

# DERIVING QUALITY CRITERIA FOR WATER AND SEDIMENT FROM THE RESULTS OF AQUATIC TOXICITY TESTS AND PRODUCT STANDARDS: APPLICATION OF THE EQUILIBRIUM PARTITIONING METHOD

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**Abstract**—The present paper summarizes an approach recently proposed in The Netherlands to use the equilibrium partitioning (EP) method to derive a coherent set of quality criteria for aquatic systems. The quality criteria refer to dissolved concentrations, the concentrations in the suspended particles, the total (dissolved + particulate) concentrations and the concentrations in the sediment. The quality criteria have been derived for standard sediment, standard water and standard suspended matter. Emphasis is laid on the relation between effect data and physicochemical data. Two types of effect data have been used, i.e. effects on aquatic toxicity (direct effects) and health related effects (product standards). Both types of data have been translated into the above mentioned criteria by means of EP. For the calculation of criteria in sediment and suspended matter solids-water partition coefficients  $K_{sw}$  have been used. Examples have been given for cadmium and hexachlorobenzene. The handled equations have been summarized in diagrams.

**Key words**—equilibrium partitioning method, quality criteria, sediment, product standard, solids-water partition coefficient

## NOMENCLATURE

- BCF = bioconcentration factor ( $l\ kg^{-1}$ )  
BCF<sub>fat</sub> = bioconcentration factor on a fat basis ( $l\ kg_{fat}^{-1}$ )  
 $C_{fat}$  = concentration of chemical in fat ( $\mu g\ kg^{-1}$ )  
 $C_{org}$  = concentration of chemicals in organisms ( $\mu g\ kg^{-1}$ )  
 $C_s$  = concentration in the solid phase ( $mg\ kg^{-1}$ )  
 $C_{sed}$  = concentration in sediments ( $mg\ kg^{-1}$ )  
 $C_{susp}$  = concentration in suspended matter ( $mg\ kg^{-1}$ )  
 $C_{tot}$  = total concentration in water, before filtration ( $\mu g\ l^{-1}$ )  
 $C_w$  = concentration in the water phase ( $\mu g\ l^{-1}$  or  $mg\ l^{-1}$ \*)  
DOC = dissolved organic carbon ( $mg_{oc}\ l^{-1}$ )  
 $f_{oc}$  = fraction of organic carbon (—)  
 $K_{oc}$  = organic carbon-referenced partition coefficient ( $l\ kg_{oc}^{-1}$ )  
 $K_{ow}$  = *n*-octanol-water partition coefficient (—)  
 $K_{sw}$  = solids-water partition coefficient ( $l\ kg^{-1}$  or  $l\ g^{-1}$ \*)  
 $r$  = empirical concentration ratio suspended matter: sediment for metals  $r = 1.5$ ; for organics  $r = 2$  (—)  
SM = concentration of suspended matter ( $mg\ l^{-1}$  or  $g\ l^{-1}$ \*)  
TOC = total organic carbon ( $mg_{oc}\ l^{-1}$ )

## INTRODUCTION

In the past the importance of sediment bound chemicals as a factor in environmental effects of chemicals

has been greatly underestimated (Maki *et al.*, 1987). Three factors probably were most responsible for the insight that discredited the overly simplistic and entrenched philosophy that emphasized only dissolved chemicals and the water column.

The first was the development of priority pollutants lists. These lists generally included a wide range of inorganic chemicals that, upon investigation, were found to be very water-insoluble. The second factor was a result of the gradual involvement of environmental chemists in the assessment process. They expressed concern about the assumption of the irreversibility of chemicals sorbed to sediments. The words bioavailability and partitioning became the key words of environmental assessment (Maki *et al.*, 1987).

The third factor was an economic factor. Activities like harbour and waterways dredging operations together with the growing awareness of soil and sediment pollution, and the associated costs for clean-up operations, showed again that prevention was cheaper than sanitation. These enormous costs urged the need for sediment quality criteria and related research in order to assess and manage the risk to health and the environment arising as a result of the production, use and disposal of chemicals that become associated with aquatic sediments.

\*See text.

One of the possible methods to assess the potential risk associated with the presence of toxic compounds in sediments is to derive sediment quality criteria for each of the individual compounds and compare the actual concentrations with the standards. Gilford and Zeller (1987) summarized the applicability of sediment quality criteria as follows:

- assess sediment quality
- deciding on remedial actions to alleviate environmental degradation related to sediment contamination
- establishing wasteload allocations
- assessing the quality of sediments in discharge impact areas
- setting requirements for ocean discharges
- evaluating disposal sites and dredge and fill permits
- assessing potential impacts on benthos
- designing and evaluating monitoring programs.

A relatively simple, and generally applicable approach to derive sediment quality criteria is the so-called equilibrium partitioning (EP) method (Shea, 1988). In the EP-method, the co-occurrence of chemicals in water and sediment are modelled as a state of thermodynamic equilibrium, usually implicitly regarded as a sorption equilibrium. In case of equilibrium sorption, the concentrations in water and sediment are related to each other through a usually simple sorption isotherm equation. Provided that such a direct relationship can be quantitatively formulated for a chemical, it is possible to estimate quality criteria for sediments from the quality criteria for water, in turn, are derived from the results of a standard set of aquatic toxicity tests.

The applicability of the EP-method hinges on the validity of this equilibrium sorption model and the availability equilibrium partitioning coefficients. The EP-approach is clearly not suitable for highly polar and charged organic chemicals for which it is not possible to model the adsorption in such a simple manner as for neutral organic chemicals (DiToro *et al.*, 1987) and for compounds which are rapidly degradable (which therefore do not pose a great sediment pollution problem). The approach for heavy metals is, in principle, the same but it is well known that speciation which may depend on many environmental factors makes it more difficult to apply it in a simple manner.

From a toxicological point of view it may be added that this approach seems to be realistic. Experiments with sediment-dwelling organisms, i.e. midges (Ziegenfuss *et al.*, 1986; Knezovich and Harrison, 1988) and oligochaetes (Connell *et al.*, 1988) indicate that toxicity of sediments can be expressed in terms of pore water concentrations. This also seems to hold true for terrestrial organisms like earthworms (Van Gestel and Ma, 1988).

The present paper is meant to summarize an approach recently proposed in The Netherlands to

use the equilibrium partitioning method to derive a coherent set of quality criteria for aquatic systems: criteria for the water phase (dissolved), for the suspended particles, for the total (dissolved + particulate) concentrations and for sediments (Fig. 1).

Emphasis is laid on the relation between effect data and physicochemical data rather than on the ecological relevance of the ecotoxicological effect parameters.

This paper focuses on the practical application of the equilibrium partitioning method as a means to relate concentrations in water, organisms and sediments, with particulate emphasis on the use of the two essential parameters that are needed for this method: the solids-water partition coefficient,  $K_{sw}$ , and the bioconcentration factor, BCF.

#### QUALITY CRITERIA FOR AQUATIC SYSTEMS DERIVED FROM TOXICOLOGICAL DATA OR PRODUCT STANDARDS

##### *General principles*

As a starting point for derivation of quality criteria for water and sediment, two sorts of data can be used:

- (1) *Toxic effect data.* By means of ecotoxicological extrapolation methods, which are not described in this paper, critical concentrations in water are derived from direct aquatic effect data. These critical concentrations are then "translated" into critical concentrations in solids by means of solids-water partition coefficients.
- (2) *Product standards.* For many chemicals, maximal allowable concentrations in, e.g. fish—generally meant to protect man—are available. These critical concentrations in organisms are "translated" into critical concentrations in water by means of bioconcentration factors. These, in turn, are "translated" into critical concentrations in solids using solids-water partition coefficients.

In the next paragraphs this bipartition has been followed to derive equations for calculating quality criteria for water and sediment. These equations hold for both metals and organic chemicals. Organic chemicals and metals are dealt with in, respectively, in the next two subsections. With both methods quality criteria can be calculated. This procedure yields two criteria for one chemical, the lowest of which is to be taken as decisive.

By definition, concentrations in water and solids are related through a partition coefficient:

$$K_{sw} = \frac{C_s}{C_w} \quad \text{or} \quad C_w = \frac{K_{sw}}{C_s} \quad (1)$$

where

$K_{sw}$  = solids-water partition coefficient ( $l\ g^{-1}$ )

$C_s$  = concentration in the solid phase ( $mg\ kg^{-1}$ )

$C_w$  = concentration in the water phase ( $\mu g\ l^{-1}$ ).

Method to derive a coherent set of quality criteria for aquatic systems: (dissolved + particulate) (Fig. 1). Relationship between effect on the effect of

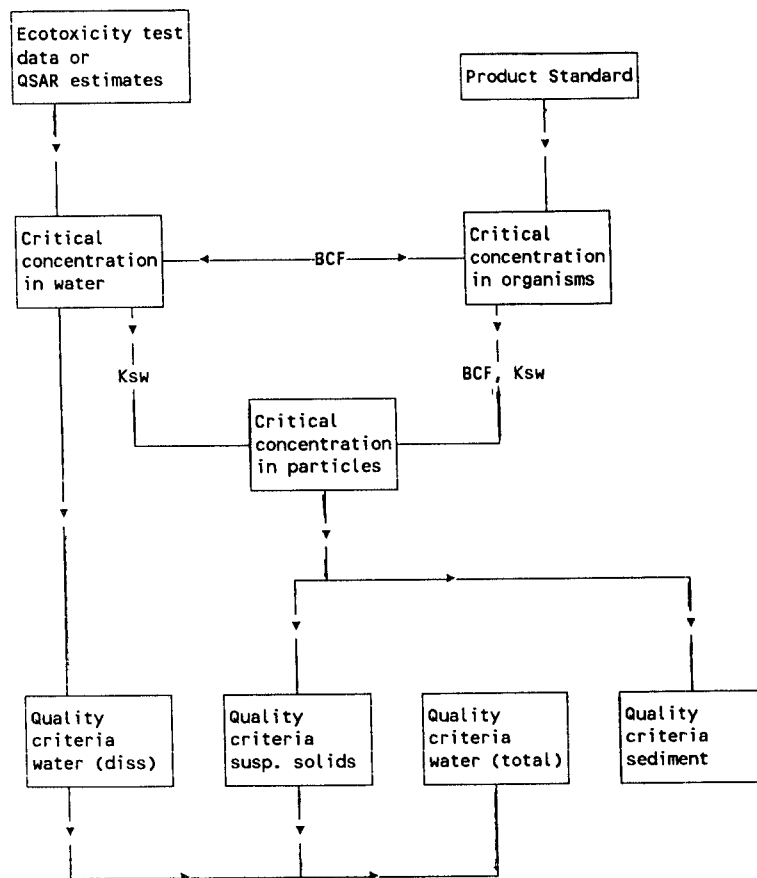


Fig. 1. Deriving a coherent set of quality criteria for aquatic systems from aquatic ecotoxicological data and product standards.

In the case of (thermodynamic) equilibrium between water and solids, values for  $K_{sw}$  can be derived theoretically, on the basis of properties of the chemical and characteristics of the solids. For organic compounds, such relationships are widely used. Presently no such general relationships are available for metals.

Alternatively, values for  $K_{sw}$  can be derived from field measurements of concentrations in water before and after filtration:

$$K_{sw} = \frac{C_{tot} - C_w}{SM \times C_w} \quad (2)$$

where

$C_{tot}$  = total concentration in water, before filtration ( $\mu\text{g l}^{-1}$ )

$C_w$  = concentration in the water phase, after filtration ( $\mu\text{g l}^{-1}$ )

SM = concentrations of suspended matter ( $\text{g l}^{-1}$ ).

\*Suspended particles in the Netherlands have fractions of lutum of approx. 40% and of organic matter of approx. 20%. Sediments in The Netherlands have fractions of lutum of approx. 25% and of organic matter of approx. 10%. All these numbers have been taken up in the Dutch definitions of standard suspended matter and standard sediment. These values may differ in other countries.

It can be inferred from field measurements (Aiking and Bruggeman, 1987) that concentrations of micropollutants in sediments differ systematically from the concentrations in the suspended solids in the water column above the sediment. For metals the concentration ratio suspended matter:sediment is approx. 1.5; for organic chemicals, this ratio is approx. 2.0\*. If the ratio of the concentrations in suspended matter and water is taken as a measure for  $K_{sw}$ , which is implicitly done when  $K_{sw}$  is empirically derived according to equation (2), the concentration in sediments  $C_{sed}$  is to be calculated as follows:

$$C_{sed} = \frac{C_{susp}}{r} = \frac{C_s}{r} = \frac{K_{sw} \times C_w}{r} \quad (3)$$

where

$C_{sed}$  = concentration in sediment ( $\text{mg kg}^{-1}$ )

$C_{susp}$  = concentration in suspended matter ( $\text{mg kg}^{-1}$ )

$r$  = empirical concentration ratio suspended matter:sediment for metals  $r = 1.5$ ; for organics  $r = 2$ .

To calculate the total (dissolved + particulate) concentration of a chemical, if a critical concentration  $C_w$

in water is given, equation (2) is used again. After rearrangement, equation (2) becomes:

$$C_{\text{tot}} = C_w \times (1 + K_{\text{sw}} \times \text{SM}). \quad (4)$$

In a similar way as for the relation between concentrations in water and suspended matter, water and biota are, by definition, related to each other through a bioconcentration factor:

$$\text{BCF} = \frac{C_{\text{org}}}{C_w} \quad (5)$$

where

BCF = bioconcentration factor ( $1 \text{ kg}^{-1}$ )

$C_{\text{org}}$  = content of chemical in organisms ( $\mu\text{g kg}^{-1}$ )

$C_w$  = concentration of chemical in the water phase ( $\mu\text{g l}^{-1}$ ).

Products standards for the consumption of fish, mussels, etc. have been established for a number of chemicals. If for these chemicals BCFs are also known, equation (5) can be used to derive a critical concentration in water  $C_w$  from critical concentrations in organisms  $C_{\text{org}}$ . For this purpose, equation (5) is rewritten into:

$$C_w = \frac{C_{\text{org}}}{\text{BCF}} \quad (6)$$

Substituting equation (6) into (3), the equation for the concentration in sediment becomes:

$$C_{\text{sed}} = \frac{C_{\text{org}} \times K_{\text{sw}}}{r \times \text{BCF}} \quad (7)$$

and similarly, the equation for the total concentration follows from substitution of equation (6) into (4):

$$C_{\text{tot}} = \frac{C_{\text{org}} \times (1 + K_{\text{sw}} \times \text{SM})}{\text{BCF}} \quad (8)$$

#### Organic chemicals

Values for the solids-water partition coefficient  $K_{\text{sw}}$  are derived from the octanol-water partition coefficient of the compound and the organic carbon content of the solid material, using the referencing procedure formulated by Karickhoff *et al.* (1979):

$$K_{\text{sw}} = K_{\text{oc}} \times f_{\text{oc}} \quad (9)$$

where

$K_{\text{sw}}$  = solids-water partition coefficient ( $1 \text{ kg}^{-1}$ )

$K_{\text{oc}}$  = organic carbon-referenced partition coefficient ( $1 \text{ kg}_{\text{oc}}^{-1}$ )

$K_{\text{ow}}$  = *n*-octanol-water partition coefficient (dimensionless)

$f_{\text{oc}}$  = fraction of organic carbon (dimensionless).

$$\log K_{\text{oc}} = 1.00 \times \log K_{\text{ow}} - 0.21 \quad (10a)$$

or, equivalently:

$$K_{\text{oc}} = 0.6 \times K_{\text{ow}} \quad (10b)$$

Combining equations (9), (10a) and (10b),  $K_{\text{sw}}$  can be written as:

$$K_{\text{sw}} = 10^{-0.21} \times K_{\text{ow}} \times f_{\text{oc}} = 0.6 \times K_{\text{ow}} \times f_{\text{oc}} \quad (11)$$

The organic carbon content  $f_{\text{oc}}$  of suspended matter can be derived from field measurements in surface waters:

$$f_{\text{oc}} = \frac{\text{TOC} - \text{DOC}}{\text{SM}} \quad (12)$$

where

TOC = total organic carbon ( $\text{mg}_{\text{oc}} \text{ l}^{-1}$ )

DOC = dissolved organic carbon ( $\text{mg}_{\text{oc}} \text{ l}^{-1}$ )

SM = concentration of suspended matter ( $\text{mg l}^{-1}$ ).

Values for the octanol-water partition coefficient  $K_{\text{ow}}$  are to be obtained from the literature.

For organic compounds, the bioconcentration factor is usually expressed on a fat basis:

$$\text{BCF}_{\text{fat}} = \frac{C_{\text{fat}}}{C_w} \quad (13)$$

where

$\text{BCF}_{\text{fat}}$  = bioconcentration factor on a fat basis ( $1 \text{ kg}_{\text{fat}}^{-1}$ )

$C_{\text{fat}}$  = concentration of chemical in fat ( $\mu\text{g kg}^{-1}$ ).

As both the fat-based bioconcentration factor and the solids-water partition coefficient are proportional to the octanol-water partition coefficient, it is theoretically expected that the ratio of  $\text{BCF}_{\text{fat}}$  and  $K_{\text{oc}}$  has the same value for all compounds. Field observations confirm this (Bruggeman *et al.*, 1985; Bruggeman, 1987). It appears that this ratio takes a value of approx. 2:

$$\frac{C_{\text{org}}/C_{\text{fat}}}{C_{\text{susp}}/f_{\text{oc}}} = \frac{\text{BCF}_{\text{fat}}}{K_{\text{oc}}} \approx 2. \quad (14)$$

Bearing in mind that  $K_{\text{oc}}$  and  $K_{\text{ow}}$  are related through equation (10b), equation (14) implies that  $\text{BCF}_{\text{fat}}$  and  $K_{\text{ow}}$  have approximately the same value:

$$\text{BCF}_{\text{fat}} \approx 2 \times K_{\text{oc}} \approx 2 \times 0.6 \times K_{\text{ow}} \approx K_{\text{ow}} \quad (15)$$

If bioconcentration factors are to be expressed on a wet weight basis, fat-based bioconcentration factors must be multiplied by the fraction of fat of the organism. Taking the value 5% as a typical fat fraction for fish (Mackay, 1982), this leads to:

$$\text{BCF} = 0.05 \times \text{BCF}_{\text{fat}} \approx 0.05 \times K_{\text{ow}} \quad (16)$$

Although this relation between  $K_{\text{ow}}$  and BCF, as developed by Mackay (1982), holds for many organic chemicals, it should be noted that deviations from this relation may be observed for instance for more polar chemicals, very hydrophobic chemicals and also for chemicals which are easily biotransformed

(Gobas *et al.*, 1987; De Bruin and Hermens, 1991; Opperhuizen *et al.*, 1985). In the case of very hydrophobic chemicals, uptake via food cannot be excluded (Bruggeman *et al.*, 1984) and this may lead to an underestimation of bioconcentration, whereas in the case of rapid biotransformation, bioconcentration may be overestimated (De Bruin and Hermens, 1991; Van Leeuwen *et al.*, 1986). As a general rule, however, chemicals that act by narcosis (cf. Veith *et al.*, 1983) are rather stable non-polar chemicals.

#### Metals

Equations (1–6) can also be applied for metals. In this case, values of  $K_{sw}$  are to be derived from the results of routine surveys of the water quality. Examples of  $K_{sw}$  values based on the Dutch Water Quality Data Base (1988) are given in Table 1. It should be stressed that  $K_{sw}$  values show a great variability and depend on many physicochemical factors, e.g. salinity, pH, dissolved oxygen concentration etc. In other countries the  $K_{sw}$  values may differ substantially from the ones presented in Table 1. BCF-values and values for  $C_{org}$  for metals are to be obtained from experimental data, reported in the literature. An illustrative example for Cd is given in the next section.

#### DISCUSSION WITH SAMPLE CALCULATIONS

In the last paragraph several equations have been given that can be used to derive quality criteria for water and sediment from effect data. Two types of effect data can be used to derive these criteria, i.e. effects on aquatic toxicity (the so-called direct effects) and health-related effects (the so-called product standards).

In order to illustrate the above-mentioned approaches examples are given for cadmium, a heavy metal, and for hexachlorobenzene (HCB), an organic micropollutant. For cadmium as well as for HCB

both types of effects, i.e. direct effects and product standards on aquatic toxicity have been used for the calculations. So at last four criteria, i.e. two criteria per substance, have been given.

However, but one criterion per substance can be used. The definite criterion can be obtained by choosing the lowest value.

#### Example 1: cadmium

For working out this example the equations of the previous section have been used. The numbers in parentheses refer to the equations in that section. In these equations the following data have been filled in:

$$\begin{aligned} K_{sw} &= 130 \text{ l g}^{-1} \text{ (see Table 1)} \\ \text{BCF} &= 100 \text{ l kg}^{-1} \text{ (fish; Ros and Slooff, 1988)} \\ C_{org} &= 50 \text{ } \mu\text{g kg}^{-1} \text{ (product standard for fish} \\ &\quad \text{consumption in The Netherlands)} \\ \text{NOEC} &= 0.1 \text{ } \mu\text{g l}^{-1} \text{ (Van Leeuwen } et al., 1985) \\ \text{SM} &= 30 \text{ mg l}^{-1}. \end{aligned}$$

(a) Starting from direct aquatic effect data (NOEC). As quality criterion for the chemical in the dissolved phase the NOEC of  $0.1 \text{ } \mu\text{g l}^{-1}$  is used:

$$\begin{aligned} C_w &= \text{NOEC} \\ &= 0.1 \text{ } \mu\text{g l}^{-1}. \end{aligned}$$

By using equation (1) the NOEC-related criterion for suspended matter has been calculated:

$$\begin{aligned} C_{susp} &= K_{sw} \times C_w \\ &= 130 \text{ l g}^{-1} \times 0.1 \text{ } \mu\text{g l}^{-1} \\ &= 13 \text{ mg kg}^{-1} \end{aligned}$$

The NOEC-related criterion for the total cadmium concentration in water has been calculated by using equation (4):

$$\begin{aligned} C_{tot} &= C_w \times (1 + K_{sw} \times \text{SM}) \\ &= 0.1 \text{ } \mu\text{g l}^{-1} \times (1 + 130 \text{ l g}^{-1} \times 30 \times 10^{-3} \text{ g l}^{-1}) \\ &= 0.49 \text{ } \mu\text{g l}^{-1}. \end{aligned}$$

Table 1. Summary of  $K_{sw}$  values based on the Water Quality Data Base (1988) for some Dutch surface waters (mean values for the period 1983–1986).  $K_{sw}$  expressed in  $\text{l g}^{-1}$

Water	Cr	Cu	Hg	Cd	Zn	Ni	Pb	As
Rijn (Lobith)	204	32	124	82	81	8.3	524	10.7
Rijn (Hagestein)	313	45	270	172	109	7.3	563	18.4
Waal	228	36	176	138	104	7.7	626	9.0
Maas (Eijsden)	164	56	188	363	215	10.9	689	10.4
Haringvliet	786	55	125	63	188	21.7	438	7.8
Westerschelde O†	324	67	170	77	58	4.3	857	7.6
Westerschelde W*	228	12	31		57	10.6	637	10.2
Ketelmeer	300	50	249	153	142	9.1	693	5.4
IJsselmeer	126	48	73	65	215	11.5	498	7.0
Nieuwe Merwede	283	40	134	119	116	6.2	865	17.9
Nieuwe Waterweg‡	320	47	205	50	81	7.5	577	11.1
Oude Maas	268	45	208	156	172	7.5	1025	8.5
Kan. Gent/Tern.‡	306	149	183	493	52	5.6	3474	17.1
Mean	296	52	164	161	122	9.1	882	10.9
Median	290	50	170	130	110	8	640	10

\*Salinity > 10,000  $\text{mg Cl}^{-1}/\text{l}$ .

†1000  $\text{mg Cl}^{-1} < \text{salinity} < 5000 \text{ mg Cl}^{-1}/\text{l}$ .

‡100  $\text{mg Cl}^{-1}/\text{l} < \text{salinity} < 500 \text{ mg Cl}^{-1}/\text{l}$ .

Other: salinity < 100  $\text{mg Cl}^{-1}/\text{l}$ .

By using equation (3) the NOEC-related criterion for cadmium in sediment has been calculated as:

$$C_{\text{sed}} = \frac{K_{\text{sw}} \times C_w}{1.5} = \frac{130 \text{ l g}^{-1} \times 0.1 \mu\text{g l}^{-1}}{1.5} \\ = 8.7 \text{ mg kg}^{-1}.$$

(b) *Starting from a product standard.* Starting from a product-standard the criterion for dissolved cadmium can be calculated by using equation (6):

$$C_w = \frac{C_{\text{org}}}{\text{BCF}} = \frac{50 \mu\text{g kg}^{-1}}{100 \text{ l kg}^{-1}} \\ = 0.5 \mu\text{g l}^{-1}.$$

The product standard-related criterion for cadmium in suspended matter has been given by using equation (7):

$$C_{\text{susp}} = K_{\text{sw}} \times \frac{C_{\text{org}}}{\text{BCF}} = 130 \text{ l g}^{-1} \times \frac{50 \mu\text{g kg}^{-1}}{100 \text{ l kg}^{-1}} \\ = 65 \text{ mg kg}^{-1}.$$

The product standard-related total concentration for cadmium in water has been calculated by using equation (8):

$$C_{\text{tot}} = \frac{C_{\text{org}} \times (1 + K_{\text{sw}} \times \text{SM})}{\text{BCF}} \\ = \frac{50 \mu\text{g kg}^{-1} \times (1 + 130 \text{ l g}^{-1} \times 30 \times 10^{-3} \text{ g l}^{-1})}{100 \text{ l kg}^{-1}} \\ = 2.45 \mu\text{g l}^{-1}.$$

Finally the product standard-related criterion for cadmium in sediment has been obtained by using equation (7):

$$C_{\text{sed}} = \frac{K_{\text{sw}} \times C_{\text{org}}}{1.5 \times \text{BCF}} = \frac{130 \text{ l g}^{-1} \times 50 \mu\text{g kg}^{-1}}{1.5 \times 100 \text{ l kg}^{-1}} \\ = 43.3 \text{ mg kg}^{-1}.$$

In this example the criteria derived from direct aquatic effect data give lower values than the criteria derived from the product standard. In other words, for cadmium quality criteria are to be derived from the *direct aquatic effect data*.

#### Example 2: HCB

The equations given in the previous section have been used to calculate the quality criteria for HCB. The numbers in parentheses refer to the equations in that section. The following data have been used:

$$\log K_{\text{ow}} = 6.18 \\ \text{BCF} = 75678 \text{ (calculated as } K_{\text{ow}}/20)$$

\*Minimum toxicity (Veith *et al.*, 1983; Hermens, 1986; Van de Naald and Bruggeman, 1986) is estimated with the equation:  $\text{LC}_{50}(\text{acute}) = 0.1/K_{\text{ow}}$ , with  $\text{LC}_{50}$  in  $\text{mol l}^{-1}$ . NOEC-values are estimated from  $\text{LC}_{50}(\text{acute})$  by dividing by a factor 100 (U.S.EPA, 1984).

$$C_{\text{org}} = 200 \mu\text{g kg}^{-1} \text{ (product standard for fish consumption in Sweden)}$$

$$\text{NOEC} = 0.19 \mu\text{g l}^{-1} \text{ (estimated using the minimum toxicity equation and extrapolation from } \text{LC}_{50} \text{ to NOEC*)}$$

$$\text{SM} = 30 \text{ mg l}^{-1} = 30 \times 10^{-6} \text{ kg l}^{-1}$$

$$f_{\text{oc}}(\text{susp}) = 0.1$$

$$f_{\text{oc}}(\text{sed}) = 0.05.$$

(a) *Starting from direct aquatic effect data (NOEC).*

The criterion for dissolved HCB, related to the estimated NOEC, has been given as:

$$C_w = \text{estimated NOEC} \\ = 0.19 \mu\text{g l}^{-1}.$$

The NOEC-related criterion for HCB has been calculated by using equations (7) and (11):

$$C_{\text{susp}} = C_w \times f_{\text{oc}}(\text{susp}) \times K_{\text{ow}} \times 10^{-0.21} = \\ = 0.19 \mu\text{g l}^{-1} \times 0.1 \times 10^{6.18} \times 10^{-0.21} \text{ l kg}^{-1} \\ = 17732 \mu\text{g kg}^{-1} \\ = 17.7 \text{ mg kg}^{-1}.$$

By using equations (8) and (11) the criterion for the total HCB concentration in water has been calculated:

$$C_{\text{tot}} = C_w \times (1 + 10^{-0.21} \times K_{\text{ow}} \times f_{\text{oc}} \times \text{SM}) \\ = 0.19 \mu\text{g l}^{-1} \times (1 + 10^{-0.21} \times 10^{6.18} \text{ l kg}^{-1} \times 0.1 \\ \times 30 \times 10^{-6} \text{ kg l}^{-1}) \\ = 0.72 \mu\text{g l}^{-1}.$$

The criterion for HCB in sediment has been obtained by using equations (7) and (11):

$$C_{\text{sed}} = C_w \times f_{\text{oc}}(\text{sed}) \times K_{\text{ow}} \times 10^{-0.21} = \\ = 0.19 \mu\text{g l}^{-1} \times 0.05 \times 10^{6.18} \text{ l kg}^{-1} \times 10^{-0.21} \\ = 8866 \mu\text{g kg}^{-1} \\ = 8.9 \text{ mg kg}^{-1}.$$

(b) *Starting point for bioaccumulation (BCF).* The criterion for dissolved HCB, related to the product standard for fish, has been calculated by using equation (6):

$$C_w = \frac{C_{\text{org}}}{\text{BCF}} = \frac{200 \mu\text{g kg}^{-1}}{75678 \text{ l kg}^{-1}} \\ = 0.0026 \mu\text{g l}^{-1}.$$

The product standard-related criterion for HCB in suspended matter has been calculated by using equations (7) and (11):

$$C_{\text{susp}} = \frac{C_{\text{org}}}{\text{BCF}} \times f_{\text{oc}}(\text{susp}) \times K_{\text{ow}} \times 10^{-0.21} = \\ = \frac{200 \mu\text{g kg}^{-1}}{75678 \text{ l kg}^{-1}} \times 0.1 \times 10^{6.68} \text{ l kg}^{-1} \times 10^{-0.21} \\ = 0.25 \text{ mg kg}^{-1}.$$

The product standard-related criterion for the total concentration of HCB in water has been obtained by using equations (8) and (11):

$$C_{tot} = \frac{C_{org} \times (1 + 10^{-0.21} \times K_{ow} \times f_{oc} \times SM)}{K_{ow}/20}$$

$$C_{tot} = \frac{200 \mu\text{g kg}^{-1} \times (1 + 10^{-0.21} \times 10^{6.18} \text{ kg}^{-1} \times 0.1 \times 30 \times 10^{-6} \text{ kg l}^{-1})}{75678 \text{ kg}^{-1}}$$

$$= 0.01 \mu\text{g l}^{-1}.$$

Finally the product standard-related criterion for HCB in sediment has been given by using equations (7) and (11):

$$C_{sed} = \frac{C_{org}}{BCF} \times f_{oc}(\text{sed}) \times K_{ow} \times 10^{-0.21} =$$

$$= \frac{200 \mu\text{g kg}^{-1}}{75678 \text{ kg}^{-1}} \times 0.05 \times 10^{6.18} \text{ kg}^{-1} \times 10^{-0.21}$$

$$= 0.12 \text{ mg kg}^{-1}.$$

In this example the product standard-related criteria give lower values than the criteria related to the direct aquatic effect data. In other words, for HCB

quality criteria are to be derived from the *product standard*.

In this way for about 120 substances ecotoxicological quality criteria have been derived for both sediment and water (Stortelder *et al.*, 1989). In this document all the values, constants and assumptions are mentioned to derive these criteria\*.

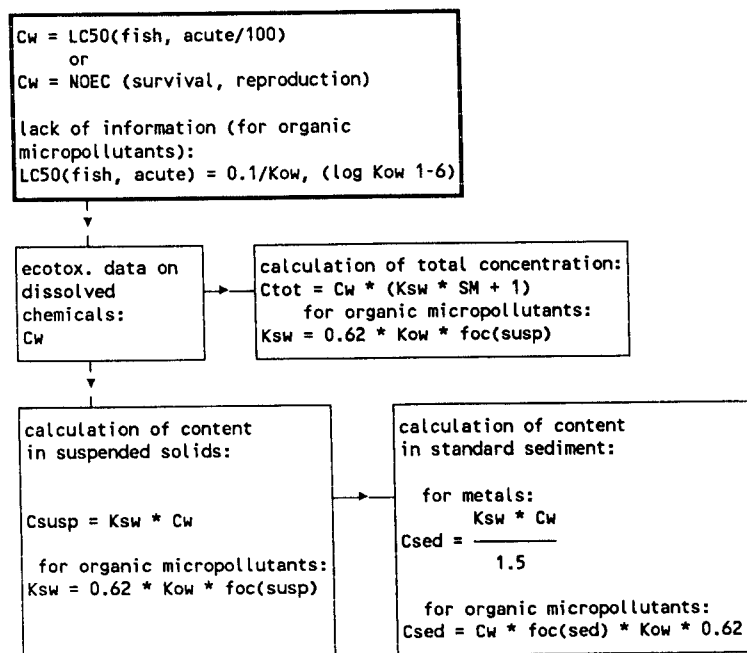
These criteria have been used to make a policy in the water management for the next 10 years in the Netherlands (Ministry of Transport and Public Works, 1989\*). However, it becomes too involved to discuss all these calculations in this paper.

SUMMARIZING DIAGRAMS

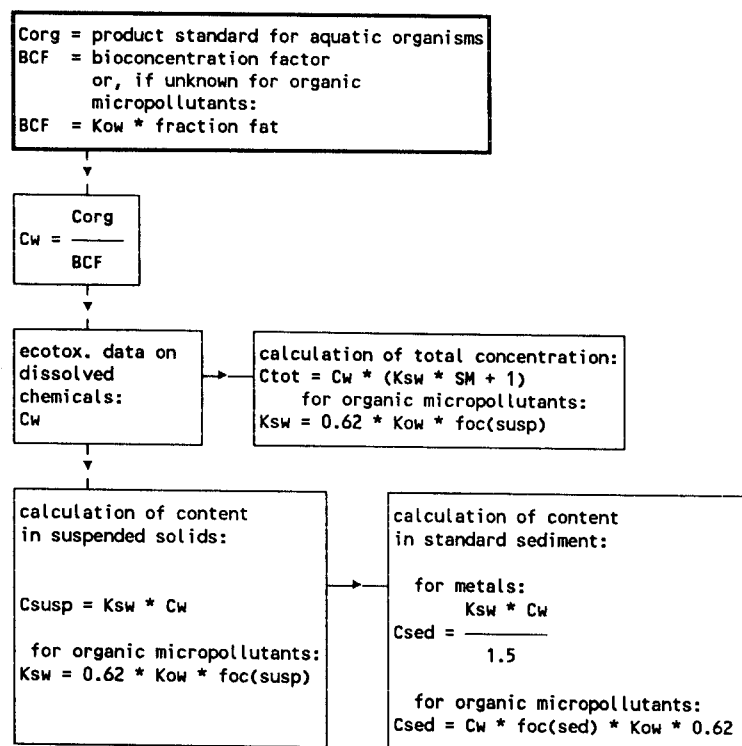
The equations handled in the previous two sections are given schematically below.

\*Summaries in English and German are available.

Direct aquatic effects (NOEC)



Scheme 1.

**Bioaccumulation effects (BCF)**

Scheme 2.

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