Feasibility of forecasting ecological performances of products in early development phases

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Abstract. Sustainability, i.e. among other things climate change and resource consumption in the product development phase, have to be increasingly taken into account. The primary energy demand of products and their influence on the greenhouse effect can be scientifically analysed through life cycle assessments. For this purpose, all product, energy and material flows must be recorded in each individual product life phase. If, for some reason, no identifiable data is (yet) available, assumptions must be made whose uncertainties may later lead to deviations in the results, some of which are difficult to assess. This can pose a major problem, as many parameters have not yet been defined or will change in the early development phase such as the production scale. In order to be able to compare the products correctly with already established products, however, the possible changes must also be considered comprehensively. An extension of the established methodology by the concept of interval arithmetic makes it possible to determine the entire spectrum of all environmental impacts potentially occurring through the product, since the existing uncertainties are considered directly in the balancing. This is illustrated by the example of an aerogel-based thermal insulation composite system, the insulating material of which is evaluated.

1. Introduction

The anthropogenic warming of the earth and the scarcity of global resources are central challenges of the current century. For this reason, intensive efforts are being made to counteract these undesirable changes. The main cause of climate change is the greenhouse gas carbon dioxide, which is essentially produced by the combustion of fossil fuels for energy supply and emitted into the atmosphere. Since the construction sector accounts for about 32% of global energy demand and 19% of global greenhouse gas emissions [1], countermeasures in the construction sector play an important role. In order to at least partially achieve the ecologically ambitious goals of reducing global greenhouse gas emissions and resource consumption, the construction industry is increasingly demanding construction products that can be manufactured with the lowest possible emissions and raw materials. One focus of research is sustainable insulation materials for building insulation, which are produced in a resource-saving manner and have particularly high insulating properties due to their particularly low thermal resistance, which can also reduce the heating energy requirement of the building. Products that appear suitable due to their very low thermal conductivity are, for example, aerogel based insulating materials, the optimization of which is currently being intensively researched.

In such a product development process, aspects of ecology as a sub-discipline of sustainability must be taken into account in addition to all technological considerations due to the increasing relevance. Due
to the increasing requirements in the above-mentioned areas, corresponding findings on the decision as to which developments should be continued and which development ideas should be abandoned are increasingly of high or even sole relevance. This increasing practical relevance, however, is associated with great difficulties in terms of the reliability and accuracy of the corresponding results. Life Cycle Assessment (LCA) is an established scientific method for assessing the environmental sustainability of products over their entire life cycle. They can be used to assess the environmental impacts of the current state of product systems and their possible future changes. However, LCA are calculated using individual values, from which the results are also calculated in the form of individual values. For example, changes in the process of the product under consideration can be calculated with the aid of scenario analyses by modelling the possible changes and recalculating these variants and documenting them as alternative results. In the early development phase of products, however, the product system is still subject to so many possible changes that the multitude of possible scenarios is so great that it is difficult to compensate for all possible alternatives. By considering the results of the individual scenarios separately in these cases, there is also the risk that too high expectations are raised in the early phase of product development, which ultimately cannot be fulfilled, and the risk that promising development ideas are abandoned prematurely due to pessimistic forecasts. In the situation described, it is therefore sensible or even necessary to dispense with statements that could lead to possible wrong decisions. However, this must not lead to a situation in which a life cycle assessment is not carried out at all in the early phase of product development. Rather, it seems logical to systematically analyse and document in which area the ecological characteristics will ultimately be located. Interval arithmetic can be used for this procedure, in which all possible and relevant uncertainties in the database are determined with the aid of intervals. Therefore, this article presents the ecological evaluation of products by the example of an aerogel-based insulating material. The procedure used is based on interval arithmetic. The results may lead to the conclusion that the procedure can be suitable to carry out balances of products of the early development phase under consideration of the existing uncertainties practice-oriented.

2. LCA and open decisions of products in early development phases
With the help of the LCA methodology, products can be ecologically assessed over their entire life cycle by modelling the corresponding product system. A product system is a limited technological system represented by unit processes and procedures. According to [2, 3] the unit process is the smallest unit for which input and output flows can be determined. The flows represent product, raw material and energy flows and can either flow within a product system between individual unit processes or between different product systems or interact with the environment across technology boundaries. Therefore, a distinction is made between elementary and product flows. Elementary flows are therefore those flows that are taken from the ecosphere and enter the product system or leave the product system and are released into the environment. These are, for example, waste that is landfilled or emissions that are released into the atmosphere. Product flows, on the other hand, are either referred to as those which originate from another product system and are fed into the product system to be analysed or which are generated as intermediate, final or co-products in the product system under consideration and passed on to other product systems.

The modelling of a product system for a product in the development phase is characterised by the fact that a large number of options are initially available for numerous individual elements whose suitability has not yet been tested in the development process. The totality of all these options, which can also be understood as "not yet conclusively made decisions", leads to a confusing variety of competing systems. So far, such possible scenarios, which can result from different decisions, have been mapped in the form of alternative models and compared separately.

3. Exemplary product system
The example describes an innovative thermal insulation composite system (ETICS), whereby it is assumed that the innovation is essentially the central highly insulating layer of the overall structure of
the ETICS and that this layer consists of two components, namely aerogel embedded in a carrier material. Such products are currently the subject of research because aerogels are known to have extreme thermal insulation properties that are counteracted by very low mechanical strength and have been developed in the EU project HomeSkin [4], for example. The above development intention raises many questions (see figure 1):

- Which carrier material is suitable? Are there alternatives?
- How is the embedding process technically implemented?
- How is the connection with the other layers of the ETICS carried out?
- What are the requirements for the layer structure and how are they fulfilled?
- Which substances / products are produced in addition to the target product and how are they treated / disposed of?

In addition, various numerical values must be specified or at least ranges must be defined in which the corresponding numerical values lie:

- Mass ratio granulate / carrier material
- Composite density
- Thickness of each individual layer of the ETICS
- Quantities of adhesives and other auxiliaries required.

The exemplary product system is limited to the manufacturing process of the innovative aerogel insulation material. The carrier material is a glass fibre mat impregnated with a dispersion. The sol consists of precursors, solvents, water and catalysts. Tetraethyl orthosilicate (TEOS) can be used as a precursor and ethanol as a solvent for the production of silica aerogels [5]. The individual TEOS compounds are linked together by chemical synthesis processes, whereby not only water but also excess ethanol is split off. The gelation gradually produces a three-dimensional, very fragile structure. The gel is first filled with water, which, after complete gelation, is removed by drying and replaced by air. This energy-intensive process is extremely critical because the drying process and the associated capillary forces shrink the carrier structure so that the walls of the gel touch each other [6]. This can lead to an undesirable restructuring of the structure, which can be largely prevented with the help of silylating agents as they can reduce the reactivity of the structure [6]. If it is possible to avoid destroying the supporting structure so that it returns to its original shape after drying, the resulting gel is called aerogel. Based on this manufacturing process, the possible scenarios that may result from this decision are presented using the example of the recycling possibilities of surplus ethanol as one of the many open questions mentioned above.
Figure 1. Open decisions modelling a product system of an innovative thermal insulation system in an early development stage.

At the time of the life cycle assessment it was still be unclear whether and, if so, to what extent ethanol could be reused. There are the following conceivable options (see figure 1):

- Excess ethanol is waste.
- Excess ethanol is reused internally, whereby the use of a primary ethanol can be avoided.
- Excess ethanol is sold.

These three possible scenarios are explained in more detail in the following chapter 3.1. to chapter 3.3.

3.1. Scenario 1: Ethanol is waste
The excess ethanol can no longer be used due to impurities or other circumstances and is not for sale, which is why it is considered as waste and is therefore be thermally recovered. Incineration generates additional emissions that are released into the atmosphere. At the same time, however, the thermal energy generated can be used, which avoids the provision of energy from fossil resources and is therefore be credited to the product system according to the credit method (see figure 2).

Figure 2. Surplus ethanol is waste and incinerated.
3.2. Scenario: Ethanol is reused

The surplus ethanol represents a benefit and can be reused with the help of an additional treatment process if necessary, e.g. in-house directly in the same company as secondary raw material in another product system. The avoided environmental impact of the product system, where the use of excess ethanol as a secondary raw material precludes the use of a primary ethanol, is counted as a negative value in the product system producing the excess ethanol (see figure 3).

![Figure 3. Surplus ethanol can be reused and replaces primary ethanol.](image)

3.3. Scenario: Ethanol is sold

The surplus ethanol cannot be reused in the same company. It is to be sold, but the intended use of the ethanol is not (yet) known. A system extension is therefore not possible and the movements occurring in the product system must be assigned. This means that the elementary flows occurring in the product system, which cannot be unambiguously attributed to either product, are to some extent attributed to the insulating material and to some extent to ethanol (see figure 4). For example, while the carrier material, the glass fibre mat, which is used exclusively for the production of the insulation and does not contribute to the production of ethanol, can be clearly assigned to the insulation, TEOS is involved both in the production of the aerogel framework produced in the insulation and in the production of the excess ethanol and is therefore assigned to both products. Since a significant difference in the operating result is to be expected between the two products, the allocation is based on economic values according to [7]. The expected sales prices must also be assumed. A sales price of € 100 is assumed for 1 m² of insulation material with a thickness of 2 cm. The resulting amount of excess ethanol is about 4 litres. The selling price for ethanol is fixed at 1.30 €/l. Thus 95% of the affected product and elementary flows are allocated to the insulating material and the remaining 5% to ethanol.
Figure 4. Ethanol can be sold. The inputs and outputs involved in the production of both products are allocated on economic rules.

4. LCA results of exemplary product system

The balancing takes into account the life cycle phases of the production phase, which include the extraction of the required raw materials, the manufacture of the required intermediate products, the transport of the insulating material to the production site and the manufacture of the insulating material. The functional unit consists of 1 m² of insulation with a thickness of 2 cm. The results consider the greenhouse potential (GWP) in kg CO₂ eq. as well as the primary energy demand. The generic data sets for the presentation of intermediate products and raw materials are taken from GaBi databases [8]. The energy demand PE in MJ total from fossil raw materials as well as from renewable energy sources (PENRT and PERT) is based on the principles according to [7]. The conventional calculation is explained in chapter 4.1., while in chapter 4.2. an interval arithmetic approach is applied.

4.1. Calculation with conventional method

Figure 5 shows the influence of the flows of the product system on the GWP of scenario 1, figure 6 illustrates the contributions to the total primary energy demand PE of scenario 1. It can be seen that the predecessor with 7.18 kg CO₂ eq. has the highest share of GWP and with 201.34 MJ the second highest contribution to PE. In addition, the energy used for production is significant with 5.47 kg CO₂ eq. or 472.62 MJ for GWP and PE. The energy requirement is based on laboratory standards. It can be assumed that the efficiency of industrial production will fall even further, which would have to be taken into account in further scenarios. The ethanol used as a solvent can be recycled as a closed loop and is therefore zero. This is not ethanol from TEOS that is thermally recycled together with other waste materials, which contributes to the incineration of 1.54 kg CO₂ eq. in the GWP (see figure 5), but for which a credit of 18.31 MJ (see figure 6) can be credited due to energy generation.
The results of the total GWP and the total primary energy demand of all three scenarios are shown in figure 7 and figure 8, the deviations of the second and third scenarios from the first scenarios in figure 9 and figure 10. The greatest environmental impacts are to be expected from the disposal of ethanol. The GWP for this scenario (scenario 1) is 20.69 kg CO₂ eq. and the total energy requirement is 781.85 MJ (cf. figure 7 and figure 8). However, if ethanol is reused internally (scenario 2), the value of the GWP decreases by 38.2 % from 20.69 kg CO₂ eq. to 12.78 kg CO₂ eq, the primary energy demand can be reduced by 21.3 % from 781.85 MJ to 615.08 MJ (see figure 7 to figure 10). However, allocation of
ethanol leads to a 10.1% reduction in GWP from 20.69 kg CO\(_2\) eq. to 18.6 kg CO\(_2\) eq. according to scenario 1, primary energy demand is reduced by 2.1% from 781.85 MJ to 765.34 MJ (see figures 7 to 10). Some of the results of the scenarios differ significantly from each other. If a statement is now made about the ecology of the insulating material and scenario 1 is presented for safety reasons, this can be too pessimistic a forecast. If, on the other hand, the statement is based primarily on scenario 2 with the lowest environmental impact, too high expectations can be placed on the environmental compatibility of the product, which ultimately cannot be fulfilled.

In addition to this open question, which already entails large differences in the results, further points, as shown in chapter 3 and figure 1, are still unclear. The consideration of further scenarios will further increase the deviations of the results and thus further complicate the problem of a reliable statement. The aim should therefore be an approach in which all "open points" are recorded as inaccuracies in the sense of interval widths. The results of the environmental impacts of the innovative insulating material carried out on the basis of the interval calculation are presented in the following.

4.2. LCA results based on interval arithmetic calculation method

In a life cycle assessment with interval arithmetic no exact values are given, but the indefinite parameters of the inputs and outputs are defined as intervals whose expected minimum and maximum values determine the limits of the interval. This eliminates the need for scenario analyses, which require a large number of balancing and modelling measures and lead to many different results. Instead of exact result values, result intervals are generated. The calculation procedure was implemented in the LCA program MultiVaLCA [9], which was developed at the Institute for Materials and Construction at the University of Stuttgart and used in the calculation presented in this study The result interval [12.05, 20.78] kg CO\(_2\) eq. results from the comparison with the interval arithmetic approach for the entire GWP. (cf. figure 11), so that the result values of scenarios 1, 2 and 3 lie within the interval limits. The result interval of the total primary energy demand PE is [564.16, 799.08] MJ and also includes the results of the three scenarios from the previous calculation (see figure 12). Thus, a reliable statement can be made with the result intervals that a GWP between 12.05 kg CO\(_2\) eq. and 20.78 kg CO\(_2\) eq. and a PE between 564.16 MJ and 799.08 MJ can be expected, taking into account the still open question of how to handle the excess ethanol.

All other uncertainties arising from open decisions can also be taken into account in a single balance sheet by also defining interval limits for the uncertain parameters.

![Figure 11. GWP contribution of flows [kg CO\(_2\) eq.] given in intervals considering all possible ethanol treatments (production stage, funct. unit: 1 m\(^2\) insulation, 2 cm thick).](image-url)
Figure 12. PE contribution of flows [MJ] given in intervals considering all possible ethanol treatments (production stage, functional unit: 1 m² insulation, 2 cm thickness).

5. Conclusion
The consideration of uncertainties by intervals usually leads to a widening of the result intervals and thus reduces the informative value of the results, but contains the existing uncertainties. In the course of the progressing development process these options can be rejected, whose unfitness for the achievement of the set goals is recognized, or decisions are made in favor of the best possible options. This reduces the overall scope of diversity. This means that once more accurate information about an uncertain parameter is available, the parameter's interval limits can be redefined and the meaningfulness of the result interval can become thus more precise thus increase step by step. Statements on ecology should only be made on the basis of results calculated in this way.

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