EVALUATION OF ENVIRONMENTAL ASPECTS OF ALTERNATIVE MATERIALS USING AN INTEGRATED APPROACH ASSISTED BY A DATABASE/EXPERT SYSTEM

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ABSTRACT. A database/expert system has been developed for (contaminated) soil, sediment, sludge, waste and construction material characterisation. The database contains results of laboratory leaching tests, various lysimeter test results and many field data. The results of leaching tests are interpreted in an expert system to make a prediction of the long-term behaviour, as test results cannot be used directly to derive this behaviour. This makes the database/expert system a unique tool to study the release behaviour of different recycled and traditional materials in different applications. Based on an understanding of release mechanisms in terms of chemical, physical and hydrological aspects in combination with insights in chemical controls, leads to a time-variable source term for different applications of reused and recycled materials, monofills and contaminated sites to be used as input to soil and groundwater impact studies. Assessing the potential environmental effects of such applications in the long-term and in different life cycles of the material is crucial for an environmentally sound use of alternative materials in construction.

Keywords: Environmental aspects, Alternative materials, Construction materials, Soil, Slag, Database, Expert system, Leaching, Long term behaviour, Modelling.

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INTRODUCTION

In recent years the pressure on primary materials for construction has increased. As a consequence, more and more alternative materials are used in Europe in different construction applications. Although alternative materials may technically prove suitable, the long-term environmental implications of several alternative materials are still uncertain. Alternative materials may perform well in the primary application, however, uncertainty exists for subsequent cycles of use (recycling, reuse in other applications and “end-of-life”). This has been partly caused by the lack of proper assessment tools. Two simple methods have been applied to address the complex issue of leaching. There are currently several tools available [1, 2, 3, 4] and have proven their potential suitability to assess different stages of the materials life cycle. Separate studies on different methods reported have known to hinder the development of a generic approach to assess environmental impact from different materials and different applications. Recent work, in which such widely different fields have been brought together by applying the same testing approach, points at many similarities in mechanisms, controlling factors for release and common aspects in scenarios. A key towards the development of a unified environmental approach in assessing impact is to bring the relevant information together in a database /expert system. This paper addresses advanced activities in that area.

RATIONAL

Leaching is the process by which constituents in a solid material, which can be soil, contaminated soil, sludge, sediment, compost, waste or a construction material, are released into the environment through contact with water. Understanding the rate and extent to which constituents of interest may be released is central to defining (i) potential environmental impacts through water-borne mechanisms including soil, groundwater and surface water contamination, (ii) human health and ecological risks from beneficial use and disposal of commercial materials and wastes, (iii) effectiveness of certain treatment processes for materials, (iv) designs and acceptance criteria for waste management facilities, and (v) degradation of structural performance of certain materials in the environment. The specific rates and extents of constituent release are a function of (i) the chemical and physical properties of the material under consideration, (ii) the chemistry of the constituent(s) of interest, (iii) characteristics of the local environment in which the material is placed, including chemical properties (e.g., pH, oxidation-reduction potential, presence of reacting constituents such as carbon dioxide) and the nature of water interaction (e.g., frequency, amount, interfacial contact area).

Fundamental understanding of leaching processes is achieved through study and research on material testing, geochemistry, constituent mass transfer, and development and verification of mathematical models to estimate long-term behaviour and characterise risks under varied environmental conditions. Extensive research and evolution in understanding fundamental aspects of leaching processes and impact evaluation has been carried out over the past two decades. This research, which has been carried out using the same consistent fundamental leaching test methods provides a sound foundation for evaluating different scenarios and associated impact assessment. Recognising the risks and environmental damage caused by uncontrolled materials use, soil contamination and waste disposal, national and regional regulatory organisations have developed widely variable, and often disparate, test methods and regulatory control frameworks to characterise leaching and make decisions about
acceptable and unacceptable use of materials, waste management practices, and contaminated site restoration needs. These regulations, which began evolving in the early 1980’s, were based on the best understanding at the time, but are largely inadequate in the context of current understanding and needs. Many circumstances that have resulted in misapplication of procedures, erroneous decisions based on inadequate science, and resulting misuse of economic resources, damage to the environment or human health impacts have been documented based on these shortcomings.

Efforts have been undertaken in the European Union and the United States to develop a more robust and scientifically sound, while practical, framework for characterisation of soils, sludges, wastes and constructions materials subject to environmental leaching and decision-making based on assessment of potential impacts. Consensus is evolving on an overarching framework and methodological details for implementation [5, 4, 6, 7]. The framework is a tiered approach, allowing the user to select the level of testing and evaluation required based on the degree of conservatism required, prior information available, and balancing costs of testing against benefits from more detailed information (e.g., reduced management costs or alternative management options). Use of this approach is beginning to emerge in both the European Union and the United States. Demand for such a system is also great in other countries (i.e., Japan). A central challenge is converting the depth and breadth of knowledge currently available to decisions on selection of characterisation methods, assessment models and decisions on acceptability, and implementation of these choices based on specific needs of a diverse set of users. A database of characterisation leaching data is a means to facilitate cross-field comparison of data. A further key aspect in such an approach is to identify the aspects besides leaching that need to be covered to be able to make a full evaluation of material behaviour in a given scenario. This is best done in an expert system, that allows tying the relevant aspects together to come to a decision on a time dependent source term description for the material in its application.

DATABASE/EXPERT SYSTEM

A database/expert system has been developed for environmental risk assessment in (contaminated) soil, sediment, sludge, waste and construction material. The first step in setting up the database has been to identify the type of questions to be answered and to ensure that data are implemented in a manner that allow the desired cross comparisons between fields, the mutual comparison between test methods and establishing relationships between lab and field. The database contains results of laboratory experiments (pH-static experiments, column leaching tests, CEN tests, availability tests and diffusion tests) on more than 600 soil, sludge, waste and construction material samples. It also contains data on lysimeter studies and relevant field data that are linked with laboratory work. This makes the database/expert system a unique tool to study the behaviour of different recycled materials, the comparison of different test on wastes and on construction materials, the comparison of data from laboratory leaching, lysimeter scale studies and field measurements. Furthermore, the system can serve as basis for modelling the chemical behaviour and release of substances in different scenarios.

In Figure 1 an outline of the expert system is given comprising software components that provide the following aspects:
1. Guidance on problem definition, selection of characterisation needs and methods, detailed methodologies (including quality control guidance, video clips and example results); existing information on characteristics and behaviour of similar materials; citations.

2. Guidance on laboratory, lysimeter and field data collection including experimental design and quality control considerations; existing information from similar pilot and field evaluations; citations.

3. Standardized data management, formatting and graphical presentation, including consistency and quality control checking.

4. Direct data evaluation, parameter derivation and comparative data sets for:
   a. pH and redox dependence of aqueous concentrations (cations, anions, DOC, ionic strength), geochemical speciation, acid/base neutralisation capacity, leaching potential (availability) from batch testing.
   b. Release as a function of time for granular materials and monolithic materials from sequential data sets (liquid-solid ratio or time from monolithic or compacted granular tank leaching, column testing, lysimeter testing), including geochemical speciation and mass transfer parameter estimation.

5. Development of a source term description that would estimate constituent release as a function of time for default or user defined use or management scenarios. This would include selection of appropriate source term models, evaluation of the effects of potential external stresses (e.g., waste mixtures, carbonation, oxidation, reduction, acidification) and uncertainty analysis.

6. Evaluation of potential impacts to soils or groundwater and risk characterisation.

7. Algorithms for comparing evaluation results and decision-making based on regulatory criteria from different jurisdictions; recommendations on reduced-testing quality control programs; recommendations on approaches to reduce constituent release.

**Scenarios**

The number of scenarios that need to be covered can be quite extended. There are, however, a limited number of typical scenarios of exposure relevant for many different materials. These can be seen as base cases. Examples of scenarios are listed in Table 1.

**Data Requirement**

The type of data that are relevant for a database/expert system on leaching cover all kinds of materials, laboratory test methods applied in various jurisdictions, pilot scale test data, field leachate data, technical properties (density, permeability, ...), hydrological information, etc. The substances for which data can be implemented range from all inorganic constituents, organic contaminants to radionuclides. There are certain minimum requirements the information to be inserted should fulfil to be meaningful. This with respect to data presentation and interpretation (e.g., using geochemical models). For this purpose data should contain pH and liquid/solid ratio or exposure-time information.
Figure 1   Outline of the database/expert system for environmental impact assessment based on release as derived from leaching tests
Table 1 Utilisation and disposal scenarios, exposure conditions and relevant test methods

<table>
<thead>
<tr>
<th>SCENARIO</th>
<th>MATERIAL(S)</th>
<th>EXPOSURE CONDITIONS</th>
<th>RELEVANT TEST(S)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Material in direct contact with drinking water (concrete pipes and basins)</td>
<td>Concrete, Copper, Plastics</td>
<td>Permanent water contact, initial high pH, carbonation</td>
<td>Tank leaching test, pH dependence test</td>
</tr>
<tr>
<td>Monolithic materials in structures exposed to fresh surface water and seawater (e.g. pillars for bridges, quays, breakwaters, locks)</td>
<td>Concrete, bricks, preserved wood</td>
<td>Permanent water contact for under water part, intermittent wetting for section above water level, carbonation</td>
<td>Tank leaching test, pH dependence test</td>
</tr>
<tr>
<td>Materials in structures exposed to fresh surface water and seawater (e.g. breakwaters)</td>
<td>Industrial slag, basalt, ...</td>
<td>Permanent water contact for under water part, intermittent wetting for section above water level, carbonation</td>
<td>Compacted granular leach test, pH dependence leach test</td>
</tr>
<tr>
<td>Materials exposed to fresh surface water (e.g. sediments)</td>
<td>Sediments, granular fill materials (MSWI bottom ash,...)</td>
<td>Permanent water contact, neutral pH</td>
<td>Compacted granular leach test</td>
</tr>
<tr>
<td>Material in contact with ground water (pilings, shafts, etc)</td>
<td>Concrete, bricks, preserved wood</td>
<td>Permanent water contact</td>
<td>Tank leaching test, pH dependence test</td>
</tr>
<tr>
<td>Monolithic material in surface structures (all forms of building on land)</td>
<td>Concrete, preserved wood, Pb sheet, Zn gutters</td>
<td>Intermittent wetting, carbonation</td>
<td>Tank leaching test, pH dependence test</td>
</tr>
<tr>
<td>Recycling in concrete as aggregate</td>
<td>Sorted construction debris, slag,</td>
<td>See above conditions for concrete applications</td>
<td>See above conditions for concrete applications</td>
</tr>
<tr>
<td>Recycling and use as unbound aggregate</td>
<td>Sorted construction debris, industrial by-products</td>
<td>Wet/dry cycles</td>
<td>Percolation test, pH dependence leaching test</td>
</tr>
<tr>
<td>Landfilling of waste and construction debris.</td>
<td>All granular and monolithic materials</td>
<td>Waste - waste interactions, buffering</td>
<td>Percolation test, pH dependence leaching test on waste mix</td>
</tr>
</tbody>
</table>

EXAMPLE CASE TO ILLUSTRATE STEPS IN THE EVALUATION

To illustrate the use of the present aspects incorporated in the database/expert system, it is best to use a realistic example. The example selected is the utilisation of MSWI bottom ash in an embankment.
Scenario Description

To evaluate the utilisation of MSWI bottom ash a number of scenario conditions need to be quantified. These include properties, such as the dimensions of the embankment (150 x 50 m; height 5 m), the infiltration rate (varies depending on the performance of the isolation system), the depth of the unsaturated zone (1m), the dispersion (longitudinal as well as in the direction of flow), material density (1600 kg/m³), the groundwater flow rate (20 m/yr) and the porosity in the subsoil (0.3). In addition, a point of compliance needs to be defined. Here we have taken a point of compliance close to the boundary of the application (20 m). For several parameters, it is possible to select default values as determined from earlier case studies [8,9]. For the infiltration, it is assumed that in the first year that the application is fully exposed to net infiltration (300 mm/yr), after that the isolation measures are assumed to work optimal for 10 years leading to a net infiltration of 50 mm/yr on average, then the deterioration sets in and for the next 20 years the average infiltration is assumed to increase to 70 mm/yr and to further increase over the following years to a long term average of 90 mm/yr. The information needed to actually assess an impact, is material leaching behaviour under a range of conditions (pH, L/S) relevant for the field scenario.

Suitable Leaching Test Methods

Worldwide many leaching tests are used [10]. Many of those largely address the same aspects of leaching under slightly different conditions. Others are very different in the concept behind the method, such as the sequential chemical extraction procedure [11]. In recent years, attempts have been made to harmonise leaching tests [1, 12, 13].

pH dependence leaching test - Based on a comparison of methods and test data the pH dependence test [2,14] has been identified before as a method that allows mutual comparison of several different test methods [1,7]. Here the properties of the method to quantify the acid neutralisation capacity and to use the data for geochemical speciation modelling are most relevant. Fresh MSWI bottom ash is known to exhibit changing chemical properties over time, of which the most important is pH, due to the uptake of CO₂ from the atmosphere. In turn, pH strongly affects leaching properties [15,16]. The element specific leaching curve (metals, oxyanions, major and minor elements and DOC) obtained with the pH dependence test can be seen as a material characteristic, a “geochemical fingerprint” of the material under study. This aspect is illustrated in Figures 2 and 3 for MSWI bottom ash by Zn, Cu, Mo, and Cl. From these few elements it is already clear that the leaching process as reflected by leaching as a function of pH is rather systematic, even for bottom ashes from widely different origin and different production dates, and is controlled by similar release mechanisms.

Significant differences in leaching behaviour are observed, when materials are treated differently, as in case of the unquenched, quenched and oxidised bottom ash [17]. The differences are not very significant for Zn, whereas substantial differences are noted for Cu. In case of unquenched ash the ultimate burn out is greater than when the ash is quenched. For Cu the association with DOC (dissolved organic carbon) is already well established as a key controlling factor [18,19] and sub-fractions of DOC have been established as relevant for Cu leaching behaviour. When these sub-fractions are selectively removed, the Cu leaching will be affected. Burnout experiments have revealed that not all carbon needs to be burnt out to significantly reduce Cu leaching. This can be explained by the fact that carbon black or elemental carbon does not affect Cu leaching [20]. The Cl leaching is obviously independent
of pH and Cl leaches completely within L/S=1. The interrelationships between pH dependence test and percolation test are very useful for the judgement of the leaching behaviour under a wide range of exposure conditions, as all relevant pH conditions (for bottom ash pH 12 – 7.8) and all relevant L/S conditions are covered (low for an embankment to moderately high L/S for a road base application).

**Percolation test** - For the percolation behaviour of (granular) materials the presentation of release and concentration as a function of the liquid to solid (L/S) ratio is the most suitable form of data presentation [3], as it allows comparison with data from larger scale experiments (e.g. lysimeter) and field data [21]. The latter does require an estimate on the amount of liquid that has passed through the material. The release behaviour as obtained in a percolation type test can be used to derive parameters for long-term prediction. A relatively simple approach for granular materials is the CSTR (Continuously Stirred Tank Reactor, a first order decay function) model, which provides a first crude estimate of release:

$$C_{L/S} = C_0 \times e^{-\kappa \frac{L}{S}}$$

In the above CSTR equation, $C_0$ is the initial concentration (as obtained in the lowest L/S fraction) and $\kappa$ is a first-order release factor. Obviously, more mechanistic models provide more accurate predictions [22,23]. This can be seen as a hierarchy in the use of models: sophisticated when needed and simple when sufficient discrimination can be obtained. In Figures 2 and 3 the percolation behaviour of Zn, Cu, Mo and Cl from MSWI bottom ash is given for material from different sources.

It illustrates the systematic behaviour in leaching from a material that is so heterogeneous in its appearance and its composition. In a validation study of EN 12457 [24], the leaching has been shown to be much more consistent for judging the material than an evaluation based on total composition [24, 25]. In Figure 4 the CSTR fits are given for Cl, Sb, Mo, S, Zn and Cu release from MSWI bottom ash. In Table 2 the parameters are given.

<table>
<thead>
<tr>
<th>PARAMETER</th>
<th>Cl</th>
<th>Sb</th>
<th>Mo</th>
<th>Cu*</th>
<th>Zn</th>
<th>SO4 as S*</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_0$</td>
<td>550</td>
<td>0.023</td>
<td>0.5</td>
<td>5</td>
<td>0.052</td>
<td>110</td>
</tr>
<tr>
<td>$\kappa$</td>
<td>0.9</td>
<td>0.1</td>
<td>1.08</td>
<td>1.75</td>
<td>0.3</td>
<td>0.01</td>
</tr>
</tbody>
</table>

This illustrates the suitability of this simple model for some, however, not for all elements of interest. The ‘kappa’ value (first order decay constant) is a release parameter from the source material. A value around 1 points at complete dissolution in the pore water, while a value approaching 0 indicates full solubility control. The Cl, Cu and Mo behaviour illustrate washout of a soluble species, whereas Sb, S and Zn indicate solubility control. In the latter case, this observation provides the option to determine through geochemical speciation modelling which phase(s) may be relevant.
Figure 2  Characterisation of the leaching behaviour of Zn and Cu from MSWI bottom ash as a function of pH and as a function of L/S.
Figure 3  Characterisation of the leaching behaviour of Mo and Cl from MSWI bottom ash as a function of pH and as a function of L/S.
Figure 4  Release modeling for Cl, Sb, Mo and Cu from MSWI bottom ash using the CSTR model. *Broken lines: CSTR model fit; C_{LS} = C_0 * e^{-k*L/S}*

In case of Cu and sulphate, the single parameter fit is not sufficient as there is apparently more than one chemical phase dictating release. This can be described by combining two independent pools of the element with separate release parameters. This aspect is addressed again in connection with the geochemical speciation modelling. From judging release behaviour of different materials, it appears that the role of key controlling factors is similar across different fields and much more information can be exchanged between fields than currently practised.

**Dynamic Monolith Leach Test and Compacted Granular Leach Test**

For the release from monolithic materials or granular materials behaving as monolithic materials in the scenario considered, the presentation of release expressed in mg/m² as a function of time is the most suitable form of data presentation. It is applicable to a wide range of materials such as bricks, stabilized waste, concrete, asphalt, tiles, metal sheeting and preserved wood. Release parameters can be derived to predict long-term behaviour [7, 13]. In the current scenario, leaching from a monolithic material is not further considered.

**L/S - Time Relationship**

The liquid solid ratio of the percolation test can be translated in a time-scale, when the variation in infiltration with time is known or estimated. For the infiltration variation as indicated in the boundary conditions for the scenario, the L/S - time relationship is given in Figure 5 for a fixed infiltration of 150 mm/yr and a variable infiltration due to isolation measures. For high applications (> 5 m), the L/S reached in 100 years is less than 1. If based on modelling of laboratory test data, solubility controlling phases can be identified, this relationship allows to relate release with time.
Figure 5  Relationship between time and L/S for specified infiltration in a given scenario.

External Influences (ANC)

In the case of MSWI bottom ash, one of the key controlling factors of release with time is the change in pH due to carbonation by CO₂ from the atmosphere and from biological degradation (organic residues in bottom ash and soil air) and self-neutralisation of bottom ash by re-mineralisation [26]. The external influences on the materials pH can be quantified through the acid neutralisation capacity data obtained in the pH dependence test parallel to the measurement of element release as a function of pH.

Using the ANC curve, the acidity (expressed in mol/kg) needed to reach any specified pH within the pH range covered by the pH dependence leaching test can be quantified. Also the pH resulting from application or exposure to a given acidity or alkalinity can be obtained. In Figure 6 this is illustrated for freshly sampled bottom ash and aged, carbonated bottom ash. In general, the buffer capacity of bottom ash is relatively not very high.

This implies that for applications of up to a meter as in road base applications, neutralisation to a final pH around 8 can be expected within 10 years. In case of an embankment as considered here, the pH will first drop to a buffered pH around pH 10.5 [17] and then in a second much longer time step decrease to around 8. For release estimates, the neutralisation of the full layer may not be the most important, as neutralisation takes place from the outside inward.

This implies that a controlling neutral pH may be reached in the base of the embankment before the full application is neutralised. This aspect needs further consideration in future field studies.
Geochemical Modelling

Understanding the controlling factors for release is crucial for long-term prediction of release. Chemical speciation modelling is a key element in obtaining such understanding. Saturation indices of potentially solubility controlling minerals in soil, sediments, wastes and construction materials are very useful in long term prediction. These saturation indices, can be calculated with geochemical models such as PHREEQC [27], ECOSAT [28] or the modelling environment ORCHESTRA [29]. The recent recognition of the concentration enhancing effect of DOC with respect to heavy metals and organic micro-pollutants, makes it desirable that these calculations include adsorption of metals by DOC, for example by using the NICA-Donnan model approach [30]. However, this type of geochemical modelling, especially when applied to many different leachates/materials with different properties, is time-consuming and requires specialist’s skills. The development of a database/expert system, in which material data are grouped in a systematic way, opens the possibility of an instantaneously coupled geochemical model, saving substantial time and effort. Modelling the chemical speciation under realistic exposure conditions will provide information on which judgements can be made on the direction and magnitude of changes in release due to external factors. Such factors can be pH change due to carbonation, redox change due to oxidation or mobilisation due to interaction with external DOC sources. Primarily, the factors relating to the own material properties will be relevant.

Modelling of chemical speciation in eluates and leachates will provide insight in the degree to which solubility is controlled by specific minerals, sorption or binding to organic matter and DOC. The capability of calculating the chemical speciation of eluate data generated by the pH dependence test (pH variation) and a percolation test (L/S variation) simultaneously offers the possibility to draw conclusions on a very large number of practical situations. In the current database version, saturation indices of over 450 possibly solubility controlling minerals are calculated using the MINTEQA2 3.11 database [31], for which a database-coupled version of the modelling environment ORCHESTRA [29] is used. The calculated
solubility indices allow for an –indicative- graphical representation, as is shown in Figure 7. In Figure 7 an example of the chemical speciation thus obtained is given for Zn, Mo and Al. Modelling pH dependence test results provides solubility control data for the relatively high L/S=10, whereas the percolation test covers the full L/S range from low L/S to L/S=10. If the same mineral phase controls solubility at different L/S and pH values, its relevance is highly probable. In case of Zn, this is apparently the case for Zinc oxide (ZnO) and Willemite (Zn$_2$SiO$_4$). Its possible relevance is further substantiated by the apparent Willemite solubility control in percolation test data for sample MBA-A (bottom ash with a very high initial pH) and the MBA1 sample series.

The latter have a much more moderate initial pH. It must be stressed that also geochemical knowledge is needed to draw conclusions on possible solubility controlling phases or processes, e.g. because formation of some minerals from the MINTEQA2 database may be kinetically hindered under field conditions. For example, Zn solubility in MSWI bottom ash may be described equally well by Zn adsorption and surface precipitation onto Fe/Al-(hydr)oxide surfaces [16,22]. In case of Mo, CaMoO$_4$, Fe$_2$(MoO$_4$)$_3$ and PbMoO$_4$ are identified as relevant controlling phases in the pH dependence test. At very low L/S in the percolation test CaMoO$_4$ is the most likely controlling phase. This phase apparently is readily depleted, which explains why Mo leaches rather easily. At higher L/S other phases as PbMoO$_4$ may become solubility limiting. In case of Al, boehmite and gibbsite are relevant phases in the pH domain ranging from pH 7 to 12. For unquenched bottom ash, Al solubility appears to be controlled by diaspore. In the percolation test, a constant concentration is measured at all L/S levels. This is a first indicator for solubility control. The geochemical modelling points at boehmite, gibbsite, amorphous Al(OH)$_3$ and diaspore as controlling phases. These minerals are all rather close together in solubility.

As discussed before, the release modelling for sulphate points at two distinct pools of sulphate in bottom ash. The solubility of sulphate as modelled by chemical speciation points at saturation with gypsum at very low L/S (the more soluble phase) and solubility control by ettringite and barite at high L/S. Until L/S=1, the rather soluble sulphate phase is depleted (about 50 mg/kg) and from L/S=1 to 10 the slower release as governed by another mineral phase (ettringite or barite) amounts to a leached amount of about 150 mg/kg. In Figure 8 the CSTR and the geochemical modelling are shown together.

As a preliminary observation, modelling chemical speciation on wide range of materials has shown that for typical elements a limited number of key mineral phases will be most prominent in a wide range of materials. Thus reducing the potential complexity of over 400 mineral phases to a much more manageable number relevant for daily practice.

**External Influencing Factors**

Laboratory testing will usually not provide information that is directly applicable to describe the behaviour of materials under field conditions. Materials may have properties that change with time due to instability of mineral phases, for instance in case of MSWI bottom ash resulting from the thermal process. Such changes need to be quantified by assessing the magnitude of pH change through the measurement of acid or base neutralization capacity, redox changes and interaction with dissolved organic matter in the scenario and the time frame under consideration. Data interpretation will always be needed to provide a prediction of long-term behaviour.
Figure 7  Geochemical modelling of MSWI bottom ashes based on pH dependence test and percolation test data extracted from the database/expert system. The model lines are an indicative graphical representation of calculated solubility indices using a database-coupled version of Orchestra as the modelling environment.
Then the magnitude of material changes with time need to be taken into account. This can be neutralization effects by carbonation resulting from exposure to atmospheric CO₂ or from exposure to the higher CO₂ concentration in soil air due to biological degradation processes. Also changes in redox may be relevant for bottom ash as metallic Al may lead to reducing conditions through H₂ formation at high pH. This may not be very relevant in a road base application with a relatively open structure and a substantial exchange with atmospheric O₂, but it may be much more relevant in an embankment scenario, particularly when the surface is sealed to reduce infiltration. A combination of neutralization and oxidation may occur simultaneously. The kinetics of such changes may not be known for the field scenario under consideration. To be able to provide an answer on possible acceptable on unacceptable release conditions, a good alternative is to test both the starting material and the material brought in its final condition by laboratory enhanced ageing or other means. In Figure 9 the leaching of Pb from MSWI bottom ash in a percolation test is shown at fixed pH values of 11.5 and pH 8. In the field the pH will change with time, which is illustrated by the drawn line (marked: actual behaviour in the field).

Figure 8  CSTR modelling of sulphate release and geochemical speciation modelling of percolation test data.

Figure 9  Evaluation of external influences on release from MSWI bottom ash for Pb.
Source Term Description

Based on an understanding of release mechanisms in terms of chemical, physical and hydrological aspects in combination with the above mentioned insights in chemical controls, leads to prediction capabilities for a variety of scenarios of soil, waste and construction material use, taking external influencing factors with time into account. The description of behaviour for different constituents for the exposure conditions of a given scenario can be integrated to lead to a new release as a function of time. Not all of the application may be exposed to the same level of infiltration. This implies that when pertinent information is available a correction can be made to account for such effects. One way of handling the data is to describe the source term in terms of release constants (CSTR model, see above). These can serve as input to an impact model, as will be outlined below.

Impact Evaluation of a Scenario Using a Variable Source Term

The source term is used as input to a chemical reaction transport model to quantify impact at specified targets. Based on a combination of ECOSAT and MODFLOW modelling, a semi-emperical meta-model was derived covering different influencing factors [9]. Input parameters for this model are CSTR-parameters \( C_0 \) and \( \kappa \) to describe the source-term, and a Kd sorption constant to describe the further transport through the aquifer. When criteria are known at the point of compliance, acceptance criteria can be derived. In this example, EU and WHO drinking water criteria are used in groundwater at 20 m next to the application. The criteria for Cu and Zn have been modified for Cu to 50 \( \mu \)g/l and for Zn to 200 \( \mu \)g/l, as the limits for drinking water are too high for an evaluation of groundwater quality. Default or adjusted Kd values for the interaction of released constituents with subsoil are needed as input values for the model (here relatively conservative estimates have been used). The other input parameters are release parameters (\( \kappa \) values) describing the source term. The acceptance values thus derived in Table 3 are expressed in mg/kg (at L/S=10). These site-specific conditions can be applied in case of specific scenario conditions.

Table 3 Acceptance limits (mg/kg at L/S=10) in an embankment scenario as a function of Drinking Water Quality (DWQ) at nearby target (POC1)

<table>
<thead>
<tr>
<th>GW flow</th>
<th>Unsat. zone</th>
<th>ACCEPTANCE LIMITS, mg/kg</th>
<th>PARAMETERS</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 m/yr</td>
<td>1 m</td>
<td>552</td>
<td>626</td>
</tr>
<tr>
<td>4 m/yr</td>
<td>5 m</td>
<td>0.049</td>
<td>0.052</td>
</tr>
<tr>
<td>20 m/yr</td>
<td>1 m</td>
<td>0.18</td>
<td>0.36</td>
</tr>
<tr>
<td>20 m/yr</td>
<td>5 m</td>
<td>1.2</td>
<td>6.4</td>
</tr>
<tr>
<td>20 m/yr</td>
<td>Kd</td>
<td>4.7</td>
<td>23.5</td>
</tr>
<tr>
<td>Zn</td>
<td>1928</td>
<td>0.27</td>
<td>250000</td>
</tr>
<tr>
<td>SO4</td>
<td>1328</td>
<td>1396</td>
<td>1928</td>
</tr>
</tbody>
</table>

Judgement against Regulatory Criteria

As soon as criteria are known, either from existing regulation or derived from site-specific modelling activities, a comparison can be made between actual test data and the acceptance values for the various regulated substances. This allows determining which substances are
most critical for a given material. Generally, of all regulated substances, a limited number of substances are critical, which provides a means to be more cost effective in quality control by measuring only critical substances in QC testing. Based on the characterisation short compliance tests can be recommended with most discriminating power for QC purposes. In all cases it is recommended to judge QC and compliance test data against characterisation information (i.e. in the same plot). Deviations in behaviour and trends are directly recognised. In Figure 10, this comparison with regulation is illustrated. The following aspects define the boundaries of the judgement box:

- Upper release boundary: regulatory limit or derived acceptance values
- Left and right pH boundary: relevant pH range for the application under consideration
- Lower release boundary: analytical detection limit.

![Graphs showing the comparison of leaching test results of Zn and Cu against regulatory limit values](image)

Figure 10  Comparison of leaching test results of Zn and Cu against regulatory limit values for a given application of MSWI bottom ash.

From this comparison, Zn is apparently not critical from a leaching perspective, whereas several bottom ashes exceed the criteria for Cu. With the site-specific information discussed above similar comparisons between lab data and derived criteria can be made.
DISCUSSION AND CONCLUSIONS

The use of alternative materials in construction can be cost effective and it can provide a competitive element in construction applications. However, the long-term environmental implications of several alternative materials in the different life-cycles of construction material consisting of or containing such alternative materials is not well covered today. As stated in the introduction, this is partly due to the lack of proper assessment tools and partly due to incompatibility of existing tools. The present study indicates that by now the proper assessment tools are in place and methodologies for mutual comparison of existing test data are available. In addition, a methodology to derive acceptance criteria for alternative materials in construction is operational. A good basis of knowledge and characterisation leaching data for a large number of potential alternative materials is available in the form of a database/expert system. The capabilities to compare different test data, to compare results at different scales of testing (lab, lysimeter and field), to couple geochemical modelling and transport modelling to uniform data in the database, to address external influences on release and to link test results to criteria are some of the valuable instruments now available.

Therefore, the database/expert system is expected to be valuable tool for waste and materials management in construction. In the CPD [32](Construction Products Directive) and the Building Materials Decree [33] the recycling, reuse and end-of-life aspect of a construction material use is not covered, which may prove a serious limitation for some materials. When a material leads to unacceptable release in later life cycle stages than those covered by the CPD, a manufacturer may want to reconsider its application from a liability point of view. The present characterisation tools provide the means to safeguard against such long-term surprises, as they can be interpreted to assess such long-term behaviour in other life-cycle stages. In that perspective the characterisation methods described here are very cost effective tools. It is recommended to derive QC testing needs from the characterisation test data in terms of relevant constituents for measurement and simplified test conditions for QC testing. Once a sufficiently established characterisation basis is available for a given material or material group, this can be used by others as reference for compliance, which avoids unnecessary duplication of work. Thus characterisation testing is limited to initial stages of material characterisation, which only needs to be repeated when the process is modified or when significant changes in source materials have occurred.

REFERENCES


Evaluation of Waste Materials  21


