Sustainable Design of novel Materials
Integration of Economic and Environmental Aspects in the Early Stages of Geopolymer Development

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Abstract
Materials, defined as solids with a function, are basic modules for products in our everyday living and work environment. Developing these products means facing a complex qualification profile, which includes, besides others, technical, economic and ecological aspects. The two latter aspects are not sufficiently included in material development, especially from a Life Cycle point of view.

In this project, Life Cycle Thinking is integrated into the development phase of materials right from the beginning, in order to identify the technical, economic, and ecological benefits and drawbacks of developed geopolymers in comparison to traditional materials. In this contribution, the authors focus on the first of three steps, the screening of raw materials for geopolymer manufacturing.

1 Introduction
The design phase of a product has to take into account differing aspects for a successful product implementation. Economic considerations are always important to product development, but also environmental aspects have become an important issue in recent years (Alting & Legarth1995). The environmental aspects will receive even more attention in the future, if an environmental product declaration (EPD) becomes obligatory for building products in the European Union (EU 2004).

In contrast to this, the main focus of many investigations of material development (basic research) is on the technical aspects like mechanical strength. In material development, economic and ecological assessment are carried out after the technical investigations are finished (T_M, Figure 1), if at all. More often, they are postponed to the subsequent phase of product development (T_M-T_P, Figure 1).

Thus, a prospective an efficient development of innovative materials is not possible.

On the example of the development of geopolymers the author presented a new approach, which integrated economic and ecological aspects in the early phases of material development. By the help of Multi Criteria Decision Analysis most promising raw materials for the production of geopolymer are identified.
2 Background Geopolymer

Geopolymers belong to a relatively new binder generation, which forms together with fillers or aggregates rock-like materials. They are formed by mixing of solid silicate-aluminate raw materials (like thermal activated clay, e.g. metakaolin) with alkali or alkali silicate solutions (alkaline activator), see Figure 2. After mixing of both components, dissolution takes place, accompanied and followed by a polycondensation. The formed polymeric network of aluminosilicates (geopolymer binder) hardens in an amorphous structure. Depending on the amount of soluble calcium oxide in the raw materials, also mineral phases may occur, similar to the hydration products of portland cement. In this respect, geopolymers represent a link between ordinary Portland Cement (OPC) and sodium silicate binders. Beside primary raw materials, like metakaolin also a broad variety of secondary raw materials can be used as solid component for the manufacturing of geopolymers. Some of the useable secondary raw materials are fly ash, slag (from different combustion processes), ceramic waste or brick scrap.
Geopolymers have been investigated for more than 25 years. Despite these long-lasting and continuous investigations, geopolymers have not yet reached a point where there is wide application. In fact, a wide range of applications is described in literature sources, but only a few niche applications can be found in the market. This is surprising, especially because geopolymers (in comparison to cement-based composite materials or ceramics) are reported to have many advantages:

- Resistance against acids
- Temperature resistance
- High strength
- High durability
- Cold setting
- Quick setting
- Stable bonding of heavy metals and harmful substances
- Simple manufacturing technique

The favorable technical properties are proved by numerous investigations, cf. (Buchwald et al. 2005). But they depend on the curing time and temperature and very strongly on the mixture composition of the chosen solid and liquid components.

Ecological and economic features of geopolymers have hardly been investigated so far. But it can be assumed that they depend very strongly on the mixture composition, too. So far, metakaolin has been applied mainly as a solid component to produce high-performance geopolymers. However, thermally activated kaolin (metakaolin) is a relatively expensive raw material. Consequently, the

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**Figure 2: Production of the geopolymer**
application fields are restricted due to the costs. In addition, due to the high energy demand metakaolin possess a relatively high environmental impact.

In contrast to this, relatively cheap industrial by-products or residues, such as blast furnace slag, fly ashes or sewage sludge ashes, can also be used as environmental advantageous solid components. These kind of solids, however, may be associated with some drawbacks regarding the technical performance, e.g. retarded setting or low mechanical strength.

The awareness of these conflicts of objectives represent a important background for the presented approach.

3 Screening Raw Materials

3.1 Goal of the screening step

The goal of the screening step is the selection of the most promising raw materials for a specific field of application under the consideration of technical, economic and ecological aspects.

3.2 Considered raw materials and samples preparation

More than 58 raw materials has been collected and tested in this 1st step.

The materials can be assigned to the following six groups:

<table>
<thead>
<tr>
<th>Secondary resources</th>
<th>Primary resources</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ceramic waste materials</td>
<td>Clays</td>
</tr>
<tr>
<td>tiles</td>
<td></td>
</tr>
<tr>
<td>sanitary porcelain</td>
<td></td>
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<tr>
<td>kiln lining material</td>
<td></td>
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<tr>
<td>Slags</td>
<td>ilitic clay</td>
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<tr>
<td>blast furnace slag</td>
<td></td>
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<tr>
<td>steel slag</td>
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<td>copper slag</td>
<td></td>
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<tr>
<td>municipal waste slag</td>
<td></td>
</tr>
<tr>
<td>Ashes</td>
<td>dolomitic clay</td>
</tr>
<tr>
<td>hard coal ash</td>
<td></td>
</tr>
<tr>
<td>soft coal ash</td>
<td></td>
</tr>
<tr>
<td>sewage sludge ash</td>
<td></td>
</tr>
<tr>
<td>Others</td>
<td>Volcanic deposits</td>
</tr>
<tr>
<td>broken down masonry</td>
<td></td>
</tr>
<tr>
<td>brick scrap</td>
<td></td>
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<tr>
<td>glass industry waste</td>
<td></td>
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<tr>
<td>Coarse raw materials, like slag, were milled smaller than 125 µm. For the comparability of laboratory results, all raw materials are activated by one standard alkaline activator (with 8 molar NaOH solution). The amount of solution has been levelled on identical paste workability. All samples were cured for one day at 40°C inside the moulds, and afterwards until strength testing without drying, at room temperature about 90% relative humidity (over water in closed boxes). Further Information to the measurement technique of the geopolymer properties are published in (Buchwald et al. 2005).</td>
<td></td>
</tr>
</tbody>
</table>
3.3 Considered indicators

In order to get a meaningful screening the right indicators were chosen for the later evaluation of the materials by intense discussion within the project team. The technical parameters were selected depending on the needs of the application; ecological and economical parameters were selected based on life cycle thinking. The following indicators were chosen for the three objective fields:

Technique
mechanical strength (including reactivity, quantitative)
resistance against acids (qualitative)
temperature resistance (quantitative)
setting time (quantitative)
workability (qualitative)

Economy
raw material costs (quantitative)
costs of the thermal activation of raw materials (qualitative)
costs of grinding raw materials (qualitative)
follow-up costs caused by slow setting (qualitative)
follow-up costs caused by high water sorption (qualitative)

Ecology/Health
availability/consumption of mineral resources (quantitative)
consumption of energy resources (qualitative)
taxic load (qualitative)
health and safety at the workplace (qualitative)

3.4 Selection of raw materials by the help of Multi Criteria Decision Analyses

The evaluation and selection of materials under the consideration of different objectives is difficult. The decision making process for the selection of the best candidates reach high complexity, if the number of alternatives are high and the number of objectives is higher than 1. In the presented geopolymers project both is true. The number of considered raw materials are high (58 different raw materials) and 14 indicators for three different objectives (economic, ecological and technical objectives, c.f. Chapter 3.3) are considered. The methods of Multi Criteria Decision Analyses (MCDA) are potentially helpful to support decision-making in complex decision situations (Zimmermann & Gutsche 1991). Besides compensatory methods (Weil et al. 2006), also a non-
compensatory method called “dominance concept” has been applied to identify the most promising candidates for a specific application fields.

The economic and ecological investigations together with the laboratory results, are stored in a database. The different quantitative and qualitative indicator values are comparable and countable, as they are normalized to values between 0 and 1. Values close to 0 are less favourable, values close to 1 are highly favourable. For each indicator, a proper scale of transformation has to be determined, cf. (Weil et al. 2006).

3.5 Results

![Figure 3: Identification of promising candidates. Crosses refer to pareto optimum, called dominant altenatives, nappe refers to pareto front.](image)

In Figure 3 the results of the non-compensatory method are shown for one selected application field. The alternatives (raw materials) in the diagram, which are far away from the origin, represent better solutions (high values), the alternatives close to the origin are suboptimal. The pareto optimums
(which is not dominate by the other alternatives) are highlighted as crosses (Figure 3). Pareto
optimums are the materials SP3, M4, SM, T2, P1, L1, S2.

In the case of the non-compensatory method the solution space is afflicted with two problems:

1 A pareto optimum does not necessarily represent a promising raw material. For instance, one
alternative from a ecological perspective is the best solution (highest value on the ecology
axis), but from a technical and economic perspective it is quite bad (low values). The
ecological advantages cannot compensate, in this case, for the technical and economic
disadvantages. To overcome this problem in general, each objective minimum requirements
has to be defined to shorten the solution space.

2 Alternatives, which are close to pareto optimum, represent interesting and valuable
candidates. In addition, every indicator value is more or less tainted with uncertainties.
To identify all valuable candidates, also under the consideration of the uncertainties, a 3-D
nappe (“pareto front”) is used to separate the promising from the less promising alternatives.
The materials on or above the nappe represents the valuable alternatives (cf. Figure 3).

After the described procedure the promising candidates can be determined. The result are compared
with the results of the compensatory method (Weil et al. 2006). Hence, after an expert discussion,
the most promising raw material are selected for the design phase of geopolymer mixtures for
specific application fields in the ongoing project.

3 Conclusions
The sustainable development of materials with enhanced properties, but also with economic and
ecologic advantages is one of the challenges of modern materials science. In practice, economic and
ecological aspects are considered rarely, which is probably due to the low level of information
available in the early phase of material development. Based on the example of the development of
g geopolymers, the authors presented a methodological approach to integrate technical, economic, and
ecological aspects in the development phase.

The presented results show that the dominance concept (non compensatory method) is a powerful
tool to separate the promising candidates from the less promising ones. The dominance concept is
especially useful if the number of alternatives and the number of objectives is high. By the
exclusion of the less promising candidates in the further approach, the workload in the laboratory
and the research and development expense can be reduce to a minimum. In addition, the integration
of Life Cycle Thinking right from the beginning allows to develop more sustainable materials for a
successful industrial application.

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4 References


