emerging contaminants in building materials.

Step	**Approach**	**Minimum information requirement**	↓ Increasing complexity, realism and cost	↓ Decreasing conservatism and uncertainty
1	Contaminant entirely in soil; Contaminant entirely in groundwater	**contaminant concentration** in building material		
2	Leached fraction in soil; Leached fraction in groundwater	**+leaching rate** (kappa)		
3	Distribution over soil and groundwater using simple adsorption models	**+adsorption coefficient** (options: function of organic matter, pH, equilibrium or non-equilibrium sorption)		
4	Distribution over soil and groundwater using advanced chemical speciation and advanced adsorption models	**+chemical speciation** reaction constants **+binding constants** to organic matter, clay and Fe- and Al-oxides and hydroxides		

Step 1

In this step we assume that nothing is known except the concentration of the new contaminant in a building material (composition). As a worst case two assumption can be worked out:

- the total contaminant present in the building material accumulates in the upper meter of the soil (in 100 years) and the concentration should comply with the environmental quality standard for soil;
- the total contaminant present in the building material accumulates in the upper meter of the groundwater (in 100 years) and should comply with the environmental quality standard for groundwater;

In this step no information is required about the leaching rate coefficient (kappa), sorption behaviour, chemical speciation, degradation, et cetera.

If the resulting critical emission value results in an acceptable protection of the environment and does not lead to unacceptable restrictions in the reuse of building materials, considerations can be made to establish a legal value. If not, data pertaining to the leaching rate needs to be collected.

Step 2

If the leaching rate of the contaminant is investigated using data from column experiments, Step 1 can be refined, by calculation of the actual exposure of the soil. If the derived critical emission value results in an acceptable protection of the environment and does not lead to unacceptable restrictions in the reuse of building materials, considerations can be made to establish a legal value. If not, more data pertaining to adsorption, biodegradation and volatilization needs to be collected.

Step 3

Reactive transport models such as PEARL or HYDRUS-1D can be used to account for adsorption, biodegradation and volatilisation of the contaminant in soil and groundwater, following the procedures described in this report. Generic soil and climate scenarios could be employed, such as was done by Verschoor et al. (2007) and in this report. A site-specific evaluation is possible in this step, but requires the measurements of site specific soil parameters. The site specific investigation could use generic chemical parameters and site specific hydraulic parameters, or site specific chemical parameters, with which specific K_d values can be interpolated, and site specific hydraulic parameters. If the derived critical emission value results in an acceptable protection of the environment and does not lead to unacceptable restrictions in the reuse of building materials, considerations can be made to establish a legal value. If not the data required to run specialized models needs to be collected. This could for example be information needed to consider chemical speciation, advanced sorption models and advanced soil hydraulic models.

An alternative course of action for this step, if the K_d has not been derived experimentally, is to use a K_d value based on quantitative structure-analysis relationships (QSAR). QSAR models are statistical and can be used to predict various physico-chemical and toxicological properties of contaminants based on the contaminants structure. K_d values based on such models could thus be used until reliable empirical data are available.

Step 4
Sophisticated reactive transport models can account for chemical speciation, specific adsorption to various soil constituent (e.g. organic matter, clay and Fe- and Al-oxides and hydroxides), kinetic adsorption and non-equilibrium water transport. These models require a large number of input parameters. It is unclear how relevant such models are for the derivation of generalized critical emission limit values. For new contaminants, it is unlikely that this information is available. The use of such models for site-specific evaluation requires that the soil properties of the site being modelled are well characterized. For generic purposes the default values used by Verschoor et al. (2007) could be adopted.

5.2 Discrepancies between PEARL and HYDRUS-1D

The derived environmental media concentrations and thus critical emission values are largely similar for most metals. For groundwater, peak concentrations are reached at a slightly later point in time when HYDRUS-1D is used. The precise cause for this discrepancy is unclear. This does not lead to large differences for contaminants whose critical emission values are dependent on groundwater concentrations. This lag between HYDRUS-1D and PEARL only leads to differences in critical emission values, when peak concentrations are simulated to occur after the cut-off time of 100 years. This is the case for vanadium, where exceedance of groundwater quality criteria is the basis for the critical emission value.

For soil, a similar relationship is present. Differences are small for contaminants that are entirely leached and present in the soil matrix within the simulation period. The soil concentrations simulated in HYDRUS-1D are generally slightly larger than those simulated in PEARL. This can be attributed to small concentration mass balance errors (≤ 3 %). This means that for certain metals, for example barium and lead, the critical emission values are slightly lower when based on HYDRUS-1D simulations.

5.3 Translation of sensitivity analyses results to policy

5.3.1 Building material application

The current critical emission values are based on a standard building scenario, which assumes a fixed height and density of the application. This scenario is simple but can lead to difficulties as the unique characteristics of the construction and the building material are not considered. It can lead to excessively stringent or lenient policy towards building materials. The sensitivity analysis shows that consideration of the leaching rate, which is dependent on application thickness, material density, leaching rate coefficient and net infiltration (equation 1), is crucial in ensuring the efficacy of derived critical emission values. To prevent too stringent or lenient critical emission values, the factors of height, density and leaching constant of the application in addition to the K_d of the contaminant in question could be considered in the regulatory process.

The consideration of these factors could be implemented by calculating soil and groundwater concentrations for different combinations of building material specifications for a range of K_d values. The outcome of these calculations can be presented in a lookup table, that contains all the combinations. A user could subsequently simply lookup which critical emission limit value corresponds to their desired application. The user defined input would thus be a leaching constant, density and height of the intended construction, a Kd-range for the contaminant of concern, and the environmental quality criteria of the contaminant. The applicant (contractor or licensing regulator) could easily derive a step 3 critical emission value.

An added benefit of this approach is that a step 3 critical emission limit value could be derived quickly for contaminants of emerging concern, that do not degrade or volatilize. The only information that would be required is a K_d range and relevant environmental quality criteria.

5.3.2 Simulation time

The sensitivity analyses also shows the importance of the considered timescale. This is because at low leaching rates contaminants may have not entirely leached from the application or are only present in the soil, which is the case for vanadium. By considering longer timescales, more relevant critical emission limit values can be derived.

This problem has been recognized by other researchers and governments. The Flemish government for example only considers peak groundwater concentrations, irrespective of the time scale at which these occur (Broos et al., 2015). Another example can be found in an investigation into the leaching caused by soil contamination (Spijker et al., 2009) where a time period of 500 years was used to determine the effects on groundwater quality. The choice of this time period was based on the findings of Verschoor et al. (2007) which indicated that protection of groundwater quality could not be guaranteed using a timescale of 100 years. Finally, the TCB also recognized this shortcoming and concluded that the consideration of longer timescale would lead to more relevant critical emission values (TCB, 2006).

5.4 Further investigations

5.4.1 Regulation based on building material application specifications

Based on the sensitivity analysis, investigating a method by which the specifics of the building material application is considered during regulation may be desirable. This would increase the flexibility of regulatory procedures and allow for tailored scenarios that consider the height and density of the building material in addition to the kappa and K_d of the contaminant under investigation. This can be incorporated in a simple lookup table that contains various combinations of the building material application specifications and a range of K_d values. A user could then lookup the critical emission value corresponding to the specifications of their building material application.

5.4.2 *Effects of increased simulation time periods*

An investigation into the effect of considering longer simulation times may also be meaningful. Certain contaminants are at most partially present in environmental media within the simulated period due to low leaching rates or high K_d. Increasing the simulated time periods can thus help clarify long-term environmental fate of contaminants and lead to environmental criteria that are meaningful for the protection of groundwater. This could be combined with an investigation into other endpoints.

5.4.3 *Consideration material specific leaching rate constants*

The sensitivity analysis shows the importance of the leaching rate on derived critical emission values. The current critical emission limit values are based on generic leaching rate constants which leads to coarse critical emission limit values. In actuality the leaching rate constants vary per metal and per building material. Based on this, it may be worthwhile to use material specific leaching rate constants for frequently used granulated building materials. This could lead to more fine-tuned and environmentally relevant critical emission limit values.

6 Conclusion

The objectives of this study are to:

1. understand the decision making process leading to derivation of the critical emission limit values;
2. understand the methods used to derive the critical emission limit values and to recalculate the critical emission limit values based on this understanding;
3. compare the newly derived results with those derived in the past by Verschoor et al. (2007) and clarify any discrepancies in results;
4. conduct a sensitivity analyses on the effect of various parameters on environmental quality.

Based on the study it has become clear which scientific and societal considerations were made when deriving the (critical) emission limit values and establishing legal standards. It is clear that the derived critical emission limit values have not been readily incorporated into legal standards due various considerations.

In this study HYDRUS-1D is used because of its ability to function as both a partition and mechanistic model and because future versions of the model are likely to include a process that can be crucial in determining the environmental fate of PFAS. Based on the modelling conducted in this study, it can be concluded that the method for the derivation of critical emission limit values has been reestablished. This can be concluded based on the agreement between the results derived in the past, using PEARL, and the results derived presently using HYDRUS-1D.

Finally, the sensitivity analysis has underscored the shortcomings of a standard scenario in terms of building material application. A standard building material application scenario has advantages for a generic and national framework but disregards the variations in building materials and their applications. This can lead critical emission limit values that are too stringent, which is the case for applications where the thickness and density are lower than standard scenario, or too lenient, which is the case for applications with a greater thickness or density than the standard scenario. This variation can be accounted for by implementing a lookup table that incorporates various building material specifications (height and density) and contaminant specifications (K_d and leaching rate constant). With such a table, a user can lookup which critical emissions correspond to the envisioned building material application. Alternatively, critical emission limit values may be derived using building material specific leaching rate constants. This could be done for the most frequently used building materials and could ensure the protection of soil and groundwater quality.

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Annex 1 Comparison of scientific and legal soil input values and emission values for building materials in the BMR

1. Conversion method

Conversion from emission from a material to areal emission from an application, which was used as the basis for legal norms in the building materials decree, and vice versa is done using equation 2.

$$I_{soil} = E_{app} = \frac{(E_{mat} - a) \cdot \rho \cdot h \cdot (1 - e^{-\kappa \cdot \frac{N_i \cdot t}{\rho \cdot h}})}{(1 - e^{-\kappa \cdot 10})} \qquad \text{Eq. 2}$$

Where:
I_{soil} is the soil input value (mg m^{-2})
E_{app} is the areal emission from the application (mg m^{-2})
E_{mat} is the cumulative emission of the material using a column test at L/S=10 (mg kg^{-1})
a is the natural leaching from clean soil (mg kg^{-1})
ρ is the building material density (kg m^{-3}); default value is 1550 kg m^{-3}
h is the application thickness (m); default values is 0.5 m
N_i is the effective infiltration (mm yr^{-1})
K is the leaching rate coefficient (-)
t is the time (yr); default value is 100 yr

ɑ and κ are dependent on the contaminant of concern and vary between the methods employed for the Building Materials Decree and the Soil Quality Regulation.

In the Building Material Decree, the areal emission from an application was calculated using specifications (e.g. thickness, density, cumulative emission) of the application. The equation was thus solved for E_{app}. For the Soil Quality Regulation the equation is solved for E_{mat} using the standard scenario. The E_{mat} is then used as the basis for legal norms.

2. Factor ɑ (background leaching)

In the Building Materials Decree the permissible leaching from building materials is reduced with factor ɑ which is the background leaching caused by the presence of the same metals in natural soil. The aim of the Building Materials Decree was to ensure that the total leaching from the two sources (building material and soil) would not lead to exceedance of Soil Target Values (negligible risk). The background leaching was derived from column leaching experiments using 25 natural soils. The variability of leaching was explained by assuming that only humus and lutum explained the variation, although for some metals the leaching was more or less constant. The background leaching was subsequently standardized for a standard soil with 10% humus matter and 25% lutum, using the regression equations derived from these experiments (see Table 8). No reference was made to the raw data.

In the Soil Quality Regulation, the background leaching of soil was neglected (factor ɑ = 0) because the protection level is derived from the maximum permissible addition (see annex 2).

Table 8 Background leaching (ɑ; mg kg^{-1}) used in the calculation of critical soil input value for the Building Materials Decree (Aalbers et al., 1993). Hu = humus (wt %), Lu = lutum (wt %)

Contaminant	Regression equation for calculation of factor a	Factor a (mg/kg) in standard soil; Hu=10 (%), Lu=25 (%)
Antimony	0.02	0.02
Arsenic	0.5 + 0.02 Hu	0.7
Barium	0.6 + 0.03 Hu	0.9
Cadmium	0.015 + 0.0006 Hu	0.021
Chromium	0.05 + 0.004 Hu	0.09
Cobalt	0.18	0.18
Copper	0.25	0.25
Lead	0.5 + 0.03 Hu	0.8
Mercury	0.016	0.016
Molybdenum	0.15	0.15
Nickel	0.25 + 0.02 Hu + 0.007 Lu	0.63
Selenium	0.03	0.03
Tin	0.03	0.03
Vanadium	0.2 + 0.02 Hu	0.4
Zinc	1 + 0.1 Hu	2

3. Kappa (leaching rate constant)

Kappa is a constant that determines the leaching rate of contaminants from building materials. The leaching rate constant depends on properties of the building material and of the contaminant. However, due to a lack of data for individual building materials an average kappa was estimated only for different contaminants and not for different building materials. Aalbers et al. (1993) suggested that the quantities of building materials on the market should be used to calculate a weighted average kappa. However, there were no data to enable such a calculation.

Kappa was derived from data of column leaching experiments with a variety of building materials (Aalbers et al., 1993). In Figure 4 the result of a (hypothetical) column leaching experiment is shown. The L/S ratio refers to the volume of water (liter) through the mass of material (kg) present in the column. The concentration is the concentration in the leachate which is sampled at specific L/S ratios. No reference has been made to the raw data.

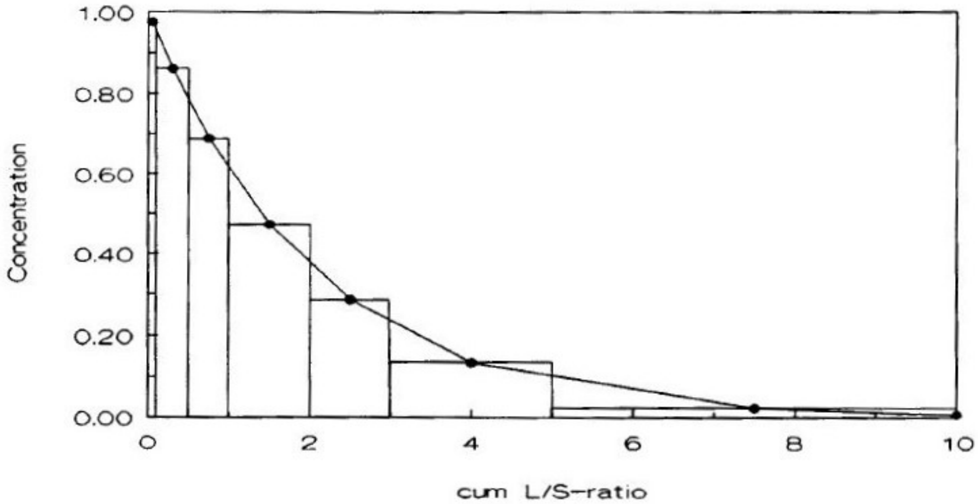

Figure 4 Graph of column leaching results used to derive the leaching rate constant kappa (Aalbers et al., 1993).

Kappa is derived with the following formula:

$$\ln(C) = \ln(C_0) - kappa * cum\ L/S \qquad \text{Eq. 3}$$

The formula logarithmicly transforms the output of the leaching experiment and produces a linear equation. The slope of the linear equation is the leaching rate constant (kappa). The datasets used to derive kappa for the Building Materials Decree differ to those used for the Soil Quality Regulation. The kappa values used by Verschoor et al. (2007) are based on unpublished results by De Wilde (1998). It is postulated that the kappa values derived by De Wilde (1998) are a combination of the data used by Aalbers et al. (1993) and new data.

Table 9 Comparison of old kappa values used by Aalbers et al. (1993) and new values used by Verschoor et al. (2007).

Contaminant	**n**	**Estimation average *old* kappa ± 95% confidence interval**	***new* kappa**
Antimony	33	0.11 ± 0.07	0.04
Arsenic	44	0.03 ± 0.05	0.01
Barium	55	0.15 ± 0.04	0.17
Cadmium	37	0.5 ± 0.10	0.32
Chromium	82	0.18 ± 0.03	0.25
Cobalt	10	0.2 ± 0.08	0.13
Copper	90	0.28 ± 0.03	0.27
Lead	52	0.27 ± 0.06	0.18
Mercury	5	0.05 ± 0.03	0.14
Molybdenum	76	0.35 ± 0.04	0.38
Nickel	37	0.29 ± 0.05	0.26
Selenium	10	0.38 ± 0.18	0.16
Tin	5	0.19 ± 0.13	0.1
Vanadium	40	0.05 ± 0.06	0.14
Zinc	41	0.28 ± 0.05	0.28

4. Comparison of critical values for the Building Materials Decree

In the table below (Table 10) a comparison is given between the values derived by Aalbers et al. (1993), the legal norms of the Building Material Regulation (BMR), the Temporary Exemption Regulation (TER) and Soil Quality Regulation (SQR). Many of the legal norms used in the BMR or TER appear to be similar to the legal norms reported in the SQR. Because the legal norms mentioned in the BMR and TER are reported as areal emission limit values, converted emission limit values are also reported, as these converted values are what were considered for the SQR. The areal emission limit values were converted to cumulative material emission limit values using equation 2, the background leaching values reported in Table 8 and the old kappa values reported in Table 9. The conversions of the areal emission limit values assume an application thickness of 0.5 m, a material density of 1,550 kg m^{-3} and net infiltration of 300 mm yr^{-1}.

Table 10 A comparison of the aerial emission limit values calculated by Aalbers et al. (1993) and the legal norms included in the BMR, TER and SQR.

Contaminant	**Areal emission values (mg m^{-2})**			**Material emission values (mg kg^{-1})**			
	Aalbers et al. (1993)	**BMR (1995)**	**TER (2004)**	**Aalbers et al. (1993)**	**BMR (1995)**	**TER (2004)**	**SQR (2007)**
Antimony	39	39	117	0.054	0.054	0.12	0.32
Arsenic	435	435		0.91	0.91		0.9
Barium	3000	6300	18900	3.9	7.2	20	22
Cadmium	12	12		0.04	0.04		0.04
Chromium	1500	1500		1.71	1.71		0.63
Cobalt	300	300		0.51	0.51		0.54
Copper	540	540		0.9	0.9		0.9
Lead	1275	1275		2.3	2.3		2.3
Mercury	4.5	4.5		0.02	0.02		0.02
Molybdenum	150	450		0.34	0.71		1
Nickel	525	525		1.27	1.27		0.44
Selenium	15	15	45	0.05	0.05	0.09	0.15
Tin	300	300		0.36	0.36		0.4
Vanadium	1020	2400	7200	1.0	1.82	4.7	1.8
Zinc	2100	2100		4.5	4.5		4.5

Annex 2 Modelling with HYDRUS-1D

1. Standard Scenario

1.1 Environmental criteria

The base scenario used is identical to the scenario used to derive emission limit values (Verschoor et al., 2007). The scenario definition was partially dependent on practical choices. The risk-based approach is the widely accepted starting point for the derivation of environmental criteria. This approach is distinct from a *stand-still* approach, which stipulates that concentrations may not increase by more than a certain percentage of current concentrations or a concentration used as an environmental criterium. Numerically, this was defined as 1% of "natural" concentrations. The risk-based approach in contrast states that concentrations may not lead to increased environmental impact. This risk-based approach is dependent on the maximum permissible addition (MPA) to an environmental compartment, which is the amount of contaminant that needs to be added to a soil or water body for an ecological effect to potentially be observed. The MPA is derived from ecotoxicological bioassays. The maximum permissible concentration (MPC) combines the MPA and the naturally occurring environmental concentration (C_b). The MPC is a concentration above which, in 5% of organisms or processes a negative effect is expected. It relies on the assumption that naturally occurring concentrations do not stress biota, and that only the added fraction need be considered. The relationship between the MPC, MPA and C_b is shown in equation 4.

$$MPC = MPA + C_b \qquad \text{Eq. 4}$$

The addition of a contaminant to an environmental compartment is dependent on multiple sources eg. contaminants may leach into groundwater from building materials but also from soils. It was decided that the MPA be dependent entirely on leaching from building materials, and that leaching from soils be neglected. This decision was based on policy maker's opinion that the ramifications related to leaching from natural sediments are acceptable and minimal, as it concerns naturally occurring metals that are predominantly bound and therefore not bioavailable (Crommentuijn et al., 1997). In contrast the contaminants present in the applied building material are assumed to be entirely bioavailable. A similar consideration was made during the derivation of emission limit values of contaminants from soils (Spijker et al., 2009). Furthermore, as background concentrations of metals differ per locality, neglecting background concentrations makes it possible to derive generic emission limit values, which was deemed desirable for national applicable standards. The current emission limit values are thus based on the entirety of the MPA being available to leaching from building materials. The input of contaminants from other sources are not considered.

In the Netherlands there are environmental quality criteria for both soil and groundwater compartments. Maximum emission limit values are derived for both compartments based on their respective MPAs. The lowest between the two derived emission limit values is subsequently used as the legal emission limit value because it provides protection for both environmental compartments. In this study the emission limit value for the protection of groundwater is evaluated using a low K_d, as this makes groundwater more susceptible to contamination and thus adequately protects groundwater quality. The emission limit values for soil are based on simulations using high K_d, as this leads to accumulation in soils and thus yields conservative emission limit values for the protection of soil. An oversight of the studies used to determine K_d values can be found in Verschoor et al. (2007). In this study a standard emission of 100 mg m^{-2} 100 yr^{-1} is used as a source term. The results of this standard emission are compared to the MPAs and subsequently used to calculate the permissible emission.

1.2 Building material application

The applied building material can vary in terms of density, leaching rate and thickness. Although there are other aspects in which building materials vary, these are the points which have been explicitly considered. The density of the building material is assumed to be 1,550 kg m^{-3}. This is based on the average density of the building materials considered in the past (Verschoor et al., 2007). Furthermore, the standard scenario is based on a granulated building material.

The leaching rate coefficient of a specific contaminant from a building material is determined experimentally through standardized column experiments. The leaching coefficient differs per metal and building material. It is furthermore dependent on physico-chemical circumstances, such as the pH of the leachate solution and the grain size of the building material after grinding it in preparation of the column experiment. In the study a single leaching coefficient was chosen per investigated metal. The chosen coefficients are the average of coefficients derived for multiple building materials. The leaching rate coefficients are used to determine concentrations in leachate at a given point in time given flow rates are constant.

The thickness of the building material in the standard scenario was chosen to be 0.5 m. In actuality the applied thickness may be greater or lesser. The chosen thickness influences the absolute amount of contaminant that is contained within an application covering a given area. As the thickness increases the contaminant reservoir increases.

1.3 Hydrological aspects

The current emission limit values are based on an infiltration rate of approximately 300 mm yr^{-1}. This rate is derived from the average of precipitation records for the period 1981 – 2000. In both HYDRUS-1D and PEARL daily precipitation rates based on the average of yearly record are used. The groundwater level in the standard scenario is 1 meter below the soil surface.

1.4 Time-scale and endpoints

Reactive transport of contaminants is a spatiotemporal process that leads to different concentrations of a contaminant in the soil profile at different times. To this end, the choice of spatial and temporal endpoints is important to consider. In the standard scenario, the relevant endpoint to be fulfilled occurs at or within a 100 years of the application of the building material. For the unsaturated zone of the soil profile, the chosen endpoint is the average concentration of the contaminant within the soil profile, 100 years post application. This means that although the peak concentration of a contaminant in soil may be higher than the MPA, if the average concentration is below the MPA at 100 years post application, the application is permitted.

For groundwater, the chosen endpoint is that the peak of the averaged concentrations of a contaminant within the top meter of groundwater may not exceed the MPA for groundwater within the first 100 years of application.

2. Model input and design

2.1 Time

The model simulations are run for a period of 100 years. As explained above, adherence to the endpoints is tested within the 100 years or at the end of the simulation (t=100). HYDRUS-1D allows the user to define an initial, minimum and maximum time step. The initial time step used is 86 s. The is a time step recommended by HYDRUS-1D based on the boundary conditions and works adequately based on comparison with smaller initial time steps. The minimum time step is set at 0.86 s and is automatically invoked by HYDRUS-1D when a smaller time step is needed for calculations. The maximum time step is 5 days and is relatively unimportant as the model chooses the optimal time step for calculations (Rassam et al., 2018; Śimûnek et al., 2008).

2.2 Waterflow boundary conditions

For the comparison between PEARL and HYDRUS-1D simulations an atmospheric upper boundary condition is used with regards to waterflow. Daily precipitation and evapotranspiration (Makkink method) records were obtained from the KNMI. The daily precipitation for a 30-year period (from 1980 onward) was compiled and averaged to produce a record equivalent to an average year of precipitation. This record is used repeatedly as the yearly atmospheric input for the 100-year period investigated.

The lower boundary condition used with respects to waterflow are a constant pressure head (h = 200 cm; ie. groundwater table at 1 m). A constant pressure head is used in HYDRUS-1D because not enough is known about the hydrological situation to for example consider regional groundwater recharge.

2.3 Soil profile

The parameters pertaining to the soil profile were largely acquired from PEARL. PEARL contains standard soil profiles, including soil hydraulic and chemical parameters, deemed representative for different European countries. The standard soils types are however relatively susceptible to leaching, as the model was developed to assess the risks associated with the leaching of pesticides. The standard soil type for the Netherlands is a sandy soil, with decreasing organic matter and clay content with depth. The modelled soil profile has a depth of 3 m and does not display heterogeneity below 1 m (Table 11).

Table 41 Soil fractions, organic matter percentages and bulk density for soil used in the standard scenario.

Soil layer (cm)	Soil fractions			Organic matter (%)	Bulk density (kg m^{-3})
	Sand	Silt	Clay		
0 – 30	0.92	0.05	0.03	4.7	1310
30 – 50	0.96	0.02	0.02	0.8	1540
50 – 70	0.95	0.03	0.02	0.19	1640
70 – 100	0.94	0.04	0.02	0.14	1650
100 – 300	0.93	0.05	0.02	0	1650

2.4 Soil profile geometry

The soil profile described in the model contains 5 layers, each having different physical, hydraulic and/ or chemical properties. In PEARL the cell sizes are 2.5 cm up to a depth of 50 cm below the soil surface. Between 50 cm and 100 cm the cell size used is 5 cm and for the remainder of the profile the cell size is 10 cm. In HYDRUS-1D, the cell sizes are scaled to be fine (~0.25 cm) at the surface, with coarseness increasing with depth. This is done to minimalize mass-balance errors and optimize runtime.

2.5 Soil hydraulic parameters

The soil hydraulic parameters used were taken from the standard Dutch soil profile described in PEARL. This study uses a single porosity Van Genuchten-Mualem model (Van Genuchten, 1980). The Van-Genuchten parameters for the different soil layers are shown in Table 12. For all soil layers a dispersion length of 5 cm is used.

Table 52 The soil hydraulic parameters of the standard soil used in model simulations.

Soil layer (cm)	Soil hydraulic parameters					
	Qr (-)	Qs (-)	Alpha (cm^{-1})	n (-)	Ks (cm yr^{-1})	I (-)
0-30	0.01	0.43	0.0249	1.507	6372	-0.14
30-50	0.01	0.43	0.0249	1.507	6372	-0.14
50-70	0.01	0.36	0.0224	2.167	4821	0
70-100	0.01	0.36	0.0224	2.167	4821	0
100-300	0.01	0.36	0.0448	2.167	4821	0

2.6 Adsorption coefficients

In the models an equilibrium sorption model and a linear sorption isotherm are used to describe sorption. In the models the temperature dependence of sorption and diffusion are not considered.

The soil chemical parameters were obtained from Verschoor et al. (2007). Verschoor et al. (2007) obtained K_d values from reviewing literature. The K_d values assigned to a soil layer decrease with depth due to changes in organic matter content (Table 13). A diffusion coefficient of $4.3 \cdot 10^{-5}$ (m^2 day^{-1}) is used for all metals. Two sets of K_d values (low and high) are used to evaluate matrix concentrations.

Table 63 The Kd values for different soil layers used during the simulations. The low Kd values were used for determining groundwater critical emission values and the high Kd for determining the soil critical emission values. For an overview of the literature used to determine Kd values see Verschoor et al. (2007).

Metal	**Kd: Low (l kg^{-1})**			**Kd: High (l kg^{-1})**		
	0 – 50 cm	**50 – 70 cm**	**70 – 300 cm**	**0 – 50 cm**	**50 – 70 cm**	**70 – 300 cm**
Antimony	10	3.3	1	550	181.5	55
Arsenic	2200	726	220	17000	5610	1700
Barium	530	175	53	1400	462	140
Cadmium	15	4.95	1.5	1700	561	170
Chromium	1200	396	120	50000	16500	5000
Cobalt	30	9.9	3	1100	363	110
Copper	30	9.9	3	830	273.9	83
Mercury	350	115.5	35	1100	363	110
Lead	400	132	40	47000	15510	4700
Molybdenum	140	46.2	14	1400	462	140
Nickel	46	15.2	4.6	1500	495	150
Selenium	200	66	20	2000	660	200
Tin	130	42.9	13	10000	3300	1000
Vanadium	70	23.1	7	2200	726	220
Zink	11	3.63	1.1	6300	2079	630

2.7 Source term building material parameters

The source term determines the absolute amount and rate at which a contaminant leaches from the building material and enters the soil system. In this study a standard emission of 100 g m^{-2} is used in the standard scenario. Based on the results of the standard emission the emission limit values are calculated.

Due to the difficulty associated with implementing a non-constant concentration boundary condition that simulates the leaching of a contaminant from a building material an alternative method is used to introduce the contaminant into the system. In this study the contaminant is introduced into the soils system using the models' capabilities to consider 1st-order decay, as was done by Verschoor et al. (2007). Since the leaching of compounds from building materials can also be described by a first-order decay function, this is an adequate approximation.

In the models, decay takes place from a "parent compound" (ie. compound present in the building material) to a "daughter compound" (ie. leached compound) at a rate equal to the leaching rate of a compound from a building material. The parent compound is added to the soil surface in PEARL and to the top cell in HYDRUS-1D. The parent compound is given as $K_d > 10^6$ l kg^{-1} so that it is not transported through the soil profile. The leaching rate, expressed as the degradation rate of the parent compound. The calculated leaching rates (K) are given in the Table 14.

Table 74 Kappa (De Wilde, 1998) and corresponding leaching rate, which has been calculated using equation 2.

Metal	**Kappa**	**Leaching rate (mm m^2 yr^{-1} kg^{-1})**
Antimony	0.11	0.041
Arsenic	0.03	0.011
Barium	0.15	0.056
Cadmium	0.32	0.119
Chromium	0.25	0.074
Cobalt	0.18	0.067
Copper	0.28	0.104
Mercury	0.05	0.019
Lead	0.27	0.100
Molybdenum	0.35	0.130
Nickel	0.29	0.108
Selenium	0.38	0.141
Tin	0.19	0.071
Vanadium	0.05	0.019
Zink	0.28	0.104

3. Translating media concentrations to emission limit values

The output concentrations in HYDRUS-1D are solute concentrations in porewater. These can be used to derive emission limit values for groundwater without alteration. Derivation of critical emission limit values for soil however requires a conversion, as environmental criteria are based on concentrations in bulk soil (Eq 5.).

$$C_{bulk} = C_{pw} \cdot \theta + C_s \cdot \rho \qquad \text{Eq. 5}$$

Where:

C_{bulk} :concentration of a contaminant in bulk soil (mass·$volume_{soil}^{-1}$);
C_{pw} :contaminant concentration in porewater (mass·$volume_{water}^{-1}$);
θ :soil moisture content ($volume_{water}$·$volume_{soil}^{-1}$);
C_s :sorbed contaminant concentration in soil (mass·$mass_{soil}^{-1}$) ;
ρ :bulk density ($mass_{soil}$·$volume_{soil}^{-1}$).

As described in Verschoor et al. (2007) the critical soil input value is calculated using a direct variation relationship (equation 6).

$$I_{crit} = EQS \cdot \frac{E_{std}}{C_{std}} \qquad \text{Eq. 6}$$

Where:

I_{crit}:critical soil input value (mass·$area^{-1}$), which is the cumulative emission from a building material application (construction) which lead to concentrations equal the environmental quality standard ;
EQS :environmental quality standard (concentration) of the relevant compartment (mass·$volume^{-1}$ or mass·$mass^{-1}$);
E_{std} :standard emission (100 mg m^{-2});

C_{std} :concentration in soil or groundwater resulting from the standard emission simulated by modelling (mass·volume^{-1} or mass·mass^{-1}).

When the emission corresponding to the EQS are calculated, these can be used to calculate the critical emission value for a product tested via a column test in a laboratory setting using equation 7 defined in the Building Materials Decree (1995).

$$E_{crit} = \frac{I_{crit} \cdot (1 - e^{-\kappa \cdot 10})}{\rho \cdot h} \qquad \text{Eq. 7}$$

Where:
E_{crit} :critical emission value expressed as the cumulative emission of a contaminant from a building material in a column experiment (mass·mass^{-1} after LS10);
I_{crit} :critical soil input value from a building material application corresponding to the environmental criteria (mass·area^{-1});
ρ :density (mass·volume^{-1}) of the building material;
h :thickness (height^{-1}) of the building application.

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