Regulatory Toxicology and Pharmacology 89 (2017) 232–239

Contents lists available at ScienceDirect

Regulatory Toxicology and Pharmacology

journal homepage: www.elsevier.com/locate/yrtph

MeClas: An online tool for hazard identification and classification of complex inorganic metal-containing materials

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ARTICLE INFO

Article history:
Received 13 February 2017
Received in revised form
12 July 2017
Accepted 14 July 2017
Available online 17 July 2017

Keywords:
Metals
Classification
Alloys
UVCB
Ores and concentrates
Labelling
Bioavailability
GHS and CLP
OSHA

ABSTRACT

MeClas is a web-based tool to generate (eco)toxicity hazard categories and corresponding classification & labelling information of inorganic metal-containing complex materials such as ores, concentrates, intermediates or alloys for which the manual application of the GHS/CLP rules is very complex and requires a high level of consistency. The tool comprises several tiers, aimed at the progressive refinement of classification through recognition of specific mineral content, speciation/mineralogy up to bioavailability corrections. Where relevant in a regional jurisdiction (EU and US), mandatory classification references are used complementary to high quality (eco)toxicity reference values (ERV/TRV) and self-classifications. MeClas addresses the GHS human health and environmental hazard endpoints, is based on an unambiguous algorithm defined under GHS/CLP, has a well defined domain of applicability and robust predictability. MeClas allows a consistent approach across companies in line with GHS ruling (and regional implementations), considering the metal specificities and related classification GHS/CLP Guidance, and the most up to date (eco)-toxicological hazard information on self-classifications and ERV/TRV.

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 Harmonised 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 harmonised 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.

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http://dx.doi.org/10.1016/j.yrtph.2017.07.015
0273-2300/

Abbreviations

ADN	European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways
ADR	European Agreement concerning the International Carriage of Dangerous Goods by Road
ATP	Adaptation to Technical Progress (to the CLP Regulation)
CLP	Classification, Labelling and Packaging of Substances and Mixtures Regulation (EC 1272/2008)
CMR	Carcinogenic, Mutagenic and Reprotoxic
ECHA	European Chemicals Agency
ERV	Ecotoxicity Reference Value
CL	Generic Concentration Limits
HP	Hazardous Properties
IMSBC	International Maritime Solid Bulk Cargoes Code
IMDG	International Maritime Dangerous Goods Code
MARPOL	Prevention of Pollution from Ships
MeClas	Metals Classification tool
OSHA	Occupational Safety and Health Administration (US)
REACH	Regulation on Registration, Evaluation, Authorisation and Restriction of Chemicals (EC, 1907/2006)
RID	Regulations concerning the International Carriage of Dangerous Goods by Rail
SCL	Specific Concentration Limits
SDS	Safety Data Sheet
STOT	Specific Target Organ Toxicity
TRV	Toxicity Reference Value
TDp	Transformation/Dissolution Protocol
UN GHS	United Nations - Globally Harmonised System of Classification and Labelling of Chemicals
UVCB	Substances of unknown or variable composition, complex reaction products or biological materials
XRD	X-ray Diffraction

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 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 (TDp) (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, 2015a) 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.

The aim of the present paper is to demonstrate that the 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. It will also describe the roles of the tool as 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.

2. Methodology

The basic principles of the MeClas tool and the outline of an example are further outlined below.

2.1. The classification rules and specificities for inorganics

2.1.1. 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 mixtures 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