Guidance sheet - Generation of Data for the bluesign® TOOL

bluesign® SYSTEM PARTNERS from the chemical industry are requested by the bluesign® TOOL entry screen to provide certain data which goes beyond the data mandatory for SDS generation. This document can be used as support when generating the necessary data.

1 Wastewater Parameters

Wastewater parameters are not required for chemicals which will not go into wastewater, e.g. a solvent-based PU coating or membrane.

1.1 Biodegradability

Gather the biodegradation (or elimination[1]) data available for the main ingredients of your product and make a worst case estimate of the biodegradability of the product itself.

In the bluesign® TOOL comments (pencil function), state whether the value refers to biodegradation or elimination. Also provide information about test method(s).

Possible information sources include:

- Raw material safety data sheets (SDS), Section 12
- https://echa.europa.eu/information-on-chemicals/registered-substances
- https://www.echemportal.org/echemportal/

[1] Biodegradation is the transformation of organic chemicals into metabolites, usually carried out by microorganisms. Ultimately, biodegradation yields inorganic metabolites, such as carbon dioxide and water. Elimination of the substance from the water phase can also occur through adsorption or volatilization, in which case the chemical remains intact. Test methods that measure carbon dioxide generation result in biodegradation values (e.g. OECD 301B). Test methods that analyze dissolved organic carbon (DOC) cannot distinguish between degradation and elimination (e.g. OECD 302B).

Note:

In the absence of better data, you can use the BOD_5/COD ratio as an estimate for biodegradability. The test should be performed according to OECD test guideline 301D.

1.2 COD or TOC

Test required.

Recommended method for COD: DIN 38409-41 or ISO 6060

Recommended method for TOC: EN 1484 or ISO 8245

1.3 Aquatic Toxicity (Fish, Daphnia, Algae)

If you have data for your product, use existing data.

If you have LC/EC50 values for all ingredients, you can use the following formula to calculate the LC/EC50 for your product and enter that value in the bluesign® TOOL.

$$\frac{\sum Ci}{L(E)C_{50_m}} = \sum_n \frac{Ci}{L(E)C_{50_i}}$$

where:

C_i	=	concentration of ingredient i (weight percentage);
$L(E)C_{50_i}$	=	LC_{50} or EC_{50} for ingredient i, in (mg/l);
n	=	number of ingredients, and i is running from 1 to n;
$L(E)C_{50_m}$	=	$L(E)C_{50}$ of the part of the mixture with test data;

Figure 1.1: LC/EC50 calculation (GHS (Rev.8), UN 2019) latest version Rev.8 2019

If you do not have the data for all ingredients, you can derive this from the GHS classification:

Aquatic acute/chronic classification	Value for bluesign® TOOL	bluesign® TOOL comment
Cat. 1	LC50/EC50 < 1 mg/L	<1 mg/L based on GHS classification
Cat. 2	LC50/EC50 > 1 mg/L	>1 - ≤10 mg/L based on GHS classification
Cat. 3	LC50/EC50 > 10 mg/L	>10 - ≤100 mg/L based on GHS classification
Not classified	LC50/EC50 > 100 mg/L	>100 mg/L based on GHS classification

Table 1: Allocation of aquatic toxicity ranges to categories (GHS (Rev.8), UN 2019)

1.4 Aquatic Toxicity to Bacteria

A value for toxicity to bacteria is no longer considered mandatory.

However, if you have data from test or literature, please enter it (OECD test method 209).

Possible information sources include:

- Raw material safety data sheets (SDS), Section 12
- https://echa.europa.eu/information-on-chemicals/registered-substances
- https://www.echemportal.org/echemportal/

1.5 P, Total

Derived by calculation based on molecular formula and recipe information, as shown below.

Example:

Auxiliary containing 30% diethylenetriaminepenta(methylenephosphonic acid)

CAS 15827-60-8

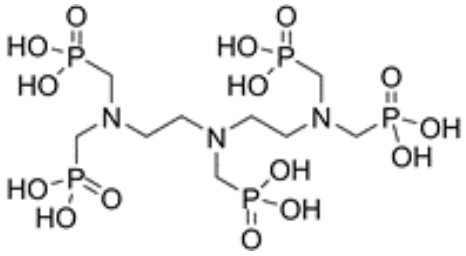

Figure 1.2: Diethylenetriaminepenta(methylenephosphonic acid)

Molecular formula: $C_9H_{28}N_3O_{15}P_5$

Molar mass: 573.20 g/mol

- w(C) = 18.86%
- w(H) = 4.92%
- w(N) = 7.33%
- w(O) = 41.87%
- w(P) = 27.02%

If 30% of the substance is used in the recipe:

>> 27.02% x 0.3 = 8.1% (value to be entered in the bluesign® TOOL)

1.6 N, Total

Derived by calculation based on molecular formula and recipe information, as shown below.

Example:

Same auxiliary as above

If 30% of the substance is used in the recipe

>> 7.33% x 0.3 = 2.2% (value to be entered in the bluesign® TOOL)

1.7 Aliphatic Hydrocarbons

Calculate from recipe with the amount of intentionally added hydrocarbons (e.g. hydrocarbons (mineral oils) for de-dusting in dyes).

1.8 Adsorbable Organic Halogens (AOX)

Derived by calculation based on molecular formula and recipe information, as shown below.

1. Determine the molecular weight and number of halogen atoms for all ingredients/substances in the mixture
2. Count every halogen atom as Cl (always take the molar mass of Cl) and divide by the total molar mass of the ingredient to determine the AOX content of the substance
3. Calculate the AOX content of a mixture based on the concentration of ingredients in the mixture and the AOX content of each ingredient

Note 1:

The value for AOX (Cl, Br and I) + F must be entered in the bluesign® TOOL.

Note 2: For reactive dyes, only the "permanent AOX" must be mentioned in the bluesign® TOOL (not the hydrolysable AOX).

Example A:

Reactive dye containing 50% Reactive Blue 198

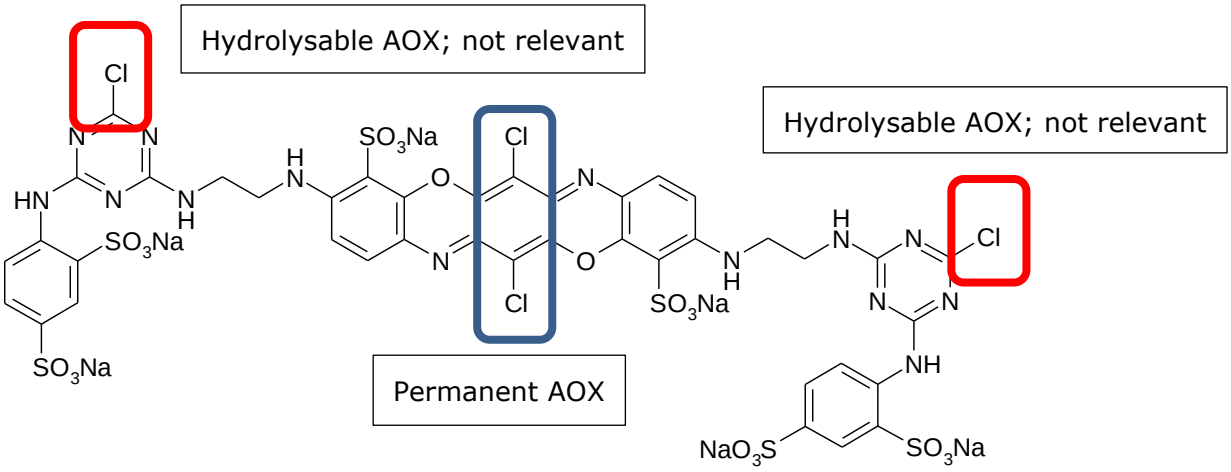

Figure 1.3: AOX relevant groups in a Reactive Blue 198 molecule

Molecular formula: $C_{40}H_{30}Cl_4N_{14}O_{20}S_6Na_6$

Molar mass: 1499 g/mol

Identify the permanent AOX (2 Cl atoms) and calculate the amount of permanent AOX:

Permanent AOX = 2 x 35.45 g/mol / 1499 g/mol x 100%= 4.7%

If 50% dyestuff is used in the recipe and no other AOX relevant ingredient is present:

>> 4.7% x 0.5 = 2.4% total AOX

Example B: Dye containing 100% Disperse Brown 19

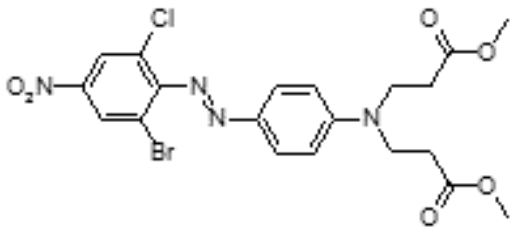

Figure 1.4: Disperse Brown 19

Molecular formula: $C_{20}H_{20}\mathbf{Br}ClN_4O_6$

Molecular mass: 527.7 g/mol

Two halogen atoms are contained (one bromine and one chlorine). For the AOX calculation, count the number of halogens and use the molecular mass of chlorine – also for the bromine atom - for your calculation:

If no other AOX relevant ingredient is present:

AOX = 2 x 35.45 g/mol / 527.7 g/mol x 100% = 13.4%

>> The amount of 13.4% is the AOX value to be entered in bluesign® TOOL.

Note:

If fluorine is contained in the molecule you must calculate the AOX content similarly.

1.9 Fluorine

Calculate from the molecule (if the molecular formula is known) or test (Wickbold incineration DIN 38405-4e).

Use the comments field (pencil function) to state the calculation or test used to obtain the value.

2 Air Emission Parameters

See also: *Guidance Sheet: Air emission management – textile finishing*.

The emission factor characterizes the emission behavior of textile auxiliaries for textile finishing in stenter processes. The emission factor allows you to compare the emission behavior of finishing agents and select low emission products and thus minimize emissions to air. Furthermore, it helps achieve better transparency, knowledge, and control of the emissions associated with textile finishing.

Two different emission factors are defined:

- **f_c:** sum parameter for total emissions of organic substances, expressed as total organic carbon (TOC) content
- **f_s:** emissions of a specific hazardous substance, expressed as mass of the substance

The emission factors can be determined by measurements or calculated.

2.1 Total Carbon Emission Factor (f_c)

Emission factors can be determined by analytical testing on different substrates in suitable labs. However, if no analytical data is available, the following simplified method can be used for the calculation of fc:

1. Calculate the TOC per ingredient
2. Allocate each ingredient to one of the following categories (see next table)
3. Calculate the contribution to the total emissions of the mixture by using the TOC factor and concentration in the mixture

Type	Intended to remain on fabric	Type of substance	TOC factor
Organic	Yes/no	VOC substances (vapor pressure >= 0.01 kPa at 20°C or boiling point <= 240°C)	100% of TOC
Organic	No	Released substances (e.g. blocking agent)	100% of TOC
Organic	Yes	Polymers	1% of TOC
Organic	No	Polymers (e.g. ethoxylates)	20% of TOC

Type	Intended to remain on fabric	Type of substance	TOC factor
Organic	Yes/no	Nonvolatile substances (vapor pressure < 0.01 kPa at 20°C or boiling point > 240°C)	20% of TOC
Organic	No/unclear	All other substances (unclear vapor pressure/boiling point)	100% of TOC
Inorganic	Yes/no	All kinds of inorganic substances	No TOC

Table 2: Substance categories for rough calculation of emission factors

Example:

Substance	CAS	Sum formula	Molecular weight (g/mol)	Fraction C in molecule	Fraction in recipe	Fraction C in mixture (TOC)	Organic/ inorganic	Kind of substance	Intended to stay on fabric?	TOC factor (%)	TOC emission factor (g/kg mixture)
Isopropyl alcohol	67-63-0	C_3H_8O	60.096	60.0%	4.0%	2.4%	Organic	VOC	no	100.0%	23.98
Substance A			264.516	45.3%	10.0%	4.5%	Organic	Polymer (ethoxylate)	no	20.0%	9.06
Substance B			87.122	55.1%	16.5%	9.1%	Organic	non-volatile substance	yes/no	20.0%	18.20
Substance C			358.563	70.3%	30.0%	21.1%	Organic	non-volatile substance	yes	20.0%	42.21
Unknown	-	-	unknown	unknown	1.0%	1.0%	Organic	unknown	no	100.0%	10.00
Water	7732-18-5	H_2O	18.015	0.0%	38.5%	0.0%	Inorganic	inorganic	no	0.0%	0.00
Sum	**-**	**-**	**-**	**-**	**100.0%**	**38.1%**	**-**	**-**	**-**	**-**	**103.45**

Figure 2.1: Example rough calculation of emission factor

2.2 Hazardous Substances Emission Factor (f_s)

For further information contact BLUESIGN.

3 Other Parameters

3.1 Density

For all chemical products the density is a mandatory parameter.

3.2 Fixation Degree

Fixation degree is mandatory for all dyestuffs. For all other products no input is required.

3.3 Toxicological Data

The following toxicological data is mandatory:

- Irritancy skin
- Irritancy eye
- Sensitization skin
- Acute oral toxicity

This data should be available from the SDS or can be derived from the GHS classification.

4 Further Reading

- Globally Harmonized System of Classification and Labelling of Chemicals (GHS): https://www.unece.org/trans/danger/publi/ghs/ghs_welcome_e.html
- GHS guidance: https://www.unece.org/trans/danger/publi/ghs/guidance.html
- OECD guidelines for the testing of chemicals: https://www.oecd.org/env/ehs/testing/oecdguidelinesforthetestingofchemicals.htm