EUROFER
European Confederation of Iron and Steel Industries

Alloys - REACH Annex VI Analytical and Spectral Data Requirements (final version dated 20082010)

Background

REACH Annex VI requires that the information given in section 2 shall be sufficient to enable each substance to be identified.

REACH recognises alloys as special preparations (i.e. special mixtures) and Annex I, 011 states that 'When assessing the risk of the use of one or more substances incorporated into a special preparation (for instance alloys), the way the constituent substances are bonded in the chemical matrix shall be taken into account'. *The constituent substances in alloys are dispersed throughout the crystal lattice (i.e. the chemical matrix) of the alloy and, furthermore, impurities are not directly associated with individual constituent substances.*

The metallic crystal structures of alloys are complex. The crystal structure adopted by an alloy is influenced by the constituent substances and their crystal structure in the unalloyed state, the relative atomic size of the constituents (which determines the extent of lattice strain and the range of solid solubility as well as the position taken up by individual atoms either in the lattice itself or in the interstices), the cooling rate from the liquid state as well as the thermal and mechanical history of the alloy. These factors give rise to the possibility of several different crystal phases with different relative distributions existing within an alloy of the same chemical composition.

This document is intended to provide guidance on suitable spectroscopic techniques for alloys - section 2.3.5 REACH Annex VI - and recommendations concerning the analytical techniques to be described under section 2.3.7 of REACH Annex VI.

REACH Annex VI Section 2.3.5 Spectral Data

In respect to the spectral data requirements demanded by REACH Annex VI section 2.3.5, Eurofer members have expressed concern about the relevance of some techniques to alloys.

Alloys are inorganic (metallic) materials where the constituent substances are bound within the crystal lattice. GC, HPLC, IR, NMR, MS and UV are **not** appropriate spectral techniques for alloys. **Methods such as XRF, XRD and ICP are more appropriate techniques for the provision of the required structural and compositional information for this type of inorganic substance and a usual practice in the metals industry.**

However, while XRD may provide structural information concerning the alloy, it is unlikely, for the reasons given above, to yield information useful for the determination of the sameness of the constituent and reference substances.

REACH Annex VI Section 2.3.7 Analytical Data

The chemical compositions of the majority of commercial alloys are defined by national, European and International standards. These standardised alloy compositions may be verified by **standardised analytical techniques**. *Examples of analytical standards for ferro-alloys and steels are provided in **Annex I.***

REACH Annex VI requires, amongst other details, that the following information must be provided in IUCLID 5 section 1.4 – Analytical information:

2.3.5. Spectral data (ultra-violet, infra-red, nuclear magnetic resonance or mass spectrum)

2.3.6. High-pressure liquid chromatogram, gas chromatogram

2.3.7. Description of the analytical methods or the appropriate bibliographical references for the identification of the substance and, where appropriate, for the identification of impurities and additives. This information shall be sufficient to allow the methods to be reproduced.

If it is not technically possible or if it does not appear scientifically necessary to give information on one or more of the items below, the reasons shall be clearly stated. For substances for which any of the items above is not suitable, data from a suitable characterisation method should be included.

The **description of the analytical methods** must be provided either in the "Analytical methods and spectral data" filed **or** as an attachment under this field (by clicking on the paper clip button, indicated in figure 1 below).

The **analytical results used to characterise the substance** must be provided in the repeating blocks under "Results of analysis" as an attachment (by clicking on the paper clip button) **or** in the "Remarks" field (figure 1).

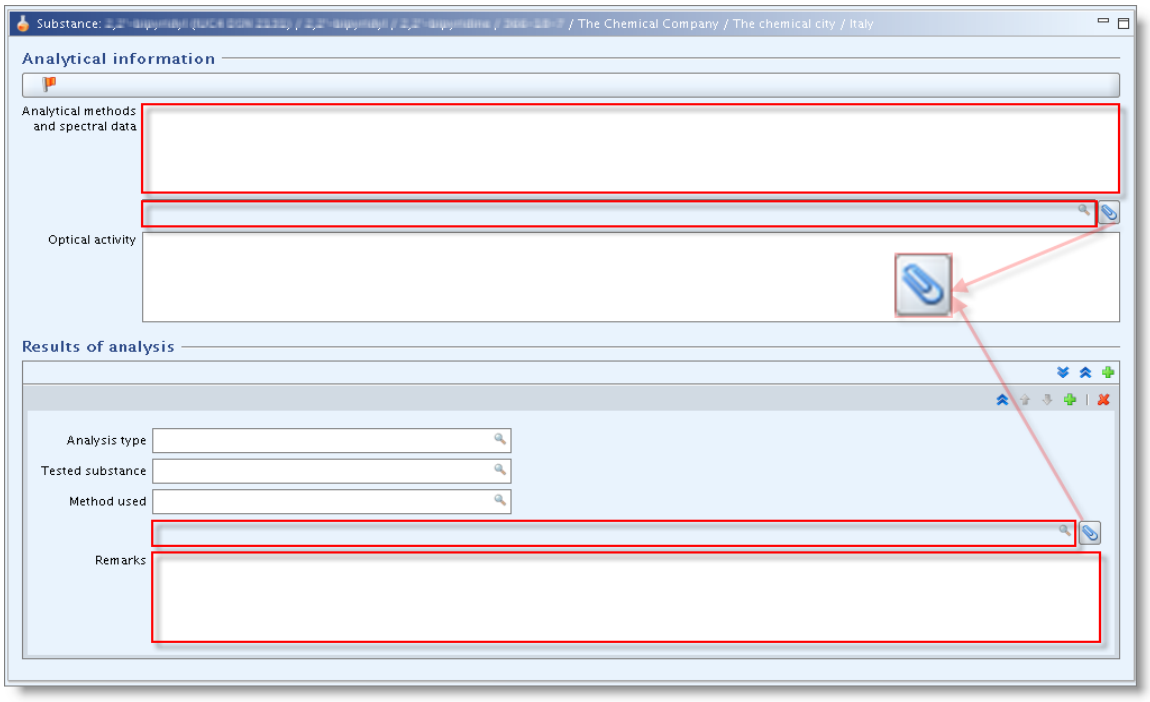

Figure 1 – Analytical Information

It is recommended that, for steel, special alloys and ferro-alloys, the following statement is entered into the "Remarks" field:-

The registered substance is inorganic and a constituent of an alloy, where the constituent substances are bound in the chemical matrix. GC, HPLC, IR, NMR, MS and UV are not appropriate spectral techniques for alloys. Methods such as XRF, XRD and ICP are more appropriate techniques for the provision of the required structural and compositional information for this type of inorganic substance and a usual practice in the metals industry.

However, while it may provide structural information concerning the alloy, XRD is unlikely to yield information useful for the determination of the sameness of the constituent and reference substances. This is due to the influence of the relative atomic size of the constituents, which determine the crystal structure adopted by the alloy, the extent of lattice strain and the range of solid solubility as well as the position taken up by individual atoms either in the lattice itself or in the interstice. In addition, the cooling rate as well as the thermal and mechanical history has a profound influence on the crystal structure of the alloy.

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Annex I – Examples of Analytical Standards for ferrous alloys

CEN/TR 10261:2008 Iron and steel - Review of available methods of chemical analysis

CEN/TR 10317:2009 European certified reference materials (EURONORM-CRMs) for the determination of the chemical composition of iron and steel products prepared under the auspices of the European Committee for Iron and Steel Standardization

CEN/TR 10345:2008 Guideline for statistical data treatment of inter laboratory tests for validation of analytical methods

CEN/TR 10350:2009 Analysis of steels and irons - Internal laboratory procedure for checking the accuracy of an analytical method by using Certified Reference Materials

CR 10299:1998 Guidelines for the preparation of standard routine methods with wavelength-dispersive X-ray fluorescence spectrometry

CR 10316:2001 Optical emission analysis of low alloy steels (routine method) - Guidelines for the preparation of standard routine method for optical emission spectrometry

CR 10320:2004 Optical emission analysis of low alloy steels (routine method) - Method for determination of C, Si, S, P, Mn, Cr, Ni and Cu

CR 10321:2003 Chemical analysis of ferrous materials - Recommendations for the drafting of standard methods of analysis employing flame atomic absorption spectrometry for the chemical analysis of iron and steel

CR 10322:2003 Chemical analysis of ferrous materials - Operational guidelines for the application of flame atomic absorption spectrometry in standard methods for the chemical analysis of iron and steel

EN 10036:1991 Chemical analysis of ferrous materials - Determination of total carbon in steels and irons - Gravimetric method after combustion in a stream of oxygen

EN 10071:1991 Chemical analysis of ferrous materials - Determination of manganese in steels and irons - Electrometric titration method

EN 10136:1991 Chemical analysis of ferrous materials - Determination of nickel in steels and irons - Flame atomic absorption spectrometric method

EN 10177:1989 Chemical analysis of ferrous materials - Determination of calcium in steels - Flame atomic absorption spectrometric method

EN 10178:1989 Chemical analysis of ferrous materials - Determination of niobium in steels - Spectrophotometric method

EN 10179:1989 Chemical analysis of ferrous materials - Determination of nitrogen (trace mounts) in steel - Spectrophotometric method

EN 10181:1989 Chemical analysis of ferrous materials - Determination of lead in steels - Flame atomic absorption spectrometric method

EN 10184:2006 Chemical analysis of ferrous materials - Determination of phosphorus in non-alloyed steels and irons - Molybdenum blue spectrophotometric method

EN 10188:1989 Chemical analysis of ferrous materials - Determination of chromium in steels and irons - Flame atomic absorption spectrometric method

EN 10200:1992 Chemical analysis of ferrous materials. Determination of boron in steel. Spectrophotometric method

EN 10211:1996 Chemical analysis of ferrous materials - Determination of titanium in steel and iron - Flame atomic absorption spectrometric method

EN 10212:1996 Chemical analysis of ferrous materials - Determination of arsenic in steel and iron - Spectrophotometric method

EN 10276-1:2000 Chemical analysis of ferrous materials - Determination of oxygen in steel and iron - Part 1: Sampling and preparation of steel samples for oxygen determination

EN 10276-2:2003 Chemical analysis of ferrous materials - Determination of oxygen content in steel and iron - Part 2: Infrared method after fusion under inert gas

EN 10315:2006 Routine method for analysis of high alloy steel by X-ray Fluorescence Spectrometry (XRF) by using a near by technique

EN 10318:2005 Determination of thickness and chemical composition of zinc- and aluminium-based metallic coatings - Routine method

EN 24159:1989 Ferromanganese and ferrosilicomanganese - Determination of manganese content - Potentiometric method (ISO 4159:1978, ed. 1)

EN 24159:1989/AC1:1989 Ferromanganese and ferrosilicomanganese - Determination of manganese content - Potentiometric method (ISO 4159:1978, ed. 1)

EN 24829-1:1990/AC:1991 Steel and cast iron - Determination of total silicon content - Reduced molybdosilicate spectrophotometric method - Part 1: Silicon content between 0,05 and 1% (ISO 4829-1:1986)

EN 24829-2:1990/AC:1991 Steel and cast iron - Determination of total silicon content - Reduced molybdosilicate spectrophotometric method - Part 2: Silicon content between 0,01 and 0,05% (ISO 4829-2:1988)

EN 24935:1991 Steel and iron - Determination of sulphur content - Infrared absorption method after combustion in an induction furnace (ISO 4935:1989)

EN 24937:1990/AC:1991 Steel and iron - Determination of chromium content - Potentiometric or visual method (ISO 4937:1986)

EN 24938:1990/AC:1991 Steel and iron - Determination of nickel content - Gravimetric or titrimetric method (ISO 4938:1988)

EN 24943:1990/AC:1991 Steel and cast iron - Determination of copper content - Flame atomic absorption spectrometric method (ISO 4943:1985)

EN 24946:1990/AC:1991 Steel and cast iron - Determination of copper content - 2,2'diquinolyl spectrophotometric method (ISO 4946:1984)

EN 24947:1991 Steel and cast iron - Determination of vanadium content - Potentiometric titration method (ISO 4947:1986)

EN 29658:1991 Steel - Determination of aluminium content - Flame atomic absorption spectrometric method (ISO 9658:1990)

EN ISO 10280:1995 Steel and iron - Determination of titanium content - Diantipyrylmethane spectrophotometric method (ISO 10280:1991)

EN ISO 10700:1995 Steel and iron - Determination of manganese content - Flame atomic spectrometric method (ISO 10700:1994)

EN ISO 10714:2002 Steel and iron - Determination of phophorus content - Phosphovanadomolybdate spectrophotometric method (ISO 10714:1992)

EN ISO 10720:2007 Steel and iron - Determination of nitrogen content - Thermal conductimetric method after fusion in a current of inert gas (ISO 10720:1997)

EN ISO 13900:2002 Steel - Determination of boron content - Curcumin spectrophotometric method after distillation (ISO 13900:1997)

EN ISO 14284:2002 Steel and iron - Sampling and preparation of samples for the determination of chemical composition (ISO 14284:1996)

EN ISO 15349-2:2003 Unalloyed steel - Determination of low carbon content - Part 2: Infrared absorption method after combustion in an induction furnace (with preheating) (ISO 15349-2:1999)

EN ISO 4934:2003 Steel and iron - Determination of sulfur content - Gravimetric method (ISO 4934:2003)

EN ISO 4945:2009 Steel - Determination of nitrogen content - Spectrophotometric method (ISO 4945:1977)

EN ISO 9556:2001 Steel and iron - Determination of total carbon content - Infrared absorption method after combustion in an induction furnace (ISO 9556:1989)

EN ISO 15350:2010 Steel and iron - Determination of total carbon and sulfur content - Infrared absorption method after combustion in an induction furnace (routine method) (ISO 15350:2000)

EN ISO 15351:2010 Steel and iron - Determination of nitrogen content - Thermal conductimetric method after fusion in a current of inert gas (Routine method) (ISO 15351:1999)

EN ISO 439:2010 Steel and iron - Determination of total silicon content - Gravimetric method (ISO 439:1994)