BASTA Methods of Calculation for substances with human toxicity and environmentally hazardous properties

2020-12-16

The methods of calculation specified below are based on the equivalent in the CLP-Regulation, (EG) no 1272/2008. To gain a better understanding of the rules help can be obtained in the Guidance on the Application of the CLP Criteria. The most recent version of this document can be found at http://echa.europa.eu/web/guest/guidance-documents/guidance-on-clp

Summation of substances with acute human toxic properties

BASTA-criteria 13

If the toxicity of a mixture is not measured, an estimate can be based on the toxicity of the chemical content (Acute Toxicity Estimate). The calculation of the ATE (Acute Toxicity Estimate)-value of the ingredients is used as a starting point to get the ATE of the mixture which is derived from available toxicity measurements. A description of how it should be done can be obtained in the Guidance on the Application of the CLP Criteria, Section 3.1

In cases where the acute toxicity of all ingredients is known, the following formula applies:

$$\frac{100}{ATE_{Bl}} = \sum_{i=1}^{N} \frac{C_i}{ATE_i} \qquad (13)$$

Where

N	is the number of substances which are classified as acute toxicity in category 1, 2 and 3 (H300, H310, H330, H301, H311 or H331)
i	represent each such substance
C_i	is the concentration in weight (%) of each such substance (i) in the product
ATE_i	is the acute toxicity for each substance (i) in the product
ATE_{Bl}	is the calculated acute toxicity of the mixture

Summation shall be performed for each relevant route of exposure for which the substances shows toxicity - oral, dermal and inhalation. Furthermore, in the case of inhalation, calculations shall be performed for each relevant form substances may have in the air (gas, vapor, mist / dust). The route that provides the most severe toxicity determines the assessment of $ATE_{Bl)}$.

Table 3.1.2 of Annex I to the CLP Regulation specifies the standard values to be used in calculating ATIBl for each Classification Category and for each route of exposure. It also displays the toxicity range where a particular value of ATE provides a certain classification category. Relevant data in the table are summarized in Table 1 below.

The product may not be registered if the ATE_{Bl} are at or below the upper limits of Acute toxicity, Category 3 for each route of exposure, and, in the case of inhalation, for each relevant form the substances might have in the air (gas, vapor, mist / dust).

If the product contains substances without any relevant data on acute human toxicity further guidance can be retrieved in CLP, Guidance on the Application of the CLP Criteria, Section 3.1.

Table 1 The relevant information for classification based on ATE_{bl} for each respective exposure route from Table 3.1.2 of CLP (EC) No 1272/2008, Annex I

Exposure route	Classification categories	A classification of Category limits/MRLs A registration may not be undertaken if the ATE_{BI} are at or below the underlined MRLs /limit	Standard values for acute toxicity estimate, ATE
Oral (mg/kg body weight)	category 1 category 2 category 3	0 < ATE ≤ 5 5 < ATE ≤ 50 50 < ATE ≤ <u>300</u>	0,5 5 100
Dermal (mg/kg bodyweight)	category 1 category 2 category 3	0 < ATE ≤ 50 50 < ATE ≤ 200 200 < ATE ≤ <u>1 000</u>	5 50 300
Inhalation of gases (ppmV)	category 1 category 2 category 3	0 < ATE ≤ 100 100 < ATE ≤ 500 500 < ATE ≤ <u>2 500</u>	10 100 700
Inhalation of vapor (mg/l)	category 1 category 2 category 3	0 < ATE ≤ 0,5 0,5 < ATE ≤ 2,0 2,0 < ATE ≤ <u>10,0</u>	0,05 0,5 3
Inhalation of dust/mist (mg/l)	category 1 category 2 category 3	0 < ATE ≤ 0,05 0,05 < ATE ≤ 0,5 0,5 < ATE ≤ <u>1,0</u>	0,005 0,05 0,5

Summation of substances with environmental hazardous properties

BASTA-criteria 17a

When determining whether the product pass or do not pass criterion 17a, the assessment should include any substances with the classification Hazardous to the aquatic environment, acute category 1 (H400). The product may not be registered if:

$$\sum_{i=1}^{N} \frac{C_i}{L_i} \geq 1 \qquad (17a)$$

where

N is the number of substances within the hazard class hazardous to the aquatic environment, category codes acute 1

i represent each such substance

C_i is the concentration in weight-% of each such substance (i) in the product.

L_i is, for each of the relevant substances (i) in the product, the specified lower concentration limits to classify a mixture, containing the substance, such as H400.

For

0,1 < $L(E)C_{50}$ ≤1	M = 1	then L_i = 25 %
0,01 < $L(E)C_{50}$ ≤ 0,1	M = 10	then L_i = 2,5 %
0,001 < $L(E)C_{50}$ ≤ 0,01	M = 100	then L_i = 0,25 %
0,0001 < $L(E)C_{50}$ ≤ 0,001	M = 1 000	then L_i = 0,025 %

0,00001 < L(E)C_{50} ≤ 0,0001 M = 10 000 then L_i = 0,0025 % etc.
where M is the multiplying factor (M-factor) according the Regulation (EC) No. 1272/2008 (CLP).

BASTA-criteria 17b

When determining whether the product pass or do not pass criterion 17b, the assessment should include any substances with the classification Hazardous to the aquatic environment, category chronic 1 (H410) and chronic 2 (H411).

The product may not be registered if:

$$\left(\sum_{i=1}^{S} \frac{C_{i,H410}}{L_{i,H410}} + \sum_{j=1}^{T} \frac{C_{j,H411}}{25} \right) \geq 1 \qquad (17b)$$

where

S is the number of substances within the hazard class hazardous for the aquatic environment, category code chronic 1 (H410)

T is the number of substances within the hazard class hazardous for the aquatic environment, category code chronic 2 (H411)

i represent each H410-substance in the product.

j represent each H411-substance in the product

$C_{i,H410}$ represent by weigh-% each H410-substance in the product.

$C_{j,H411}$ represent by weigh-% each H411-substance in the product.

$L_{i,H410}$ are, for each of the H410-substance, the lower concentration limit to classify a mixture which contains substances, such as H411.
In the classification of a substance such as H410 or H411 the following cases occur:

Case 1: The classification is based on the relevant data for chronic toxicity and the substance **is not** rapidly degradable

If the substance has a chronic toxicity-value for fish, crustaceans or algae (NOEC or EC_{10}[1]) ≤ 0,1 mg/l it is classified as H410. If the substance cannot be classified as H410 it gives each chronic toxicity value for fish, crustaceans or algae 0,1 < (NOEC or EC_{10}) ≤ 1 (mg/l) the classification H411. Test methods for rapid degradability recommends standard tests according to the OECD, see Annex II of CLP Regulation Guidance on the Application of the CLP Criteria.

$L_{i,H410,}$ in case A is due to an H410-substance (i = 1 to S) of the chronic toxicity, so that if

0,01 < (NOEC or EC_{10}) ≤ 0,1	M = 1	then $L_{i,H410}$ = 2,5 %
0,001 < (NOEC or EC_{10}) ≤ 0,01	M = 10	then $L_{i,H410}$ = 0,25 %
0,0001 < (NOEC or EC_{10}) ≤ 0,001	M = 100	then $L_{i,H410}$ = 0,025 %
0,00001 < (NOEC or EC_{10}) ≤ 0,0001	M = 1 000	then $L_{i,H410}$ = 0,0025 %
0,000001 < (NOEC or EC_{10}) ≤ 0,00001	M = 10 000	then $L_{i,H410}$ = 0,00025 % etc.

where the toxicity values are expressed in mg/l and M is the multiplying factor (M-factor) according the Regulation (EC) No. 1272/2008 (CLP).

[1] Use primarily NOEC. If such a value is missing, EC10 may be used. See OECD 2006

Case 2: The classification is based on the relevant data for chronic toxicity and the substance **is** rapidly degradable

If the substance has a toxicity value for fish, crustaceans or algae (NOEC or EC_{10}[2]) ≤ 0,01 mg/l, it is classified as H410. If the substance cannot be classified as H410 it gives each chronic toxicity value for fish, crustaceans or algae 0,01 < (NOEC or EC_{10}) ≤ 0,1 (mg/l) the classification H411.

$L_{i,H410,}$ in case B is due to an H410-substance (i = 1 to S) of the chronic toxicity, so that if

0,001 < (NOEC or EC_{10}) ≤ 0,01	M = 1	then $L_{i,H410}$ = 2,5 %
0,0001 < (NOEC or EC_{10}) ≤ 0,001	M = 10	then $L_{i,H410}$ = 0,25 %
0,00001 < (NOEC or EC_{10}) ≤ 0,0001	M = 100	then $L_{i,H410}$ = 0,025 %
0,000001 < (NOEC or EC_{10}) ≤ 0,00001	M = 1 000	then $L_{i,H410}$ = 0,0025 %
0,0000001 < (NOEC or EC_{10}) ≤ 0,000001	M = 10 000	then $L_{i,H410}$ = 0,00025 % etc.

where the toxicity values are expressed in mg/l and M is the multiplying factor (M-factor) according the Regulation (EC) No. 1272/2008 (CLP).

Case 3: There are no adequate chronic toxicity data available

If the substance is not rapidly degradable and/or the experimentally determined BCF≥ 500 (or in the cases when BCF are missing, but logK_{OW} ≥ 4) it may be classified as H410 if the substance simultaneously has an acute toxicity value of, 96 hours LC_{50} for fish, 48 hours EC_{50} for crustaceans or 72 hours ErC_{50} for algae, ≤ 1 mg/l. If the substance cannot be classified as H410 it may be classified as H411 if the acute toxicity value is 1 < L(E)C_{50} ≤ 10 (mg/l).

$L_{i,\ H410,}$ in case C is due to an H410-substance (i = 1 to S) of the chronic toxicity, so that if

0,1 < L(E)C_{50} ≤1	M = 1	then $L_{i,H410}$ = 2,5 %
0,01 < L(E)C_{50} ≤ 0,1	M = 10	then $L_{i,H410}$ = 0,25 %
0,001 < L(E)C_{50} ≤ 0,01	M = 100	then $L_{i,H410}$ = 0,025 %
0,0001 < L(E)C_{50} ≤ 0,001	M = 1 000	then $L_{i,H410}$ = 0,0025 %
0,00001 < L(E)C_{50} ≤ 0,0001	M = 10 000	then $L_{i,H410}$ = 0,00025 % etc.

where the toxicity values are expressed in mg/l and M is the multiplying factor (M-factor) according the Regulation (EC) No. 1272/2008 (CLP).

BASTA-criteria 17c

Criterion 17c: This is a collection criterion made for products that do not meet the criteria for chronic 1 (H410), chronic 2 (H411) or chronic 3 (H412). A summation includes substances classified as chronic 1 (H410), chronic 2 (H411), chronic 3 (H412), chronic 4 (H413). To meet the requirement the sum of the containing substances must be below 25%.

When determining whether the product pass or do not pass criterion 17c, the summation should include any substances with the classification Hazardous to the aquatic environment, category chronic 1 (H410), chronic 2 (H411), chronic 3 (H412) and chronic 4 (H413). The product may not be registered if

$$\left(\sum_{i=1}^{M}\frac{C_{i,H410}}{L_{i,H410}}+\sum_{j=1}^{N}\frac{C_{j,H411}}{L_{j,H411}}+\sum_{k=1}^{O}\frac{C_{k,H412}}{L_{k,H412}}+\sum_{l=1}^{P}\frac{C_{l,H413}}{L_{l,H413}}\right)\geq 1 \quad (17c)$$

where

M,N,O, P are the number of substances which meets the criteria for H410, H411, H412 and H413 respectively in the product.

i, j, k, l represent each substance which respectively meets the criteria for H410, H411, H412 and H413 in the product.

[2] Use primarily NOEC. If such a value is missing, EC10 may be used. See OECD 2006

$C_{i,H410}$, $C_{j,H411}$,$C_{k,H412}$ $C_{l,H413}$ are the concentration (in weight-%) of each substance which meets the criteria for H410, H411, H412 and H413 respectively in the product.

$L_{i,H410}$,$L_{j,H411}$,$L_{k,H412}$ $L_{l,H413}$ are for each H410-, H411-, H412- and H413-substance respectively, the specified lower concentration limits to classify a mixture as environmentally hazardous with H413.

If a substance is listed in table 3.1 in Annex VI to the Council Directive (CLP) (Regulation (EC) No. 1272/2008 are specified with a specified concentration limit, then it applies.

If these substances do not have any specified concentration limits in table 3.1 in Annex VI to the Council Directive (CLP) (Regulation (EC) No. 1272/2008, then it is applicable to all of these environmental hazard classes that L_x = 25 % where x stands for i, j, k and l. This is the normal case and then the calculation is:

$$\frac{\sum_{x=1}^{N} C_x}{25} \geq 1 \qquad \text{(17c in normal cases)}$$

where

N	is the number of substances which are classified as environmentally hazardous H410, H411, H412 or H413 respectively in the product.
x	represent each such substance in the product.
C_x	is the concentration in weight-% of substance x in the product.

If the product contains substances without relevant data for acute aquatic toxicity further guidance can be found in the CLP (EC) No 1272/2008, Chapter 3.1. It stipulates that the QSAR models, read-across or grouping are methods that can be used to produce aquatic toxicity data if they meet the set requirements. These recommendations are similar to those used in REACH. For QSAR models, there is the guidance from ECHA: *Guidance on Information Requirements and Chemical Safety Assessment*, Chapter R.6: *QSARs and grouping of chemicals*. If these recommendations are followed the model-values may be used in place of the experimental data.