UFOPLAN-Project FKZ 360 01 064

# SELECTION AND USE OF CHEMICALS IN SMALL AND MEDIUM SIZED ENTERPRISES

## ANALYSIS OF THEIR SUSTAINABILITY

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# Selection and use of chemicals in small and medium sized enterprises

Analysis of their sustainability degree

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# ABBREVIATIONS

| | |
|---|---|
| APEO | Alkylphenol ethoxylate |
| BCF | Bioaccumulation factor |
| BDG | Butyldiglykol |
| BDK | 2,2-dimethoxy-1,2-diphenyl-ethanone |
| BAT | Best Available Technique |
| CHC | Chlorinated hydrocarbons |
| CLP | Classification, Labelling and Packaging |
| DEHP | Bis (2-ethylhexyl) phthalate |
| DIDP | di-"isodecyl" phthalate |
| DINP | di-"isononyl" phthalate |
| EDC | Endocrine Disruptor |
| HDDA | 1,6-Hexanedioldiacrylate |
| ITX | Isopropylthioxanthone |
| SME | Small and medium sized enterprises |
| LC50 | LC = Lethal concentration; LC 50 –concentration at which 50% of the exposed individuals of a population show lethal effects |
| SC | Solvent component |
| MDI | 4,4'-Methylenediphenyldiisocyanate |
| MIPS | Material Intensity Per Service unit |
| MQL | Minimal Quantity Lubrication |
| n.d. | No data |
| Pa | Pascal |
| PBT/vPvB | Persistent Bioaccumulating and Toxic (PBT)<br>very Persistent und very Bioaccumulating (vPvB) |
| PC | Polycarbonate |
| PE | Polyethylene |
| PP | Polypropylene |
| PVA | Polyvinylacetate |
| PVP | Polyvinylpyrrolidone |
| SDS | Safety Data Sheet |
| SubChem | Substitution of hazardous chemicals |
| TEDX | The Endocrine Disruption Exchange, Inc. |
| TPA | Textile processing aid |

# 1 BACKGROUND AND AIMS

The criteria for the sustainable selection and use of chemicals were developed by the Umweltbundesamt between 2008 and 2010 and reflect the current state of the expert discussion. They were compiled in a guide for small and medium sized enterprises (SME)[1]. These criteria and the systematic approach outlined in the guide were to be further tested and analysed within the scope of the current project using practical examples and reference experiences[2].

Besides some fundamental systematic aspects regarding the guide's applicability[3], it was tested and discussed in close cooperation with two SMEs, how they could select and scrutinize their chemicals using the sustainability criteria of the guide.

The UFOPLAN-project was carried out in cooperation between Ökopol (project management), Öko-Institut e.V. and the Kooperationsstelle Hamburg IFE GmbH.

# 2 RESULTS OF THE PRACTICAL EXAMPLES

## 2.1 Method

The project team targeted enterprises for cooperation which not only conducted substance innovations in the past, but which are currently also faced with the challenge of having to substitute some of the substances they use. In close cooperation with the consultant team and the practitioners, the enterprises' concrete practical examples were assessed using the guide.

As a result an answer to the question whether a selected chemical is more sustainable than another was obtained. In addition, potential problems in understanding and/or applying the guide itself were identified.

The results of the analysis are documented in the following using flow texts and simple graphs. The colours green, yellow and red are used in accordance with the guide's systematic approach.

[1] http://www.umweltbundesamt.de/uba-info-medien/4168.html

[2] In the entire document the term „guide" is used when referring to the work conducted in the context of the project to develop the UBA guide „sustainable chemicals".

[3] Among others it was tested if and which complementary aspects should be implemented in the guide in order to allow an assessment of mixtures and mineral fibres.

The colours signify the following, irrespective of which criterion or sub-criterion is assessed:

- Green: there is no need to act. Based on the available information, it could be demonstrated that there is no concern from the substance for the assessed sub-criterion.
- Yellow: there is a need to act. Based on the available information, there is a concern from the substance in relation to the assessed sub-criterion.
- Red: there is an urgent need to act. The available information shows that there is a high concern from the substance in relation to the assessed sub-criterion, e.g. due to its properties.
- White: there are no data to develop an indicator value or to operationalise the criterion. In this case there is a need to generate or obtain more information for the assessment.

## 2.2 Case study UHU GmbH & Co KG

### 2.2.1 Characterisation of the enterprise (regarding SME characteristics)

The UHU GmbH & Co. KG[4] is a medium sized enterprise with approximately 450 employees. The production site Bühl is located in Baden-Württemberg. The company has further business locations and distribution partners in more than 125 countries globally. In 1994 UHU became a wholly owned subsidiary of the Bolton Group. The Bolton group is an international enterprise which produces and markets a broad range of brand products and consumer products globally. The portfolio ranges from foodstuffs, household cleaning products and glues to body care and beauty products.

The company UHU has 80 years of experience in developing, manufacturing and marketing high quality adhesives for various applications for private consumers. Since the invention of the UHU all-purpose glue – the first ready-to-use adhesive made of synthetic resins – the brand name “UHU” has become a synonym for adhesives and glues in general. UHU can offer a comprehensive portfolio of different adhesives due to its continuous development of new products and progressive adhesive technologies.

On the company’s website (http://www.uhu.com/de/home.html) information on the various product groups are provided. The different application areas are introduced from a consumer perspective. Currently, the product portfolio consists of glues and adhesives for different glueale materials. The product types differ significantly in their chemical composition. In many product categories, both solvent-borne and water-borne products are offered.

[4] For better readability the abbreviated company name “UHU” is used in the following instead of “UHU GmbH & Co. KG”.

Due to historical reasons, UHU's production site is located in the middle of the small town of Bühl. This is one of the reasons, why safety and cleanliness are a natural principle of everyday practice. In addition, several projects were carried out to reduce solvent and $CO_2$ emissions as well as to reduce waste amounts and water consumption. Product related research and development aims to achieve strategic innovations, new technologies and the continuous optimization of existing products (e.g. the optimization of product composition).

The topic "sustainability" has become more and more important for the company. Awareness is built on the already firmly integrated activities improving the environmental performance. Respective measures are introduced in all company areas – starting with product development, production processes up to the use and disposal of products by the consumer.

UHU continuously works towards the best consumer and environmental protection on a world-wide scale. Among others, one of the company's strategic goals is not only to fulfil the existing legal requirements but also to implement measures reaching beyond them. From the beginning, UHU has been developing glues for children, parents and the do-it-yourself area. UHU will continue its efforts towards innovative and "safe" products to answer the demand of their customers with concrete solutions in the future.

### 2.2.2 Description of the assessed products and processes (selection of hot spots, starting situation, alternatives)

UHU's core business is the production of final products, which are sold to private consumers and professional users. Therefore, the products should be of high quality, easy and safe to use and as environmentally friendly as possible. Therefore, avoiding or substituting hazardous substances which are contained in the products is one of the core goals of UHU's research and development activities. For chemicals which are used as processing aids but are not included in the end products, worker protection issues are more in the foreground.

All products' packaging materials used by UHU can be recycled and a large share is manufactured from recycled materials. Further ideas pursued by UHU were also tested using the guide "sustainable chemicals" for a comparative analysis and assessment of materials.

The following substitution cases were analysed using the guide:

- Substitution of phenolphthalein by thymolphthalein,
- Substitution of cyclohexane by a solvent mixture based on solvent naphtha, light,
- Use of the organic solvents ethanol, acetone, ethyl acetate and methyl acetate,
- Use of inorganic silica acids.

### 2.2.3 Results from applying the guide criteria „sustainable chemistry“

In the following the results of the individual substitution cases are presented regarding the assessment of the criteria “substance lists”, “physical-chemical properties”, “hazardousness for humans”, “hazardousness for the environment” and “mobility of the substance”. Thereafter, the assessment results for the criteria “substance origin”, “greenhouse gas potential” and “resource consumption” are presented in a common scheme for all cases.

## Criteria on substance lists, PC-properties, hazardousness for humans and the environment and mobility

Substitution of phenolphthalein by thymolphthalein

**Table 1** shows the results from applying the substance-related criteria to the colorimeters (pH indicator) phenolphthalein and the substitute thymolphthalein.

Table 1: Comparison of phenolphthalein and thymolphthalein using the guide’s substance-related criteria 1 to 5

| Criterion | Phenolphthalein | Thymolphthalein |
|---|---|---|
| Contained in lists of problematic substances | Substance is mentioned in one or more lists | Substance is not mentioned in any list |
| Physical-chemical properties | No critical physical-chemical properties | No critical physical-chemical properties |
| Hazardousness for humans | | |
| Hazardous via inhalation, ingestion and eye contact | Substance may cause severe damage to human health. | Substance is not hazardous to human health |
| Hazardous via dermal contact | Substance is only slightly hazardous to human skin. | Substance is only slightly hazardous to human skin |
| Endocrine disruption | Substance is included in the list of endocrine disrupters | More information is necessary |
| Hazardousness for the environment | | |
| PBT/vPvB and toxicity | More information is necessary | More information is necessary |
| Mobility of the substance | | |
| Release potential in water | High water solubility | Low water solubility |
| Release potential to air | More information is necessary | More information is necessary |
| Long range transport | More information is necessary | More information is necessary |
| Release potential at the workplace | Dusty | Dusty |

The use of thymophthalein clearly improves the sustainability regarding the criteria "lists of problematic substances" and "hazardousness for humans". Phenolphthalein is a substance of very high concern on the REACH candidate list. It may cause severe chronic health damage. Both aspects do not apply to thymolphthalein.

The mobility assessment requires further information on both substances. Due to its low water solubility thymolphthalein has a better evaluation of the sub-criterion "release potential to water" than phenolphthalein.

Based on the available data, UHU's substitution of phenolphthalein with thymolphthalein could be evaluated using the guide's criteria without ambiguity[5].

UHU ceased the use of phenolphthalein even before the revision of its classification – although its concentration in the product remained under the declaration threshold and therefore did not influence the product labelling – and used thymolphthalein instead.

Substitution of cyclohexane by solvent naphtha, light

**Table 2Fehler! Verweisquelle konnte nicht gefunden werden.** presents the results from applying the substance-related criteria to compare the sustainability of the use of cyclohexane and its alternative solvent naphtha, light.

Table 2: Comparison of cyclohexane and solvent naphtha, light using the guide's substance-related criteria 1 to 5

| Criterion | Cyclohexane | Solvent Naphtha, light |
|---|---|---|
| Contained in lists of problematic substances | Substance is mentioned in one or more lists | Substance is not mentioned in any list |
| Physical-chemical properties | Substance is flammable | Substance is flammable |
| Hazardousness for humans | | |
| Hazardous via inhalation, ingestion and eye contact | Substance is not hazardous to human health | Substance is not hazardous to human health |
| Hazardous via dermal contact | Substance is hazardous to skin | Substance is only slightly hazardous to human skin |
| Endocrine disruption | More information is necessary | More information is necessary |
| Hazardousness for the environment | | |
| PBT/vPvB and toxicity | Substance is classified R50/53 | Based on available data it cannot be excluded that the substance is a PBT/vPvB. |
| Mobility of the substance | | |
| Release potential in water | High water solubility | Low water solubility |

[5] "without ambiguity" means that several criteria indicate a higher level of sustainability and that there are no concrete indications that there are contrary effects to be expected in the areas which could not yet be finally evaluated due to data gaps.

| Criterion | Cyclohexane | Solvent Naphtha, light |
|---|---|---|
| Release potential to air | High vapour pressure | High vapour pressure |
| Long range transport | No indication of long range transport, probably quick degradation in the atmosphere | Substance is not persistent in air |
| Release potential at the workplace | Not dusty | Dusty |
| Release potential from product | Use in mixtures; intended release from products | Use in mixtures; intended release from products |

For the criterion “lists of problematic substances” and the criteria “hazardousness for the environment” and “mobility” the alternative substance solvent naphtha, light has better results than cyclohexane. Some smaller differences are visible for the alternative solvent naphtha regarding its “hazardousness for humans”. Both substances can be released from the products. For end-using consumers this is hardly of relevance because only small packages for the use of small amounts are produced.

For both substances lifecycle data could be obtained. No differences could be seen regarding their assessment (c.f. next chapter). Based on the available data, UHU could assess the substitution of cyclohexane with solvent naphtha, light using the guide’s criteria without ambiguity.

Use of organic solvents

UHU uses different organic solvents for its mixtures. To test the guide, the substance related criteria were used for the substances acetone, ethanol, methyl acetate and ethyl acetate. **Table 3** shows the comparison results for acetone and ethanol.

Table 3: Comparison between acetone and ethanol using the guide’s substance-related criteria 1 to 5

| Criterion | Acetone | Ethanol |
|---|---|---|
| Contained in lists of problematic substances | Substance is not mentioned in any list | Substance is not mentioned in any list |
| Physical-chemical properties | Substance is flammable | Substance is flammable |
| Hazardousness for humans | | |
| Hazardous via inhalation, ingestion and eye contact | Substance is not hazardous to human health | Substance is not hazardous to human health |
| Hazardous via dermal contact | Substance is only slightly hazardous to human skin | Substance is only slightly hazardous to human skin |
| Endocrine disruption | More information is necessary | More information is necessary |
| Hazardousness for the environment | | |
| PBT/vPvB and toxicity | No PBT/vPvB, low aquatic toxicity | No PBT/vPvB, low aquatic toxicity |

| Criterion | Acetone | Ethanol |
|---|---|---|
| Mobility of the substance | | |
| Release potential in water | High water solubility | High water solubility |
| Release potential to air | High vapour pressure | High vapour pressure |
| Long range transport | More information is necessary | More information is necessary |
| Release potential at the workplace | Not dusty | Not dusty |
| Release potential from product | Use in mixtures; intended release from products. | Use in mixtures; intended release from products |

The assessment of the other two solvents – methyl acetate and ethyl acetate – had similar results.

The evaluation shows that the solvents used by UHU are not recorded on lists of problematic substances. The critical property "high vapour pressure" is necessary due to the function as a solvent. The same applies to the release potential from products, which results in a "red" category for the criterion. This has a lower relevance due to the small amounts used and the small packages produced.

When the substances are used in the production, standards for the protection of workers' health and the environment as well as general safety standards are fulfilled (e.g. gas hunting, activated carbon filters). The problematic property "high water solubility" does not critically influence the assessment, because the substances are not classified for the environment

There is no action need related to the criteria "hazardousness for humans" and "hazardousness for the environment". The four solvents don't exhibit relevant differences regarding the assessed sustainability criteria and they don't indicate additional action needs.

Use of inorganic silica

UHU uses silica in its formulations. **Table 4** shows the results from applying the substance-related criteria to silica.

Table 4: Assessment of silica using the using the guide's substance-related criteria 1 to 5

| Criterion | Assessment | Reasoning |
|---|---|---|
| Contained in lists of problematic substances | Substance is not mentioned in any list | Substance is not mentioned in any list |
| Physical chemical-properties | No critical physical-chemical properties | No classification |

| Criterion | Assessment | Reasoning |
|---|---|---|
| Hazardousness for humans | | |
| Hazardous via inhalation, ingestion and eye contact | Substance is not hazardous to human health | No classification |
| Hazardous via dermal contact | Substance is only slightly hazardous to human skin | No classification |
| Endocrine disruption | More information is necessary | No indication for endocrine disruption but also no evidence for absence of effects |
| Hazardousness for the environment | | |
| PBT/vPvB and toxicity | No PBT/vPvB, low aquatic toxicity | According to the SDS the substance does not fulfil the PBT/vPvB criteria and the aquatic toxicity is > 10 mg/l. |
| Mobility of the substance | | |
| Release potential in water | Low water solubility | Not soluble in water |
| Release potential to air | Low vapour pressure | Vapour pressure not applicable |
| Long range transport | No long range transport to remote areas | Substance is not persistent. |
| Release potential at the workplace | Dusty | Assumption: Silica is used as coarse powder, the dust settles. |
| Release potential from product | Firmly bound (reactive) | Used in mixtures (UHU) but due to the physical-chemical properties, no release is expected. |

The application of the criteria shows no action need for silica in relation to the evaluated aspects of risks.

UHU pointed to the discussion on nanomaterials and planned measures e.g. the notification requirements in France regarding the content of nanomaterials in consumer products. Many associations reacted to the publication of the background paper by the Federal Environment Agency on the risks and opportunities of nanotechnologies for man and the environment.

It is not yet possible to answer the increasingly important question of whether or not the use of nanotechnologies and nanomaterials is sustainable based on the information in the safety datasheets. Among others, more detailed information on the particle size is needed from the suppliers. The current version of the guide does not provide any criteria on nanomaterials. This is an important possibility to further elaborate the guide.

### Criteria on the greenhouse gas potential and resource use

For the assessment of the greenhouse gas potential and the resource uses related to the substances evaluated using the guide, it is necessary to apply data from life-cycle analyses. The guide recommends two databases in its

Annex 3. One is the ProBas[6] database of the Federal Environment Agency which contains information on different materials and processes. The other is a database by the Wuppertal institute on climate, environment and energy (Wuppertal Institut für Klima, Umwelt, Energie GmbH) called MIPS[7]. MIPS is an abbreviation for material input per service unit. Both databases were searched for information on the following substances and polymers: acetone, ethanol, methyl acetate, ethyl acetate, silica, phenolphthalein, thymolphthalein, cyclohexane and polymers (including recyclates) and renewable raw materials.

**Greenhouse gas potential, energy consumption, water consumption and waste generation**

**In the publicly accessible databases recommended in the guide, only little information was available on a few substances and one polymer. For one additional substance (cyclohexane) information on a similar substance was used as first orientation (this step requires expertise, which cannot be expected from enterprises).**

**Table 5** and **Table 6** present the data obtained from the databases and how they influenced the overall assessment.

The following results and conclusions should be taken into account:

- The values of $CO_2$-equivalents, energy consumption, waste generation and water consumption did not differ mucht for the substances.
- The values triggering a “yellow” assessment are very close to the borders defined for the category “green”. Considering the uncertainties connected to lifecycle data the difference between two substances placed into different assessment categories are rather small.

Note: The lifecycle data presented in the table refer to 1 kg of a substance. The values should not be used for a direct comparison because it is necessary to relate it to the substance amount which is actually used in the specific application. Only if lifecycle data are corrected with regard to the used amounts can the comparison be meaningful (this aspect is also described in the guide). When UHU tested the guide this additional step could not be performed because information from suppliers, which would have been needed to make the assessment, could not be obtained within time.

The information provided in the public databases ProBas and MIPS were not sufficient to compare virgin materials and recycling materials. No information was available on recyclates. For the further assessment of this question it would have been necessary to model recycling processes – a task which is not feasible for small and medium sized enterprises because detailed knowledge of the processes of recycling companies is needed.

[6] ProBas is a library of lifecycle data of substances; http://www.ProBas.umweltbundesamt.de/php/index.php.

[7] MIPS (Material input per service unit is a measure for the use of natural resources of a product or a service considering the entire lifecycle; http://www.wupperinst.org/de/projekte/themen_online/mips/index.html.

Table 5: Lifecycle data for five substances and a polymer for the assessment of the criterion greenhouse gas potential

| | Acetone | Ethanol | Methyl acetate* | Ethyl acetate* | Cyclohexane | LDPE |
|---|---|---|---|---|---|---|
| Surrogate data | | | Data for acidic acid (p.a.) | Data on acidic acid and ethylene | Data on benzene | |
| $CO_2$-equivalents (100 years) in kg(*1) | 2.16 | 0.97 | 2.59 | 2.31 | 1.76 | 2.04 |

For substances marked with an asterix (*) no data was found. Here, surrogate data are used from structurally similar substances or data from educts for the synthesis of these compounds. (*1): Orienting values for the greenhouse gas potential (in kg $CO_2$-equivalents) l: > 50; 1 – 50 / < 1 kg/kg/substance.

Table 6: Lifecycle data on five substances and polymers for the assessment of the criterion resource use

| | Acetone | Ethanol | Methyl acetate* | Ethyl acetate* | Cyclohexane | LDPE |
|---|---|---|---|---|---|---|
| Surrogate data | | | Data for acidic acid (p.a.) | Data on acidic acid and ethylene | Data on benzene | |
| Energy consumption in MJ | No data available | < 0.0001 | 7.9 | 7.58 | No data available | 76.2 |
| Water consumption in l (ProBas) (*1) | 82 | 3.4 | 2.4 | 2.85 | 84 | 47 |
| Water consumption (MIPS) (*1) | 18.72 | 25 (Note 3) | No data available | No data available | 28 | 162 |
| Waste generation in kg (*2) | 0.034 | -0.637 | 1.91 | 1.30 | 0.017 | 0.017 |

For substances marked with an asterix (*) no data was found. Here, surrogate data were used from structurally similar substances or data from starting substances the compounds' syntheses. For water consumption data were used from two lifecycle databases: ProBas (Database of the Federal environment Agency) and MIPS (Data of the Wuppertal Institute for climate, environment and energy; (*1): Orienting values for water consumption: > 100 / 5 – 100 / < 5 l water / kg substance; (*2): Orienting values for waste generation: > 50 kg / 50 – 1 kg / < 1 kg waste / kg substance.

### Sub-criterion renewability of resources

In the guide, the following advice was provided on how enterprises could obtain a first impression on the sub-criterion „renewability of resources“[8].

Table 7: Indications from the guide on the assessment of the sub-criterion “renewability of resources”

| Assessment | RED | YELLOW | GREEN |
|---|---|---|---|
| Sub-criterion: Renewability of resources | Non-renewable and scarce raw materials | Non-renewable raw materials available in large amounts. Renewable resources used in excess or produced with high resource consumption | Renewable raw materials used below the amount that is regenerated, wastes |
| Indicator Type of raw material – preliminary evaluation | E.g. fossil raw materials the stocks of which are limited. Raw materials which are difficult to reach (e.g. underground mining, deep drilling, high efforts for purification, etc.), e.g. beryllium | Non-scarce fossil raw materials (some minerals and gases) which can be obtained with comparably low efforts (surface mining, low refinement efforts) e.g. Iron | Sustainably used raw materials, recovered substances from wastes e.g. gelatine |
| | | Renewable raw materials (origin: plants or animals) can be yellow or green | |
| | A case-by-case assessment is necessary | | |

The results of the assessment show that mineral oil based polymers are categorized as “red”. In the second group - materials based on recyclates - the assessment derives the category “green” because the substance are recovered from wastes. For the assessment of materials based on renewable raw materials further information is necessary to decide if a material should be assigned to the category “yellow” or “green” category. Missing data relates particularly to the origin of raw materials.

## 2.3 Case study Kilian industrial nameplates GmbH

### 2.3.1 Characterisation of the enterprise (regarding SME-characteristics)

The company KILIAN industrial nameplatesGmbH [9] located in Hamburg develops solutions for industrial nameplates and signs. Among others, the company produces nameplates for the labelling of machines, vehicles and tools.

KILIAN employs 36 persons and is located in Hamburg-Langenhorn in the middle of a water protection area. Due to the fact that KILIAN is the only company in Germany that is allowed to manufacture inside a protected area, there are specific requirements regarding land use.

[8] Based on this a detailed assessment is envisaged in the guide which could not be performed during the project due to time constraints.

[9] In the following text the short name “KILIAN” is used instead of “Kilian industrial signs GmbH” to improve the readability

### 2.3.2 Description of the assessed products and processes (selection of hot spots, starting situation, alternatives)

KILIAN's entire production takes place inside the industrial plant. A rather small amount of hazardous substances is stored onsite in authorized storage areas with a drainage system.

In the 60ies and 70ies large amounts of volatile chlorinated hydrocarbons (CHC) were used as degreasing agents for metals and as cold cleaner in Germany. Volatile chlorinated hydrocarbons quickly evaporate, they are heavier than air and they can penetrate even concrete floors. Soil pollution was therefore unavoidable in the production of industrial signs, even if the substances were used appropriately and as intended.

Emissions of long-lived halogenated substances are a potential hazard for human health (they are suspected carcinogens) and contribute to the destruction of the ozone layer.

However, processing with CHC-solvents has been an established part of many of the manufacturing processes carried out at the company. It was not possible in all cases to exchange all the installation or manufacturing procedures. Therefore, it was important for KILIAN to find a CHC-free alternative cleaner or an alternative process. After having applied a crystal oil, finally the alternative, coco-based ester oil Estisol 242 was found as a high-performance alternative. It is still successfully used today.

The industrial signs should be durable and robust against mechanical and chemicals influences. The normal production process is carried out as follows: The metal sheets are partly etched with acids. Other parts of the metal sheets are covered by a bitumen separation layer to protect them from the acid attack. Then, the entire sign is covered with lacquer, which enters the deepened parts and is burnt into the material at 130°C. Thereafter the bitumen separation layer including the burnt-in lacquer is removed without damaging those areas where the lacquer is etched into.

The cleaning was originally preformed with two different processes – one process with a crystal oil and another with tetrachloroethylene. Until the substitution with the plant oil ester Estisol 242 as cleaning agent, the removal of the lacquered bitumen layer was carried out as follows:

The signs were placed into a multi-chamber bath (pre-cleaning I, c.f. **Figure 1**) which contained an "AII-product" (crystal oil). The cleaner penetrated the lacquer and attacked the bitumen. The bitumen macerated and caused the lacquer to crack. The soaked layers were manually removed with scrapers and wipes afterwards. Any remaining bitumen was removed in a small, continuously operated installation with an "AIII-product" (pre-cleaning, c.f. **Figure 2**). Approximately 400 litres of cleaner were used per year. In the third cleaning step using butyldiglycol (BDG) and water, grease-free surfaces were obtained. Grease-free surfaces are particularly important in case a second lacquering step is performed.

The process using tetrachloroethylene was carried out according to this procedure.

Figure 1: Pre-cleaning I at the company Kilian

For the implementation of a new process without CHC and without aromatic compounds the process involving the crystal oil and the tetrachloroethylene should be substituted. Plant oil esters from different suppliers were tested. The product by the company Haltermann (Estisol 242) achieved the best results regarding the removal of the bitumen separating layers.


Figure 2: Pre-cleaning II at the company Kilian

After only 5 to 10 minutes residence time the lacquered bitumen layer had macerated and decomposed into flakes. These flakes can be removed with low mechanical effort. The plant oil esters are positive with regard to workers' and environmental protection but also the smell is much more pleasant than of the AII and AIII cleaners. After applying the plant oil esters for manual cleaning the automatic pre-cleaning was also changed.

### 2.3.3 Retrospective assessment of the used substances and the conducted substitution

The past several substances and processes were evaluated with regard to their optimization potential for workers' protection and environmental protection.

The guide was used to assess the following three areas of action:

- Substitution of tetrachloroethylene by plant oil esters,
- Substitution of solvent naphtha (petroleum), medium aliph. as component of the crystal oil, by plant oil esters,
- Substitution of naphtha (petroleum), hydrodesulfurized heavy as component of the crystal oils by plant oil esters.

### 2.3.4 Results from applying the criteria of the guide "sustainable chemistry"

#### Criteria on substance lists, PC-properties, hazardousness for humans and the environment and substance mobility

Substitution of tetrachloroethylene with the plant oil ester Estisol 242

**Table 8** presents the results from using the substance-related criteria of the guide to compare tetrachloroethylene and the plant oil ester Estisol 242.

Table 8: Comparison of tetrachloroethylene and Estisol 242 using the guide's substance-related criteria 1 to 5

| Criterion | Tetrachloroethylene (CAS 127-18-4) | Plant oil ester Estisol 242 (no CAS-Nr.) |
|---|---|---|
| Contained in lists of problematic substances | Substance is mentioned in one or more lists | Substance is not contained in any list |
| Physical-chemical properties | R 10 | No physical-chemical properties of concern |
| Hazardousness for humans | | |
| Hazardous via inhalation, ingestion and eye contact | R40 suspected carcinogen | Substance is not hazardous to human health |
| Hazardous via dermal contact | Damages health via uptake through the skin | Not irritating to skin |
| Endocrine disruption | More information is necessary | More information is necessary |
| Hazardousness for the environment | | |
| PBT/vPvB and toxicity | No PBT/vPvB but persistent and very toxic | No PBT/vPvB, not classified for the environment |
| Mobility of the substance | | |
| Release potential in water | Toxic to the aquatic environment, long-term damage to the aquatic environment | Low water solubility |
| Release potential to air | High vapour pressure | Low vapour pressure |
| Long range transport | More information is necessary | Demonstrated to be not persistent |
| Release potential at the workplace | Not dusty | Not dusty |

| Criterion | Tetrachloroethylene (CAS 127-18-4) | Plant oil ester Estisol 242 (no CAS-Nr.) |
|---|---|---|
| Release potential from product | No release potential | No release potential |
| Origin of substance: environmental and social standards | More information is necessary | More information is necessary |

For almost all criteria the substitution was an improvement. Tetrachloroethylene is listed in many substance lists because depending on the different environmental influences, very hazardous substances may be formed. It is a suspected carcinogen and it can damage human health via skin absorption. For the coco-based plant oil esters no adverse human health effects are known.

The substance tetrachloroethylene is critical regarding the release potential to air and to water and therefore is categorized "red" for these criteria. The plant oil esters do not have comparable high release potentials (category “green”). They are rapidly degraded in water and due to their low vapour pressure are hardly released to air.

For the assessment of the criteria “long range transport” and “origin of the substance; environmental and social standards” the information basis for tetrachloroethylene is insufficient. The environmental and social standards at the origin of coco-based plant oil esters can also not be determined due to the lack of data. KILIAN’s attempts to obtain respective information have not been successful since years. It was also not possible to increase the pressure on the supplier, because the product was selected for use due to its good cleaning results and no alternative producers exist.

KILIAN unambiguously concluded that the substitution of tetrachloroethylene by the coco-based plant oil ester improves the sustainability. Naturally, a comprehensive and complete assessment would require collection of the missing data and determination of the missing indicators.

Substitution of solvent naphtha (petroleum), medium aliph, with plant oil esters

**Table 9** presents the results of comparing solvent naptha with the substitute plant oil ester Estisol 242 using the substance-based criteria of the guide.

For almost all criteria, improvements could be achieved. Solvent naphtha has narcotic effects and can cause dizziness. Ingestion may cause lung damage. The plant oil esters do not have hazardous properties for human health.

The release potential to air and water is critical for solvent naphtha. It is toxic to aquatic organisms and causes long term effects in the aquatic environment. Due to the medium vapour pressure a release potential to air exists. Both aspects are evaluated as of low relevance for the plant oil esters: the biological degradability in water is high and due to the low vapour pressure, the release potential to air is low as well.

Table 9: Comparison between solvent naphtha and Estisol 242 using the guide's substance-related criteria 1 to 5

| Criterion | Solvent naphtha (petroleum), medium aliph. CAS: 64742-88-7 | Plant oil ester Estisol 242 (no CAS-Nr.) |
|---|---|---|
| Contained in lists of problematic substances | Substance is mentioned in one or more lists | Substance is not listed |
| Physical-chemical properties | R 10 | No physical-chemical properties of concern |
| Hazardousness for humans | | |
| Hazardous via inhalation, ingestion and eye contact | R 65a | Substance is not hazardous to human health |
| Hazardous via dermal contact | R 66 | Not irritating to skin |
| Endocrine disruption | More information is necessary | More information is necessary |
| Hazardousness for the environment | | |
| PBT/vPvB and toxicity | No PBT/vPvB; R51/53 | No PBT/vPvB, not classified for the environment |
| Mobility of the substance | | |
| Release potential in water | Low water solubility | Low water solubility |
| Release potential to air | Medium vapour pressure | Low vapour pressure |
| Long range transport | More information is necessary | Demonstrated to be not persistent |
| Release potential at the workplace | Not dusty | Not dusty |
| Release potential from product | No release potential | No release potential |
| Origin of substance: environmental and social standards | More information is necessary | More information is necessary |

For the evaluation of the long range transport potential, information on solvent naphtha (petroleum) is missing, such as on the persistence or indications of atmospheric transport mechanisms.

There is also a lack of information on the origin of the substance and the environmental and social standards for its production. Indicators for the assessment could be the degree to which the production is environmentally friendly, the workplace conditions and if the production is sustainable. The assessment of the environmental and social standards cannot be performed for the coco-based plant oil esters because, although repeatedly requested from the supplier, no such information is available.

Based on the available data and with the help of the guide, the substitution of solvent naphtha (petroleum), medium aliph, with the coco-based plant oil ester was unambiguously evaluated by KILIAN as a step towards more sustainability.

In order to make a comprehensive assessment, it is necessary, however to obtain the missing data and assess the remaining criteria.

Substitution of naphtha (petroleum), hydrodesulfurized heavy with plant oil esters

**Table 10** presents the comparison result of Naphtha (petroleum), hydrodesulfurized heavy and its substitute plant oil ester Estisol 242.

Table 10: Comparison of naphtha (petroleum) with Estisol 242 using the guide's substance-related criteria 1 to 5

| Criterion | Naphtha (petroleum), hydrodesulfurized heavy (CAS: 64742-82-1) | Plant oil ester Estisol 242 (no CAS-Nr.) |
|---|---|---|
| Contained in lists of problematic substances | Substance is mentioned in one or more lists | Substance is not listed |
| Physical-chemical properties | R 10 | No physical-chemical properties of concern |
| Hazardousness for humans | | |
| Hazardous via inhalation, ingestion and eye contact | R 65a | Substance is not hazardous to human health |
| Hazardous via dermal contact | R 66 | Not irritating to skin |
| Endocrine disruption | More information is necessary | More information is necessary |
| Hazardousness for the environment | | |
| PBT/vPvB and toxicity | No PBT/vPvB; R51/53 | No PBT/vPvB, not classified for the environment |
| Mobility of the substance | | |
| Release potential in water | Low water solubility | Low water solubility |
| Release potential to air | High vapour pressure | Low vapour pressure |
| Long range transport | More information is necessary | Demonstrated to be not persistent |
| Release potential at the workplace | Not dusty | Not dusty |
| Release potential from product | No release potential | No release potential |
| Origin of substance: environmental and social standards | More information is necessary | More information is necessary |

For almost all criteria an improvement could be achieved by the application of the coco-based plant oil esters. Naphtha (petroleum), hydrodesulfurized heavy is listed on the lists of HELCOM (Commission for the protection of the marine environment of the Baltic Sea)[10] and the Water Framework Directive[11].

10 http://www.helcom.fi/home/en_GB/welcome/

11 http://ec.europa.eu/environment/water/water-framework/ priority_substances.htm

Due to its low flashpoint, naphtha can form explosive mixtures. It has some narcotic effect and may cause dizziness in humans. No hazards to human health are known of the coco-based plant oil esters.

The release potential to air and water is critical for naptha. Both these aspects are not critical for the plant oil esters. They are well degradable in water and due to the low vapour pressure the release potential to air is very low.

For naphtha (petroleum) information on long range transport is missing. There is also an information gap on the origin of the substance and the environmental and social standards for the production of naphtha and the coco-based plant oil esters.

Based on the available data and with the help of the guide the substitution of naphtha (petroleum), hydrodesulfurized heavy, with the coco-based plant oil ester was unambiguously evaluated by KILIAN as a step towards more sustainability. In order to make a comprehensive assessment it is necessary, however to obtain the missing data and assess the remaining criteria.

### Criteria on the greenhouse gas potential and the resource use

For the identification of greenhouse gas emissions and resource uses related to the manufacture of the two substances, information from lifecycle analysis databases are necessary. The guide recommends two databases (Annex 3). The database ProBas[12] of the German Federal Environment Agency contains information on different materials and processes and the database of the Wuppertal Institute for Climate, Environment and Energy GmbH (MIPS)[13] are also referred to. For the assessment of greenhouse gas potentials and resource use the guide was applied to 2 substances / materials.

### Greenhouse gas potential, energy consumption, water consumption and waste generation

The databases recommended by the guide contain information only on one of the assessed substances (naphtha). No specific information is contained for solvent naphtha, tetrachloroethylene or the substitute plant oil ester Estisol 242.

Although it is possible to use information from related substances as a first approximation, this step requires expertise which cannot be expected from an enterprise the size of KILIAN. The case study showed that this criterion cannot be applied by the company.

**Table 11** and **Table 12** present the data obtained on naphtha and the respective assessment result. The data on tetrachloroethylene was taken from sources which are not mentioned in the guide. Therefore and in accordance with the principles provided in the guide, a direct comparison of the data is not possible.

12 http://www.ProBas.umweltbundesamt.de/php/index.php
13 http://www.wupperinst.org/de/projekte/themen_online/mips/index.html MIPS means material input per service unit.

For the criteria greenhouse gas potential and resource use only first approximations can be obtained for the assessment, if only the recommended data sources are used. Considering the annual use amount of naphtha by Kilian and the assessment result in a “green” category (generated only for a first orientation) it is likely that these criteria are less relevant and are given less weight in the overall sustainability assessment by KILIAN. Nevertheless, it should be taken into account that a direct comparison of the original substances and their substitutes would be necessary but is not possible based on the available data.

Table 11: Lifecycle analysis data on the greenhouse gas potential

| | Naphtha (petroleum), hydrodesulfurized heavy | Solvent naphtha (petroleum), medium aliph. | Tetrachloro-ethylene | Coco-based plant oil ester Estisol 242 |
|---|---|---|---|---|
| Used reference substances (if available)[14] | | | | |
| $CO_2$-equivalents (100 years) in kg | 4.08E-01 | n.d.[15] | 2.9E-5 | n.d. |

Table 12: Lifecycle analysis data on the energy consumption, water consumption and waste generation er

| | Naphtha (petroleum), hydrodesulfurized heavy | Solvent naphtha (petroleum), medium aliph. | Tetrachloroethylene | Coco-based plant oil ester Estisol 242 |
|---|---|---|---|---|
| Used reference substances (if available) | | | | |
| Energy consumption in MJ | n.d. | n.d. | 32.6 | n.d. |
| Water consumption in litre | 2.12 | n.d. | 0.123 | n.d. |
| Waste generation in kg | 0.115 | n.d. | n.d. | n.d. |

Similarly to the other case study (company UHU) it was observed that information on primary and recycling materials was insufficient to perform the originally intended comparison of using primary materials and recycled materials. A comprehensive evaluation of this issue would hence require modelling of the recycling processes.

### Sub-criterion renewability of raw materials

Based on the guide’s advice for a first evaluation of the sub-criterion renewability of raw materials[16] the following materials were assessed:

- Naphtha, solvent naphtha and tetrachloroethylene
- Plant oil ester Estisol 242

[14] Data for related substances (reference substance) was used in case no information was available in the databases on the substance or substance group

[15] The blue fields filled with “n.d.” indicate that in the databases no data was available (no data).

[16] Based on this work a detailed assessment is planned using the guide, which could not be performed due to the insufficient data currently available.

The assessment of the first group of substances resulted in a “red” category because they are produced from primary raw materials, the supply of which is limited (mineral oil). The second group, the plant oil esters are produced based on renewable raw materials and according to an expert evaluation a “yellow” assessment result is appropriate. This is explained by the fact that although the raw materials are renewable and available in large amounts, they are frequently grown in mono cultures which over exertsthe soils.

The substitution decision by KILIAN is supported by this assessment because the raw materials are used only to a small extent for technical applications. An English publication on the aspect supported the assumption that the technically used amounts of the raw materials are not significant compared to other uses.[17]

## 2.4 Experiences from the application of the guide in the two enterprises

A number of observations and experiences were collected from the practical application of the guide by the companies UHU and KILIAN. They are valuable for the use and further development of the guide.

### 2.4.1 Strengths of the current version of the guide:

- In its current form, the guide raises awareness in enterprises on the different aspects of sustainability.
- In particular the decision makers who have to make human resources for substitution measures available can take a new perspective on the topic.
- The “golden rules” in the guide – a summary of orienting principles – present the topic “sustainable chemicals” in an attractive form and create an incentive to learn more about it.
- The structure of the guide and the comparably low number of criteria is useful to operationalise the topic “sustainability”. This is particularly true for the substance-related and use-related criteria.[18]
- The presentation of the individual topics on normally 2-3 pages provides a quick and comprehensive entry point to the topic and compiles the most important aspects neatly.
- The first criterion (lists of problematic substances) enables a quick identification of critical substances, which should be prioritized for substitution.

[17] Bertz, K.: Vegetable Oil Based Fatty Acid Ester Production; Herausgeber: Kooperationsstelle Hamburg, Studie, Hamburg 1997

[18] Due to resource constraints, main assessment areas had to be defined. Therefore, the eight substance-related criteria were in the focus of attention.

- Some topics are very familiar to the corporate every-day work (workers protection, physical-chemical substance properties). This allows directly relating parts of the guide's criteria/indicators to information in the company. The references to legally required classifications (R-phrases; H-statements) allow an evaluation based on available data in substances inventories.
- Since the assessment of the substance-related criteria (PC-properties, workers and environmental hazards) is based on the classification a quick screening of all substances used in the company is possible (portfolio screening).
- For many criteria, quantification is offered by the guide, which does not yet exist in similar tools. The quantified indicators enable companies to make an orienting evaluation of their substances. For example up to now no orienting values were available for the assessment of water consumption of individual substances.
- The system to present the results in a traffic light system with the addition of the colour white for data gaps is welcomed because it is easy to use and signal colours from everyday life are used.
- For all criteria already after a short research time it is possible to decide if the available data is sufficient to make a decision (result: white or a colour).
- If sufficient data is available for a first evaluation, after only a short research time an orienting evaluation is possible. However, it is important to highlight that the "result colour" of the individual criteria is only a facet of the entire picture. Only the overall picture can be interpreted with regard to potential action needs. The colours indicate where to start with an assessment of possible improvements.

### 2.4.2 Weaknesses of the guide in its current form:

- Whereas the "golden rules" and the individual chapters of the guide were welcomed, the enterprises' employees stated that the guide as a whole contains too much information. This means in particular: when the guide is browsed through, its attractive design raises interest. This is a big advantage. However, having decided to look into details and to read from the beginning, the large amount of detailed information can cause the reader to stop after a relatively short time.
- The relevance of the criterion "mobility" is not understood by the employees. Additional explanation and examples would be useful, e.g. an indication to problems of pesticides leaching to ground water.
- The on-going intense discussion on nanomaterials has led to a demand for respective information in the supply chain and/or the need to notify in certain countries (e.g. France). This is not addressed by the guide.

- The guide is illustrated with the example substance “formaldehyde”. The use of this substance is avoided or prohibited in many sectors. For readers in these sectors it is surprising that the substance has a comparably positive sustainability profile in the guide.
- It is not clear to the users what consequences should be implemented following an assessment of substances using the “golden rules” or the individual criteria.
  This is surprising as the presentation of a sustainability assessment’s benefits is emphasized in the guide. Clarifying this issue can only be achieved, by including additional illustrative examples according to the consultant team.

### 2.4.3 Problems in obtaining data

- The availability and accessibility of information for the assessment differs for the different criteria. The first four substance-related criteria can be established using easily accessible information from lists of problematic substances and the chemical classification.
- The evaluation of the hazardousness for the environment requires information on the PBT/vPvB-properties, which is normally not provided by the suppliers with the safety data sheets. The same applies to endocrine disrupting properties in relation to human health. This disappoints the guide’s users and their readiness to work with the guide decreases.
- The data search gets cumbersome for the criteria greenhouse gas potential, resource use and social responsibility in the supply chain (origin of substances). The danger of user disappointment and demotivation is high.
- The recommended, publicly accessible databases with lifecycle analysis data contain information only for a limited number of chemicals. More comprehensive databases are not usually free.
- The use of the criterion “resource use”, sub-criterion “renewability of raw materials” can be applied without in-depth research but only using the information in the guide. However, no distinction between the category “yellow” and “green” is possible. If for example the use of renewable raw materials instead of mineral oil-based ones should be distinguished, additional information is necessary.

## 2.5 Overarching results / recommendations from the case studies

The guide in its current form creates interest for the complex topic “sustainable chemicals” in enterprises. It offers useful information and is attractive enough to incite the responsible persons and exerts to assess the use of substances in their companies. However, personnel that is not specifically educated on this

issue and responsible persons who are not familiar with the topic are partly overstrained.

In order to ensure a broad applicability of the guide the following is proposed for a revision:

- The “golden rules” should be moved to the first sections of the guide.
- The barriers for a complete reading of the guide could be reduced if the presentation of the sub-aspects “relevance”, “applicability of the criterion”, “information basis” and “assessment” are significantly shortened in the individual sections (the comprehensive texts in the current version of the guide could be moved to an annex).
- The orienting values for the greenhouse gas potential could be more distinctive and meaningful if the differentiation was slightly changed between “yellow” and “green” (the orienting value for the category “green” should be: < 5 kg $CO_2$-equivalents/kg substance (current value: < 1 kg $CO_2$-equivalents / kg substance) and that for the “yellow” category should be changed respectively).
- For the cases where a differentiation between “yellow” and “green” is difficult, examples could illustrate how a decision can be made using further information (e.g. additional information on the how renewable raw materials are grown).
- It should be clarified that the values from lifecycle analyses only allow a first approximation and the values always need to be related to the functional unit. In many cases a case-by-case assessment will require detailed research.
- The evaluation of the criteria “origin of a substance”, “greenhouse gas potential” and “resource use” is difficult because the necessary data can hardly be obtained and interpreted. If the guide is revised the possibility of making a first approximation using more easily available information should be checked.
- Although comprehensive databases such as EcoInvent are normally with costs, it appears useful to recommend their application in the guide. Here it should also be indicated that the comparison of information from lifecycle analyses requires significant efforts.
- First decision support for the evaluation of nanomaterials should be included in the guide. Companies analysing their portfolio should at least be supported in identifying whether or not they use nanomaterials at all. This check could be carried out using the EU-Commission’s definition of a “nanomaterial” published in October 2011.
  *“A nanomaterial is a natural, incidental or manufactured material containing particles in an unbound state or as an aggregate or as an agglomerate and where, for 50 % or more of the particles in the number size distribution, one or more external dimensions is in the*

*size range 1 nm - 100 nm."* (European Commission, 2011[19]). The number size distribution should be provided for solid materials in the safety data sheet or in technical documents. If this is not the case, the users of the guide could request information on the size from the supplier.

- It should be checked if it is possible to point out how and which information which already exists in the enterprises can be used for the assessment. This could be e.g. classification and labelling data in the enterprises' substance inventories. With this data the criteria "hazardous physical-chemical properties" and "hazardousness for humans" could be evaluated quickly for a high number of substances.
- Examples for information requests to suppliers could be evaluated and used as examples. Making respective draft letters available in the guide for information requests should be considered.
- Practical examples in an annex of the guide could increase the attractiveness for enterprises. Examples are convincing if they clearly present the concrete improvements achieved, e.g. regarding the protection of workers, the environment and consumers. Also, actions that secure the medium and long-term sourcing of products and substances decrease corporate costs or improve the company's image in the supply chain and in the general public would be useful (e.g. Results from the assessment of phenolphthalein substitution: the substance is listed on a list of problematic substances which constitutes a high urgency for action. Consequence: substitution with thymolphthalein. Advantages for the company: long-term availability of the substitute / higher acceptance because the substance is used in a consumer product / no disadvantage regarding costs (due to low use amount).
- The guide should be provided as modular internet version with a simple dialogue and user navigation.
- Enterprises should be advised to use the guide and individual modules for their internal training activities.
- Support could be provided to enterprises on how they could communicate their use of the guide for sustainable chemicals to external customers and the general public. This could become part of the overall sustainability reporting.
- In addition, a dynamic and up-to-date reference to a list of experts, consultants or workshops offered by pertinent associations and chambers to train the use of the guide could support companies to obtain the necessary know-how for its efficient and appropriate use.

[19] European Commission: "COMMISSION RECOMMENDATION of 18 October 2011 on the definition of nanomaterial", Pub. L. No. 2011/696/EU (2011) EU-Commission. Retrieved from http://eur-lex.europa.eu/LexUriServ/LexUriServ.do?uri=OJ:L:2011:275:0038:0040:EN:PDF.

The guide in its current form well contributes to the initiation of a discussion in small and medium sized enterprises on their use of sustainable chemicals. If and when this leads to a substitution of problematic substances, cannot be judged based on the experience obtained in the project. The implementation of the proposed changes, specifically the easy-to-use internet application could increase the attractiveness of the guide significantly. The chances for implementation of the guide in the companies would be significantly increased by this, according to the consultant team's opinion.