Classification of inorganic UVCB
Variability and grouping of individual streams

Introduction

One UVCB actually embraces a number of similar substances resulting from the same or similar source materials and/or processes or process steps. This is illustrated in Figure 1 below.

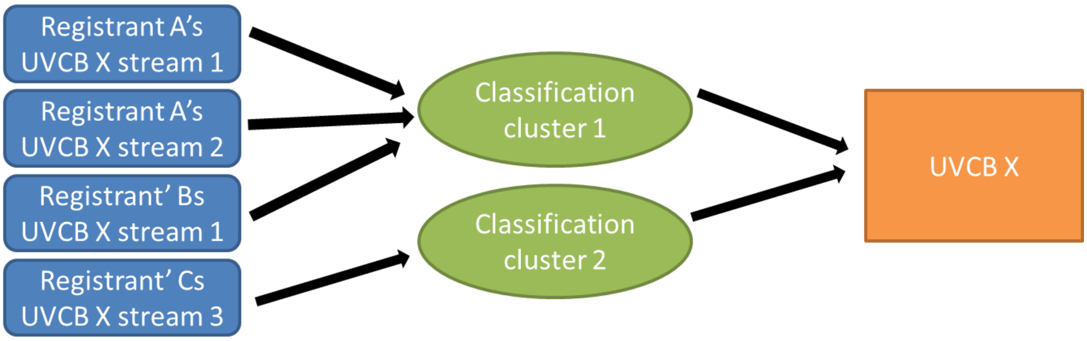

Figure 1: Variability of inorganic UVCB substances across individual registrants and grouping approach for classification and Registration Dossier preparation

Within one UVCB substance, the variability in elemental composition and/or no/limited variability in mineralogical composition can potentially lead to different hazard and risk profiles (note that the within-UVCB variability is smaller than the between-UVCB variability). Therefore, there is a need to differentiate more hazardous from less hazardous individual streams within the UVCB. In principle, individual stream specific (e.g. less severe) classifications can be reported for SDS and labelling purposes. Generic groups within one UVCB - each group with a common worst-case classification profile - are nevertheless developed and reported in IUCLID to increase general understanding of the Variability of the UVCB and to allow companies to easily derive a worst-case classification for possible new streams.

The objective of this section is to describe an approach to subcategorize a UVCB substance in several clusters by grouping individual stream[1]s based on hazard properties, risk management consequences, chemical composition and process information for classification purposes. These categories can also validate substance composition ranges and hence, substance identity.

Approach

UVCB substances are chemically characterized by their **known but variable elemental composition** and their structure can be sometimes characterized by means of their **(un)known (and sometimes variable), characteristic constituting minerals**, crystals, or other species defining a mineralogical (crystallographic) composition.

The overall concept to subcategorize the UVCB substance by grouping individual streams is based on a weight-of-evidence approach taking into account following lines of evidence in order of importance:

- The hazard classification and resulting risk management consequences (e.g. for transport[2] or in the framework of SEVESO or permitting) of individual streams
- The chemical elemental composition of individual streams
- Process information of individual streams

Figure 2 outlines the overall approach schematically.

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[1] A stream results from a particular process, which can be formed from variable sources, leading to a UVCB produced or used in a particular process and formed from variable sources.

[2] United Nations. 2012. European Agreement concerning the International Carriage of Dangerous Goods by Road. ADR applicable as from 1 January 2013

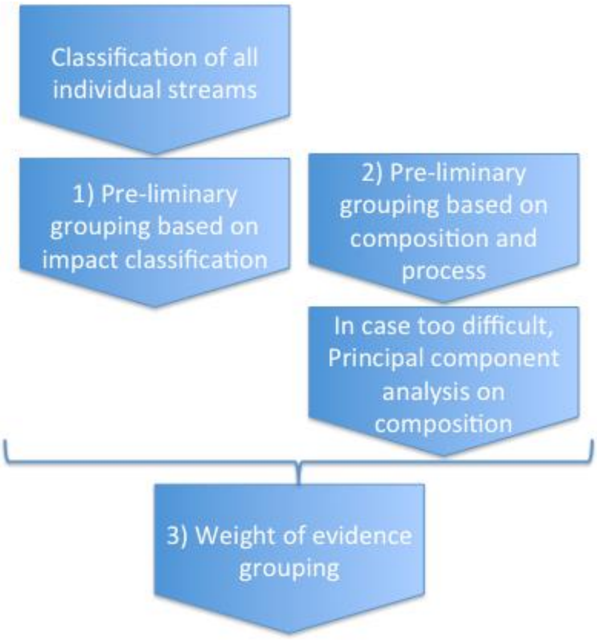

Figure 2: Approach grouping of individual streams

Step 1: Hazard/risk management driven grouping

Classification can trigger (additional) risk management measures for transport, under the SEVESO Directive or national legislation (e.g. permitting). Individual streams with similar risk management measures are to be grouped whereas individual streams with different risk management measures are to be split. For example, CMR-substances trigger risk management measures under several national or regional worker safety regulations. It is consequently relevant to distinguish individual streams with CMR properties from those without CMR properties. Moreover, when grouping for classification purposes there is no need to further distinguish between C-substances, CM-substances, CMR-substances, etc. because the practical risk management consequences are not significantly different.

Figure 3 outlines the most relevant environmental and human health classification endpoints in combination with risk management measures consequences. Note that for permitting, differences occur between different national regulations and only the overall tendency/principle is covered.

These hazard and resulting risk management consequences lead to a preliminary grouping of individual streams. This provides one line of evidence in the final grouping in step 3.

		Transport & packing	Permits	SEVESO
Hazardous to the aquatic environment -	Acute Cat 1, Chronic Cat 1,2	YES		YES
	Cat 3,4	NO		NO
Hazardous to the ozon layer		NO		NO
Acute Toxicity	Cat 1,2,3	YES	YES	YES
	Cat 4	NO		NO
Skin corrosion/irritation	Cat 1 (1A, 1B, 1C)	YES	YES	NO
	Cat 2, 3	NO		NO
Serious eye damage/eye irritation	Cat 1, 2A, 2B	NO		NO
Respiratory or skin sensitization	Cat 1	NO		NO
Germ cell mutagenicity	Cat 1A, 1B, 2	NO	YES	NO
Carcinogenicity	Cat 1A, 1B, 2	NO	YES	NO
Reproductive toxicity	Cat 1A, 1B, 2	NO	YES	NO
Specific target organ toxicity single exposure	Cat 1, 2, 3	NO		NO
Specific target organ toxicity repeated exposure	Cat 1, 2	NO		NO
Aspiration hazard	Cat 1, 2	NO		NO

Figure 3: Rationale behind hazard/risk management driven grouping

Step 2: Composition/process-driven grouping

A preliminary grouping based on elemental and/or mineralogical composition and/or process can be done qualitatively or quantitatively. Quantitative grouping is sometimes of added value in case many elemental constituents driving hazard and risk are present and/or many individual streams are present.

Qualitative grouping

Analysing overview tables of individual streams and their composition allow identifying groups of individual streams with similar relative elemental composition. For each group, the presence (or absence) of the driving elemental constituents can be characterised and used to interpret the characteristics of the group and try to link it to specific process related information. This provides another line of evidence in the final grouping in step 3.

Quantitative grouping

Principal component analysis (PCA) converts possibly correlated elemental concentrations into a set of values of uncorrelated variables called principal components. In this way, the multidimensional data set of elemental concentrations is reduced to two dimensions.

Since the elemental concentrations are typically log-normally distributed, the PCA will produce better results if the elemental concentrations are linearised. A log-normal transformation can, however, not be employed since many zero values are present in elemental concentration data sets when working with a cross-registrant set of streams with varying feed material and processes or process steps. Consequently, it is recommended to use a rank-transformation. In a rank transformation, the values are sorted from smallest to largest and a rank is assigned to each value starting with one for the smallest, two for the second smallest, etc. A rank transformation will normalise all elemental concentrations to the same scale and provides a more robust analysis (since the effect of outliers is minimized).

To avoid that the number of variables (i.e. elemental concentrations) exceeds the number of observations (i.e. individual streams), a selection of elements may be required. Priority is given to process driving elements and classification driving elements.

The results of the PCA are displayed in so-called biplots. Biplots are a type of exploratory graph used in statistics, a generalization of the simple two-variable scatterplot. A biplot allows information on both samples (i.e. individual streams) and variables (i.e. elemental concentrations) of a data matrix to be displayed graphically. Samples/individual streams are displayed as points while elemental concentration/variables are displayed as axes. There are three sources of information within a biplot:

- the information contained in the position and distances among the points. With the points the same arguments apply as in any other point-based plot such as dotplot or scatterplot: it is assumed that points lying close by have similar values. Therefore interesting graphical elements in a biplot are the same as in a dotplot or scatterplot: gaps, groups and outliers are easy to recognize.
- the length of the axes and the angles between them: the length of the axes express the contribution in the two main principal components. The angles between the axes are also interpretable. Though they do not give exact estimates of the correlation between projected axes, small angles between projected axes imply a high correlation. The direction of axes gives the sign of correlation. Perpendicular angles imply low correlation.
- the position of points corresponding to the axes. Points located near the high end of the axe direction have relative high values for that variable/elemental concentration and vice versa.

In summary, biplots allow to identify groups of individual streams with similar relative elemental composition. For each group, the presence (or absence) of the driving elemental constituents can be characterised and used to interpret the characteristics of the group and try to link it to process related information. This provides another line of evidence in the final grouping in step 3.

Step 3: Weight-of-evidence grouping

The final grouping of individual streams is based on weighing preliminary groupings based on hazard (classification) and risk (risk management measures impact of classification) and preliminary groupings based on chemical composition and process information.