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**Water quality — Characterization of  
analytical methods — Guidelines for  
the selection of a representative matrix**

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ISO copyright office  
CP 401 • Ch. de Blandonnet 8  
CH-1214 Vernier, Geneva  
Phone: +41 22 749 01 11  
Fax: +41 22 749 09 47  
Email: [copyright@iso.org](mailto:copyright@iso.org)  
Website: [www.iso.org](http://www.iso.org)

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## Foreword

ISO (the International Organization for Standardization) is a worldwide federation of national standards bodies (ISO member bodies). The work of preparing International Standards is normally carried out through ISO technical committees. Each member body interested in a subject for which a technical committee has been established has the right to be represented on that committee. International organizations, governmental and non-governmental, in liaison with ISO, also take part in the work. ISO collaborates closely with the International Electrotechnical Commission (IEC) on all matters of electrotechnical standardization.

The procedures used to develop this document and those intended for its further maintenance are described in the ISO/IEC Directives, Part 1. In particular, the different approval criteria needed for the different types of ISO documents should be noted. This document was drafted in accordance with the editorial rules of the ISO/IEC Directives, Part 2 (see [www.iso.org/directives](http://www.iso.org/directives)).

Attention is drawn to the possibility that some of the elements of this document may be the subject of patent rights. ISO shall not be held responsible for identifying any or all such patent rights. Details of any patent rights identified during the development of the document will be in the Introduction and/or on the ISO list of patent declarations received (see [www.iso.org/patents](http://www.iso.org/patents)).

Any trade name used in this document is information given for the convenience of users and does not constitute an endorsement.

For an explanation of the voluntary nature of standards, the meaning of ISO specific terms and expressions related to conformity assessment, as well as information about ISO's adherence to the World Trade Organization (WTO) principles in the Technical Barriers to Trade (TBT) see [www.iso.org/iso/foreword.html](http://www.iso.org/iso/foreword.html).

This document was prepared by Technical Committee ISO/TC 147, *Water quality*, Subcommittee SC 2, *Physical, chemical and biochemical methods*.

Any feedback or questions on this document should be directed to the user's national standards body. A complete listing of these bodies can be found at [www.iso.org/members.html](http://www.iso.org/members.html).

## Introduction

This document has been prepared for the validation of analytical methods applied to the water quality field. It enables a laboratory to determine the characteristics of a material suitable for determination of the performances of an analytical method itself.

It is not intended to provide an exhaustive inventory of all published recipes, but to propose a selection of recipes supporting the characterization of the performances of analytical methods used by a laboratory. For this reason, a restricted number of recipes are proposed. References giving access to other recipes are available in the Bibliography.

This document includes four recipes for preparing marine waters and five recipes for waste waters with controlled characteristics.

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# Water quality — Characterization of analytical methods — Guidelines for the selection of a representative matrix

## 1 Scope

This document specifies representative materials suitable for the determination of the performance characteristics, including uncertainty, during the initial assessment of a quantitative method, used in a laboratory, for physico-chemical water analysis.

This document focuses on five main types of water:

- waters intended for consumption (5.2);
- natural waters (5.3);
- waste waters (5.4);
- marine waters (5.5);
- recreational waters (5.6).

NOTE Other more specific or less common types of water can be incorporated in any of the above types provided appropriate justifications. The characteristics of the standard matrix are compatible with the characteristics of the samples handled.

## 2 Normative references

The following documents are referred to in the text in such a way that some or all of their content constitutes requirements of this document. For dated references, only the edition cited applies. For undated references, the latest edition of the referenced document (including any amendments) applies.

ISO 5667-3, *Water quality — Sampling — Part 3: Preservation and handling of water samples*

ISO 6107 (all parts), *Water quality — Vocabulary*

## 3 Terms and definitions

For the purposes of this document, the terms and definitions given in ISO 6107 (all parts) and the following apply.

ISO and IEC maintain terminological databases for use in standardization at the following addresses:

- ISO Online browsing platform: available at <https://www.iso.org/obp>
- IEC Electropedia: available at <http://www.electropedia.org/>

### 3.1 General vocabulary

#### 3.1.1 matrix

set of constituents of the test sample, except the *analyte* (3.2.1)

Note 1 to entry: By extension, a matrix defines a group of waters characterized by similar analytical behaviour in relation to the analytical method used.

### 3.1.2

#### **accepted reference value**

value that serves as an agreed-upon reference for comparison, and which is derived as:

- a) a theoretical or established value, based on scientific principles;
- b) an assigned or certified value, based on experimental work of some national or international organization;
- c) a consensus or certified value, based on collaborative experimental work under the auspices of a scientific or engineering group;
- d) when a), b) and c) are not available, the expectation of the (measurable) quantity, i.e. the mean of a specified population of measurements

Note 1 to entry: In the specific context of this document, the accepted reference value (or conventionally true value) of the sample is provided according to possibilities by:

- the value from a certified reference material certificate,
- the consensus value obtained from an inter-laboratory comparison,
- the arithmetic mean of the repeated measurement values according to the reference method,
- the target value by adding analyte to a representative matrix of the scope in question.

[SOURCE: ISO 5725-1:1994, 3.5]

### 3.1.3

#### **reference material**

material, sufficiently homogeneous and stable with respect to one or more specified properties, which has been established to be fit for its intended use in a measurement process

[SOURCE: ISO Guide 35:2017, 3.1]

### 3.1.4

#### **certified reference material**

*reference material* (3.1.3), accompanied by a certificate, one or more of whose property values are certified by a procedure which establishes traceability to an accurate realization of the unit in which the property values are expressed, and for which each certified value is accompanied by an uncertainty at a stated level of confidence

[SOURCE: ISO/TS 13530:2009, 3.2.7]

### 3.1.5

#### **assessment procedure**

procedure related to the establishment of the specifications for the performance of a new method and/or experimental verification that a method meets theoretically derived quality criteria

## 3.2 Terms related to analytical methods

### 3.2.1

#### **analyte**

subject of the analytical method

### 3.2.2

#### **analytical method**

unambiguously written procedure describing all details required to carry out the analysis of the *analyte* (3.2.1), namely: scope and field of application, principle and/or reactions, definitions, reagents, apparatus, analytical procedures, calculations and presentation of results, performance data and test report

[SOURCE: ISO/TS 16489:2006, 3.3]

**3.2.3****quantitative analytical method**

analytical method for measuring the quantity of *analyte* (3.2.1) contained in the test sample

Note 1 to entry: The result can consist of a quantity in a given quantity of test sample.

**3.2.4****limit of detection**

output signal or value above which it can be affirmed, with a stated level of confidence, for example 95 %, that a sample is different from a blank sample containing no determinand of interest, and which could be estimated by different means and shall be verified in the intended matrix

[SOURCE: ISO 6107-2:2006, 60, modified — “and which could be estimated by different means and shall be verified in the intended matrix” has been added.]

**3.2.5****limit of quantification****LOQ**

lowest value of a determinand that can be determined with an acceptable level of accuracy, which could be estimated by different means and shall be verified in the intended matrix

Note 1 to entry: For each matrix, this limit is related to the pair [*analyte* (3.2.1), method].

**3.2.6****reasonable dilution**

dilution conditions for reducing the concentration of a substance in a matrix without substantially modifying the intrinsic characteristics of the matrix

**3.2.7****matrix blank values**

values of a given parameter obtained using a test conducted on a matrix giving rise to a result below the *limit of detection* (3.2.4) for the *analyte* (3.2.1) in question

**3.2.8****scope of the analytical method**

combination of the various types of matrix and the *analyte* (3.2.1) concentration range covered, to which the analytical method applies

Note 1 to entry: In addition to an indication of all the satisfactory performance conditions for each factor, the scope of the analytical method may also include warnings in respect of known interferences from other analytes, or inapplicability to some matrices or conditions.

**3.3 Terms related to matrix****3.3.1****influence parameter**

intrinsic characteristic of the matrix, independent of the *analyte* (3.2.1) concentration, a variation of which is liable to modify the analytical result

**3.3.2****representative matrix**

sample for which all the intrinsic characteristics are characteristic of a type of water or the source of a group of samples

**3.3.3****salinity**

mass in grams of solid substances contained in one kilogram of sea water, when the bromide and iodide ions are replaced by their chloride equivalent, carbonates converted into oxides and all the organic matter oxidized

### 3.3.4

#### **leachate**

water which has percolated through tipped refuse or other specified permeable material

Note 1 to entry: See [Annex D](#).

[SOURCE: ISO 6107-7:2006, 23]

## 4 Principle

The purpose of this document is to specify the concept of a representative matrix and its characteristics with a view to studying the performance of an analytical method.

For each analyte under test, the scope of an analytical method includes all the matrices under test, their descriptive parameters, and the concentration ranges of the influence parameters for which the method is applicable. The laboratory should define its requirements beforehand in respect of the scope of the analytical method, selecting the materials most in line with requirements.

**WARNING — The definition of the scope is entirely dependent on the analyst (the validation or characterization study manager) and their knowledge acquired while developing the method. It is sometimes preferable to segment a scope rather than seek to validate an overly general method. In this case, a validation file should be compiled for each scope.**

See [Figure 1](#).

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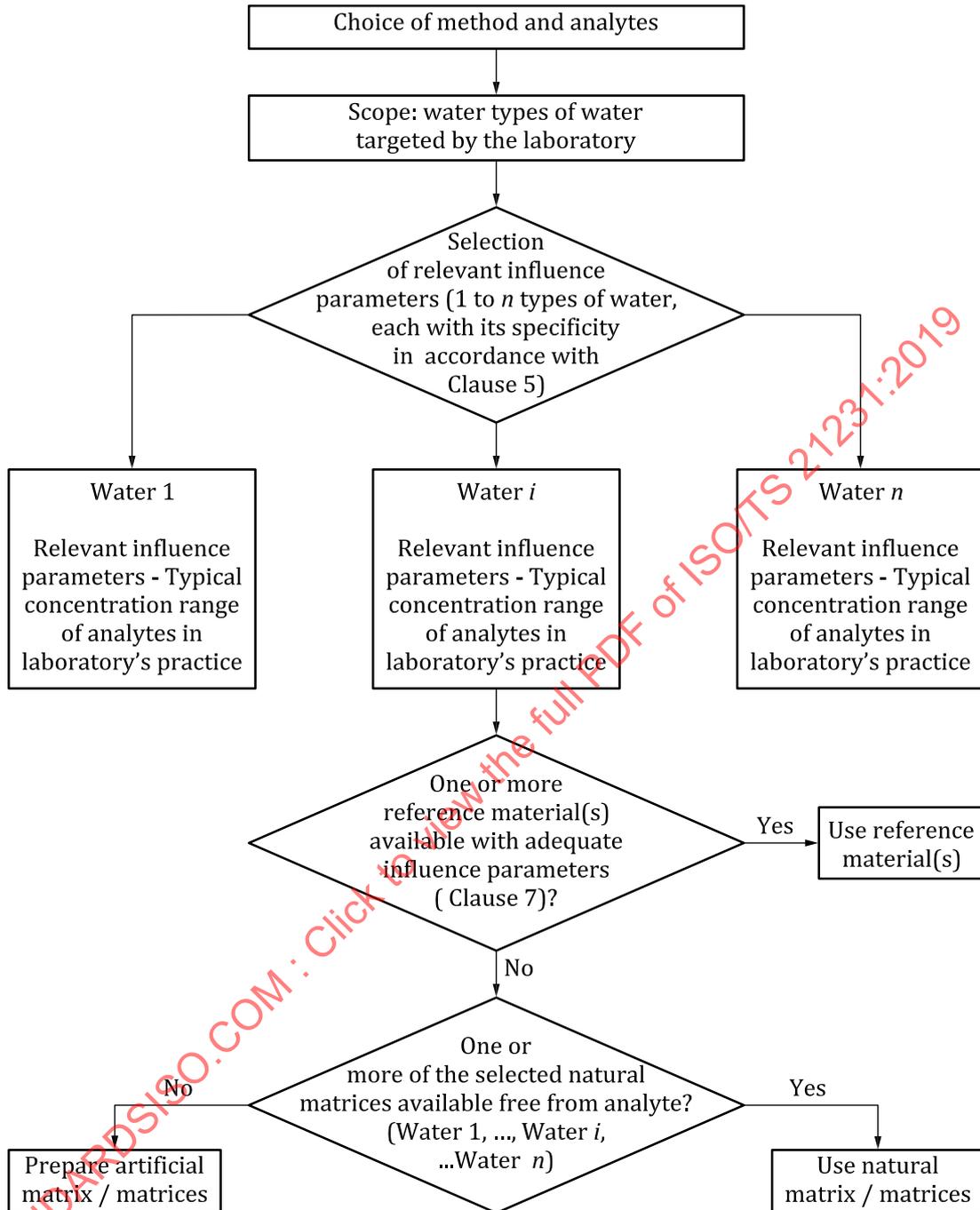


Figure 1 — Summary flow chart

## 5 Influence parameters

### 5.1 Common parameters for all matrices

The following influence parameters are liable to have an impact on analysis procedures. They shall help classify the types of water on which the laboratory has validated its method or determined performance characteristics.

- pH;
- ion composition and/or conductivity;

- salinity;
- dissolved organic carbon (DOC) and/or total organic carbon (TOC);
- colour or turbidity;
- suspended particular matter (SPM) content.

During the validation or characterization study, it is up to the laboratory to:

- define, for its practice, the characteristic ranges associated with each of the above parameters;
- justify, if applicable, the lack of influence thereof on the characterized method;
- complement this list with other characteristic parameters based on the methods and the source of the samples analysed, using for example [Annex A](#) or [Annex C](#).

## 5.2 Water intended for consumption

Water intended for human and livestock consumption is water considered to be fit for drinking.

Drinking water belongs to this category. It includes groundwater that has been chlorinated in the resource.

The minimum additional characteristics to be included for this category are:

- disinfectant presence and content (distributed waters or groundwater chlorinated in the resource);
- CO<sub>2</sub> content (natural mineral water), if relevant to subsequent specified analysis requirements.

## 5.3 Natural waters

Natural waters are waters taken from the natural environment not undergoing to any treatment other than the addition of reagents for analyte preservation.

Surface waters and groundwater belong to this category. Brackish waters with salinity lower than 30 g/l are incorporated in this category.

Rainwater, which is generally not intended for consumption, are incorporated in this category.

## 5.4 Waste waters

Waste waters can originate from any combination of household, industrial or commercial activities. They include collected run-offs and those from any spillage or infiltration from the waste water collection system, including the contents of storm water tanks or ponds, discharged into collection systems or into the environment.

NOTE 1 Waste waters can be collected in common systems or in separate systems.

NOTE 2 For the purposes of this document, the definition of waste water also includes untreated sanitary waters.

NOTE 3 National or local regulations can include lists of substances of concern in relation to sewer discharges.

[Annex C](#) gives a list of examples of additional characteristics associated with some sectors of activity.

Some waste waters may have a high salinity.

## 5.5 Marine waters

Sea water consists of a large number of compounds distributed over the following categories: gases, particulate matter, colloids, and dissolved elements (see Reference [7]).

The dissolved elements consist of 92 natural chemical elements, approximately two-thirds of which are present in ultra-trace amounts and are difficult to detect. Sea water is characterized in that the relative proportions of its 11 main constituents are substantially constant (Dittmar's law [8]) within 1 %. Dittmar's law can thus be used to determine the salinity of sea water by measuring only one of its components.

The average salinity of sea water is 35 g/kg. It is generally between 30 g/kg (North Atlantic) and 40 g/kg (Red Sea) but exhibits extreme values in closed or semi-closed seas (6 g/kg in the Baltic Sea, 330 g/kg in the Dead Sea). The pH of sea water is approximately 8,2.

## 5.6 Recreational waters

Recreational waters are bathing, swimming pool, thermal bath and spa waters. They may be sourced from natural waters or waters intended for human consumption and are characterized, in addition to the influence parameters defined in 5.2, by the potential presence of specific disinfection products and by-products, and the potential presence of sulfur compounds.

## 6 Selection of characteristic parameters of a matrix

### 6.1 General

For the purposes of characterization of the applicability and the performances of an analytical method to a matrix, the laboratory shall describe the limits of the ranges associated with the characteristic parameters discussed in this clause.

### 6.2 All waters

The parameters are those defined in 5.1.

### 6.3 Waters intended for consumption

In addition to the characteristics listed in 5.1, waters intended for consumption are characterized by:

- their free and total chlorine content;
- the nature and content of disinfection reagents and by-products;
- their CO<sub>2</sub> content, if relevant.

Refer to [Annex A](#) for more detailed characterization of waters intended for human consumption.

### 6.4 Natural waters

In addition to the characteristics listed in 5.1, natural waters are characterized by:

- the sampling location, including the sampling depth;
- the identified surrounding anthropic pressures.

In the case of groundwater used as drinking water resources, which are treated in situ, free and total chlorine content should be verified.

### 6.5 Waste waters

In addition to the characteristics listed in 5.1, waste waters are characterized by:

- the original activity sector (see [Annex C](#));

- the connected activity sectors in the case of municipal waste water treatment plants (MWWTP) discharges.

## 6.6 Marine waters

In addition to the characteristics listed in [5.1](#), marine waters are characterized by:

- the sampling location, including sampling depth;
- their salinity.

## 6.7 Recreational waters

In addition to the characteristics listed in [5.1](#), recreational waters are characterized by:

- the sampling location;
- the nature and content of disinfection reagents and by products.

## 7 Available materials

### 7.1 General

The laboratory shall select study matrices for one or more of the above water types from, in order of preference:

- reference materials if the matrix is sufficiently characterized;
- supernumerary material from interlaboratory tests if stable and sufficiently characterized;
- material obtained by spiking with the real matrix free from the analytes of interest;
- material obtained by spiking a reasonable dilution of a real matrix, after adjusting the characteristics modified by the dilution;
- material obtained by spiking of an artificial matrix based on a recipe (see [Annex B](#)).

At least three different representative samples of each water type should be studied to provide a realistic evaluation of performance of the method on the selected water type. Wherever possible, the method performances shall be characterized on a non-artificial sample.

### 7.2 Material obtained by reasonable dilution of a real matrix

When the laboratory cannot select a real matrix free from analyte(s) of interest, but it is possible to select a real matrix containing the analyte(s) of interest at a concentration lower than  $10\times$  the limit of quantification (LOQ) defined for the method under examination, a representative matrix can be prepared by diluting the low-concentration real matrix, so as to lower the concentration of analyte(s) of interest to less than the LOQ defined for the method.

The dilution factor,  $f$ , shall be lower than 10. For this dilution, a water free from analyte(s) of interest having a similar composition to the chosen matrix (major elements and influence factors) shall be used.

Before dilution, the selected matrix shall be characterized on the basis of the influence parameters chosen for the study. After dilution, these parameters shall be readjusted if required using solid state reagents or stock solutions of solid state reagents so that the value of each influence parameter remains within the scope defined by the laboratory.

### 7.3 Artificial material

Artificial materials can be prepared according to [Annex B](#), after adjusting the influence parameters selected based on a bibliographic study, and/or on [Annex C](#), within the concentration range defining the scope of the method.

### 7.4 Analyte-specific blank values in matrices

For some analytes, such as heavy metals, no analyte-free natural or artificial matrix can be obtained. After proper justification, the laboratory should study LOQ as follows.

- Determine  $LOQ_{MQ}$  on ultrapure water.
- Calculate  $LOQ_{water\ i}$  by correcting  $LOQ_{MQ}$  using the recovery of the analyte in the intended matrix, i.e. water by using [Formula \(1\)](#):

$$LOQ_{water\ i} = \frac{LOQ_{MQ}}{\rho_{water\ i}} \quad (1)$$

where

- $LOQ_{water\ i}$  is the LOQ of the method for the analyte in water type  $i$ ;
- $LOQ_{MQ}$  is the LOQ of the method for the analyte in ultra pure water;
- $\rho_{water\ i}$  is the mean recovery of the method for the analyte in water type  $i$ .

## 8 Report

The quantitative analytical method assessment report, for a given matrix, shall include, in addition to the information requested by the assessment procedure:

- a) the name of the tested matrix according to the typology defined in [Clause 5](#);
- b) the characteristic parameters of the matrix according to [Clause 6](#) and the associated representative ranges (scope);
- c) the influence parameters tested, the justification for their selection and the representative contents;
- d) the source of the matrix and, if applicable, its preparation method.

## Annex A (informative)

### Characterization of waters intended for human consumption and mineral waters

Water intended for human consumption produced, is generally characterized by:

- the absence of suspended solids;
- a relatively low organic content (TOC < 4 mg/l);
- a conductivity at 25 °C between 50 µS/cm and 1 100 µS/cm and
- a pH between 6 and 9.

Waters sampled during the production cycle, or at distribution point, often show traces of oxidants used to disinfect resource water, usually chlorine, chlorine dioxide or ozone at levels between 0,2 mg/l and 2 mg/l. Depending on the parameters to be analysed, it may be necessary to eliminate these traces of oxidants by a neutralizing agent, usually sodium thiosulfate pentahydrate added to reach a concentration between 20 mg/l and 200 mg/l.

The oxidant addition may also generate disinfection by-products, mainly trihalomethanes, bromates, chlorates.

Mineral waters show generally the same figures, without addition of oxidant, but some of them are also characterized by:

- high mineralization level (higher than 2 g/l);
- presence of carbon dioxide (sparkling waters), or
- presence of sulfides (thermal waters).

To select a representative model water for the validation of a method dedicated to the analysis of water intended for human consumption, the data listed above, and, where their presence might influence on the analytical protocol, the presence of ions representative of the catchment zone, nature and concentration, according to the geological characteristics thereof is taken into account.

## Annex B (informative)

### Examples of preparation of artificial matrices and representative characteristics

#### B.1 Overview

This annex gives examples of formulae that may be used to prepare various water types in a reproducible manner, to be used for the validation of analytical method.

NOTE In case of use for quality control (QC), suitable procedure for homogeneity and stability checking can be found, if necessary, in ISO Guide 80<sup>[19]</sup>.

#### B.2 Equipment

**B.2.1 Balance accurate to 1/10 mg.**

**B.2.2 Common laboratory glassware.**

**B.2.3 Non-actinic glassware for storage of stock solutions.**

**B.2.4 Flask with screw cap**, for degassing beer.

**B.2.5 Laboratory mixer**, comprising an inert container and a lid, for waste water preparations.

#### B.3 Reagents

All reagents used for a formula should be of sufficient quality (at least “analysis quality”). Unless otherwise indicated, water compliant to ISO 3696 shall be used to implement these formulae.

Some reagents are specific to one of the formulae.

**B.3.1 Boric acid**,  $\text{H}_2\text{BO}_3$ , anhydrous.

**B.3.2 Nitric acid**,  $\text{HNO}_3$ ,  $c(\text{HNO}_3) = 15,8 \text{ mol/l}$ ,  $\rho = 1,4 \text{ kg}$ .

**B.3.3 Ammonium chloride**,  $\text{NH}_4\text{Cl}$ , anhydrous.

**B.3.4 Potassium bromide**,  $\text{KBr}$ , anhydrous.

**B.3.5 Aluminium chloride hexahydrate**,  $\text{AlCl}_3 \cdot 6\text{H}_2\text{O}$ .

**B.3.6 Magnesium chloride hexahydrate**,  $\text{MgCl}_2 \cdot 6\text{H}_2\text{O}$ .

**B.3.7 Anhydrous calcium chloride**,  $\text{CaCl}_2$ .

**B.3.8 Strontium chloride hexahydrate**,  $\text{SrCl}_2 \cdot 6\text{H}_2\text{O}$ .

**B.3.9 Potassium chloride**, KCl, anhydrous.

**B.3.10 Sodium chloride**, NaCl, anhydrous.

**B.3.11 Sodium fluoride**, NaF, anhydrous.

**B.3.12 Sodium hydroxide**, NaOH, solution 0,10 mol/l.

**B.3.13 Sodium hydrogen carbonate**, NaHCO<sub>3</sub>, anhydrous.

**B.3.14 Barium nitrate**, Ba(NO<sub>3</sub>)<sub>2</sub>, anhydrous.

**B.3.15 Manganese nitrate hexahydrate**, Mn(NO<sub>3</sub>)<sub>2</sub>·6H<sub>2</sub>O.

**B.3.16 Copper nitrate trihydrate**, Cu(NO<sub>3</sub>)<sub>2</sub>·3H<sub>2</sub>O.

**B.3.17 Zinc nitrate hexahydrate**, Zn(NO<sub>3</sub>)<sub>2</sub>·6H<sub>2</sub>O.

**B.3.18 Lead nitrate**, Pb(NO<sub>3</sub>)<sub>2</sub>, anhydrous.

**B.3.19 Potassium acid phosphate**, (KH<sub>2</sub>PO<sub>4</sub>), anhydrous.

**B.3.20 Sodium sulfate**, Na<sub>2</sub>SO<sub>4</sub>, anhydrous.

**B.3.21 Ferric sulfate**, Fe(SO<sub>4</sub>)<sub>3</sub>, anhydrous.

**B.3.22 Magnesium sulfate**, MgSO<sub>4</sub>, anhydrous.

**B.3.23 Urea**, (NH<sub>3</sub>)<sub>2</sub>CO.

**B.3.24 Kaolin.**

Argillaceous rock containing kaolinite, hydrous aluminium silicate (2SiO<sub>2</sub>, Al<sub>2</sub>O<sub>3</sub>, 2H<sub>2</sub>O). This rock is friable, impermeable and refractory.

**B.3.25 Degassed beer.** Industrially produced commercial drink, obtained by fermenting a mixture of cereal grains, malt and hops. "Low-calorie" quality (<1 180 J/ml).

Transfer the beer into a closed container with capacity 20 % greater than the quantity of beer to be degassed. Close, shake vigorously, then release the pressure by slightly loosening the cap. Leave to rest in the refrigerator for 24 h.

Bring to ambient temperature before use.

**B.3.26 Microcrystalline cellulose**, dried to constant mass at 105 °C and kept in a desiccator.

**B.3.27 Dry salt for marine aquarium.**

A commercial mixture of mineral salts for marine aquariums, such as sold in pet shops for example, dried to constant mass at 105 °C and kept in a desiccator.

**B.3.28 Yeast**, *Saccharomyces cerevisiae*, also called baker's yeast, fresh.

**B.3.29 Peptone.**

An animal protein digestate used in the preparation of biological culture media, containing  $\geq 12$  % nitrogen.

**B.4 Marine waters****B.4.1 General**

These formulae enable preparation of a solution containing mineral salts in comparable proportions to a sea water, corresponding to a typical heavy metal-enriched sea water, that is reproducible and usable when it is necessary to simulate a marine water.

Preparation of stock solutions is required.

**B.4.2 Stock solutions****B.4.2.1 Stock solution No. 1**

In a 1 l volumetric flask, place 500 ml of water. Dissolve:

MgCl <sub>2</sub> ·6H <sub>2</sub> O:	555,6 g
CaCl <sub>2</sub> :	57,9 g
SrCl <sub>2</sub> ·6H <sub>2</sub> O:	2,1 g

Adjust to 1 l with water. Store in a carefully stoppered amber glass flask.

**B.4.2.2 Stock solution No. 2**

In a 1 l volumetric flask, place 500 ml of water. Dissolve:

KCl:	69,5 g
NaHCO <sub>3</sub> :	20,1 g
KBr:	10,0 g
H <sub>3</sub> BO <sub>3</sub> :	2,7 g
NaF:	0,3 g

Adjust to 1 l with water. Store in a carefully stoppered amber glass flask.

**B.4.2.3 Stock solution No. 3**

In a 1 l volumetric flask, place 500 ml of water. Dissolve:

Ba(NO <sub>3</sub> ) <sub>2</sub> :	0,994 g
Mn(NO <sub>3</sub> ) <sub>2</sub> ·6H <sub>2</sub> O:	0,546 g
Cu(NO <sub>3</sub> ) <sub>2</sub> ·3H <sub>2</sub> O:	0,396 g
Zn(NO <sub>3</sub> ) <sub>2</sub> ·6H <sub>2</sub> O:	0,151 g
Pb(NO <sub>3</sub> ) <sub>2</sub> :	0,066 g

Adjust to 1 l with water. Store in a carefully stoppered amber glass flask.

NOTE Larger quantities of stock solutions can be prepared by proportionally adapting the above formulations.

### B.4.3 Preparation

#### B.4.3.1 Artificial marine water[7], [10]

In a 1 l volumetric flask, place 800 ml of water. Dissolve:

NaCl: 24,534 g

Anhydrous Na<sub>2</sub>SO<sub>4</sub>: 4,094 g

Add 20 ml of stock solution No. 1 and 10 ml of stock solution No. 2. Shake vigorously. Adjust to 1 l. Adjust the pH to 8,2 with a few drops of 0,1 N sodium hydroxide solution (B.3.12).

The artificial marine water thus prepared has the following composition:

	Concentration (g/l)
NaCl:	24,534
Na <sub>2</sub> SO <sub>4</sub> :	4,09
KCl:	0,695
NaHCO <sub>3</sub> :	0,201
KBr:	0,100
H <sub>3</sub> BO <sub>3</sub> :	0,027
NaF:	0,030
MgCl <sub>2</sub> :	5,20
CaCl <sub>2</sub> :	1,16
SrCl <sub>2</sub> :	0,025

This preparation should be used immediately after preparation.

#### B.4.3.2 Heavy metal-enriched artificial marine water[11]

Add 1 ml of stock solution No. 3 to 1 l of artificial marine water (B.4.2.1).

The heavy metal-enriched artificial marine water thus prepared has the following composition:

	Concentration (g/l)
NaCl:	24,534
Na <sub>2</sub> SO <sub>4</sub> :	4,09
KCl:	0,695
NaHCO <sub>3</sub> :	0,201

KBr:	0,100
H <sub>3</sub> BO <sub>3</sub> :	0,027
NaF:	0,030
MgCl <sub>2</sub> :	5,20
CaCl <sub>2</sub> :	1,16
SrCl <sub>2</sub> :	0,025
Ba(NO <sub>3</sub> ) <sub>2</sub> :	0,000 994
Mn(NO <sub>3</sub> ) <sub>2</sub> ·6H <sub>2</sub> O:	0,000 546
Cu(NO <sub>3</sub> ) <sub>2</sub> ·3H <sub>2</sub> O:	0,000 396
Zn(NO <sub>3</sub> ) <sub>2</sub> ·6H <sub>2</sub> O:	0,000 151
Pb(NO <sub>3</sub> ) <sub>2</sub> :	0,000 066

This formula should be used immediately after preparation.

#### B.4.3.3 Artificial marine water as per Kester<sup>[15]</sup>

Dissolve in 750 ml of distilled water:

Compound	NaCl	Na <sub>2</sub> SO <sub>4</sub>	KCl	NaHCO <sub>3</sub>	KBr	H <sub>3</sub> BO <sub>3</sub>	NaF
Mass (g)	23,926	4,008	0,677	0,196	0,098	0,026	0,003

Add:

Solution <sup>a</sup>	Volume (ml)
MgCl <sub>2</sub> ·6 H <sub>2</sub> O: 1 mol·l <sup>-1</sup>	53,27
CaCl <sub>2</sub> ·2 H <sub>2</sub> O: 1 mol·l <sup>-1</sup>	10,33
SrCl <sub>2</sub> ·6 H <sub>2</sub> O: 0,1 mol·l <sup>-1</sup>	0,90

<sup>a</sup> Solutions with precise concentrations of silver nitrate.

Make up to 1 kg with distilled water.

This water has a salinity of 35,00 g/kg.

**B.4.3.4 Controlled-salinity artificial marine waters as per Grasshoff**<sup>[15], [16]</sup>

**B.4.3.4.1 Artificial marine water as per Grasshoff — Formula 1**

Dissolve in 500 ml of distilled water (solution G1a):

Compound	NaCl	Na <sub>2</sub> SO <sub>4</sub>	KCl	NaHCO <sub>3</sub>	KBr	H <sub>3</sub> BO <sub>3</sub>	NaF
Mass (g)	23,9	4,0	0,7	0,2	0,1	0,03	0,003

Dissolve in 455 ml of distilled water (solution G1b):

Compound	MgCl <sub>2</sub> ·6 H <sub>2</sub> O	CaCl <sub>2</sub> ·2H <sub>2</sub> O	SrCl <sub>2</sub> ·6H <sub>2</sub> O
Mass (g)	10,8	1,5	0,025

Mix solutions G1a and G1b, measure the salinity of the mixture (S approximately 35).

**B.4.3.4.2 Artificial marine water as per Grasshoff — Formula 2**

Dissolve in approximately 800 ml of distilled water:

Compound	NaCl	NaHCO <sub>3</sub>	MgSO <sub>4</sub> ·7 H <sub>2</sub> O
Mass (g)	32	0,2	14

Make up to 1 l with distilled water: salinity is equal to 34,2 (chlorosity = 19,4 g/l).

**B.5 Waste waters**

**B.5.1 General**

Waste waters can have very variable compositions depending on their source. The formulations suggested below contain compounds in concentrations such as those that can be found in treated urban waste water discharges. They are not intended to represent all waste waters, but can provide a laboratory material enabling assessment of the initial performances and performances over time of the analytical methods on a reproducible and inexpensive material.

If the laboratory wishes to refine the prepared material in order to adapt its representativeness to certain types of discharges, it may select the relevant substances or interfering substances using the substance lists provided in [Annex C](#).

**B.5.2 WWTP water**<sup>[9]</sup>

Place approximately 500 ml of water in the container of the mixer. Set the mixing speed to the lowest.

Add in this order:

Microcrystalline cellulose ( <a href="#">B.3.26</a> ):	0,400 g
Dry salt for marine aquarium ( <a href="#">B.3.27</a> ):	2,000 g
Kaolin ( <a href="#">B.3.24</a> ):	0,080 g
Degassed beer ( <a href="#">B.3.25</a> ):	120,0 ml

Mix for 30 s. Transfer quantitatively to a 2 l volumetric flask and adjust.

This solution may be kept in the refrigerator for 24 h. Preservative additives described in ISO 5667-3 should be added depending on the analytical method to be assessed.

The typical characteristics of this effluent are listed in [Tables B.1](#) and [B.2](#).

### B.5.3 Discharge water

#### B.5.3.1 Source of the formula

This formula has been used by INERIS since 2005 (see Reference [17]). The values have been chosen regarding applicable national French regulation setting the technical requirements relating to collection and waste water treatment plans:

- suspended solids are represented by microcrystalline cellulose in the proportion of 250 mg/l;
- the total nitrogen content of 10 mg/l will be obtained using a mixture of urea and ammonium chloride;
- the total phosphorus content of 1 mg/l will be obtained using  $\text{KH}_2\text{PO}_4$ .

Aluminium and iron are not part of the monitoring of discharge waters and do not appear in the IOW databases (International Office for Water). On the other hand, they are regularly present in interlaboratory test materials, for example those supplied by AGLAE (General Association of Analysis and Testing Laboratories). Based on the study of contents between June 2003 and May 2004, a typical content of 200  $\mu\text{g/l}$  for each of these is proposed, expressed as total metal, for a given range of:

Al ( $\mu\text{g/l}$ ): 170 to 775

Fe ( $\mu\text{g/l}$ ): 130 to 590

As this model is intended for studying the performances of methods in a limited catchment area or in a specific industrial sector, it is always created based on drill water or water for consumption in the geographical area concerned; this is why only anthropogenic parameters are adjusted by means of reagents. Its composition in terms of main elements is to be recorded.

#### B.5.3.2 Preparation

Place approximately 500 ml of water in the container of the mixer. Set the mixing speed to the lowest.

Add in this order:

Microcrystalline cellulose ( <a href="#">B.3.26</a> )	500 mg
Urea ( <a href="#">B.3.23</a> ) and ammonium chloride ( <a href="#">B.3.3</a> )	Equiv 20 mg nitrogen each
$\text{KH}_2\text{PO}_4$ ( <a href="#">B.3.19</a> )	Equiv 2 mg phosphorus
$\text{AlCl}_3 \cdot 6\text{H}_2\text{O}$ ( <a href="#">B.3.5</a> )	Equiv 400 $\mu\text{g}$ aluminium
$\text{Fe}(\text{SO}_4)_3$ ( <a href="#">B.3.21</a> )	Equiv 400 $\mu\text{g}$ iron

Mix for 30 s. Transfer quantitatively to a 2 l volumetric flask and adjust. Check the characteristic parameters of the prepared effluent; adjust if necessary using the reagents above.

This solution may be kept in the refrigerator for 24 h. Preservative additives described in ISO 5667-3 should be added depending on the analytical method to be assessed.

The typical characteristics of this effluent are listed in [Tables B.1](#) and [B.2](#).

#### B.5.4 Artificial effluent 1<sup>[12]</sup>

To 1 l of deionized water, add:

Compound	Microcrystalline cellulose	Urea	Yeast	NaCl	K <sub>2</sub> HPO <sub>4</sub>	CaCl <sub>2</sub>	MgSO <sub>4</sub>
QS	0,400 g/l	0,03 g/l	0,11 g/l	0,007 g/l	0,028 g/l	0,028 g/l	0,028 g/l

Mix and check the characteristic parameters of the prepared effluent; adjust if necessary using the reagents above.

The typical characteristics of this effluent are listed in [Tables B.1](#) and [B.2](#).

This solution should be prepared daily. Preservative additives described in ISO 5667-3 should be added depending on the analytical method to be assessed.

#### B.5.5 Artificial effluent 2<sup>[11]</sup>

To 1 l of deionized water, add:

Compound	Peptone	Urea	Yeast	NaCl	K <sub>2</sub> HPO <sub>4</sub>	CaCl <sub>2</sub>	MgSO <sub>4</sub>
QS	0,16 g/l	0,03 g/l	0,11 g/l	0,007 g/l	0,028 g/l	0,028 g/l	0,028 g/l

NOTE 0,9 ml of the food product Viadox®<sup>1)</sup> can replace the peptone. Before dilution, it has the following characteristics: COD: 260 g/l, BOD: 155 g/l, Kjeldahl nitrogen: 26 g/l, NH<sub>4</sub><sup>+</sup>: 7 g/l PO<sub>4</sub><sup>3-</sup>: 3,6 g/l (see References [\[12\]](#) and [\[14\]](#)).

The typical characteristics of this effluent are listed in [Table B.1](#).

Check the characteristic parameters of the prepared effluent; adjust if necessary using the reagents above.

This solution should be prepared daily. Preservative additives described in ISO 5667-3 should be added depending on the analytical method to be assessed.

#### B.5.6 Artificial effluent 3<sup>[13]</sup>

A commercial mixture comprising meat, vegetable extracts and sugars (Viadox®) can constitute an anthropogenic model of dissolved organic matter. It contains 42 g/l carbohydrates, 173 g/l protein, and 0,77 mg/l fat (see Reference [\[14\]](#)).

Artificial waste water can be prepared based on Viadox®, by diluting at 1 % in mineral water. Dissolved organic matter is simulated by 1 g of yeast.

The typical characteristics of this effluent are listed in [Tables B.1](#) and [B.2](#).

Check the characteristic parameters of the prepared effluent; adjust if necessary using the reagents in [B.4.1](#).

This solution should be prepared daily. Preservative additives described in ISO 5667-3 should be added depending on the analytical method to be assessed.

#### B.5.7 Typical values of the characteristic parameters of waste water formulae

The typical values of the characteristic parameters of the waste water formulae described in [B.5](#) were measured on formulae that were reconstituted based on water for consumption distributed in

1) Viadox® is an example of a suitable product available commercially, solution of a product similar to OXO®, VEGEMITE®, or BOVRIL®. This example is given only as information for the convenience of users of this document and does not constitute an endorsement by ISO of this product.

the Commune of Verneuil-en-Halatte (France, Oise), natural water or based on deionized water if the formula specifies this.

Two types of parameter were measured:

- the influence parameters defined in [5.4](#);
- the characteristic parameters commonly measured in a regulatory framework.

The parameters other than those defined in [5.4](#) are given to enable the laboratory to link the formulae to the samples it normally examines.

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Table B.1 — Typical values obtained for the influence parameters for the waste water formulae described in B.5[19]

Water	Days	pH	Conductivity µS/cm at 25 °C	SPM mg/l	TOC mg/l	DOC mg/l	Cl <sup>-</sup> mg/l	PO <sub>4</sub> <sup>-</sup> mg/l	SO <sub>4</sub> <sup>-</sup> mg/l	NO <sub>3</sub> <sup>-</sup> mg/l	NH <sub>4</sub> <sup>+</sup> mg/l	Na mg/l	K mg/l	Mg mg/l	Ca mg/l
WWTP water (B.5.2)	D0	4,69	1 877	235	1,784	1,735	520	270	72,6	1,03	<0,02	274	39,8	36,9	13,6
					1,800	1,714					<0,02	280	40,8	37,6	11,8
	D+2	5,44	1 884	261	1,796	1,783	514	25,9	72,0	0,94	<0,02	281	39,3	36,3	11,5
	D+3	5,62	1 874	256	1,801	1,757	511	20,8	72,6	0,95	<0,02	265	36,8	34,1	11,4
	D+7	4,45	1 884	382	1,748	1,728	533	19,3	74,2	0,89	<0,02	285	40,2	40,1	11,8
					1,737	1,722									
Discharge water (B.5.3)	D0	7,63	674	253	76,1	3,02	25,5	1,98	33,1	24,6	0,76	12,6	3,88	11,8	102
					76,3	2,91					0,80	13,6	3,99	12,1	111
	D+2	7,81	692	234	75,6	3,91	25,6	1,87	33,4	24,7	0,75	13,5	3,91	11,8	107
	D+3	7,75	680	240	69,9	3,20	25,8	1,91	33,3	24,8	0,72	13,7	3,69	11,6	103
	D+7	7,88	678	242	73,2	3,85	26,7	1,86	34,7	26,2	0,84	13,9	3,73	13,9	69,8
					64,6	2,73									
Artificial effluent 1 (B.5.4)	D0	6,44	122	338	73,8	8,46	18,1	21,2	10,8	<0,05	0,13	2,95	8,25	2,56	7,89
					75,1	8,87					0,14	3,01	8,39	2,59	8,30
	D+2	7,09	154	402	88,1	8,28	18,1	18,2	10,7	<0,05	0,07	2,99	8,35	2,58	12,8
	D+3	7,11	146	418	91,2	8,07									
	D+7	7,18	149	488	68,8	8,78	18,1	17,7	10,8	<0,05	0,07	3,22	7,87	2,46	12,1
					71,2	7,47									
					104	10,6	18,7	19,1	11,1	<0,05	0,32	2,74	7,70	2,66	7,93
					108	9,3									

Table B.1 (continued)

Water	Days	pH	Conductivity at 25 °C µS/cm	SPM mg/l	TOC mg/l	DOC mg/l	Cl <sup>-</sup> mg/l	PO <sub>4</sub> <sup>-</sup> mg/l	SO <sub>4</sub> <sup>-</sup> mg/l	NO <sub>3</sub> <sup>-</sup> mg/l	NH <sub>4</sub> <sup>+</sup> mg/l	Na mg/l	K mg/l	Mg mg/l	Ca mg/l
Artificial effluent 2 (B.5.5)	D0	6,37 at 25,1 °C	164	38,0	196	177	21,0	27,8	16,2	<0,05	1,40	8,38	10,9	2,54	6,73
	D+2	6,74 at 23,9 °C	231	55,2	192	180	21,2	16,7	16,3	<0,05	1,55	8,67	11,0	2,58	7,26
	D+3	6,89 at 23,1 °C	270	48,6	169	143	141	15,9	16,1	<0,05	1,53	8,51	12,1	2,46	7,21
	D+7	7,17 at 21,8 °C	458	69,7	152	128	21,1	15,8	16,9	<0,05	17,4	8,48	12,3	2,33	6,97
	D0	6,81 at 25,7 °C	3,900	349	640	438	1,072	27,4	13,5	4,10	<0,02	807	25,0	25,6	73,3
	D+2	6,69 at 23,9 °C	4,020	403	542	399	1,075	25,3	13,7	<0,05	<0,02	724	24,4	25,8	79,5
	D+3	6,89 at 23,1 °C	4,040	449	492	360	1,066	10,5	13,1	<0,05	23,8	699	20,8	22,3	73,7
D+7	6,82 at 21,8 °C	4,060	556	477	340	1,092	9,3	13,5	<0,05	31,2	678	22,0	25,3	46,1	
					328	175									

Table B.2 — Typical values obtained for the characteristic parameters for the waste water formulae described in B.5

Water	Days	COD mg/l	BOD5 mg/l	COD/ BOD5 ratio	TKN mg/l	NO <sub>2</sub> <sup>-</sup> mg/l	P <sub>tot</sub> mg/l	Pb mg/l	Sb mg/l	Se mg/l	Sn mg/l	Ti mg/l	Zn mg/l
WWTP water (B.5.2)	D+2	6,520	4,560	1,4	36	<0,05	12,2	<0,002	<0,005	0,000 2	<0,005	0,700	<0,010
Discharge water (B.5.3)	D+2	275	73	3,8	<1	<0,05	0,44	0,010	<0,005	0,001 6	<0,005	<0,010	0,743
Artificial effluent 1 (B.5.4)	D+2	470	130	3,6	15	<0,05	7,00	<0,002	<0,005	0,000 1	<0,005	0,025	<0,010
Artificial water 2 (B.5.5)	D+2	415	250	1,7	70	<0,05	7,40	<0,002	<0,005	0,000 3	<0,005	0,085	<0,010
Artificial water 3 (B.5.6)	D+2	1,460	700	2,1	109	0,47	19,2	<0,002	<0,005	0,000 3	<0,005	0,041	0,014

Water	Days	Al mg/l	As mg/l	Ca mg/l	Cd mg/l	Co mg/l	Cr mg/l	Cu mg/l	Fe mg/l	Hg mg/l	K mg/l	Mg mg/l	Mn mg/l	Na mg/l	Ni mg/l
WWTP water (B.5.2)	D+2	1,520	<0,005	13,0	<0,002	<0,003	<0,005	<0,005	0,035	<0,000 5	52,3	31,6	0,007	237	<0,010
Discharge water (B.5.3)	D+2	0,073	<0,005	110	<0,002	<0,003	<0,005	0,722	0,092	<0,000 5	2,99	11,5	<0,005	12,4	0,240
Artificial effluent 1 (B.5.4)	D+2	0,062	<0,005	8,18	<0,002	<0,003	<0,005	<0,005	<0,025	<0,000 5	6,13	2,78	<0,005	2,36	<0,010
Artificial water 2 (B.5.5)	D+2	0,020	<0,005	8,23	<0,002	<0,003	<0,005	<0,005	<0,025	<0,000 5	8,63	2,74	<0,005	7,15	<0,010
Artificial water 3 (B.5.6)	D+2	<0,020	<0,005	74,3	<0,002	<0,003	<0,005	<0,005	<0,025	<0,000 5	42,2	31,6	0,005	684	<0,010

## Annex C (informative)

### Occurrence of chemical substances in waste water, by industrial activity sector

#### C.1 Sources

Substances generated by industrial activities have been identified through an investigation on the discharge of hazardous substances into surface water by a representative of set Installations Classified for Protection of the Environment (ICPEs) launched in France in 2002 and completed in 2007 (see Reference [5]).

Substances for which occurrence is recorded at final discharge of WWTPs were identified during an exhaustive investigation conducted between 2009 and 2013 (see Reference [6]).

During these investigations, an extensive list of substances was searched.

- Alkylphenols: nonylphenols, octylphenols
- Aniline: 2-chloroaniline, 3-chloroaniline, 4-chloroaniline, 3,4-dichloroaniline, 4-chloro,3-nitroaniline
- BTEX: benzene, ethylbenzene, isopropylbenzene, toluene, xylenes (all isomers)
- Chlorobenzenes: chlorobenzene, 1,2-dichlorobenzene, 1,3-dichlorobenzene, 1,4-dichlorobenzene, 1,2,3-trichlorobenzene, 1,2,4-trichlorobenzene, 1,3,5-trichlorobenzene, 1,2,4,5-tetrachlorobenzene, pentachlorobenzene, hexachlorobenzene, 1-chloro-2-nitrobenzene, 1-chloro,3-nitrobenzene, 1-chloro,4-nitrobenzene
- Chlorophenols: 2-chlorophenol, 3-chlorophenol, 4-chlorophenol, 2,4-dichlorophenol, 2,4,5-trichlorophenol, 2,4,6-trichlorophenol, pentachlorophenol, 4-chloro, 3-methylphenol
- HVOCs: dichloromethane, trichloromethane, carbon tetrachloride, 1,1-dichloroethane, 1,2-dichloroethane, 1,1,1-trichloroethane, 1,1,2-trichloroethane, 1,1,2,2-tetrachloroethane, hexachloroethane, 1,1-dichloroethylene, 1,2-dichloroethylene, trichloroethylene, tetrachloroethylene, 2-chlorotoluene, 3-chlorotoluene, 4-chlorotoluene, 3-chloroprene (allyle chloride), Hexachlorobutadiene, hexachloropentadiene, vinyl chloride
- Metals: arsenic, cadmium, chromium, copper, lead, mercury, nickel, zinc
- PAH: anthracene, fluoranthene, naphthalene, Benzo [a] Pyrene, Benzo [k] Fluoranthene, Benzo [b] Fluoranthene, Benzo [g,h,i] Perylene, Indeno [1,2,3-cd] Pyrene
- Polybrominated diphenyl ethers (congeners 47, 99, 100, 154, 153, 183, 209)
- OTC: monobutyltin cation, dibutyltin cation, tributyltin cation, triphenyltin cation
- Pesticides: Alachlor, Atrazine, Simazine, Trifluralin, Chlorfenvinphos, Chlorpyrifos, Diuron, Isoproturon, alpha Endosulfan, beta Endosulfan, alpha Hexachlorocyclohexane, gamma Hexachlorocyclohexane
- PCB: congeners 28, 52, 101, 118, 138, 153, 180
- C10-C13 SCCP, Biphenyl, Epichlorhydrin, Tributylphosphate, Chloroacetic acid, 2-nitrotoluene, DEHP

## C.2 Industrial activities

Table C.1 gives a list of industrial activity sectors where hazardous substances are potentially present in aqueous discharges from establishments carrying out the said industrial activity.

**Table C.1 — Industrial activity sectors and sub-sectors**

Sector No.	ACTIVITY SECTORS	ACTIVITY SUB-SECTORS
1	SLAUGHTERHOUSES	/
2	OIL and GAS INDUSTRY	2.1 Refining plans 2.2 Oil and gas storage sites and terminals 2.3 Oil and gas industries: mixing and conditioning facilities for petroleum products 2.4 Oil and gas industries: synthesis and conversion facilities for petroleum products (excluding petrochemicals)
3	WASTE TREATMENT AND STORAGE INDUSTRY	3.1 Collection, pretreatment or treatment of hazardous waste 3.2 Non-hazardous waste storage facilities 3.3 Urban wastes incineration units 3.4 Tank washing 3.5 Other non-hazardous waste treatment sites
4	GLASS INDUSTRY	4.1 Glass melting 4.2 Crystal works 4.3 Other activities
5	THERMAL ELECTRIC POWER PLANTS	/
6	CHEMICAL INDUSTRY [Fine chemistry, mineral chemistry, organic chemistry, chlorochemicals, cosmetics, petrochemicals, fertilizer production, manufacture of explosives, pharmaceuticals (excluding galenics), phytopharmaceutical products].	
7	MANUFACTURE OF GLUES AND ADHESIVES	/
8	MANUFACTURE OF PAINTS	/
9	MANUFACTURE OF PIGMENTS	/
10	PLASTICS INDUSTRY	/
11	RUBBER INDUSTRY	/
12	TEXTILE INDUSTRY	12.1 Finishing 12.2 Bleaching
13	PAPER INDUSTRY	13.1 Preparation of chemical pulp 13.2 Preparation of non-chemical pulp 13.3 Manufacture of paper/cardboard
14	METALLURGY	14.1 Steelworks 14.2 Ferrous metal casting 14.3 Non-ferrous metal casting 14.4 Production and/or processing of non-ferrous metals

Table C.1 (continued)

Sector No.	ACTIVITY SECTORS	ACTIVITY SUB-SECTORS
15	PHARMACEUTICAL INDUSTRY: formulation of pharmaceutical products	/
16	PRINTING INDUSTRY	/
17	AGRI-FOOD INDUSTRY (Products of animal origin)	/
18	AGRI-FOOD INDUSTRY (Products of plant origin)	18.1 Wine production 18.2 AGRI-FOOD INDUSTRY (products of vegetal origin) excluding wine production
19	TANNERY AND LEATHERWORKS	/
20	METALLUGY INDUSTRY	/
21	SURFACE TREATMENT, COATING	/
22	TIMBER INDUSTRY	/
23	CERAMICS AND REFRACTORY MATERIALS	
24	MUNICIPAL WASTE WATER TREATMENT PLANTS	

[Table C.2](#) gives an overview of the occurrence of the investigated substances in each industrial sector. Substances are noted:

- R: when the substance has been found on a regular basis;
- O: when the substance has been found occasionally;
- /: when the substance has not been found in the sector or sub-sector.

When the occurrence of a substance in an industrial sector varies according to the sub-sector concerned, the indications take this into account.

When a substance listed under [C.1](#) has not been found in any sector, this substance is not part of [Table C.2](#).

For industrial sector of chemical industry (sector 6), no occurrence data are given in [Table C.2](#), due to the large variety of individual situation, not leading to a unique tendency. The interfering substance should be derived from the overview of the activity of each facility.

Table C.2 — Occurrence of substances by sectors and sub-sectors

SUBSTANCE	SECTOR																							
	1	2	3	4	5	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	
Alkylphenols: non-ylphenols	/	R: 2.2	R: 3.1, 3.2, 3.3, 3.5 O: 3.4	R: 4.1, 4.2, 4.3	0	/	/	/	/	R	R: 12.1, 12.2	R: 13.3	R: 14.1, 14.2, 14.3, 14.4	R	R	0	R: 18.1, 18.2	R	R	R	R	/	R	
Alkylphenols: octylphenols	/	R: 2.2	O: 3.1 R: 3.2	O: 4.3	/	/	/	/	/	R	/	/	O: 14.3	/	/	/	/	0	0	0	/	/	R	
BTEX: benzene	/	R: 2.1, 2.2	R: 3.4 O: 3.1	/	/	/	/	/	/	/	O: 12.1	/	O: 14.1	/	R	/	/	0	/	/	0	0	R	
BTEX: ethylbenzene	0	/	R: 3.4 O: 3.2, 3.5	/	/	/	R	/	/	/	/	/	/	/	/	/	/	0	/	/	/	/	/	
BTEX: isopropylbenzene	/	/	O: 3.4	/	/	/	/	/	/	/	/	/	/	/	/	/	/	0	/	/	/	/	/	
BTEX: toluene	0	O: 2.2, R: 2.4	R: 3.1, 3.4 O: 3.2, 3.3, 3.5	/	/	R	R	/	/	R	O: 12.1	O: 13.3	O: 14.3	/	R	/	/	R	0	0	0	/	0	
BTEX: xylenes (all isomers)	/	O: 2.2, R: 2.4	R: 3.4 O: 3.1, 3.5	/	0	0	R	0	/	/	O: 12.1	/	O: 14.3	/	0	/	/	R	/	/	/	/	0	
Chlorobenzenes: chlorobenzene	/	/	O: 3.4	/	/	/	0	/	/	/	/	/	/	/	/	/	/	/	/	/	/	/	/	
Chlorobenzenes: 1,2-dichlorobenzene	/	R: 2.4	/	/	/	/	/	/	/	/	/	/	/	/	/	/	/	/	/	/	/	/	/	
Chlorobenzenes: 1,3-dichlorobenzene	/	R: 2.4	/	/	/	/	/	/	/	/	/	/	/	/	/	/	/	/	/	/	/	/	/	
Chlorobenzenes: 1,2,3-trichlorobenzene	/	R: 2.4	/	/	/	/	/	/	/	/	/	/	/	/	/	/	/	/	/	/	/	/	R	
Chlorobenzenes: 1,2,4-trichlorobenzene	/	/	/	/	/	/	/	/	/	/	/	/	/	/	/	/	/	/	/	/	/	/	R	

Table C.2 (continued)

SUBSTANCE	SECTOR																							
	1	2	3	4	5	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	
Chlorobenzenes: 1,2,4,5-tetra- chlorobenzene	/	/	/	/	/	/	/	/	/	/	/	/	/	/	/	/	/	/	/	/	/	/	R	
Chlorobenzenes: pentachloroben- zene	/	/	0: 3.4	0: 4.1	/	/	0	/	/	/	0: 12.1	/	/	/	/	/	/	/	/	/	/	/	R	
Chlorobenzenes: hexachloroben- zene	/	0: 2.1	0: 3.3	/	/	/	/	/	/	/	0: 12.1	/	/	/	/	/	0: 18.2	/	/	0	/	/	R	
Chlorophenols: 2,4,6-trichlorophe- nol	0	/	0: 3.3	/	/	/	/	/	/	/	/	/	/	0	/	/	/	/	/	/	/	/	/	
Chlorophenols: 4-chloro,3-meth- ylphenol	/	R: 2.4	/	/	/	0	/	/	/	/	/	/	/	/	/	/	/	R	/	/	/	/	/	
Chlorophenols: pentachlorophenol	/	/	R: 3.3 O: 3.1, 3.2, 3.4	0: 4.1	/	0	0	/	/	/	/	R: 13.2, 13.3	0: 14.2, 14.3	/	/	/	R: 18.1	/	/	/	0	0	R	
HVOC: dichlo- romethane	0	R: 2.3, 2.4	R: 3.1, 3.4	R: 4.3	/	R	R	/	/	R	/	/	/	/	/	/	/	/	0	0	/	/	/	
HVOC: trichlo- romethane	R	R: 2.4 O: 2.1	O: 3.1, 3.3, 3.4, 3.5	O: 4.1, 4.2, 4.3	/	R	/	0	/	/	R: 12.1, 12.2	R: 13.2 O: 13.1	O: 14.1, 14.2, 14.4	R	/	R	R: 18.1, 18.2	0	R	R	/	R	R	
HVOC: carbon tetrachlo- ride	/	/	O: 3.4, 3.5	/	/	/	/	/	/	/	/	/	/	/	/	/	O: 18.2	0	R	0	/	/	R	
HVOC: 1,2-dichlo- roethane	/	/	0: 3.4	/	/	/	/	/	/	/	/	/	/	/	/	/	/	/	/	/	/	/	R	
HVOC: trichlo- roethane	/	/	/	/	/	/	/	/	/	/	R: 12.1, 12.2	/	/	/	/	/	/	/	/	/	/	/	/	
HVOC: 1,1-dichlo- roethylene	/	R: 2.4	/	/	/	/	/	/	/	/	/	/	/	/	/	/	/	/	/	/	/	/	/	