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SIM: Chemicals in materials

A database tool for identifying harmful substances in products

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Over the last few years there has been a sharp increase in international statutory regulations on harmful substances in products, not least on account of a UN environmental programme. Importers of products face an enormous challenge in identifying potentially harmful substances in bought-in products. The DEKRA SIM database offers support in some cases.

Baseline situation

Prohibitions and restrictions of harmful substances in products have existed in Germany and Europe for some time, e.g. for toys, food contact materials and similar product groups. With its rules concerning SVHCs in products, the requirements of the REACH regulation were greatly expanded in 2007.

A focus is also being increasingly placed on harmful substances in products in the international arena. The UN environmental programme founded the strategic SAICM initiative in 2006, which in turn launched the “Chemicals in Products” programme (CiP) in 2009. The focus of this programme is an improvement of the information flow on chemicals in products.

Few companies have such a high degree of vertical integration that they know all the substances their products contain. Invariably mixtures and components are bought in whose composition is not fully known. The extreme case in this spectrum is dealers who buy their products in Asia primarily according to price criteria.

Challenges exemplified by REACH

Art. 33 REACH requires that EU suppliers inform their customers if an article contains a substance from the candidate list (< 0.1%). In addition, pursuant to Art. 7 para. 2 he may be required to report the candidate substances in imported products to the ECHA.

For every article the company must also know whether a substance from the candidate list is present. As the candidate list is updated twice a year, the company regularly update the information on its articles.

The company must take two further factors into account which have a decisive influence on the amount of work involved:

- Complexity of the product: the more individual parts incorporated, the more difficult it to know all candidate substances it contains.
- Changes in the product portfolio: the more often new articles are adopted in the range, the more complex the check for candidate substances becomes.

These differences in the company’s orientation (aircraft manufacturer vs promotional dealer) also exert a strong influence on the task solving approach.

Approach

The use of chemicals in products strongly depends on the materials used. The harmful substances to be be anticipated in products made of metal differ from those in products made of plastic. In the case of plastic products the harmful substances they may contain depend on the type of plastic (PP, ABS or PVC, etc.).

For this reason, DEKRA developed the so-called “SIM database”, which specifies for each substance in the candidate list the materials in which it is typically present. This information was derived mainly from reliable literature and our own expertise and observations, e.g. generated in the DEKRA laboratory.

Currently the SIM database lists over 120 materials, including approx.

- 50 polymers
- 15 natural substances and tissues
- 10 mineral materials
- 15 metals and alloys
- 30 electronic components

Candidate list inclusion date	Stoffname	Eigenschaft	EC-No	CAS-No	"Plastik" Thermoplaste Mat. 1	Mat. 2	Mat. 3	Mat. 4	Mat. 5	Mat. 6	Mat. 7	Mat. 8	Mat. 9	Mat. 10	Mat. 11	Mat. 12	Mat. 13	Mat. 14	Mat. 15	Mat. 16	Mat. 17	Mat. 18	Mat. 19	Mat. 20	Mat. 21	Mat. 22	Mat. 23	Mat. 24	Mat. 25	Mat. 26
CORAP 2017	(1-Methylethyl)-1,1-biphenyl		247-156-8	25640-78-2																										
CORAP 2017	(bis(2-Ethylhexyl)tetrabromphthalat)		247-426-5	26040-51-7																										
CORAP 2015	[1,3 (oder 1,4)-Phenylenbis(1-methylethyliden)]bis[tert.-butyl]peroxid	PBT, vPvB	246-678-3	25155-25-3																										
06/12	[4-[[4-Anilino-1-naphthyl][4-(dimethylamino)phenyl]methylen]cyclohexa-2,5-dien-1-yliden] dimethylammoniumchlorid (C.I. **Basic Blue** 26) [mit ≥ 0.1% of Michler's Keton (EG Nr. 202-027-5) bzw. Michler's Base (EG Nr. 202-959-2)	Carc. 1B	219-943-6	2580-56-5	1	1	1	1	1	1	1	1			1	1	1	1	1	1		1								1
					C	C	C	C	C	C	C	C			C	C	C	C	C	C		C								C
06/12	[4-[4,4'-Bis(dimethylamino) benzhydryliden]cyclohexa-2,5-dien-1-yliden]dimethylammoniumchlorid (C.I. **Basic Violet** 3) [mit ≥ 0.1% of Michler's Keton (EG Nr. 202-027-5) bzw. Michler's Base (EG Nr. 202-959-2)]	Carc. 1B	208-953-6	548-62-9									1	1																
													C	C																
CORAP 2015	1-(2-Hydroxy-5-nonylfenylkete)-phenylethanonoxim	PBT, vPvB	-	244235-47-0																										
CORAP 2014	1,1,1,3,3,3-Hexamethyldisilazan	-	213-668-5	999-97-3																										
CORAP 2014	1,1,1-Trihydroxymethylpropyltriacrylat, Trimethylolpropantriacrylat	EqC	239-701-3	15625-89-5																										
CORAP 2013	1,1'-Iminodipropan-2-ol, Diisopropanolamin	CMR, EqC	203-820-9	110-97-4																										
Rol (-)	1,2,3-Trichlorbenzol		201-757-1	87-61-6																										
06/11	1,2,3-Trichlorpropan	Carc. 1B	202-486-1	96-18-4																										
CORAP 2015	1,2,4-Triazol	CMR	206-022-9	288-88-0																										
Rol (-)	1,2,4-Trichlorbenzol (TCB)	PBT	204-428-0	120-82-1																										
CORAP 2014	1,2-Benzoldicarbonsäure, Benzyl C7-9-verzweigte und lineare Alkylester	CMR	271-082-5	68515-40-2																										
CORAP 2014	1,2-Benzoldicarbonsäure, di-C11-14-verzweigte und lineare Alkylester, C13-reich	CMR	271-089-3	68515-47-9								2			3	3	3	3	3											
06/11	1,2-Benzoldicarbonsäure, Di-C6-8-verzweigte Alkylester, C7-reich	Repr. 1B	276-158-1	71888-89-6								A			A	A	A	A	A										
Rol	1,2-Benzoldicarbonsäure, Di-C6-10 Alkylester, 1,2-Benzoldicarbonsäure, gemischte Decyl-, Hexyl- und Octyldiester mit ≥ 0.3% Dihexylphthalat (EG Nr. 201-559-5)	Repr. 1B	271-094-0 272-013-1	68515-51-5 68648-93-1								2			3	3	3	3	3											
												A			A	A	A	A	A											
06/11	1,2-Benzoldicarbonsäure, Di-C7-11-verzweigte und lineare Alkylester (DHNUP)	Repr. 1B	271-084-6	68515-42-4								2	1	1	3	3	3	3	3			1						1		
												A	B	B	A	A	A	A	A			A						B		
CORAP 2014	1,2-Benzoldicarbonsäure, di-C9-11-verzweigte und lineare Alkylester	CMR	271-085-1	68515-43-5											1	1	1	1	1											
06/14	1,2-Benzoldicarbonsäure, dihexylester, verzweigt und linear	Repr. 1B	271-093-5	68515-50-4								1			A	A	A	A	A											
												A			2	2	2	2	2											
12/12	1,2-Benzoldicarbonsäure, dipentylester, verzweigt und linear	Repr. 1B	284-032-2	84777-06-0								2			2	2	2	2	2											
												A			A	A	A	A	A											

Contents

The SIM database for SVHC lists the following groups of substances:

- substances of the candidate list
- substances of the Registry of Intentions
- substances of the CORAP[1]

The EG No., CAS No. and SVHC chemical property (e.g. Carc. 1B) are listed for each substance.

If the substance is to be expected in a material, the database contains a qualitative statement of the probability of occurrence:

- 1: low
- 2: medium
- 3: high

For many substances additional information is available on the concentration in which the substance typically occurs in the material:

- A: high
- B: medium
- C: low
- D: < 0.1%

The SIM database can be used as a tool for risk assessment and minimisation, as shown in the following. It enables the user to evaluate a product in terms of the risk of candidate substances. He must, however, know or be able to identify the materials which the product contains.

Risk minimisation

As a rule it is difficult to achieve 100% compliance regarding harmful

[1] Community Rolling Action Plan

substances in products, as this would require a large number of laboratory tests.

In many cases it makes sense to select an approach to risk minimisation by listing the various influencing factors with their risks. Supplier management and incoming goods inspection must be configured to effectively minimise the risks and restrict lab tests to only a small proportion of the products.

This could be as follows:

- 100 suppliers with a total of 3,000 articles
- thereof 50 non-EU suppliers
- thereof 20 suppliers who do not submit a valid test report
- thereof 15 “B suppliers”
- thereof 50 articles which acc. to SIM database have an increased risk for candidate substances
- sample analysis focuses on anticipated substances according to SIM database.

Further influencing factors must be taken into consideration in risk assessment:

- **Type of substance regulation:** A breach of restrictions pursuant to Annex XVII REACH are severely penalised and should be subject to stricter controls than candidate substances (here only obligation to inform).
- **Customer requirements:** the consequences of incomplete declaration may differ depending on the customer.

This means that each company decides for itself the optimum method of risk minimisation.

Process integration

Manufacturers usually have tools for supplier management, incoming goods inspection and customer communication.

To ensure effective use of the SIM database it should be incorporated into the existing processes, or the processes should be adapted to achieve optimum risk minimisation.

The database should be adjusted to the product portfolio. Some companies insist on mapping each article number in the database. For others it suffices to form product groups and map these.

The supplier evaluation should, of course, also contain aspects of harmful substance management. A simple confirmation that the product contains no candidate substances is less meaningful than a questionnaire in which the supplier must state how he prevents candidate substances from getting into the product.

Finally, the company should define a decision-making process specifying when which documents are required and when laboratory tests are necessary.

For the customer’s benefit, the process should specify the information to be provided and in which manner (deadlines, form, updating, etc.).

Possible applications

A SIM database can used for various different purposes.

Product design

At this stage companies which develop their own products can effectively avoid harmful substances in the product. A SIM database can help by listing the potential harmful substances per material. The designer/engineer can then decide whether another substance should be used or whether a stipulation should be adopted in the material requirement that it may not contain these harmful substances.

This is of significance in particular for substances which were already selected for Annex XIV of REACH and whose use in the near future will only be permitted with prior approval.

For companies which design their products themselves, but have them manufactured in Asia, the database information enables them to specify the choice of materials to their suppliers and thus avoid harmful substances in the product.

Product selection

Companies who buy modules or whole products can use the SIM database to scan the products for harmful substances prior to ordering. On the basis of the material list, the supplier can be obliged to submit test reports or explain how the introduction of a harmful substance was prevented.

In this phase an importer also has the option of rejecting products whose materials are subject to high risk.

Supplier communication

If the company has clear picture of the harmful substances which may be contained in a product, it can focus communications with the supplier on these risks. Agreements can be made with the supplier to minimise the concentration of harmful substances in the products.

Testing

The company can also use the information of a SIM database to check the plausibility of statements and documents of suppliers. For example, it can recognise if critical substances have not been included in the submitted lab reports.

Sample analysis

If the company itself orders lab tests to be carried out, the information from the database can be used to

better focus them on the harmful substances which occur in the material. This enables substantial cost savings.

Customer communication

A further possibility is to conduct customer communications with the results of a SIM database. The company selects, as it were, a "worst-case" approach: it notifies the customer of all substances that could potentially be contained in the product, and preventive measures specified in Art. 33. A company can thus fulfil its disclosure obligation even without lab data and reliable supplier information.

Whether this approach is practicable strongly depends on the sector and consumer group.

Outlook

The SIM database is not limited to candidate substances. It can also be used, e.g. for the restrictions according to Annex XVII of REACH.

A further deployment scenario is CMR substances[2] which are regulated by the Toy Safety Directive. Here again, the large number of listed substances can be greatly reduced by the material selection procedure.

Summary

The selected procedure for assignment of harmful substances to materials in which they may occur has already been proposed in a number of guidelines of the EU and member states. We have had over 5 years of positive experience with the database. The sharp jump in the number of candidate substances (particularly Dec. 2012) were also reflected in the database. In particular sectors which have hitherto received little information from their suppliers on harmful substances in products will benefit from this approach.

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[2] Carcinogens, mutagens and reproduction toxic materials