



MECLAS (MEtals CLAssification tool)

**for the classification of complex inorganic materials
from the metals sector**

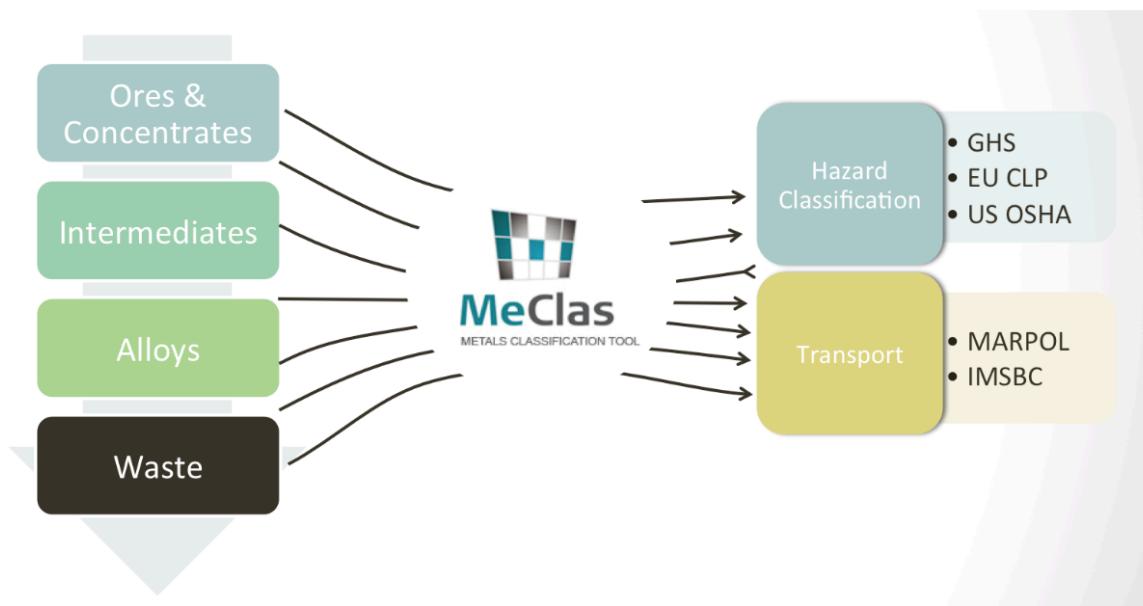
19 September 2018

TECHNICAL USER MANUAL

MeClas version 5.2

MeClas - the smartest way to fulfil your classification obligations

- Tool to determine the classification of your complex inorganic materials like ores and concentrates, complex intermediates, alloys or UVCBs
- Tiered approach
- Using the most updated information on toxicity references and self classifications available following classification guidance and legal ruling



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1. Introduction

The identification and characterisation of the hazards of a chemical is a key step in chemicals management, and as such part of all the regulatory schemes aiming at assuring safe use of chemicals. Identifying and communicating hazards are pivotal in the Globally Harmonized System of Classification and Labelling of Chemicals (GHS), which is an international United Nations (UN) system that addresses classification of chemicals by types of hazard and proposes harmonized hazard communication elements, including labels and safety data sheets (UN, 2015). Its main objectives are to harmonize and enhance human health and environment protection levels and to facilitate international trade in chemicals. The provisions of the UN GHS are implemented by the different jurisdictions. For example, the European Regulation on Classification, Labelling, and Packaging of substances and mixtures or CLP regulation EC 1272/2008 (EC, 2008) has applied the UN GHS conditions within the EU, taking into account the existing classification schemes. The OSHA Hazard Communication Standards (US, 2012) are the alignment to the UN GHS in the United States.

The goal of the UN GHS is to identify the intrinsic hazards found in substances and mixtures and to convey hazard information about these hazards (UN, 2015). This requirement also applies for complex inorganic materials like UVCBs (ores and concentrates, intermediates, slags) and mixtures such as alloys that need to be classified and labelled before being placed on the market or transported. The UN Model Regulations for Transport of Dangerous Goods and related legal instruments (e.g. ADR, RID, ADN, IMDG Code, MARPOL Annex V, IMSBC) refer to GHS criteria for some of their hazard classes. Finally, some of the Hazardous Properties criteria of Annex III of the EU Waste Framework Directive refer directly to the EU CLP criteria.

Complex inorganic materials present a number of specificities rendering their hazard characterisation and classification challenging.

- **Related to their composition:** Typically, inorganic UVCBs contain a variable number of metal constituents of which their elemental composition can be highly variable or, in some cases, their speciation/mineralogical composition. Chemical speciation allows knowing the the different chemical forms or minerals of metals in a sample. This variability precludes the selection of a representative sample for toxicity testing. In this context, it is recommended to assess the hazard of the UVCB, based on the hazards of its constituents.
- **Related to their definition and legal status:** complex inorganic materials can be considered differently (e.g. as substance or mixtures) in different jurisdictions which may result in different classification rulings and timings for implementation to be applied.
- **Related to their inorganic nature:** aspects like speciation/mineralogy, solubility/bioavailability, the presence of a matrix and the physical form will affect the hazard properties. For environmental endpoints, the GHS and CLP guidance include specific ruling for inorganics compounds and metals such as: Transformation Dissolution testing (TD_p) (UN GHS, Annexes 9.7 and 10 and Annex IV of the CLP) which allow different classification entries for massives and powders.
- **Related to data-sharing aspects:** classification of complex inorganic materials requires having access to the most recent harmonised and/or reliable self-classification, but also to high quality Ecotoxicity Reference Values (ERV) / Toxicity Reference Values (TRV) (definitions, see ECHA, 2015) for different inorganic metals (and metal compounds) and natural occurring minerals

MeClas is a web-based tool that was developed to address the specific challenges associated with the human health and environmental hazard assessment and classification of complex inorganic materials. It has been made freely available for industries and authorities after registration since 2010 and is accessible at www.meclas.org. Physical hazards are not in the scope. The tool is compliant with the UN GHS (UN, 2015), EU-CLP (EC, 2008) and US OSHA (US, 2012) requirements and mainly relies on the hazards of its constituents. It includes links to (EU REACH based) up-to-date ERV/TRVs, a tiered assessment approach and a series of features that are crucial for the classification of metals and complex inorganic materials, which – to date – the current (commercial) classification tools do not include.

MeClas tool is able to deal with the complexity and specificity of the toxicological and ecotoxicological hazard identification and classification of complex inorganic materials, whilst providing full recognition to information on inorganic specificities. MeClas also has the role of facilitator of consistent and harmonised classification of these complex materials throughout the industry and the supply chain and as platform for relevant data-sharing (self-classifications and ERV/TRV, read-across of speciation/mineralogy and bioavailability tests). Finally, the tool ensures a continuous update and information process on both classification ruling and ERV/TRVs.

The scientific principles behind MeClas are published in Verdonck et al. (2017).

1.1. History

In 2009, ARCHE developed an initial classification spreadsheet tool for complex materials, aimed at providing an automated expert judgement system for the hazard identification and classification of complex inorganic materials. The tool was subsequently amended to be suitable for assessing appropriate hazard identification and classification of ores and concentrates, complex intermediates, and has been proven to be relevant and efficient - but also "data hungry" (e.g. (eco)toxicity reference values have to be provided). The original tool includes several tiers, aiming for a progressive refinement of the classification through recognition of *speciation*, specific *mineral content* and the availability of *test data on the complex material in question*. However, it does not include an extensive database on toxicity reference data sets; neither it does include more complex features such as correction for Transformation Dissolution data (for the environmental classification, see Section 0) or bio-elution (for Human Health classification, see Section 0) and/or labelling guidance. The original spreadsheet tool had several limitations:

- It has been circulated widely in different versions, meaning that most of them are no longer up to date and no longer fulfil all refinement requirements
- Most complex materials, such as ores and concentrates, UVCB intermediates, slags with a unique EINECS number, and many other complex materials with unique EINECS numbers, will require hazard assessment and appropriate classification. These complex materials contain a spectrum of different metals (compounds) and minerals going beyond what is covered by the REACH consortia, thereby requiring extensive physico-chemical, toxicity and ecotoxicity reference data sets. Consortia do not usually have automatic access to such data from other metals/consortia
- As more (self-) classifications and toxicity reference values become available over time as a result of test- or data-gathering obligations under REACH and CLP, the tool requires continuous and rigorous updating,
- A user can only use predefined compositions and cannot define its own composition for its materials.

In view of this complexity, considering the above-mentioned limitations of the original tool, MeClas (Metals Classification tool) was developed to

- Deal with the complexity of the hazard classification of complex inorganic UVCBs
- Ensure consistent classification of complex inorganic UVCBs throughout the industry
- Provide full recognition to metal specific aspects
- Provide a platform for relevant data sharing between metal consortia (self-classifications and ecotoxicity reference values) and between metal consortia and companies (read-across of speciation and bio-availability tests)

Several versions were developed since then:

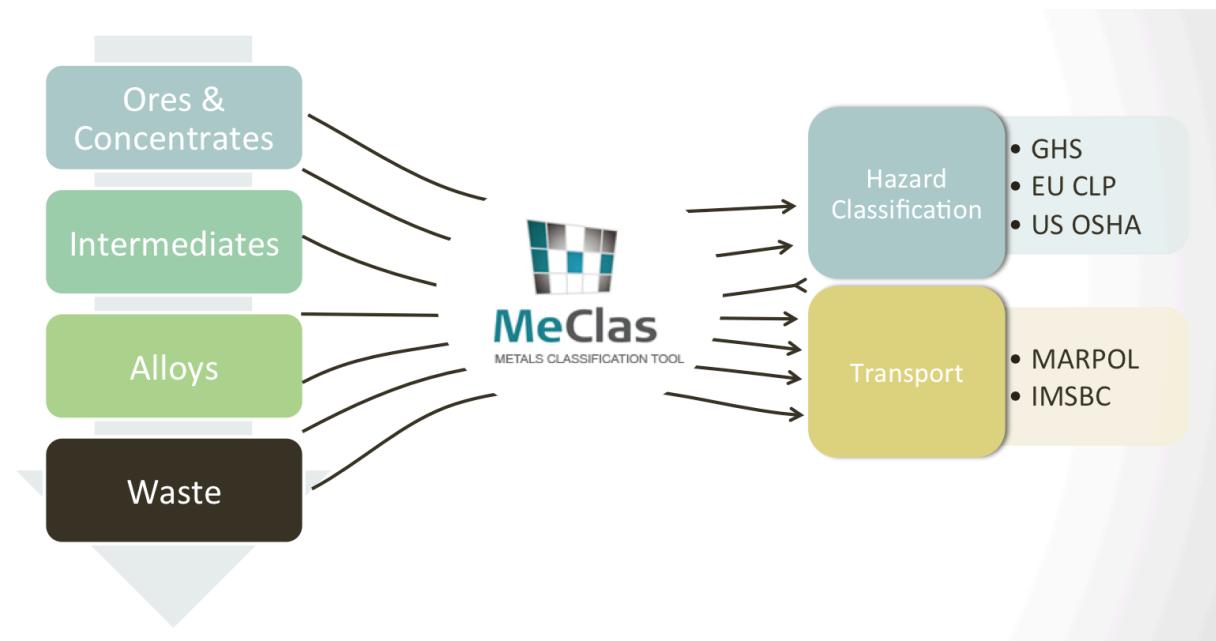
Version	Date	Main features
Version 1.0	Q3 2010	Spreadsheet tool translated into online tool
Version 2.0	Q4 2012	CLP 2nd ATP updates on environment and sensitization bio-accessibility correction for oral route module GHS mixture ruling module
Version 3.0	Q4 2014	Ores and Concentrates module

		Marpol transport module
Version 4.0	Q3 2015	Alloys module GHS database of self-classifications module US OSHA mixture ruling + database module EU older DSD/DPD classification module removed
Version 5.0	Q2 2018	New IT architecture allowing easier access for long term maintenance and updates, improved graphical user-interface (filtering options, copy operations, extended intermediate calculations Tier 2 human health inhalation (SWERF correction for SiO ₂)

2. Scope

MECLAS is therefore facilitating the hazard ID for complex metal materials under CLP throughout the metal industry. MECLAS is built on a limited number of simple and basic principles:

- A **tiered and inorganic specific approach**, allowing refinement in accordance with the following (not necessarily sequential) steps:
 - Tier 0: elemental concentrations only (and worst-case speciation and worst-case 100% solubility)
 - Tier 1: speciation data and mineralogical evidence (and worst-case 100% solubility)
 - Tier 2: correction based on release/solubility test data on the complex material and/or bio-elution
- A **up-to-date database** including the official EU harmonised (Annex VI of the CLP and subsequent ATPs) and self-classifications, specific concentration limits, the M-factors, ecotoxicity reference values (ERVs) values,...
- An **open building block structure**, enabling the inclusion of specific side modules if relevant (e.g. for Ores and Concentrates, for Transport Classification, additional reference lists (e.g. Japan), alloys, etc.). The core engine contains the CLP (and UN-GHS) hazard ID rulings and US OSHA, forming the base of the MECLAS tool.
- **Confidentiality assurance** for proprietary information: Confidentiality of proprietary data is assured by having the ERVs for such substances hidden



3. Technical background

3.1. *The classification rules and specificities for inorganics*

3.1.1 The generic application of classification mixture rules

As a general rule, available hazard data on a (or a similar) complex inorganic material as a whole should primarily be used to determine classification where applicable (EC, 2008). In case such data is lacking, the hazard assessment has to be based on the hazard of data on the individual ingredients (in case of mixtures) or constituents (in case of substances) to classify the material or mixture for the relevant hazard, using the so-called “mixture rules”. These mixture rules are either based on additivity or summation calculation rules (for endpoints like acute toxicity, skin irritation/corrosion or aquatic toxicity) or based on generic cut-offs. Those cut-offs are the minimum concentrations for a substance triggering classification. When a classified substance is present in a concentration above the generic cut-off value it contributes to the mixture classification even if it does not trigger classification of the mixture directly. In addition, for some human health hazards as for example carcinogenicity, mutagenicity or reproductive toxicity, generic or specific concentration limits are used in CLP. Specific concentration limits and generic concentration limits are limits assigned to a substance indicating a threshold at or above which the presence of that substance in another substance or in a mixture as an identified impurity, or individual constituent leads to the classification of the substance or mixture as hazardous (ECHA, 2015). For environmental aquatic hazards, M-factors are used in application of the summation method for the classification of mixtures containing substances that are classified as very toxic. For acute aquatic toxicity for example, the sum of the concentrations (in %) of all Acute category 1 classified ingredients (each multiplied by their acute M-factor) is calculated and if the sum exceeds 25%, the whole mixture is classified as Acute category 1.

These mixture rules are the “backbone” calculation module of MeClas and typically require information on the hazard categories for classification according to GHS/CLP, the concentration of the ingredients in the mixture (in %), the generic/specific concentration limits and M factors where necessary.

Decision trees on how to use these mixture rules should be applied for different complex inorganic materials like alloys (mixtures), UVCB ores and concentrates and intermediates (substances) have been included in MeClas.

3.1.2 Inorganic specific classification ruling

For inorganics, there are a number of specificities to consider in addition to the general classification rules originally developed for organic substances.

First, the ingredients of a complex inorganic material can be analysed in two ways, i.e. through elemental or speciation/mineralogical analysis. Elemental analysis is usually determined using ICP (Inductively Coupled Plasma spectroscopy). Speciation/mineralogical analysis is determined using sequential extraction/metal analysis and mineralogical analysis (e.g. XRD and microscopes equipped with EDS (Energy Dispersive Spectrometry) or WDS (Wavelength Dispersive Spectrometry) or Quantitative Evaluation of Minerals by SCANning electron microscopy – QEMSCAN) analysers. In contrast to organic materials, the elemental composition is often used as the primary key in defining a complex inorganic material because it is 1) more readily available for inorganic materials compared to a speciation/mineralogical analysis (it is indeed used in practice to determine the cost of the material), 2) more accurate/objective than a speciation/mineralogical analysis (from the analytical point of view), and 3) more complete as more trace elements can be measured,

which is particularly useful for elements not detected in speciation/mineralogical analysis. Elemental composition is to be coupled with speciation information for an appropriate hazard assessment.

Second, the hazard of complex inorganic materials is often determined by their solubility in various liquid media or the release of the toxic ion from the surface of the material. For example, in aqueous media the materials will undergo interactions that affect the release/solubilisation of metal ions, their partitioning between soluble and solid fractions and the prevailing metal species. It is thus necessary to consider whether toxic soluble metal species are likely to be formed and if so whether they are likely to be formed rapidly enough to cause concern. The rate and extent of the formation of soluble metal ions and metal compounds are known as “transformation/dissolution (T/D)” and this determines the aquatic bioavailability of the material tested. It can vary extensively between different compounds and the metal itself, and is therefore an important intrinsic factor in determining the appropriate environmental hazard class for the material in its given form. Therefore, the environmental hazard classification of inorganic complex materials can be refined in case information on T/D, generated following the guidance described in Annexes 9.7 and 10 of the UN GHS (2007), is available. To determine the acute aquatic hazard for metals, acute ERVs (derived from acute toxicity data) are typically compared with dissolution concentrations for a 7 days period, while the assessment of the chronic aquatic hazard considers comparison of chronic ERVs (derived from chronic toxicity data) with 28 days dissolution data. For metals, the loading can be related to a surface, thereby measuring a release/surface. A reduction or increase due to a matrix effect manifests itself as a change in the release/surface, independently from the shape or the form. It is this loading level which yields the level of metal ion equivalent to the available toxicity levels that can then be used to determine the acute or long-term aquatic hazard category appropriate for classification. Examples are described in Skeaff & Beaudoin (2014) for Nickel matte and Nickel ores and concentrates and in Skeaff et al. (2008) for alloys.

Similarly, for human health, one may consider the release of the metal ion in surrogate biological fluids (e.g. in gastric fluids) to estimate the bioavailable fraction of the metal that could cause systemic effects after oral exposure (Henderson et al., 2014). Discussions are ongoing with the EU regulatory authorities on how to best integrate bioavailability considerations in the context of CLP and achieve a standardised protocol to generate bioavailability estimates in vitro.

Thirdly, different classification entries are allowed for two different physical inorganic forms (both under GHS and CLP), i.e. for “metal massive form” or the “powder form” (particles < 1 mm), for environmental hazards.

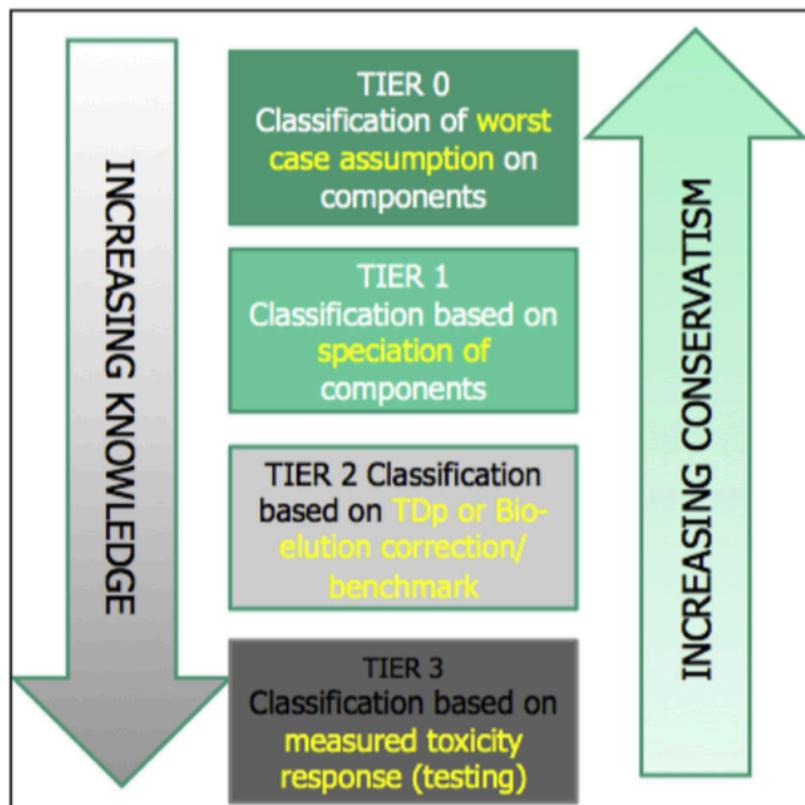
3.2. *The databases for harmonised classifications/self-classifications*

The MeClas tool is based on a number of databases that are at least yearly updated to ensure the latest and complete data is made available, i.e. 1) international industry-wide science-based self- classification GHS database (irrespective of regional implementations), 2) the EU CLP database including the official EU harmonised classifications (Annex VI of the CLP and subsequent updates in ATPs), specific concentration limits (SCL), M-factors and, where the classifications are not harmonised, completed with self- classifications from GHS self-classification database, and 3) the US database including IARC database for carcinogenicity (WHO, 2014) and, when not harmonised or for other endpoints, completed with self-classifications from GHS self-classification database. All databases in the tool are built on quality screened acute/chronic eco- toxicity (ERVs) at different pH values (i.e. pH 6, 7 and 8) and human health (TRVs) reference values. The tool is built in a flexible way and easily allows the addition of additional datasets, e.g. to allow compliance with GHS implementation in other countries such as Korea or Japan.

3.3. *Tiered approach: from elemental to bioavailable concentrations*

MeClas makes the best use of information (elemental, speciation or bioavailability data) using a tiered approach, depending on the level of information that is available. The better quality information is available, the higher the tier, reducing thereby the conservatism of the assessment and increasing its precision. This

This section outlines how the hazard of complex inorganic materials can be assessed and defined in a tiered way starting from a “minimum” material identity data set and worst-case assumptions to a more advanced material identity data set up to actual toxicity testing in Tier 3 (which is outside MeClas).



3.3.1 Tier 0 (worst case level)

Classification based on elemental analysis (and worst classifiable speciation and 100% solubility assumptions)

This first Tier is solely based on the quantification of the **elemental concentrations** of the constituents/ingredients in the complex inorganic materials. Elemental analysis is usually determined using ICP (inductively Coupled Plasma spectroscopy).

Tier 0 can be used for screening purposes or in case speciation/mineralogical data and bioavailability data are lacking. It can also be used for those (trace) elements for which speciation data are lacking (in case of incomplete speciation/mineralogical analysis). On the other hand, it is not recommended to use Tier 0 when complete speciation/mineralogical data or bioavailability are available (it is proposed to move to Tier 1).

The Tier 0 hazard classification generated by MeClas will be based on the worst-case classification species for every element of the material, to ensure its conservatism.

For example, for a UVCB including chromium (Cr), in the absence of speciation data that would allow to move to Tier 1, the tool will assume that the Cr is present as CrVI (CrO_3). This is indeed the species with the most severe classification in Annex VI of the CLP (e.g. compared to the CLP Annex VI group entry for “Cr compounds”). Another example can be given for arsenic (As) in UVCBs: MeClas will by default assume As_2O_3 because this is indeed the species with the most severe classification. MeClas will subsequently derive the classification based on the mixture toxicity rules as described in UN GHS (2015) or EU CLP (2008).

3.3.2 Tier 1 (correcting for chemical speciation):

Classification based on speciation/mineralogy of elements (and worst-case 100% solubility assumptions)

The second tier (Tier 1) requires more knowledge on speciation and is based on the determination of the **metal speciation/mineralogy**. Metal speciation/metal mineralogy can be assessed from sequential extraction/metal analysis and mineralogical analysis (XRD and microscopes equipped with EDS (Energy Dispersive Spectrometry) and WDS (Wavelength Dispersive Spectrometry) analyzers. The determination of the speciation requires in-depth knowledge of metal particularities.

However, the speciation results can easily be entered in MeClas. Speciation results usually come in two formats. Speciation results are usually expressed as a percentage relative to the total mixture or a percentage relative to the metal element. Input to MeClas requires the speciation results be expressed as percentage relative to the metal element. The tool subsequently classifies the inorganic materials based on elemental and speciation data and the mixture rules as laid down in UN GHS (2015) or EU CLP (2008). For example, **Error! Reference source not found.** shows that nickel is 100% distributed as massive, metallic Ni in the case study example (100% relative to Ni).

The example figure below illustrates that speciation results usually come in two formats.: either as relative % to the total mixture (e.g. Lead metal: 0.11%, Litharge 0.09% and Galena 0.09%) or relative % to the metal element, defined as distribution (e.g. Pb metal 42.78%, Litharge 31.85%, Galena 25.37%). Distribution percentages should not exceed 100% for each element. The classification is then based on elemental and speciation data.

Elemental Analysis

Cu	TOT %	0.60
As	TOT %	0.00
Fe	TOT %	12.20
Ni	TOT %	0.03
Pb	TOT %	0.84
Co	TOT %	0.21
Sb	TOT %	<0.01
Sn	TOT %	<0.01
Zn	TOT %	0.86
Mo	TOT %	
Ag	TOT %	<0.002
Se	TOT %	
Sr	TOT %	
Te	TOT %	
Bi	TOT %	
Cd	TOT %	
SiO ₂	KEM %	45.30
Al ₂ O ₃	TOT %	13.20
Cr ₂ O ₃	TOT %	0.19
K ₂ O	TOT %	3.70
MgO	TOT %	6.80
MnO	TOT %	0.30
Na ₂ O	TOT %	1.10
CaO	TOT %	11.00

Speciation Analysis

% relative to element		% relative to total mixture		
Distribution of iron				
CuFeS	0,42	CuFeS	Calcopyrite	0,44
FeCr ₂ O ₄	1,03	FeCr ₂ O ₄	Chromite	0,63
CoFeS	0,19	CoFeS	Villanovite	0,08
Cu	0,04	Cu	Copper	0,26
Fe ₂ SiO ₄	37,89	Fe ₂ SiO ₄	Fayalite	16,4
FeCo	4,91	FeCo	Fe-alloy	0,67
KAl ₂ Si ₃ O ₁₀	2,09	KAl ₂ Si ₃ O ₁₀	K-Al-silicate	32,11
Si(Fe,Al,Ca)O ₂ -3	11,87	Si(Fe,Al,Ca)O ₂ -3	Glass	9,65
CaSiO _x	32,78	Pb	Lead	0,11
ZnFeS	4,22	PbO	Litharge	0,09
Fe ₃ O ₄	4,54	PbS	Galena	0,09
Distribution of zinc				
FeCr ₂ O ₄	2,56	CaSiO _x	Ca-silicate	37,61
ZnFeS	53,93	ZnFeS	Sphalerite	1,33
Fe ₂ SiO ₄	17,88	Fe ₃ O ₄	Magnetite	0,54
KAl ₂ Si ₃ O ₁₀	2,26			
CaSiO _x	14,30			
Si(Fe,Al,Ca)O ₂ -3	9,07			
Distribution of lead				
Pb	42,78			
PbO	31,85			
PbS	25,37			
Distribution of copper				
CuFeS	49,61			
FeCr ₂ O ₄	0,09			
Cu	42,17			
FeCo	6,35			
KAl ₂ Si ₃ O ₁₀	0,94			
Si(Fe,Al,Ca)O ₂ -3	0,84			

Reference sample

These percentages
need to be filled out
in distribution

3.3.3 Tier 2 (correction for bioavailability):

Classification based on elemental analysis and measured release/solubility (T/D for environment and bioelution for human health)

Hazards classification of inorganic materials can be further refined by comparing the released bioavailable metal concentrations after specific time periods with ecotoxicological endpoints, using metal release data from T/D, or human health endpoints, using metal release from in vitro bioelution tests. Bioaccessibility is defined as the “fraction of a substance that dissolves under surrogate physiological conditions” and therefore is “potentially available” for absorption into systemic circulation. Bioelution refers to the in vitro extraction methods used to measure the degree to which a substance is released in artificial biological fluids (e.g. synthetic sweat, simulated gastric juice etc.), i.e. a substance’s bioaccessibility. In situations where the bioavailability of a substance/material is not known or where it is not feasible to determine this in vivo, bioaccessibility may be used to conservatively estimate bioavailability.

Classification is subsequently corrected by considering the bioavailable elemental and/or speciation concentration instead of the 100% soluble constituent concentration as in Tiers 0 and 1. For example, a material containing 1% cobalt metal of which only 0.2% is released after 28 days (long term aquatic hazard) will result in an available, soluble cobalt concentration of 1% x 0.2% or 0.002% to be further considered in the environmental mixtures rules (EC, 2008; UN, 2015).

Transformation dissolution tests (TDp) are conducted to determine the rate and extent to which metals and sparingly soluble metal compounds can produce soluble, available ionic and other metal-bearing species in aqueous media under a set of standard laboratory conditions, representative of those generally occurring in the environment. Bio-elution tests are conducted to estimate the bioaccessible fraction, i.e. the fraction of the material soluble under physiological conditions, by measuring the dissolution of the material in artificial biological fluids. Classification is then corrected by considering the bio-available elemental and/or speciation concentration instead of the 100% soluble constituent concentration as in Tiers 0 and 1.

Elemental Analysis			Speciation Analysis			Bioelution Analysis-oral route		
			% relative to element			concentration		
Cu	TOT %	0.60				Cu	ug/L	1,10
As	TOT %	0.00				As	ug/L	<DL
Fe	TOT %	12.20				Fe	ug/L	8,20
Ni	TOT %	0.03				Ni	ug/L	0,03
Pb	TOT %	0.84				Pb	ug/L	1,8
Co	TOT %	0.21				Co	ug/L	0,02
Sb	TOT %	<0.01				Sb	ug/L	<DL
Sn	TOT %	<0.01				Sn	ug/L	<DL
Zn	TOT %	0.86				Zn	ug/L	<DL
Mo	TOT %					Mo	ug/L	<DL
Ag	TOT %	<0.002				Ag	ug/L	<DL
Se	TOT %							
Sr	TOT %							
Te	TOT %							
Bi	TOT %							
Cd	TOT %							
SiO ₂	KEM %	45,30						
Al ₂ O ₃	TOT %	13,20						
Cr ₂ O ₃	TOT %	0,19						
K ₂ O	TOT %	3,70						
MgO	TOT %	6,80						
MnO	TOT %	0,30						
Na ₂ O	TOT %	1,10						
CaO	TOT %	11,00						
Distribution of zinc								
				FeCr ₂ O ₄	2,56			
				ZnFeS	53,93			
				Fe ₂ SiO ₄	17,88			
				KAlSiO _x	2,26			
				CaSiO _x	14,30			
				Si(Fe,Al,Ca)O ₂₋₃	9,07			
Distribution of lead								
				Pb	42,78			
				PbO	31,85			
				PbS	25,37			
Distribution of copper								
				CuFeS	49,61			
				FeCr ₂ O ₄	0,09			
				Cu	42,17			
				FeCo	6,35			
				KAlSiO _x	0,94			
				Si(Fe,Al,Ca)O ₂₋₃	0,84			
Distribution of iron								
				CuFeS	0,42			
				FeCr ₂ O ₄	1,03			
				CoFeS	0,19			
				Cu	0,04			
				Fe ₂ SiO ₄	37,89			
				FeCo	4,91			
				KAlSiO _x	2,09			
				Si(Fe,Al,Ca)O ₂₋₃	11,87			
				CaSiO _x	32,78			
				ZnFeS	4,22			
				Fe ₃ O ₄	4,54			

3.3.4 Tier 3: Classification based on toxicity testing

This approach is based on actual (eco-)toxicity testing, and the results can be directly used for classification. This tier is not included in the MeClas tool.

3.4. How is this tiered approach built in MeClas?

3.4.1 Format of a composition

Each composition is built with the elemental analysis as the primary identity key. There are several reasons to use the elemental composition as the primary key in defining a complex inorganic material:

- Elemental analysis is usually more readily available than speciation analysis
- Elemental analysis is more accurate than speciation/mineralogical analysis (from the analytical point of view)
- Elemental analysis is often more complete: more trace elements are measured which are often not detected in speciation/mineralogical analysis

The format of each composition is built following the tiered approach:

Reference composition name				Show details	Filter Composition	Calculate			
Element	Concentration	Classification	Source	% distribution	Formula	TDP 7days	TDP 28days	Bio-elution oral	SWERF inhalation
Ag	0.00200	Ag massive (>1 mm)	not classified		Ag	0.00000	0.00000		
		Ag (other not classified compounds/species)	not classified		Ag				
		Ag compounds (e.g. AgCl, AgI, AgBr)	self classification EPMF		Ag				
		Ag nano-powder (<100 nm)	self classification EPMF		Ag				
		Ag powder (<1 mm and >100 nm)	self classification EPMF		Ag				
		Ag ₂ CO ₃	self classification EPMF		Ag ₂ CO ₃				
		Ag ₂ O	self classification (ECHA dissemination website)	100.00000	Ag ₂ O				
		Ag ₂ SO ₄	self classification EPMF		Ag ₂ SO ₄				
		AgNO ₃ (aq)	self classification EPMF		AgNO ₃				
		AgNO ₃ (solid)	Annex VI		AgNO ₃				

Tier 0,1,2 → Tier 1 → Tier 2

If only the concentration of the different elements of the complex material is available, then the only classification option is to use Tier 0, which is the worst-case calculation. If, besides concentrations, the speciation column distribution is also filled out, then a Tier 1 approach can be made. When TDP and bio-elution results are available, a Tier 2 approach can be calculated.

Note: For Tiers 1 and 2, the distribution percentages ALWAYS have to be filled in (even when there is only one form of a specific species). For example, Ag element is in the form of AgNO₃ for 100%.

3.4.2 How does it work in the background?

In MECLAS, the elements are linked to mineral or speciation forms, which in turn are linked to classification entries.

1. Link Elements to Mineralogy/Species

To link the elements to the appropriate species/minerals, the results from worst-case assumptions (e.g. in Tier 0, selection of the species with the worst classification), user expert judgment or species/mineralogical analysis (as in Tier 1) is used: e.g.

- As: 100% in the form of FeAs
- Cu: 49% in the form of Cu₂S and 51% in metal form
- Pb: 98.65% in the form of PbO; 1.05% in the form of PbS and 0.30% in the metal form

In the case of several species, the percent of distribution can be calculated:

e.g. Pb in the form of Pb metal (4%) and PbO (1%) => percent contribution is respectively 80% Pb metal and 20% PbO. In the case of multiple samples/contributions, the worst case can be taken.

If, for some elements, no mineralogical data are available, the metal, oxide, sulfide or sulphate forms are assumed.

2. Link mineral/species to classification entry

The minerals/species are then linked to classification entries, e.g.

- PbO links to the “Pb compounds” classification
- SbSnO links to the “Sb compounds” classification

Some minerals are linked to several classification entries, e.g. PbAsO links both to the “Pb compounds” and the “As compounds” classification.

Metal in inter-metallic forms (such as alloys) can often be considered as “metal form”. It is up to the user to decide if read-across can be made to a similar compound
 – FeZnO could link to the “ZnO” classification entry
 – CoNiSbSO₄ could link to both the “NiSO₄” and “CoSO₄” classification entry (and also to the “Sb compounds” classification)

A link can also be made to different physical forms (if available): the “metal massive form” or the “powder form” (particles < 1 mm).

3. Molecular weight conversion

All elemental percentages have been transformed to the molecular weight of the relevant classification entry, e.g.

1. For As compounds other than arsenic trioxide and arsenic pentoxide, the molecular weight of As metal is used (“Arsenic compounds”, with the exception of those specified elsewhere in Annex VI)
2. For PbO, use of the molecular weight of Pb metal (“Pb compounds” entry; a PbO entry does not exist)
but ZnO: conversion to molecular weight of ZnO (“ZnO” entry)
3. PbCuO: conversion to the molecular weight of Pb metal (“Pb compounds” classification) and CuO (copper(II)oxide classification)

4. Substance classification database

Once the speciation/mineralogical composition is calculated (each species% relative to total material), the mixture rules can be applied using the classification of each species.

3.5. Legal context and rules

Following legal frameworks are implemented in MECLAS:

Legal framework	Geographical area	Mixture ruling	Background database of harmonized and self-classifications
GHS	International	Implemented	Self-classifications
CLP	European Union	Implemented	Annex VI + ATPs + self-classifications
OSHA	United States Canada	Implemented	GHS + IARC monographs vol 1-112 for carcinogenicity

Other regional implementations of GHS may be considered in MECLAS in the future.

3.5.1 International

The Globally Harmonised System (GHS) is an international standardised system for classifying chemicals and communicating their health and environmental hazards to consumers, workers, transport workers and emergency responders. The system is undergoing worldwide implementation at national or regional level. It also provides a basis for the harmonization of rules and regulations on chemicals at national, regional and worldwide level. Its main aims are to facilitate international trade in chemicals and to maintain the existing level of protection of human health and the environment. The UN GHS incorporates a “building block” approach to facilitate implementation, leaving it to the discretion of legislators to decide on the extent of implementation. The drawback of this building block approach is that classification rules may still differ between regions.

3.5.2 European Union

The CLP is the Regulation on the Classification, Labelling and Packaging of substances and mixtures. This Regulation aligns the previous EU legislation on Classification and Labelling of Substances (Dangerous Substances Directive DSD, 67/548/EEC) and Preparations (Dangerous Preparations Directive DPD 1999/45/EC) to the UN GHS. The CLP Regulation was published in the Official Journal on 31 December 2008 and entered into force on 20 January 2009. According to the Regulation, the deadline for substance classification according to the new rules is December 2010, while for mixtures the deadline is June 1, 2015. The CLP Regulation will ultimately replace the existing rules for Classification and Labelling of substances and preparations (DSD and DPD) after this transitional period.

The legal text of the CLP can be found on: <http://eur-lex.europa.eu/LexUriServ/LexUriServ.do?uri=CELEX:32008R1272:EN:NOT>

The guidance (2011) developed by ECHA for the application of the CLP criteria can be found on:

<http://echa.europa.eu/web/guest/support/guidance-on-reach-and-clp-implementation>. This includes specific guidance for the environmental classification of metals and metal compounds.

Discussions on the “removal from the water column” are still ongoing. In the meantime, reference is made to ECHA CLP Guidance (2009) on “removal from the water column”.

3.5.3 United States and Canada

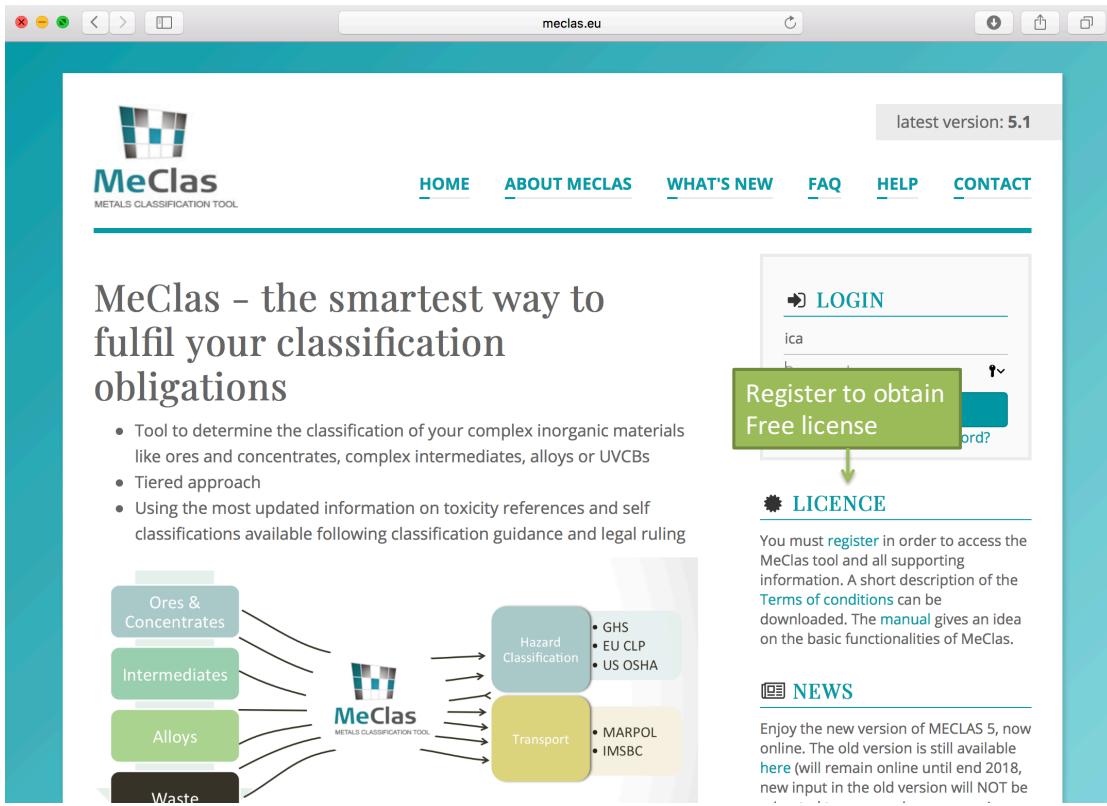
OSHA (Occupational Safety and Health Administration) is part of the United States Department of Labor. OSHA assures safe and healthful working conditions for men and women by setting and enforcing standards and providing training, outreach, education and assistance. The OSHA classification is based on GHS, with exception of the carcinogenicity endpoint. This endpoint is covered by the IARC Monographs, a list of chemicals, complex mixtures and agents that can increase the risk of human cancer. The agents classified by the IARC Monographs, volumes 1-112 are implemented in the MeClas database.

3.6. *Validity of MeClas*

The compliance of MeClas to the five OECD principles for establishing the validity of QSAR (Quantitative Structure Activity Relationships) models for use in regulatory assessment of chemical activity is assessed for validity: defined endpoint, unambiguous algorithm, a defined domain of applicability, predictive measure and if possible, a mechanistic interpretation. More detailed information can be found in Verdonck et al. (2017).

4. How to use MeClas?

4.1. Registration



The screenshot shows the MeClas homepage with a teal header. In the top right corner, it says "latest version: 5.1". Below the header, there are navigation links: HOME, ABOUT MECLAS, WHAT'S NEW, FAQ, HELP, and CONTACT. A "LOGIN" button is visible on the right. A green box highlights the "Register to obtain Free license" button. Below this, a "LICENCE" section is shown with a note about registering for access. A "NEWS" section at the bottom right discusses the new version 5.1.

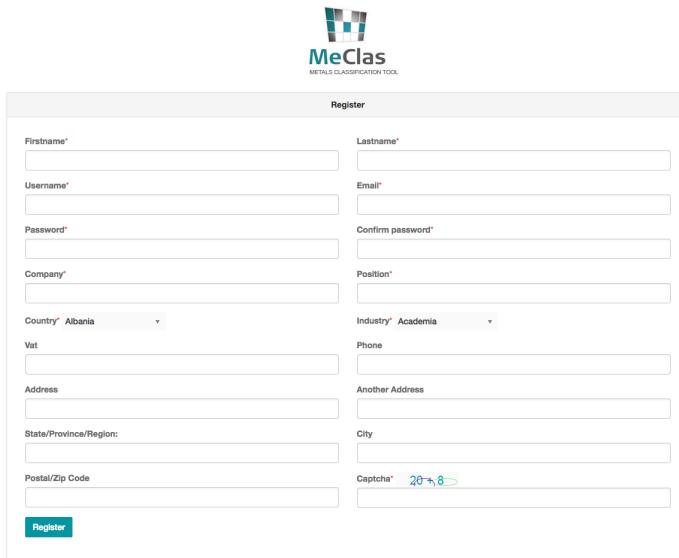
MeClas – the smartest way to fulfil your classification obligations

- Tool to determine the classification of your complex inorganic materials like ores and concentrates, complex intermediates, alloys or UVCBs
- Tiered approach
- Using the most updated information on toxicity references and self classifications available following classification guidance and legal ruling

Ores & Concentrates, **Intermediates**, **Alloys**, **Waste** → **Hazard Classification**: GHS, EU CLP, US OSHA

→ **Transport**: MARPOL, IMSBC

In order to use MeClas, please first register in order to create an account by filling in the form below.

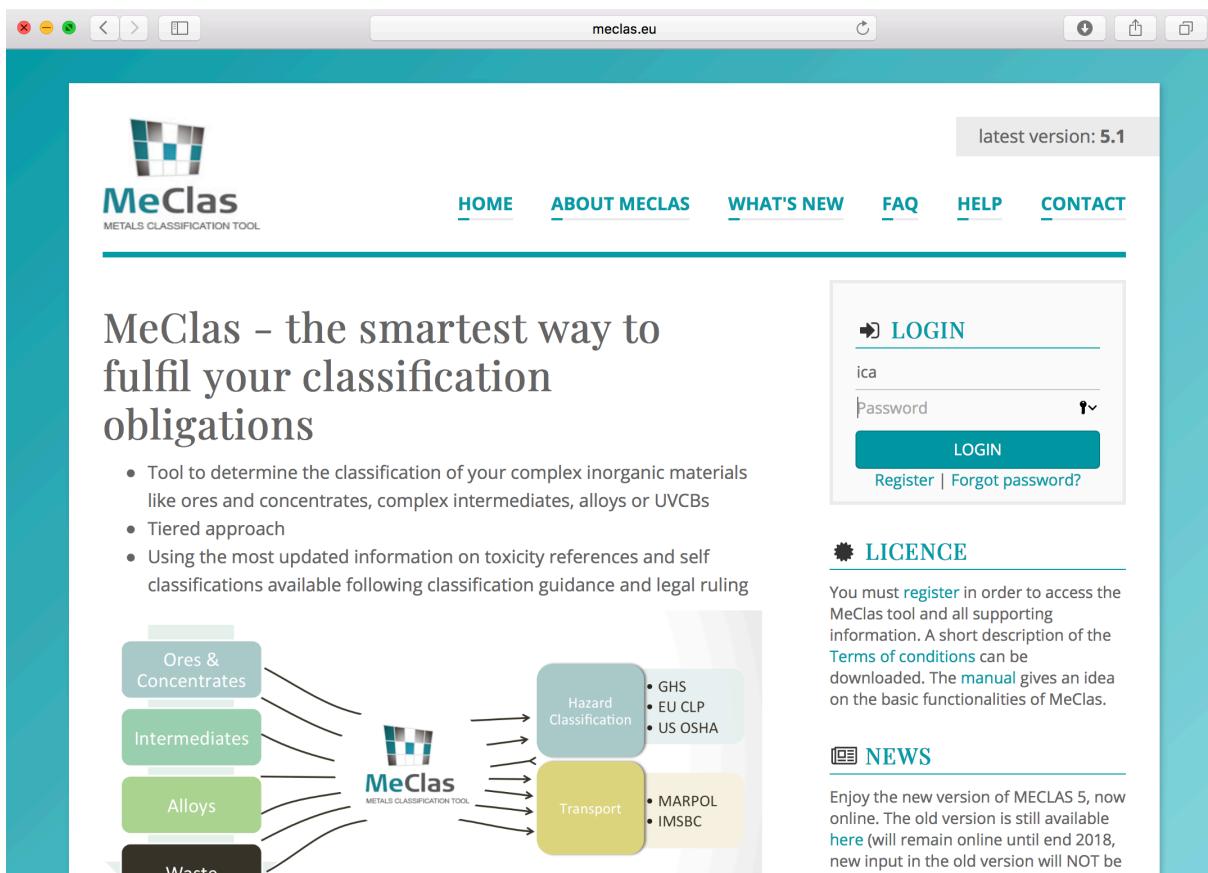


The form has fields for Firstname*, Lastname*, Username*, Email*, Password*, Confirm password*, Company*, Position*, Country*, Industry*, Vat, Phone, Address, Another Address, State/Province/Region, City, Postal/Zip Code, and Captcha*. A "Register" button is at the bottom.

On the MeClas website (www.MeClas.eu), users can log in by entering their username and password. In order to use the tool, a registration and acceptance of the terms of conditions is required. More general information about MeClas can be found in the toolbar: version number, FAQ, what's new page. Questions can be asked and further information can be requested by filling out the form in the CONTACT tab.

When the maximum number (5) of free compositions is reached, an upgrade is possible. Funding members can enter an unlimited amount of compositions. Please send an email to info@meclas.eu in order to find out how to upgrade the account.

4.2. Login



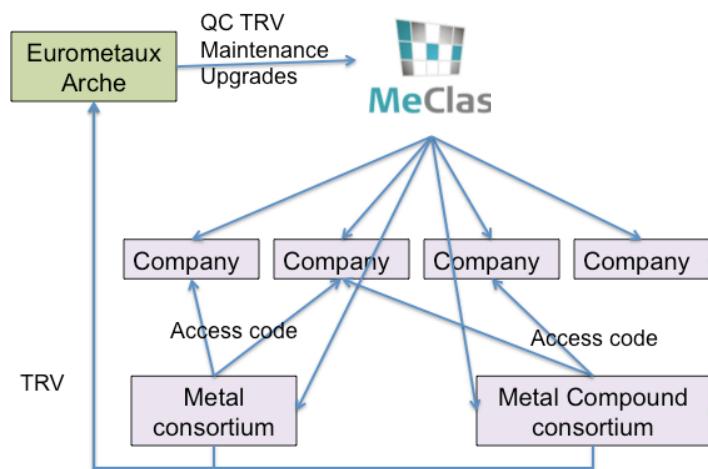
When logged in, the company can view its profile by clicking 'Profile'. The name of the user and the organisation, the position, e-mail and phone number of the registrant can be filled in or edited. The password can also be changed. If the user has forgotten his password, he can leave his e-mail address and will receive an e-mail with further information on how to obtain a new password.

After logging in, an extra tab will pop up (TOOL).

4.3. MeClas Users

There are several actors/type of users involved in MeClas:

- Eurometaux and Arche are the **MeClas managers**: they collect self-classifications from metal (compound) consortia and update the background database in MeClas. They also maintain the software and organise updates with input from the Steering Committee meeting.
- **Companies**: individual companies can use MeClas to create their own company-specific compositions (called reference compositions). These compositions can only be accessed by the company.
- **Metal (compound) consortia**: Moreover, for metal and metal compounds, Consortia can create reference compositions, which can be shared with the companies. The companies can only import the reference composition if the access code or share code is known. The companies can only adapt the elemental concentrations of the reference composition (only exception is for ores and concentrates where the speciation/mineralogy can also be adapted).



MECLAS consequently enables:

1. Companies to create and manage their own company-specific (ref) compositions
2. Consortia (or Technical Lead Companies) to create and manage reference compositions
3. Companies to edit and manage company-adapted versions of the Consortia reference compositions

The first and second points are covered by the same functionality. The third point is further elaborated below.

For some complex metal materials, due to the intrinsic similarities of the composition depending on the process or source, a complete mineralogical analysis for all batch samples from all companies is not required. Samples can therefore be selected and fully analyzed for representative UVCB processes and original materials (= Representative Compositions, Reference Compositions/Samples). In view to characterize a reference composition, the following points need to be considered:

- For each complex mixture, the range in elemental compositions within and across all companies should be assessed and compared.
- For each complex mixture, detailed information on the different process conditions (if any) should be evaluated in view of potential differences in resulting mineralogy (i.e. speciation). For each specific process type, a representative sample can be selected and the metal species and/or mineralogical forms can be determined (by means of XRD analysis).

Consequently, **the speciation/mineralogical pattern determined for a sample that is representative of a particular process or source and conditions is the same for all materials produced or mined according to the same process, source or conditions**. Since the mineralogical composition is expressed as a relative percentage for each element, a higher concentration for a particular element will automatically lead to a higher concentration of the corresponding mineral/species.

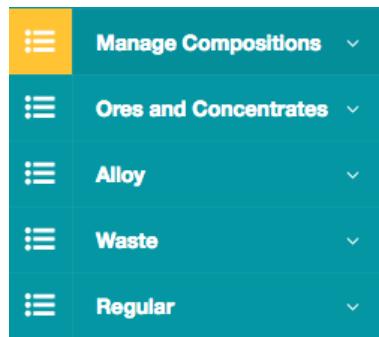
Even so, the bioavailability/solubility pattern determined for a sample that is representative of a particular process (source & conditions) is the same for all materials produced according to the same process. The release is expressed as a relative percentage for each element. Consequently, a higher concentration for a particular element will automatically lead to a higher concentration of the releasing mineral/species.

The table hereunder summarizes the two paragraphs above.

Testing	By	Read-cross within one UVCB (from one company to another company)
Elemental analysis	For each UVCB: by each company and for multiple batchesstreams	None
Speciation/mineralogical analysis	In case of refining the hazard identification of an UVCB: by consortium or company for one or more carefully selected representative materials	From reference composition to all company compositions (for which source and process conditions is the same)
TDP or bio-elution analysis	In case of further refining the hazard identification of an UVCB: by consortium or company for one or more carefully selected representative materials	From reference composition to all company compositions (for which source and process conditions is the same)

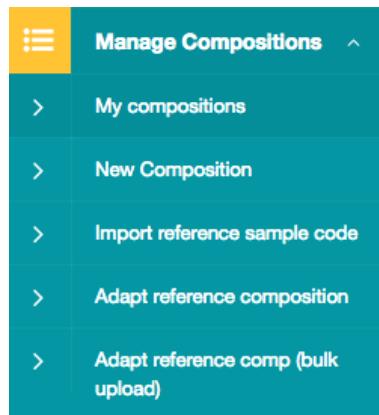
4.4. Input user interface: material composition

Select one of the following options in the TOOL tab:



4.4.1 Manage compositions

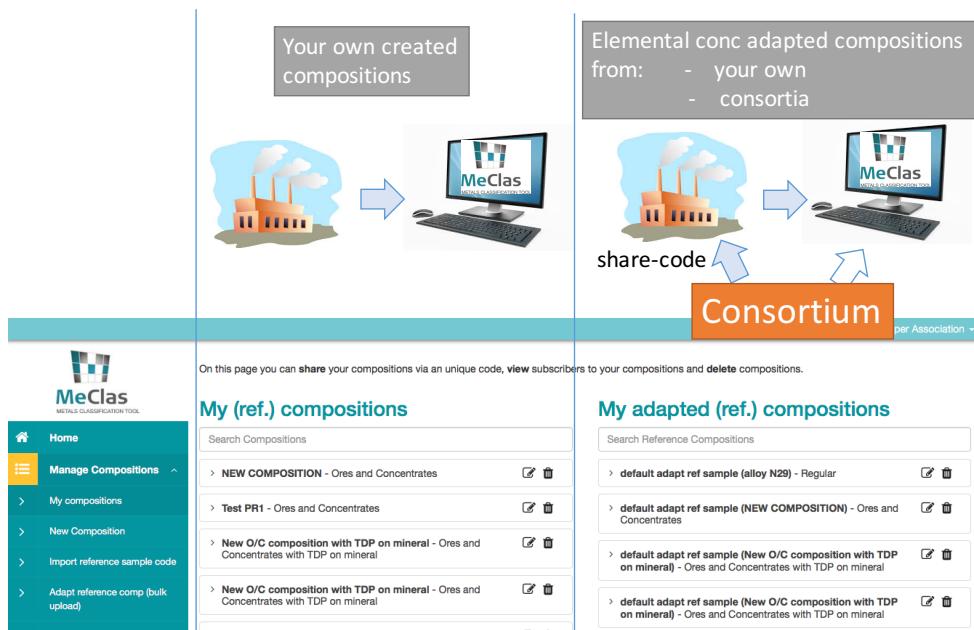
Select one of the following possibilities in the TOOL > MANAGE COMPOSITIONS tab:



4.4.1.1. My compositions

As a consequence of the different MeClas users (see section 4.3), MeClas defines two types of compositions (see figure below):

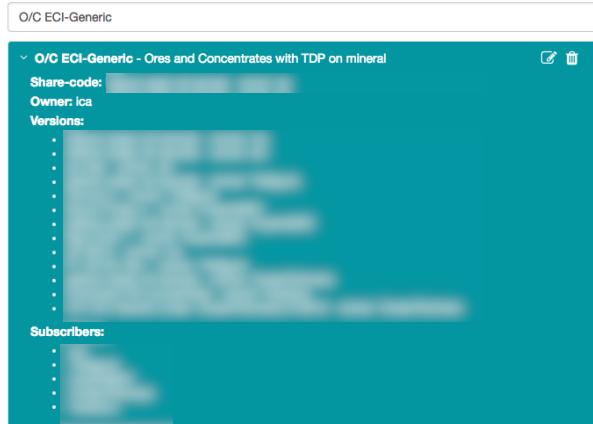
- **My (reference) compositions:** these compositions are created and managed by you. They are not visible to other MeClas users unless you shared the share code with them.
- **My adapted (reference) compositions:** these adapted compositions are alternative versions of reference compositions either created by yourself or obtained via share code from consortia.



To **edit** a composition, click the edit icon.

To **share** compositions, click the arrow icon and share the share-code. The user receiving the sharing code cannot edit the composition. The user can only run elemental adaptations of the reference compositions (the reference composition is not changed). These adapted reference compositions are so-called versions. In this box you can also **view** subscribers to references compositions and their version names of the adapted reference composition.

My (ref.) compositions



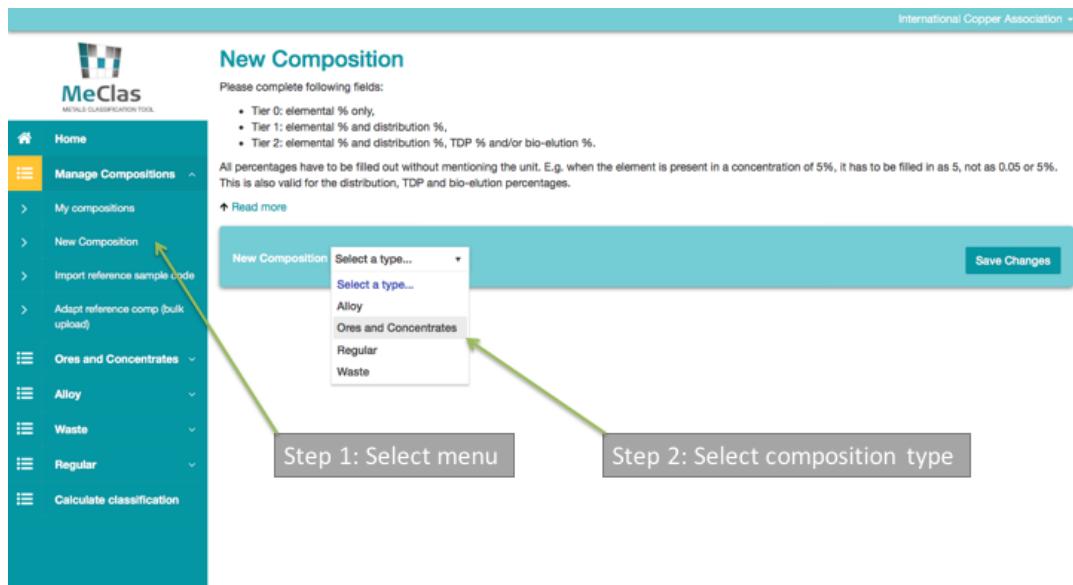
This screenshot shows the "My (ref.) compositions" page. It includes a search bar at the top and a list of compositions. One item is expanded to show its details:

- O/C ECI-Generic - Ores and Concentrates with TDP on mineral**
- Share-code:** [REDACTED]
- Owner:** Ica
- Versions:** [REDACTED]
- Subscribers:** [REDACTED]

To **delete** compositions, click the trash icon. Note that when compositions are deleted, the users who are subscribed to this composition (via a share code) will also lose their data!

4.4.1.2. New composition

A new (reference) composition can be created by clicking the link ‘new composition’ (step 1) and selecting the composition type (step 2). The “regular” composition type is the most generic, exhaustive and common type to be used for inorganic materials. An user may also select “ores and concentrates”, “alloys” or “waste” composition type. These composition types are 1) more simplified (compared to the “regular” composition type) and 2) have specific features (e.g. in a “waste” composition, an user can input percolation test results).



The concentration of the different elements can be filled out. Information about the distribution, TDp and bio-elution can also be entered. Fill out the following fields:

- Tier 0: elemental % only,
- Tier 1: elemental % and distribution %,
- Tier 2: elemental % and distribution % and TDp % (7 days and/or 28 days test) and/or bio-elution %.

Please keep in mind that changes are not saved automatically. Click the “save changes” button to save what you have edited.

International Copper Association →

New Composition
 Complete
 Elemental composition
 Speciation composition
 TDP if relevant
 and save

New Composition Ores and Concentr... ▾

Save Changes

Reference composition name: New composition

Ores and Concentrates with TDP on Mineral Show details

Filter Composition

Unknown acute toxicity oral route (%)

Unknown acute toxicity dermal route (%)

Unknown acute toxicity inhalation route (%)

pH of TDP test

Surface area (m²/g) from reference material tested in TDP test

Surface area (m²/g) of other than tested sample

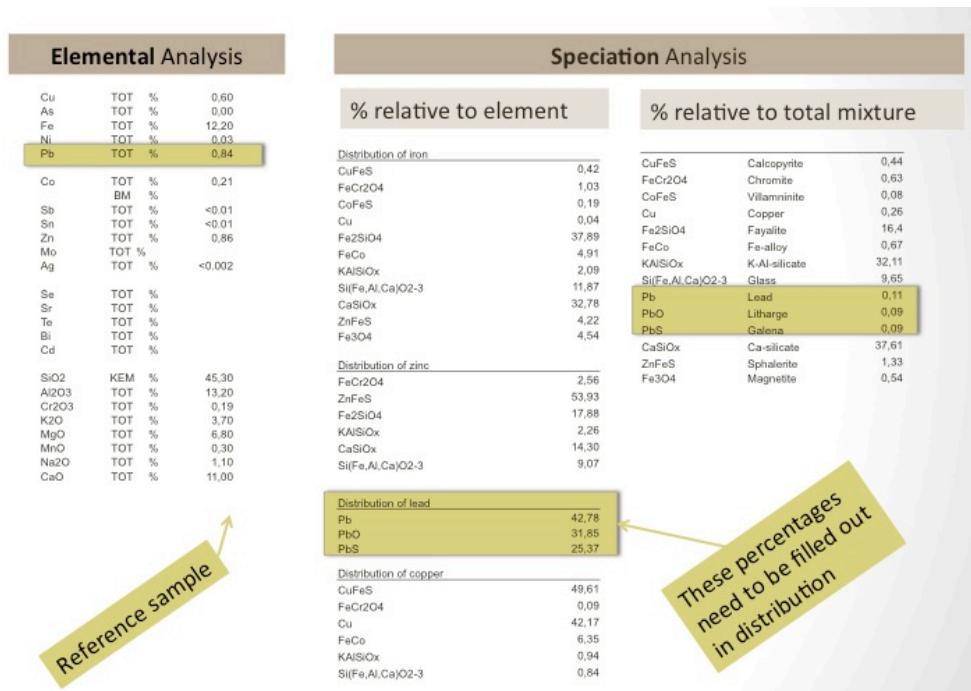
Element	Concentration	Classification	Source	% distribut...	Formula	TDP 7days	TDP 28days	Bio-el...
Ag		Ag massive (>1 mm)	not classified	0.00000	Ag	-100.00000	-100.00000	100.00000
		Ag compounds (e.g. AgCl, AgI, AgBr)	self classification EPMF	0.00000	Ag			100.00000
		Ag ₂ CO ₃	self classification EPMF	0.00000	Ag ₂ CO ₃			100.00000
			self					

Elemental percentage

All numbers should be filled out without mentioning the unit (%). For example, when Ag is present in a concentration as 5 % AgNO₃, it should be entered as 5 (not as 0.05 or as 5%). This is also valid for the elemental, TDp and bio-elution percentages.

Distribution percentage

Distribution percentages relate to the speciation (Tier 1), and should not exceed 100% for each element. As demonstrated in the Figure below, distribution percentages should not relate to the total composition of the metal mixture, but should relate to the element/metal.



By default, 100 % distribution for the worst-case species is applied for each element. If detailed information is available about the species/mineral in which each element appears in the composition, one can manually change the distribution percentages (and remove the 100 % next to the worst-case form to avoid double calculations). If this kind of information is not available, maintain the default value as a worst-case approach.

The sum of the distribution percentages of each element must be equal to 100%. This example can be filled out but is not possible (sum is 400%):

Al		Al massive/Al compounds	not classified	Al	100
		Al powder (pyrophoric)	Annex VI	Al	100
		Al powder (stabilised)	Annex VI	Al	100
		Al silicate	not classified	Al ₂ SiO ₅	100

This, on the other hand, is correct (sum is 100%):

Al		Al massive/Al compounds	not classified	Al	1
		Al powder (pyrophoric)	Annex VI	Al	80
		Al powder (stabilised)	Annex VI	Al	19
		Al silicate	not classified	Al ₂ SiO ₅	19

Note: For Tiers 1 and 2, the distribution percentages must ALWAYS be filled in and the sum must equal 100 %. If you don't have information about the exact species, you can use the default species as a worst-case assumption.

Al		Al massive/Al compounds	not classified	Al	
		Al powder (pyrophoric)	Annex VI	Al	100.00000
		Al powder (stabilised)	Annex VI	Al	
		Al silicate	not classified	Al ₂ SiO ₅	

If an element or (self-)classification entry is missing, please send an email to info@meclas.eu. The new entry will be evaluated (quality control) by Eurometaux's selected quality control group, for inclusion in MeClas.

TDP percentage

In the column with TDP percentages a default value of 100% (related to complete solubility and noted in MeClas as "100") for every element is initially filled out for the 7 days test. These predefined percentages can be replaced by actual TDP translation factors derived from TDP test results. The TDP translation factors that should be entered correspond to the % solubility at 1, 10 or 100 mg/L sample loading (7 days test results) or 0.1 or 1 mg/L sample loading (28 days test results) for each tested metal. The % solubility can be calculated from the mean metal release and the maximum metal release expected from the sample composition (taken into account the sample loading rate).

In MeClas (link is in description under "New composition"); a simple excel calculator sheet is provided that can be used to calculate the value that should be entered in the TDP column. Expand the 'Read more' section to download the TDP % calculator.

Below you can find a screen shot of the calculator sheet mentioned above. Dependent on the sample loading rate (1-10-100 mg/L) that was assessed the top, middle or bottom panel should be used to calculate the TDP translation factor. For each tested metal, fill out the mean TDP result ($\mu\text{g}/\text{L}$) and the metal concentration (%) that was initially present in the sample (fields that should be completed are highlighted in orange). The TDP translation factor that should be entered in MeClas appears then in the yellow field.

Loading rate 1 mg/L - 7 or 28 days

Element	T/D result, mean ($\mu\text{g}/\text{L}$)	Concentration in original tested sample (%)	Maximum expected ($\mu\text{g}/\text{L}$) = Theoretical content at 1 mg/L	Solubility (%) = Translation factor
	200	40	400	50

Loading rate 10 mg/L - 7 or 28 days

Element	T/D result, mean ($\mu\text{g}/\text{L}$) - 10 mg/L	Concentration in original tested sample (%)	Maximum expected ($\mu\text{g}/\text{L}$) = Theoretical content at 10 mg/L	Solubility (%) = Translation factor
	2000	40	4000	50

Loading rate 100 mg/L - 7 or 28 days

Element	T/D result, mean ($\mu\text{g}/\text{L}$) - 100 mg/L	Concentration in original tested sample (%)	Maximum expected ($\mu\text{g}/\text{L}$) = Theoretical content at 100 mg/L	Solubility (%) = Translation factor
	20000	40	40000	50

If the release of one of the tested metals is below the detection limit, zero should be filled out as TDP percentage. For metals where no TDP results are available, the default value of 100 should be maintained to avoid an underestimation of the classification result. Note that the TDP translation factor for metal powder can be entered in the same field as for metal massive.

Bio-accessibility percentage

General note: The methodology and regulatory acceptance for bio-elution correction is still ongoing and will be updated as soon as more information becomes available. For the moment, only the "oral route" bio-accessibility correction is implemented. For SiO₂, a correction for the "inhalation route" is also implemented. For more information, the reader is referred to the Eurometaux roadmap on bio-elution.

The bio-elution percentages that should be filled out in MECLAS correspond to the % solubility at 200 mg/L sample loading for each tested metal. An excel calculator sheet can be found in MeClas (link is in description under "New composition") after expanding the 'Read more' section.

Below you can find a screen shot of the calculator sheet mentioned above. For each tested metal fill out the mean bio-elution result ($\mu\text{g}/\text{L}$) and the metal concentration (%) that was initially present in the sample (fields that should be completed are highlighted in orange). The bio-elution translation factor that should be entered in MeClas appears then in the yellow field.

Sample loading 200 mg/L

Element	bio-elution result, mean ($\mu\text{g}/\text{L}$)	Concentration in original tested sample (%)	Maximum expected ($\mu\text{g}/\text{L}$) = Theoretical content at 200000 $\mu\text{g}/\text{L}$	Solubility (%) = Translation factor
Pure metal	1272	100	200000	0.636
UVCB	1.8	0.84	1680	0.1071429

μg metal released from Material	1.8
μg metal present per μg Material tested	1680
μg metal released from pure metal	1272
μg pure metal tested	200000

$$\begin{aligned} \text{Relative bio-accessibility} &= (\mu\text{g} \text{ metal released from UVCB} / \mu\text{g} \text{ metal present per } \mu\text{g} \text{ UVCB tested}) \\ &/ (\mu\text{g} \text{ metal released from pure metal} / \mu\text{g} \text{ pure metal tested}) \end{aligned}$$

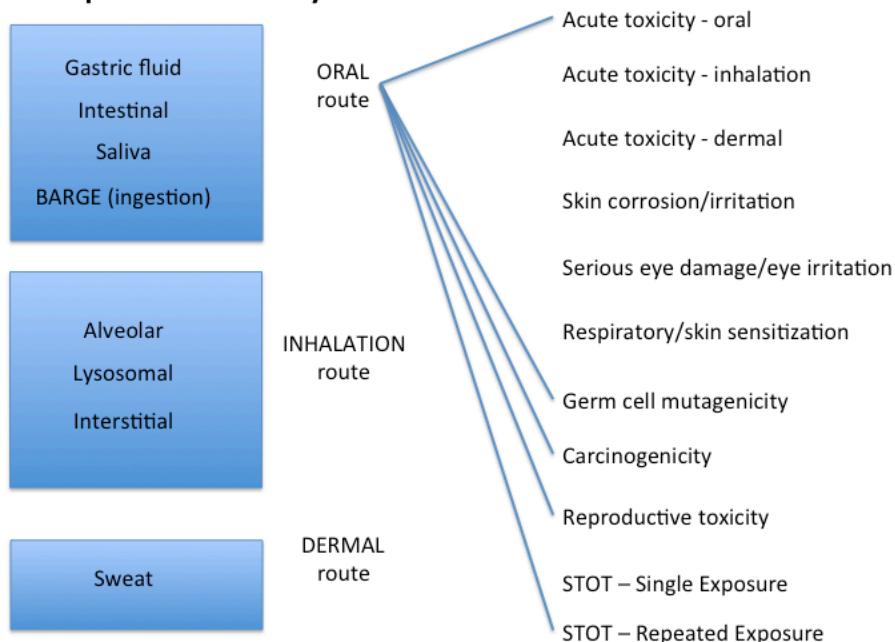
0.1684636
16.846361 %

In case of "oral route" bio-elution tests (such as gastric fluid, intestinal, saliva, BARGE), one can assume that the measured metals in the gastric fluid will be present in the form of soluble metal compounds. Bio-elution

percentages should then be filled out in the row of the soluble compound (in general the sulphate form is used for gastric test). The value of zero should be entered for the other compounds of that metal. If the bio-elution for one of the tested metals is below the detection limit, zero should be filled out as bio-elution percentage. For metals where no bio-elution results are available a default value of 100 should be entered in the row that corresponds with the speciation form selected for Tier 1.

It is important to note that currently the “oral route” bio accessibility correction is done for following human health endpoints in scheme below. In case chronic endpoints (e.g. carcinogenicity) are caused by other than oral route, the user should not use oral route correction.

Endpoints affected by Tier 2 human health bio-elution corection



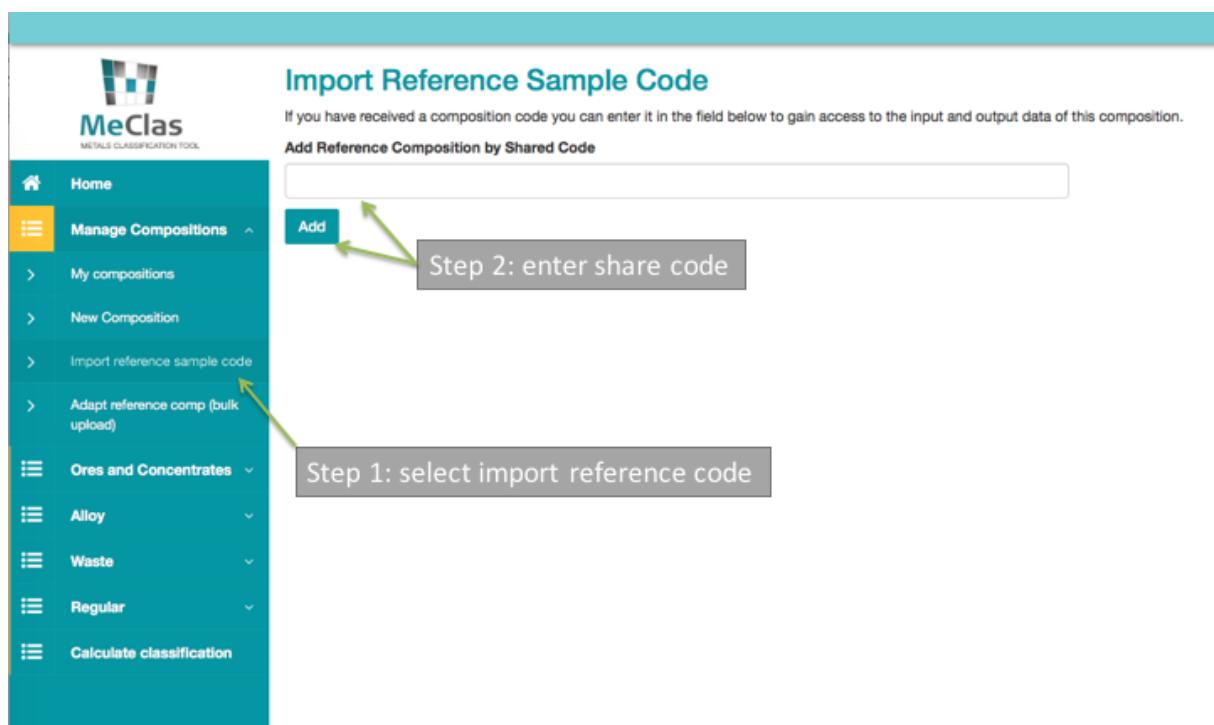
4.4.1.3. Create adapted reference compositions

There are two scenarios to create adapted reference compositions:

- You would like to adapt a reference composition from a consortium (or another company): then, you have to use “**import reference composition code**” menu option
- You would like to adapt a reference composition of your own: then, you have to use “**Adapt reference composition**” menu option

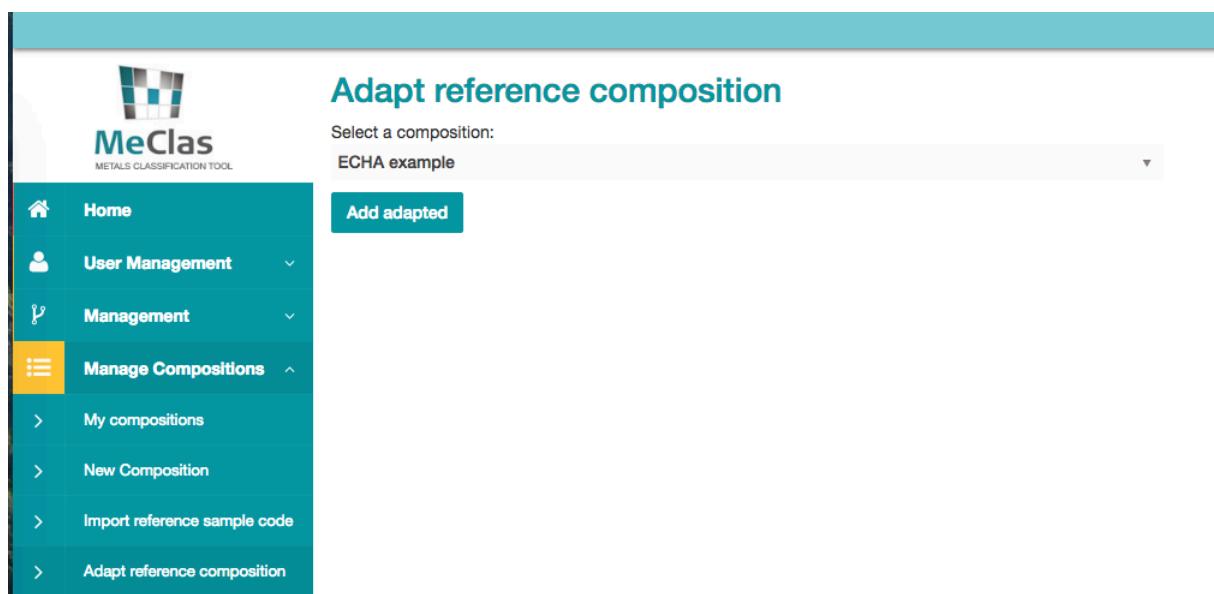
Import reference composition code

Go to the “import reference sample code” link in the ‘My compositions’ menu. If you have received a share code from a consortium (or another company), it can be entered in the field to gain access to the input data of this reference composition. The company is asked whether it wants to add this composition to the input and output list. Click ‘yes’.



Adapt reference composition

Go to the “adapt reference composition” link in the “My compositions” menu. Now you can select one of your own compositions you would like to adapt.

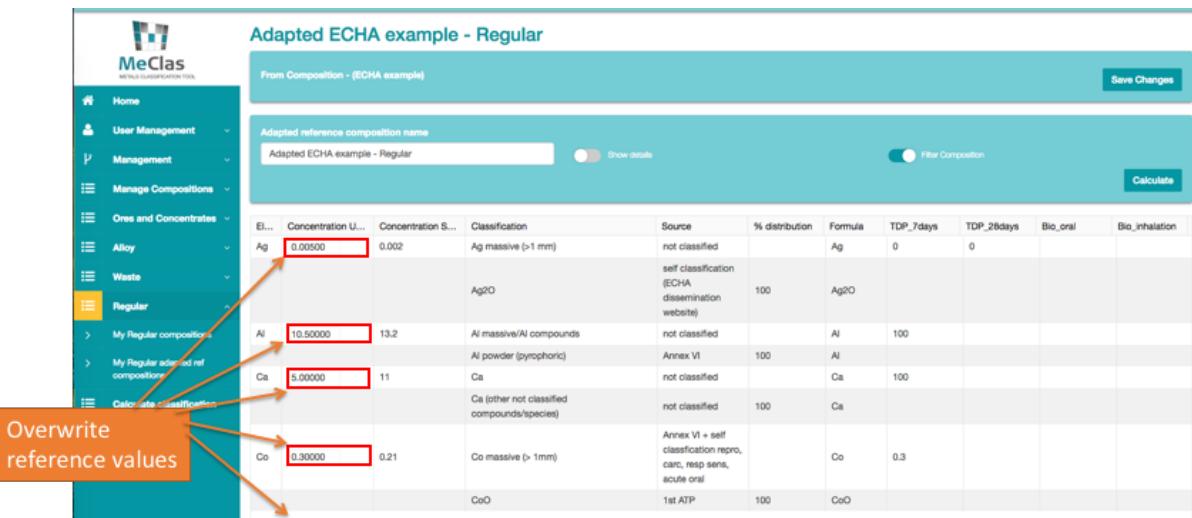


4.4.1.4. Edit adapted reference composition (run elemental adapted versions of a reference composition)

To view or adapt the composition go to ‘My compositions’ and select the adapted reference composition in the right hand overview.

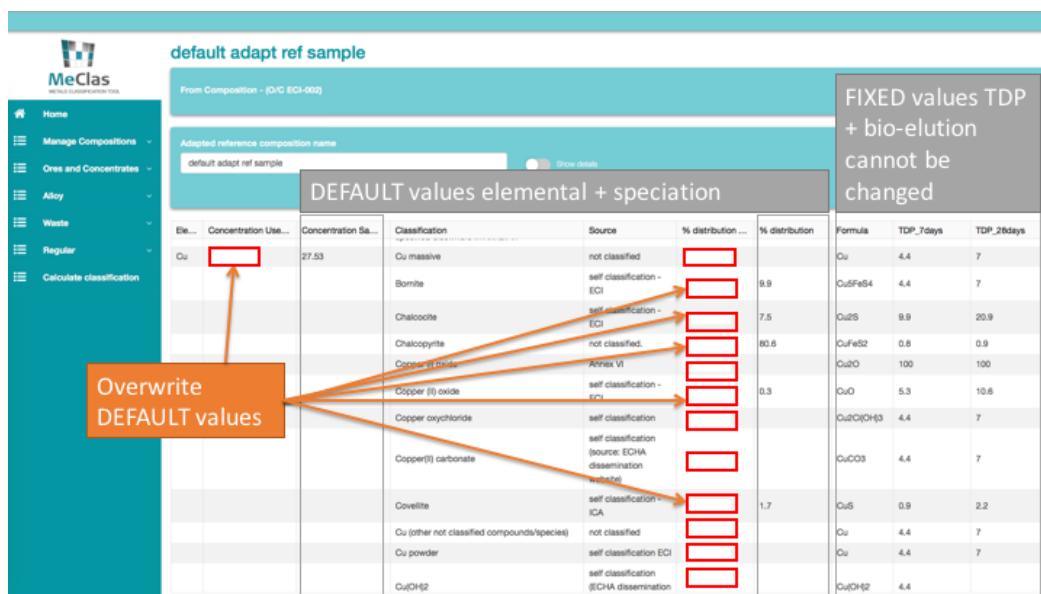
The objective of the input sheet is to adapt the elemental composition of a reference composition. For this, input specific elemental concentrations will overwrite reference elemental concentrations from the reference composition. The adapted company-specific classification is then calculated. If input boxes are left blank, the value of the reference composition for that element is considered. However, if you do not wish to assume the reference concentrations, overwrite the value from the reference sample by inserting zero ("0"). Note that the changes are user-specific and will not overwrite the default values from the reference samples. Other users that share the same reference sample will not be able to view your adaptations.

All elemental percentages have to be filled out without mentioning the unit. For example, when the element is present in a concentration of 5%, it should be entered as 5, not as 0.05 or 5%. The sum of the percentages of the elements should be equal to 100%.



Element	Concentration Unit	Concentration Sample	Classification	Source	% distribution	Formula	TDP_7days	TDP_28days	Bio_oral	Bio_inhalation
Ag	0.00000	0.002	Ag massive (>1 mm)	not classified		Ag	0	0		
Al	10.50000	13.2	Al2O3	self classification (ECHA dissemination website)	100	Al2O3				
Ca	5.00000	11	Ca	not classified		Ca	100			
Co	0.30000	0.21	Co massive (> 1mm)	Annex VI + self classification repro, carc, resp sens, acute oral		Co	0.3			
			CoO	1st ATP	100	CoO				

Only elemental concentrations can be adapted. Only for the ores and concentrates composition type, the mineralogy can also be adapted (see screenshot below).



Element	Concentration Sample	Classification	Source	% distribution	Formula	TDP_7days	TDP_28days
Cu	27.53	Cu massive	not classified		Cu	4.4	7
		Bornite	self classification - ECI	9.9	Cu ₃ FeS ₄	4.4	7
		Chalcocite	self classification - ECI	7.5	Cu ₂ S	9.9	20.9
		Chalcopyrite	not classified	80.6	Cu ₂ FeS ₂	0.8	0.9
		Copper(II) oxide	self classification - ECI	0.3	Cu ₂ O	100	100
		Copper oxychloride	self classification		Cu ₂ O	5.3	10.6
		Copper(II) carbonate	self classification (source: ECHA dissemination website)		Cu ₂ O(OH) ₃	4.4	7
		Covellite	self classification - ICA	1.7	Cu ₂ CO ₃	4.4	7
		Cu (other not classified compounds/species)	not classified		Cu ₂ S	0.9	2.2
		Cu powder	self classification ECI		Cu	4.4	7
		Cu ₂ OH ₂	self classification (ECHA dissemination website)		Cu	4.4	7

4.4.1.5. Adapt reference composition (bulk upload)

This functionality will be further updated in the future.

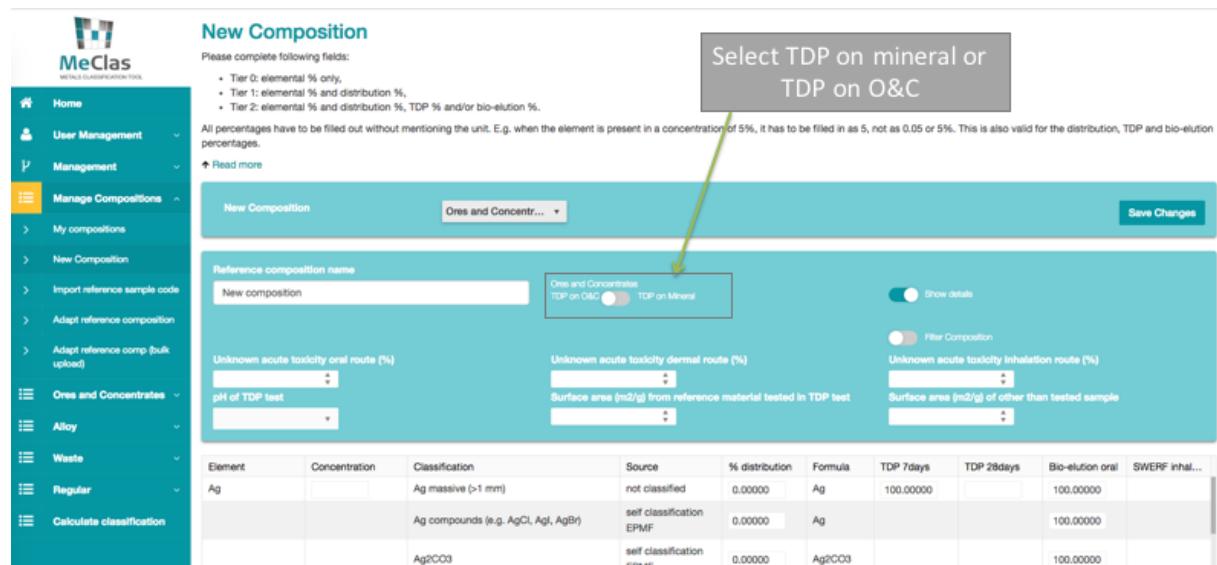
4.4.2 Composition types

The “regular” composition type is the most generic, exhaustive and common type to be used for inorganic materials. An user may also select “ores and concentrates”, “alloys” or “waste” composition type. These composition types are 1) more simplified (compared to the “regular” composition type) and 2) have specific features. The specific features are discussed in this section. For the regular features, the reader is referred to previous and next sections.

4.4.2.1. Ores and concentrates

The editing and managing of O/C compositions (Ores/Concentrates) is very similar to regular compositions. The reader is therefore referred to previous section. The main differences are:

- The speciation is limited to relevant speciation and minerals present in ores and concentrates
- Tier 0 is not relevant for ores and concentrates
- The user can choose to specify TDP% for each mineral separately (TDP done on minerals) or for each element (TDP done on the O/C as a whole, as is the case in regular compositions). This needs to be selected when creating a new O/C composition.



The screenshot shows the 'New Composition' interface for 'Ores and Concentrates'. A callout box highlights the 'Select TDP on mineral or TDP on O&C' option. The 'TDP on Mineral' radio button is selected. The table below lists elements and their properties, showing two rows for silver (Ag).

Element	Concentration	Classification	Source	% distribution	Formula	TDP 7days	TDP 28days	Bio-elution oral	SWERF inhal...
Ag		Ag massive (>1 mm)	not classified	0.00000	Ag	100.00000		100.00000	
		Ag compounds (e.g. AgCl, AgI, AgBr)	self classification EPMF	0.00000	Ag			100.00000	
		Ag ₂ CO ₃	self classification EPMF	0.00000	Ag ₂ CO ₃			100.00000	

This selection does NOT impact a Tier 1 assessment. The selection can impact a Tier 2 assessment. The screenshot below further illustrates the difference between the two options.

TDP on O&C							
Element	Concentration	Classification	Source	% distribution	Formula	TDP 7days	TDP 28days
Cu	26.70000	Cu massive	not classified		Cu	1.20330	1.82360
		Bornite	self classification - ECI	5.20000	Cu ₅ FeS ₄		
		Chalcocite	self classification - ECI	1.80000	Cu ₂ S		
		Chalcopyrite	not classified.	78.20000	CuFeS ₂		
		Copper (I) oxide	Annex VI		Cu ₂ O		
		Copper (II) oxide	self classification - ECI		CuO		
		Copper oxychloride	self classification		Cu ₂ Cl(OH) ₃		
		Copper(II) carbonate (source: ECHA dissemination website)	self classification		CuCO ₃		
		Covellite	self classification - ICA	13.30000	CuS		

TDP on mineral							
Element	Concentration	Classification	Source	% distribution	Formula	TDP 7days	TDP 28days
Cu		Cu massive	not classified		Cu		
		Bornite	self classification - ECI		Cu ₅ FeS ₄	4.40000	7.00000
		Chalcocite	self classification - ECI		Cu ₂ S	9.90000	20.90000
		Chalcopyrite	not classified.		CuFeS ₂	0.80000	0.90000
		Copper (I) oxide	Annex VI		Cu ₂ O	100.00000	100.00000
		Copper (II) oxide	self classification - ECI		CuO	5.30000	10.60000
		Copper oxychloride	self classification		Cu ₂ Cl(OH) ₃	4.40000	7.00000
		Copper(II) carbonate (source: ECHA dissemination website)	self classification		CuCO ₃	4.40000	7.00000
		Covellite	self classification - ICA		CuS	0.90000	2.20000

The decision tree menu provides flow charts and reference to sources for more information.

4.4.2.2. Alloys compositions

The editing and managing of alloy compositions is very similar to regular compositions. The main difference is:

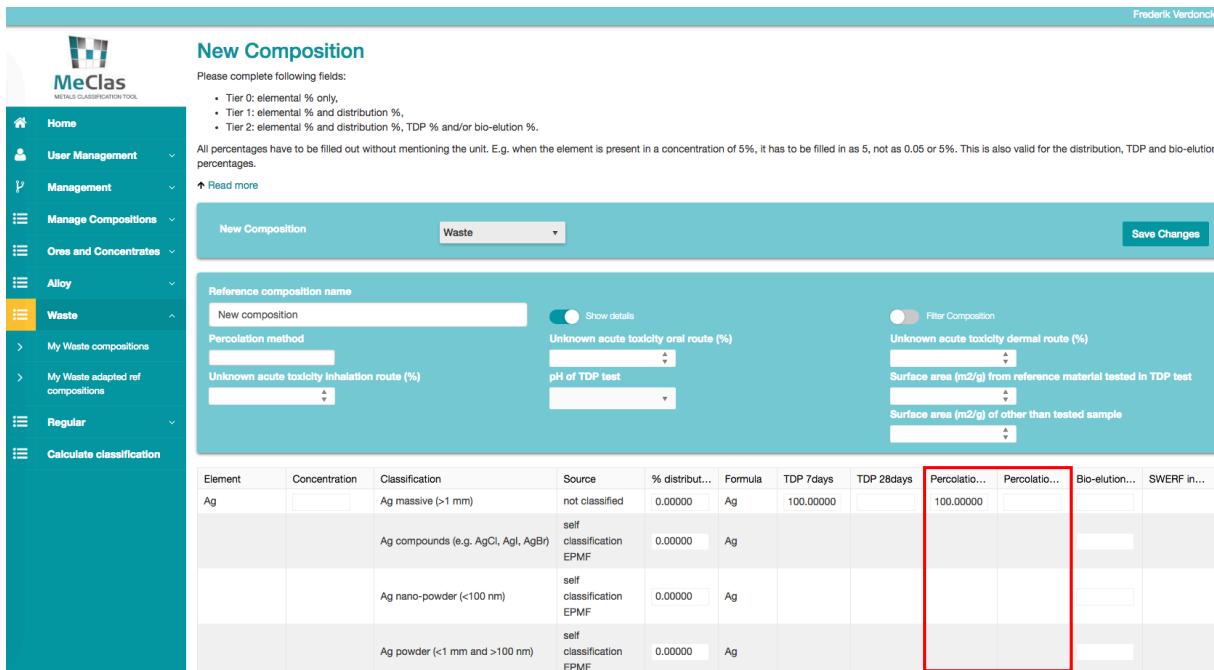
- The speciation is limited to relevant speciation present in alloys
- Tier 0 is not relevant for alloys

The decision tree menu provides flow charts and reference to sources for more information.

4.4.2.3. Waste compositions

The editing and managing of waste compositions is very similar to regular compositions. The main difference is:

- The speciation is limited to relevant speciation present in waste
- It is possible in Tier 2 to add other than TDP solubilization tests (e.g. percolation tests, see screenshot below). When both TDP and percolation tests are available, TDP take precedence over the percolation tests (given its regulatory weight).



The screenshot shows the 'New Composition' page of the MeClas tool. On the left is a sidebar with navigation links: Home, User Management, Management, Manage Compositions, Ores and Concentrates, Alloy, Waste (selected), My Waste compositions, My Waste adapted ref compositions, Regular, and Calculate classification. The main area has a teal header 'New Composition' and a dropdown 'Waste'. A 'Save Changes' button is in the top right. Below is a 'Reference composition name' input ('New composition') and a 'Show details' toggle. There are two rows of input fields: 'Percolation method' (Unknown acute toxicity oral route (%)) and 'Unknown acute toxicity inhalation route (%)'. To the right are filters for 'Unknown acute toxicity dermal route (%)', 'Surface area (m²/g) from reference material tested in TDP test', and 'Surface area (m²/g) of other than tested sample'. At the bottom is a table with columns: Element, Concentration, Classification, Source, % distribut..., Formula, TDP 7days, TDP 28days, Percolatio..., Percolatio..., Bio-elution..., and SWERF in... . The table contains four rows for different forms of silver (Ag).

Element	Concentration	Classification	Source	% distribut...	Formula	TDP 7days	TDP 28days	Percolatio...	Percolatio...	Bio-elution...	SWERF in...
Ag		Ag massive (>1 mm)	not classified	0.00000	Ag	100.00000		100.00000			
		Ag compounds (e.g. AgCl, AgI, AgBr)	self classification EPMF	0.00000	Ag						
		Ag nano-powder (<100 nm)	self classification EPMF	0.00000	Ag						
		Ag powder (<1 mm and >100 nm)	self classification EPMF	0.00000	Ag						

4.5. Output user interface: hazard classification and labelling

The classification can be calculated by

- Selecting “calculate classification” from the “Tool” menu
- Selecting “calculate” when editing/viewing a composition

Once the calculation classification sheet has loaded, a metal mixture and the tier are automatically selected but can be amended. Depending on the input, a suggested Tier is selected. More information about the different tiers can be found in Section 3.

The calculated output is the classification and labelling of the material according to GHS (UN, 2015) and different regional formats like the EU CLP (EU, 2008) and US OSHA (US, 2012) for each toxicological and ecotoxicological endpoint.

Tier 1

Endpoint	EU-CLP	GHS	US/Canada
Acute toxicity-oral	Not classified	Cat. 5	Cat. 5
Acute toxicity-dermal	Not classified	Not classified	Not classified
Acute toxicity-inhalation	Not classified	Not classified	Not classified
Skin corrosion/irritation	Not classified	Not classified	Not classified
Serious eye damage/eye irritation	Not classified	Not classified	Not classified
Respiratory or skin sensitisation	Resp./Skin Sens. Cat. 1; H334/H317	Resp./Skin Sens. Cat. 1; H334/H317	Resp./Skin Sens. Cat. 1; H334/H317
Germ cell mutagenicity	Not classified	Not classified	Not classified
Carcinogenicity	Cat. 1B; H350	Cat. 1B; H350	Cat. 1A; H350
Reproductive toxicity	Cat. 1A; H360	Cat. 1A; H360	Cat. 1A; H360
Specific target organ toxicity - single exposure	Not classified	Not classified	Not classified
Specific target organ toxicity - repeated exposure	Cat. 1; H372	Cat. 1; H372	Cat. 1; H372
Aspiration hazard	Not classified	Not classified	Not classified
Hazardous to aquatic environment - ACUTE	Acute Cat. 1; H400	Acute Cat. 1; H400	
Hazardous to aquatic environment - CHRONIC	Chronic Cat. 2; H411	Chronic Cat. 2; H411	

EU-CLP

Signal word: Danger



MARPOL

Endpoint	Classification
harmfull to the marine environment (HME)	Classified

IMSBC

Endpoint	Classification
Materials hazardous only in bulk (MHB) - part toxic solid	Classified

3

In the example above, the three outputs (GHS, CLP and OSHA) give similar results except for acute toxicity and carcinogenicity. The difference for acute toxicity is due to the non-existence of Cat. 5 under CLP. And the difference for carcinogenicity can be explained because US-OSHA is referring to the -in this case- more precautionary IARC database for carcinogenicity of elemental arsenic.

The implications for transport: MARPOL and IMSBC (toxic solid part only) are also given. The results can be printed or exported in pdf or spreadsheet format.

A summary report with the assumptions and the classification result (CLP, GHS and US OSHA) can be exported/downloaded in PDF or Excel.

4.6. In-between calculations in excel export

The intermediate calculations are transparently given in an overview spreadsheet (for each tier). The concentration of each species is given along with its classification and, for some endpoints, more intermediate calculation results (e.g. concentration ATEi ratio in case of acute toxicity).

This overview contributes to the overall transparency of the calculations and allows the user to fully understand the contribution of different drivers.

Classification Entry	Concentrati on (%)	CLP - EU		CLP - EU		CLP - EU		CLP - EU	
		Classification Acute Toxicity - oral - CLP	Conc/ATEi	Classification Acute Toxicity - dermal - CLP	Conc/ATEi	Classification Acute Toxicity - inhalation - CLP	Conc/ATEi	Classification Acute Toxicity - oral - CLP	Conc/ATEi
Ag massive (>1 mm)	0,2		0			0			0
Al massive/Al compounds	0,15		0			0			0
As	0,9	Cat. 3; H301	0,009			0 Cat. 3; H331	1,8		
Au	0,002		0			0			0
CaO	0,28		0			0			0
CdS	0,025	Cat. 4; H302	0,00005			0			0
Co powder (<1 mm and non-respirable)	0,3173	Cat. 4; H302	0,0006346	0		0	0		0
CoS	1,05		0			0			0
Chalcocite	43,2		0			0			0
Copper (I) oxide	0,87	Cat. 4; H302	0,001732962			0			0
Cu massive	1,6		0			0			0
Fe/Fe compounds (e.g. FeS2)	15		0			0			0
MnO2	0,13	Cat. 4; H302	0,00025319			0 Cat. 4; H332	0,084396714		
MoS2	0,0001		0			0			0
Ni massive	5,5		0			0			0
lead compounds with the exception of those specified elsewhere in Annex VI	7,5	Cat. 4; H302	0,015			0 Cat. 4; H332	5		
Metal sulfides/sulphates	25,00		0			0			0
Sb compounds, with the exception of the tetroxide (Sb2O4), pentoxide (Sb2O5), trisulphide (Sb2S3), pentasulphide (Sb2S5) and those specified elsewhere in Annex VI	0,17	Cat. 4; H302	0,00034			0 Cat. 4; H332	0,113333333		
Selenium compounds except cadmium sulphoselenide	0,46	Cat. 3; H301	0,0046			0 Cat. 3; H331	0,92		
SiO2 non-crystalline	1,71		0			0			0
Sn	0,36		0			0			0
ZnS	6,41		0			0			0
				ATEmix(oral)		ATEmix(dermal)		ATEmix(inhalation)	
Total (Sum or maximum)	133,3324559		3163,48052			0,0000		12,6299	
Mixture rules classification outcome		CLP - EU		CLP - EU		CLP - EU		CLP - EU	
Mixture rule		Not classified		Not classified		Not classified		Not classified	
		ATEmix ORAL > 2000 mg/kg		ATEmix DERMAL > 2000 mg/kg		ATEmix INHALATION > 5 mg/L			

5. Disclaimer

The MECLAS tool aims to generate classifications for complex metal mixtures. Although prepared with great care, flawless operations cannot be guaranteed. Users of the MECLAS tool need to be aware of this. By using the MECLAS tool, users accept full responsibility for their calculations. Neither Arche, Eurometaux nor the data providers can take liability for (mis)use of the results.

6. References

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7. Glossary

ADN is the European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways

ADR is the European Agreement concerning the International Carriage of Dangerous Goods by Road

ATP means Adaptation to Technical Progress (to the CLP Regulation)

Alloy means a metallic material, homogeneous on a macroscopic scale, consisting of two or more elements so combined that they cannot be readily separated by mechanical means; alloys are considered to be mixtures for the purposes of the GHS draft Regulation;

Aspiration means the entry of a liquid or solid chemical product into the trachea and lower respiratory system directly through the oral or nasal cavity, or indirectly from vomiting;

Carcinogen means a chemical substance or a mixture of chemical substances which induce cancer or increase its incidence;

CAS means "Chemical Abstract Service";

CLP means Classification, Labelling and Packaging of Substances and Mixtures Regulation (EC 1272/2008)

CMR means Carcinogenic, Mutagenic and Reprotoxic

Competent authority means the authority or authorities or bodies established by the Member States to carry out the obligations arising from the GHS draft Regulation;

Contact sensitiser means a substance that will induce an allergic response following skin contact. The definition for "contact sensitiser" is equivalent to "skin sensitiser";

Corrosive to metal means a substance or a mixture which by chemical action will materially damage, or even destroy, metals;

Dermal corrosion: see skin corrosion;

Dermal irritation: see skin irritation;

Downstream user means any natural or legal person established within the Community, other than the manufacturer or the importer, who uses a substance, either on its own or in a preparation, in the course of his industrial or professional activities. A distributor or a consumer is not a downstream user. A re-importer exempted pursuant to Article 2(7)(c) REACH Regulation shall be regarded as a downstream user;

Dust means solid particles of a substance or mixture suspended in a gas (usually air);

EC50 means the effective concentration of substance that causes 50% of the maximum response;

ECHA means European Chemicals Agency;

EC Number or (ECN) is a reference number used by the European Communities to identify dangerous substances, in particular those registered under EINECS;

EINECS means "European Inventory of Existing Commercial Chemical Substances";

ERV means Ecotoxicity Reference Value;

EU means the "European Union";

Eye irritation means the production of changes in the eye following the application of test substance to the anterior surface of the eye, which are fully reversible within 21 days of application;

GCL means Generic Concentration Limits;

GESAMP means the "Joint Group of Experts on the Scientific Aspects of Marine Environmental Protection of

IMO/FAO/UNESCO/WMO/WHO/IAEA/UN/UNEP”;

GHS means the “Globally Harmonised System of Classification and Labelling of Chemicals”;

Hazard categories means the division of criteria within each hazard class;

Hazard class means the nature of the physical, health or environmental hazard;

Hazard statement means a phrase assigned to a hazard class and category that describes the nature of the hazards of a hazardous substance or mixture, including, where appropriate, the degree of hazard;

HP means Hazardous Properties;

IARC means the “International Agency for Research on Cancer”;

IMO means the “International Maritime Organisation”;

IMDG means International Maritime Dangerous Goods Code;

IMSBC means International Maritime Solid Bulk Cargoes Code;

Intermediate means a substance that is manufactured for and consumed in or used for chemical processing in order to be transformed into another substance (hereinafter referred to as "synthesis");

Label means an appropriate group of written, printed or graphic information elements concerning a hazardous product, selected as relevant to the target sector (s), that is affixed to, printed on, or attached to the immediate container of a hazardous product, or to the outside packaging of a hazardous product;

Label element means one type of information that has been harmonised for use in a label, e.g. pictogram, signal word;

LC50 (50% lethal concentration) means the concentration of a chemical in air or of a chemical in water which causes the death of 50% (one half) of a group of test animals;

LD50 means the amount of a chemical, given all at once, which causes the death of 50% (one half) of a group of test animals;

L(E)C50 means LC50 or EC50;

MARPOL means the “International Convention for the Prevention of Pollution from Ships”;

MeClas means Metals Classification tool;

Mist means liquid droplets of a substance or mixture suspended in a gas (usually air);

Mixture means a mixture or solution of two or more substances which do not react; Note: Mixture and preparation are synonymous

Mutagen means an agent giving rise to an increased occurrence of mutations in populations of cells and /or organisms;

Mutation means a permanent change in the amount or structure of the genetic material in a cell;

NOEC means the “no observed effect concentration”;

OECD means the “Organisation for Economic Cooperation and Development”;

OSHA means the “Occupational Safety and Health Administration”;

Pictogram means a graphical composition that includes a symbol plus other graphic elements, such as a border, background pattern or colour that is intended to convey specific information;

Precautionary statement means a phrase and/or pictogram that describes recommended measure(s) to minimise or prevent adverse effects resulting from exposure to a hazardous substance or mixture due to its use;

QSAR means “quantitative structure-activity relationships”;

REACH database means the classification & labelling inventory established under Article 113 of the proposed

REACH Regulation;

REACH Regulation means the Regulation (EC) No... concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals;

Recommendations on the Transport of Dangerous Goods, Manual of Tests and Criteria means the latest revised edition of the United Nations publication bearing this title, and any published amendment thereto;

Recommendations on the Transport of Dangerous Goods, Model Regulations means the latest revised edition of the United Nations publication bearing this title, and any published amendment thereto;

Respiratory sensitiser means a substance that induces hypersensitivity of the airways following inhalation of the substance;

RID means The Regulations concerning the International Carriage of Dangerous Goods by Rail [Annex 1 to Appendix B (Uniform Rules concerning the Contract for International Carriage of Goods by Rail) (CIM) of COTIF (Convention concerning international carriage by rail)], as amended;

SAR means "Structure Activity Relationship";

SCL means Specific Concentration Limits;

SDS means "Safety Data Sheet";

Serious eye damage means the production of tissue damage in the eye, or serious physical decay of vision, following application of a test substance to the anterior surface of the eye, which is not fully reversible within 21 days of application;

Signal word means a word that indicates the relative level of severity of hazards to alert the potential reader of the hazard; the following two levels are distinguished: (a) *Danger* means a signal word indicating the more severe hazard categories; (b) *Warning* means a signal word indicating the less severe hazard categories.

Skin corrosion means the production of irreversible damage to the skin following the application of a test substance for up to 4 hours;

Skin irritation means the production of reversible damage to the skin following the application of a test substance for up to 4 hours;

Skin sensitiser means a substance that will induce an allergic response following skin contact. The definition for "skin sensitiser" is equivalent to "contact sensitiser";

STOT means Specific Target Organ Toxicity;

Substance means a chemical element and its compounds in the natural state or obtained by any manufacturing process, including any additive necessary to preserve its stability and any impurity deriving from the process used, but excluding any solvent which may be separated without affecting the stability of the substance or changing its composition;

Supplemental label element means any additional non-harmonised type of information supplied on the container of a hazardous product that is not required or specified under the GHS. In some cases this information may be required by other competent authorities or it may be additional information provided at the discretion of the manufacturer/distributor;

Symbol means a graphical element intended to succinctly convey information;

TRV means Toxicity Reference Value;

TD_p means Transformation/Dissolution Protocol;

UNCETDG/GHS means the "United Nations Committee of Experts on the Transport of Dangerous Goods and on the Globally Harmonised System of Classification and Labelling of Chemicals";

UN GHS means United Nations - Globally Harmonised System of Classification and Labelling of Chemicals

UNEP means the "United Nations Environment Programme";

UVCB means Substances of unknown or variable composition, complex reaction products or biological materials

XRD means X-ray Diffraction

WHO means the “World Health Organisation”;