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Committee of Experts on the Transport of Dangerous Goods and on the Globally Harmonized System of Classification and Labelling of Chemicals

Sub-Committee of Experts on the Globally Harmonized System of Classification and Labelling of Chemicals

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Item 3 (h) of the provisional agenda
Classification criteria and related hazard communication: other issues

Amendment of the guidance on calculating specific heats of combustion for composite formulations in Chapter 2.3

Transmitted by the expert from Sweden*

Background

1. GHS Chapter 2.3 on Aerosols contains guidance on how to calculate the specific heat of combustion for a "composite formulation", see section 2.3.4.2 of that chapter. While the essence of equation is correct the way it is cast may lead to confusion and miscalculations, which may in turn lead to misclassifications.

2. There is a proposal from CEFIC and EIGA to amend Chapter 2.3 in order to include chemicals under pressure, see ST/SG/AC.10/C.4/2018/3. That document contains the corresponding guidance in its section 2.3.3. The expert from Sweden proposes that the guidance section is amended to provide mathematical consistency of the equation and logical flow of the surrounding text.

Discussion

3. The main problem with the current equation is the use of the symbol "w_i%" to denote a fraction. A fraction is a number between zero and one, not to be confused with a percentage

* In accordance with the programme of work of the Sub-Committee for 2017–2018 approved by the Committee at its eighth session (see ST/SG/AC.10/C.3/100, para. 98 and ST/SG/AC.10/44, para. 14).

which is one hundred times the fraction. The symbol "w_i%" is thus misleading in relation to what is actually meant, which is a fraction.

4. There is also inconsistent use of "specific heat of combustion" (an entity expressed in kJ/gram) versus "heat of combustion" (an entity expressed in kJ/mole), which may cause confusion. And for clarity it may be better to use brackets instead of subscripts to denote dependency on the variable *i*, since a subscript already appears in the denotation of the specific heat of combustion (Δh_c). Furthermore, the introduction that explains the difference between a practical and a theoretical combustion seems rather to be an explanatory comment to the calculation procedure, and therefore would probably fit better after the calculation procedure has been introduced.

Proposal

5. The expert from Sweden proposes the section to be cast as follows (text to be deleted in bold strike-through, new text in bold underline, note that equation denotations are proposed to be changed accordingly although for clarity have not been underlined):

2.3.3 ***Guidance on specific heat of combustion***

~~**The specific heat of combustion (Δh_c), in kilojoules per gram (kJ/g) is the product of the theoretical heat of combustion (ΔH_c) and the combustion efficiency, usually less than 1.0 (a typical efficiency is 0.95).**~~

For a composite formulation, the specific heat of combustion **of the product** is the summation of the weighted **specific** heats of combustion for the individual components, as follows:

$$\Delta h_c(\text{product}) = \sum_{i}^{n} [w(i) \times \Delta h_c(i)]$$

Where:

Δh_c(product) = specific heat of combustion (kJ/g) **of the product**;

Δh_c(i) = specific heat of combustion (kJ/g) of component i in the product;

w(i) = mass fraction of component i in the product;

n = total number of components in the product

The specific heat**s** of combustion**, which are given in kilojoules per gram (kJ/g),** can be found in the scientific literature, calculated or determined by tests (see ASTM D 240, NFPA 30B.). **Note that experimentally measured heats of combustion usually differ from the corresponding theoretical heats of combustion, since the combustion efficiency normally is less than 100% (a typical combustion efficiency is 95%).**

6. For clarity, the section as proposed would read:

"**2.3.3** ***Guidance on specific heat of combustion***

For a composite formulation, the specific heat of combustion of the product is the summation of the weighted specific heats of combustion for the individual components, as follows:

$$\Delta h_c(\text{product}) = \sum_{i}^{n} [w(i) \times \Delta h_c(i)]$$

Where:

Δh_c(product) = specific heat of combustion (kJ/g) of the product;

$\Delta h_c(i)$ = specific heat of combustion (kJ/g) of component i in the product;

w(i) = mass fraction of component i in the product;

n = total number of components in the product

The specific heats of combustion, which are given in kilojoules per gram (kJ/g), can be found in the scientific literature, calculated or determined by tests (see ASTM D 240, NFPA 30B.). Note that experimentally measured heats of combustion usually differ from the corresponding theoretical heats of combustion, since the combustion efficiency normally is less than 100% (a typical combustion efficiency is 95%).".