How to generate data for the bluesign® bluetool (or the PSF)?

The bluesign® bluetool rates chemical products as blue (ok), grey (ok, with restrictions) or black (banned). In order to make the rating, you will be asked to provide certain data for your products. This document can be used as support, when generating the necessary data.

1. Wastewater parameters

Biodegradability

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

Specify whether the value refers to biodegradation or elimination in the bluetool comments (pencil function). Also give information about test method(s) if available.

Possible information sources include:

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

Note that in the absence of better data, you can use the BOD5/COD ratio as an estimate for biodegradability. The test should be performed according to OECD test guideline 301D.

*Biodegradation is the transformation of organic chemicals to 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 measuring carbon dioxide generation result in biodegradation values (e.g. OECD 301B). Test methods analyzing dissolved organic carbon (DOC) cannot distinguish between degradation and elimination (e.g. OECD 302B).

COD or TOC
Test required.
Recommended method for COD: DIN 38409-41 or ISO 6060
Recommended method for TOC: DIN EN 1484 or ISO 8245

BOD5
Test required.
Recommended method: DIN EN 1899-1 or ISO 5815 (5 days)

Aquatic toxicity (fish, daphnia, algae)

If you have data for your product, use that.

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 into the bluetool.

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

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;

For reference, see GHS, UN 2015, Section 4.1.3.5.2 (p. 228)

If don't have the data for all ingredients you can derive this from the GHS classification:

Aquatic acute/chronic classification	Value for bluetool	bluetool 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

For reference, see GHS, UN 2015, Section 4.1.2 (p. 219)

Aquatic toxicity against bacteria

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

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

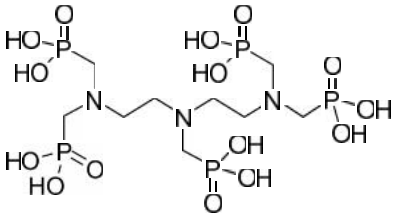
Possible information sources include:
- Raw material safety data sheets (SDS), Section 12
- https://echa.europa.eu/information-on-chemicals/registered-substances
- http://www.echemportal.org/echemportal/index.action

P, total

Calculate from molecular formula and recipe, as shown below.

Example: Auxiliary containing 30% Diethylenetriaminepenta(methylenephosphonic acid) CAS 15827-60-8

Molecular formula: C9H28N3O15P5
Molecular mass: 573.2012 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 bluetool

N, total
Calculate from molecular formula and recipe

Example: same auxiliary as above

Molecular formula: C9H28N3O15P5
Molecular mass: 573.2012 g/mol
•w(C) = 18.86 %
•w(H) = 4.92 %
•w(N) = 7.33 %
•w(O) = 41.87 %
•w(P) = 27.02 %

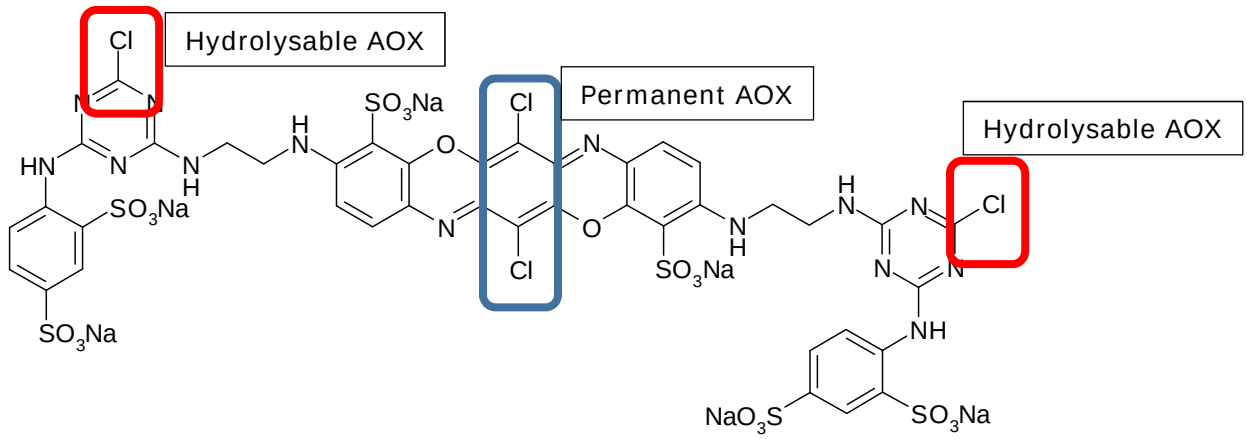
If 30% of the substance is used in the recipe
➔ 7.33% x 0.3 = 2.2% → Value to be entered in the bluetool

Aliphatic hydrocarbons
Calculate from recipe

Adsorbable organic halogens (AOX)
Calculate from molecular formula and recipe

Note: For reactive dyes, hydrolysable, permanent and total AOX should be calculated separately and entered in the bluetool. (Hydrolysable AOX is not relevant for other substances.)

Example A: Reactive dye containing 50% Reactive Blue 198



Molecular Formula: C40H30Cl4N14O20S6.6Na
Change to: C40H36Cl4N14O20S6

Calculate total amount of AOX (Permanent + Hydrolysable):

M(C40H36Cl4N14O20S6) = 1367.0156 g/mol
•w(C) = 35.15 %
•w(H) = 2.65 %
•w(Cl) = 10.37 %
•w(N) = 14.34 %
•w(O) = 23.41 %
•w(S) = 14.07 %

If 50% dyestuff in recipe is used
➔ 10.37% x 0.5 = 5.20% AOX -> Value to be entered in bluetool

Calculate the amount of permanent AOX:

M(C40H36Cl2N14O20S6) = 1296.1096 g/mol
•w(C) = 37.07 %
•w(H) = 2.80 %
•w(Cl) = 5.47 %
•w(N) = 15.13 %
•w(O) = 24.69 %
•w(S) = 14.84 %

If 50% dyestuff in recipe is used
➔ 5.47% x 0.5 = 2.74 % AOX -> Value to be entered in the bluetool comments (pencil function) as “amount of permanent AOX”

Calculate the amount of hydrolysable AOX:

Molecular formula: C40H36Cl2N14O20S6
Molecular weight: 1296.1096 g/mol

•w(C) = 37.07 %
•w(H) = 2.80 %
•w(Cl) = 5.47 %
•w(N) = 15.13 %
•w(O) = 24.69 %
•w(S) = 14.84 %

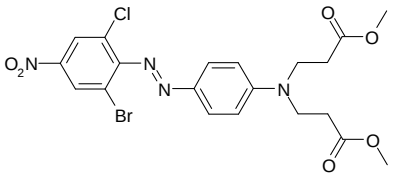
If 50% dyestuff in recipe is used

➔ 5.47% x 0.5 = 2.74% AOX -> Value to be entered in the bluetool comments (pencil function) as “amount of hydrolysable AOX”

Example B: Dye containing 100% Disperse Brown 19

AOX values are based on chlorine (Cl). If the molecule contains halogens other than chlorine (Br, F, I) it should be replaced by chlorine in the molecular formula for the purpose of AOX calculation, as shown below.

Molecular formula: C20H20BrClN4O6
Molecular weight: 527.7590 g/mol



•w(C) = 45.52 %
•w(H) = 3.82 %
•w(Br) = 15.14 %
•w(Cl) = 6.72 %
•w(N) = 10.62 %
•w(O) = 18.19 %

The amount of 15.14% may not be used as AOX value.

First, replace Br with Cl:

C20H20BrClN4O6 → C20H20Cl2N4O6

Molecular formula: C20H20Cl2N4O6
Melocular weight: 483.3080 g/mol

•w(C) = 49.70 %
•w(H) = 4.17 %
•w(Cl) = 14.67 %
•w(N) = 11.59 %
•w(O) = 19.86 %

The amount of 14.67% is the AOX value to be entered in bluetool.

Fluorine

Dyestuffs: Calculate as above (AOX, conversion to Cl).
Fluorocarbons: Calculate from molecule as above (no conversion to Cl) or test (Wickbold incineration DIN 38405-4e)

Use the Comments field (pencil function) to specify which calculation or test was made.

2. Irritancy and sensitization

Irritancy skin

If you have data for your product, use that.

If not, you can derive this information from the GHS classification.

Classified as Skin corrosion/irritation Cat. 1, 2 or 3 → positive
Not classified as skin corrosion/irritation → negative
Comment in bluetool: “based on GHS classification”

Irritancy eye

If you have data for your product, use that.

If not, you can derive this information from the GHS classification:

Classified for Serious eye damage/eye irritation Cat. 1, 2, 2A or 2B → positive
Not classified for Serious eye damage/eye irritation → negative
Comment in bluetool: “based on GHS classification”

Sensitization skin

If you have data for your product, use that.

If not, you can derive this information from the GHS classification:

Classified for Skin sensitizer Cat. 1, 1A or 1B → positive
Not classified for Skin sensitizer → negative
Comment in bluetool: “based on GHS classification”

Note: For disperse dyes a negative test result is required for registration for Class A (Test methods: OECD 406, OECD 429).

3. Toxicity

Acute oral toxicity

If you have data for your product, use that.

If you have LD50 values for the relevant ingredients (classified as acute oral and present at <1%) you can use the following formula to calculate the value for your product. ATE corresponds to the LD50 value.

$$\frac{100}{ATEmix} = \sum_{n} \frac{C_i}{ATE_i}$$

where:

C_i = concentration of ingredient i;

n ingredients and i is running from 1 to n;

ATE_i – Acute toxicity estimate of ingredient i;

For reference, see: GHS, UN 2015, Part 3, Section 3.1.3.6.1 (p. 119)

If you don't have data for all relevant ingredients, you can derive this information from the GHS classification, as shown in the table below.

Table 3.1.2: Conversion from experimentally obtained acute toxicity range values (or acute toxicity hazard categories) to acute toxicity point estimates for use in the formulas for the classification of mixtures

Exposure routes	Classification category or experimentally obtained acute toxicity range estimate (*see Note 1*)	Converted acute toxicity point estimate (*see Note 2*)
Oral (mg/kg bodyweight)	0 < Category 1 ≤ 5	0.5
	5 < Category 2 < 50	5
	50 < Category 3 ≤ 300	100
	300 < Category 4 ≤ 2000	500
	2000 < Category 5 ≤ 5000	2500

For reference see: GHS, UN 2015, 6th rev. ed., Part 3, Section 3.1.3.3, p. 117

Example: Acute tox. Oral Cat. 4 → 500 mg/kg

4. Air emission parameters

Only relevant for products used in textile finishing (e.g. stenter processes).

Air emissions can be expressed using two different values: the emission factor (real value) or the total organic carbon (TOC) content (a worst case estimate).

- The emission factor for a chemical product is defined as the amount of organic and inorganic substances (in grams) released into the atmosphere per kilogram product, during the finishing process, under defined conditions (curing time, temperature, textile substrate). The emission factor is expressed as total content of carbon measured in the off-gas. The emission factor is thus a real measured value.

- The TOC content of a chemical product is the total amount of organic carbon present in the product; that is, all the organic carbon that could potentially be released into the atmosphere. Obviously, this can be a substantial overestimation. In reality, many substances will not be released due to low volatility for example. The TOC content is thus a theoretical worst case value, which is generally higher than the measured emission factor.

How to determine the emission factor?

The determination of emission factors requires a complex infrastructure, which is not available at most testing facilities. Based on our current knowledge, the German test institutes listed below offer this service.

Modern Testing Services
Provinostr. 52
86153 Augsburg
Germany
Phone: +49 (0) 821 / 569796-0 Fax +49 (0) 821 / 569796-90
http://www.mts-germany.eu
Mail: s.ruderisch@mts-germany.eu

TÜV SÜD Industrie Service GmbH
Niederlassung Nürnberg
Abteilung Umwelt Service
Edisonstraße 15
90431 Nürnberg
Germany
Phone: +49 911 6557-278 Fax: +49 911 6557-249
mailto:katharina.brandt@tuevsued.de
http://www.tuev-sued.de/is

How to determine the TOC content?

The TOC content of a chemical product can be calculated based on its chemical composition. The proportion of carbon within a substance is calculated, based on its molecular formula. Then, using the concentration of the substance in the recipe, the TOC for the product can be calculated. Below two examples are given. In the first example, a simple phenol solution is used to show the principle of the calculation. The second example is a more realistic composition for a finishing auxiliary. Although the calculation is in principle straightforward, it requires the molecular formula and concentration of all ingredients to be known, so that the proportion of carbon can be calculated. As some finishing auxiliaries consist of multi-constituent substances with undefined/varying molecular structures (e.g. reaction mass of …), calculating the proportion of carbon may be difficult. In this case you can:

- Make an estimate about the proportions of the different possible molecular structures, based on the reactants, conditions, etc. (cf. specification); the estimate should reflect a worst case TOC (highest possible)
- Ask your supplier for the above information, or for the TOC content of a particular (multi-constituent) substance

Example 1: 200 mg/kg phenol solution in water

Formula: C6H6O
Molar mass of phenol: (6 x 12 + 6 x 1 + 16) g/mol = 94 g/mol
Carbon mass per mol of phenol: 6 x 12 g/mol = 72 g/mol
Carbon mass portion of phenol mass: (72 g/mol)/(94 g/mol) = 0.766
Phenol concentration of the solution: 200 mg/kg
Theoretical TOC of standard solution: 0.766 x 200 mg/kg = 153.2 mg/kg

Example 2: Multi-constituent substance

30% Siloxanes and Silicones, 3-[(2-aminoethyl)amino]propyl Me, di-Me, hydroxy-terminated (CAS 75718-16-0)
70% water

➔ Define main constituents of Siloxanes and Silicones, 3-[(2-aminoethyl)amino]propyl Me, di-Me, hydroxy-terminated (CAS 75718-16-0) and their concentration (mg/kg).
➔ Calculate carbon mass proportion and TOC as in Example 1.

5. Components of high concern

APEO

- NPEO, OPEO
- NP, OP

To be tested if relevant: softeners, detergents, surfactants, etc.

Condensation products of fatty acid derivatives with AEEA (Aminoethylethanolamine)

These substances are widely used as surfactants, sequestering agents, softening agents, chelating agents, etc.

They are not impurities, but intentionally added ingredients.

Check your recipe or ask your supplier to clarify if AEEA derivatives were used as ingredients.

- If yes, the product cannot be approved.
- If no, presence of these substances as impurity is unlikely. (Testing may be needed if the information cannot be obtained by the supplier or cannot be trusted.)

6. Substances listed in the bluesign® system substance list (BSSL)

Substances listed in the bluesign® BSSL

Go through the BSSL and see if any of the substances could be present in your product, for example as:

- intentionally added component (e.g. preservation agents)
- impurity from raw materials (e.g. PAH, quinoline in disperse dyes)
- impurity from the production process (e.g. residues of catalyst or solvent, residual monomer in polymer products)

All suspected BSSL relevant impurities should be analyzed.