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and the Environment
Ministry of Health, Welfare and Sport

Guidance for the derivation of environmental risk limits

Part 9. Recalculation of standards to Dutch characteristics;
Equilibrium partitioning method

version 1.0

Colophon

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1 Standard soil, sediment and suspended matter

The methodology for derivation of environmental risk limits (ERL) for soil and sediment in this report, makes use of the characteristics for Dutch standard soil, Dutch standard sediment and Dutch standard suspended matter[1] as they have been used in the past for ERL derivations at the Dutch national level. These characteristics are: the percentage of organic matter, which is proportional to the percentage organic carbon, the percentage of clay (lutum), and the concentration of suspended matter in surface water. The ERLs should be expressed on the basis of Dutch characteristics.

Note that an ERL that is expressed in standard soil or sediment should be recalculated to local soil or sediment conditions when a local concentration is compared with an ERL [1]. Using Dutch standard conditions for all ERLs is thus a way of expressing ERLs, a systematization that enables comparison of values for different compounds, rather than a generic value that should be valid for all soils and sediments in the Netherlands.

In the WFD [2] and REACH [3] guidance documents, compartment characteristics have values that differ from the standards used in the Netherlands. Table 1 summarizes the different parameter and their values.

Table 1 Characteristics of standard soil, standard sediment and standard suspended matter used in The Netherlands compared to REACH and WFD guidance.

	The Netherlands				REACH & WFD		
Compartment	%o.m [-]	%o.c. [-]	%clay [-]	C_{susp} [mg/L]	%o.m [-]	%o.c. [-]	C_{susp} [mg/L]
soil	10	5.88	25	–	3.4	2	–
suspended matter	20	11.8	40		17[a]	10	15
sediment	10	5.88	25		8.5[a]	5	–

a: Values for %o.m. calculated from %o.c. using Eq. **Error! Reference source not found.**, since REACH guidance presents only %o.c. values.

Sources used in Table 1:

- All Dutch values based on VROM [1],
- REACH values based on Table R.16-9 [3],
- WFD values on WFD EQS guidance [2].

[1] Suspended matter should be distinguished from dissolved organic carbon (DOC). The former are non-dissolved particles, consisting of both an organic and an inorganic component, the latter are smaller particles (e.g. not isolated after filtration over 0.45 µm) consisting of organic components.

2 Recalculation of standards to Dutch characteristics

2.1 Equilibrium partitioning method

This report explains the use of the equilibrium partitioning (EqP) method within the framework of environmental standard derivation in The Netherlands. The procedure outlined is identical to the guidance given in REACH for the soil, sediment and suspended matter compartments. The WFD guidance cites REACH on this subject. However, because Dutch standard soil, standard sediment and standard suspended matter have different values for the organic matter content, a recalculation to Dutch standard characteristics for soil, sediment and suspended matter is included as an additional step in the EqP method.

2.1.1 *General equations needed in conversions*

The two following equations are needed in some of the conversion steps described in this report.

$$K_{p,\,susp\text{-}water} = K_{oc} \times Foc_{susp,REACH} \quad (1)$$

$$\%\,o.m. = 1.7 \times \%\,o.c. \quad (2)$$

2.1.2 *Calculation of $K_{comp\text{-}water}$*

In the EqP method outlined in REACH guidance R.16 [3], the 'dimensionless' partition coefficient $K_{comp\text{-}water}$ is used, in units of $m^3\ m^{-3}$. This parameter is also called the total compartment-water partition coefficient. It is calculated, for each compartment of interest according to the equations given in section R.16.5.3.3, pages 31 and 32. The default values for compartment-specific characteristics ($Fair_{comp}$, RHOsolid, etc.) from REACH [Table R.16-9, p.49] [3] should be used in these equations; their values are listed in the list of variables and default values ERL Report 11. The selection of the K_{oc} value that is used in EqP calculations, is described in ERL Report 02.

$$Kp_{comp} = K_{oc} \times Foc_{comp} \quad \text{with } comp \in \{soil, sed, susp\} \quad (3)$$

$$K_{comp-water} = \frac{Ctotal_{comp}}{Cporew_{comp}} \quad (4)$$

$$K_{comp-water} = Fair_{comp} \times K_{air-water} + Fwater_{comp} + Fsolid_{comp} \times \frac{Kp_{comp}}{1000} \times RHOsolid \quad (5)$$

with comp $\in$ {soil, sed, susp}

$$K_{air-water} = \frac{H}{R \times TEMP} \quad (6)$$

2.1.3 *EqP for soil*

The calculation of the MPC_{soil} in REACH by equilibrium partitioning follows the same route as for sediment:

- The MPC_{soil} is calculated according to EqP from the QS (quality standard) for aquatic organisms, $QS_{fw,\ eco}$, using Equation 7.
- When the MPC_{soil} is calculated using EqP and log K_{ow} > 5 for the compound of interest, MPC_{soil} is divided by 10. This correction factor is applied because EqP only considers uptake via the water phase. Extra uncertainty due to uptake by ingestion of food should be covered by the applied assessment factor of 10.

$$MPC_{soil,\ EU,\ EqP,\ ww} = \frac{K_{soil-water}}{RHO_{soil}} \cdot QS_{fw,\ eco} \cdot 1000 \qquad (7)$$

$$MPC_{soil,\ EU,\ EqP,\ dw} = \frac{RHO_{soil}}{Fsolid_{soil} \times RHOsolid} \times MPC_{soil,\ EU,\ EqP,\ ww} \qquad (8)$$

The values for the environmental compartment characteristics (*viz.* $Fsolid_{soil}$ and RHO_{soil}) have been taken from REACH guidance [section R.16.6.4, p. 49]; these are also listed in ERL Report 11. The formulae, parameters and default characteristics necessary to calculate the density are also mentioned in section R.16.6.4 and will not be repeated here.

2.1.4 *EqP for sediment*

Following WFD guidance, bulk-sediment characteristics are used in EqP calculations for sediment [2, section 5.2.1.2, p. 97], in contrast to REACH, where suspended matter characteristics are used for the sediment compartment. There is no methodological difference behind the choice for suspended matter, because in both cases the equilibrium partitioning method is used. When departing from the same concentration in water, the calculated dry weight concentration in 'REACH-sediment' will be higher, due to the higher organic matter content of suspended matter (10%) compared to sediment (5%) within REACH.

Sediment standards that have been derived using EqP, based on a $QS_{water,\ eco}$, have to be converted to Dutch standard sediment (for characteristics, see Table 1. This is done using Eq. 21.

When a sediment standard is based on toxicity data for benthic organisms, these data have already been normalised to the organic matter content of Dutch standard sediment (see ERL Report 04). Further recalculation is then not necessary.
The calculation of the $QS_{sediment}$ by equilibrium partitioning according to WFD (REACH equations).

- The $QS_{sediment,\ EU\ EqP,\ dw}$ is calculated according to EqP from the QS for aquatic organisms, $QS_{fw,\ eco}$, using Eqs. 9 and 10, or in the case of marine sediment, from $QS_{sw,\ eco}$.
- When the $QS_{sediment}$ has been calculated using EqP and log K_{ow} >5 for the compound of interest, $QS_{sediment}$ is divided by 10. This correction factor is applied because EqP only considers uptake via the water phase. Extra uncertainty due to uptake by ingestion of food should be covered by the applied assessment factor of 10.

- It should be noted that in the case of metals, only empirically derived values for $K_{susp\text{-}water}$ should be derived [WFD EQS guidance section 1.2.1.2 p. 128].

$$QS_{sediment, EU, EqP, ww} = \frac{K_{sed\text{-}water}}{RHO_{susp}} \times QS_{fw, eco} \cdot 1000 \quad (9)$$

$$QS_{sediment, EU, EqP, dw} = \frac{RHO_{sed}}{Fsolid_{sed} \times RHOsolid} \times QS_{sediment, EU, EqP, ww} \quad (10)$$

The default values for sediment characteristics ($Fsolid_{susp}$, RHO_{susp}, etc.) have been taken from REACH guidance [section R.16.6.4, p. 48]; these are also listed in ERL Report 11. The formulae, parameters and default characteristics necessary to calculate the density are also mentioned in REACH guidance section R.16.6.4 and will not be repeated here.

2.2 Recalculation of water standards to suspended matter

If it is necessary to express a water standard as a concentration in suspended matter, follow the method given in the WFD EQS guidance, Section 3.8.1, page 71 [2].

$$QS_{susp} = QS_{water, dissolved} \cdot K_{p, susp-water} \quad (11)$$

2.3 Recalculation of standards from dissolved to total concentrations

In case the ERLs derived using this guidance should be expressed as total concentrations, use the following equation.

2.3.1 Organic compounds

$$QS_{water, total} = QS_{water, dissolved} \cdot (1 + K_{p, susp\text{-}water} \cdot C_{susp,\ Dutch\ standard} \cdot 10^{-6}) \quad (12)$$

In this equation, characteristics for Dutch standard suspended matter should be used: $C_{susp, Dutch\ st.}$ = 30 mg/L. $K_{p, susp\text{-}water}$ is calculated using Eq. 1.for the substance of interest.

If the standard should be expressed using EU characteristics, $C_{susp, WFD}$ is 15 mg/L for freshwater and $C_{susp\ marine, WFD}$ is 3 mg/L for marine water.

2.3.2 Metals

In case ERLs for metals have been derived using the added risk approach and a standard expressed as dissolved concentration should be converted into a total concentration, take care to convert both $MPA_{water, dissolved}$ and $C_{b, dissolved}$ into a total concentration since:

$$QS_{water, dissolved} = C_{b, dissolved} + MPA_{water, dissolved} \quad (131)$$

$$QS_{water, total} = C_{b, total} + MPA_{water, total} \quad (14)$$

2.4 Recalculation of standards from total to dissolved concentrations

In case ERLs for water are encountered that have been expressed at total water concentrations and it is desirable to express these as dissolved concentrations use the following equations.

2.4.1 *Organic compounds*

$$QS_{\text{water, dissolved}} = QS_{\text{water, total}} \quad \frac{1}{1 + K_{\text{p, susp-water}} \times C_{\text{susp, Dutch standard}} \times 10^{-6}} \qquad (15)$$

In this equation, characteristics for Dutch standard suspended matter should be used: $C_{\text{susp, Dutch standard}}$ = 30 mg/L. $K_{\text{p, susp-water}}$ is calculated using Eq. 1.for the substance of interest.

In case $QS_{\text{water, total}}$ is not a Dutch standard, the C_{susp} value used to express that standard should be known and entered in Eq. 15. If the standard is to be expressed using EU (WFD) characteristics, $C_{\text{susp, WFD}}$ is 15 mg/L for freshwater and $C_{\text{susp marine, WFD}}$ is 3 mg/L for marine water.

2.4.2 *Metals*

Recalculation for metals is performed using the same equation as described in the previous section.

- In case the added risk approach has been followed to derive the $QS_{\text{water, total}}$, and this standard is expressed as the sum of background concentration (C_b) and the added fraction ($MPA_{\text{water, total}}$), $QS_{\text{water, total}}$ can be converted to $QS_{\text{water, dissolved}}$ using Eq. 15 with the Kp_{susp} for the metal in question.
- In case the standard expresses only the added fraction ($MPA_{\text{water, total}}$) convert the MPA into $MPA_{\text{water, dissolved}}$ using Eq. 15. A background concentration (C_b) of the metal in the water body to which the standard should apply should be available, as a dissolved concentration. If C_b is available as total concentration, convert it to $C_{\text{b, dissolved}}$ in the same manner. Calculate the standard as
  $QS_{\text{water, dissolved}} = C_{\text{b, dissolved}} + MPA_{\text{water, dissolved}}$.

2.5 Recalculation to Dutch standard soil and sediment

The resulting standards for sediment and soil are expressed with the characteristics of suspended matter and soil, according to REACH guidance. These values should be recalculated to Dutch standard sediment and soil. Both standard sediment and soil contain 10% organic matter, which is equivalent to 5.88% organic carbon, calculated using Eq. 2. See also Table 1. There are two options that are outlined in the next sections.

2.5.1 *Recalculation departing from a standard in water*

The soil or sediment standard derives from a standard in water and is calculated using EqP (section 2.1). In this situation, the ERL for soil or sediment should be calculated using the correct o.c. content from the start of the calculation. A stepwise description is given here (see section 2.1 and subsections for detail):

- the value for Kp_{soil} or Kp_{susp} should first be calculated using an organic carbon content of 5.88%, using Eq. 3;
- next, convert this partition coefficient into SI units: m^3/kg;
- calculate $K_{\text{air-water}}$ (Eq.6) in SI units, which is needed as input for the next step;
- Use Eq. 5 to calculate $\underline{K}_{\text{soil-water}}$ for recalculation to Dutch standard soil or $K_{\text{susp-water}}$ for recalculation to Dutch standard sediment;

– Finally, calculate the Dutch standards using Eq. 16 and 17 for soil and Eq. 18 and 19 for sediment. The final standard is to be expressed as a dry weight concentration.

$$MPC_{soil, NL, EqP, ww} = QS_{fw, eco} \times \frac{K_{soil-water}}{RHO_{soil}} \times 1000 \qquad (16)$$

$$MPC_{soil, NL, EqP, dw} = MPC_{soil, NL, EqP, ww} \times \frac{RHO_{soil}}{Fsolid_{soil} \times RHOsolid} \qquad (17)$$

$$JG\text{-}MKE_{sediment, NL, EqP, ww} = QS_{fw, eco} \times \frac{K_{sed-water}}{RHO_{susp}} \times 1000 \qquad (18)$$

$$JG\text{-}MKE_{sediment, NL, EqP, dw} = JG\text{-}MKE_{sediment, NL, EqP, ww} \times \frac{RHO_{sed}}{Fsolid_{sed} \times RHOsolid} \qquad (19)$$

Parameter defaults and explanation of variables are presented in ERL Report 11.

2.5.1.1 Old versus new method: differences explained

The differences between concentrations calculated to standard soil, sediment, and sediment with suspended matter characteristics are caused by the differences in the fraction water of the compartment, since the fraction organic matter of Dutch standard soil and Dutch standard sediment is the same.

In the previous guidance [4] for Dutch ERL derivation standards in soil and and sediment that were derived from a standard in water, were recalculated to recalculated to Dutch characteristics in a different way. The final standard in soil standard in soil or sediment was corrected with the ratios for organic carbon carbon content, equal to the method explained in section 2.5.2. In this way, the way, the fraction of water in the dimensionless partition coefficients ($K_{soil-water}$ ($K_{soil-water}$ and $K_{sed-water}$) used in this EqP method, were neglected. See

Table 2 Difference between ERLs derived by equilibrium partitioning from water-based quality standards using the former [4] and current recalculation to Dutch standard characteristics. Ratios between the old and new method are shown for Dutch soil and sediment standards and a series of K_{oc} values.Table 2 for an overview of the differences caused by the two methods. The effect is more apparent for substances with low K_{oc} values, that occur for a substantial mass fraction in the water phase. The effect is also more prominent for sediment than for soil, since sediment (with suspended matter characteristics) contains 4.5 times more water than soil, following REACH parametrization.

In general, for soil, the Dutch standard values are lower using the new method, but for substances with a log K_{oc} = 2, the difference is only 4%, and this becomes less with increasing K_{oc}.
For sediment, the Dutch standard values are higher using the new method, with an effect of approximately 2.5% at log K_{oc} = 3 and this becomes less as K_{oc} increases.

Table 2 Difference between ERLs derived by equilibrium partitioning from water-based quality standards using the former [4] and current recalculation to Dutch standard characteristics. Ratios between the old and new method are shown for Dutch soil and sediment standards and a series of K_{oc} values.

log Koc	**Ratio MPC_{soil} old/new method**	**Ratio $QS_{sediment}$ old/new method**
1	1.36	0.646
2	1.04	0.844
3	1.00	0.976
4	1.00	0.997
5	1.00	0.997

2.5.2 *Recalculation departing from a standard in soil or sediment*

In this situation, a standard in soil or sediment is available that should be normalised to an organic carbon content. If this soil or sediment standard is based on studies with soil or sediment organisms, the normalisation of the results of the toxicity experiments (e.g. EC50s, NOECs, EC10s) should be directly performed to the desired organic carbon content. See Table 1 for the correct o.c. percentages per framework and compartment.

In case there are no underlying data for the soil or sediment standard, the standard is normalised using the Eqs. 20 and 21.

$$MPC_{Dutch\ st.soil,dw} = MPC_{soil,\ EU,\ dw} \times \frac{Foc_{Dutch\ st.soil}}{Foc_{soil,\ EU}} \qquad (20)$$

$$MPC_{Dutch\ st.sed,dw} = MPC_{sed,\ EU,\ dw} \times \frac{Foc_{Dutch\ st.sediment}}{Foc_{sediment,\ EU}} \qquad (21)$$

Care should be taken to retrieve the correct organic carbon content used in the derivation of the EU standard. E.g. a standard put forward in REACH or biocides framework may be termed $PNEC_{sediment}$, but might have been derived using characteristics for suspended matter. Parameter defaults and explanation of variables are presented in ERL Report 11.

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Appendix 1. Abbreviations

EC	European Commission
EC_x	concentration that causes x% effect on a test organism
ECHA	European Chemicals Agency
Eq	equation
EqP	equilibrium partitioning
EQS	environmental quality standard
ERL	environmental risk limit
EU	European Union
EU-RAR	European Union-risk assessment report
MPA	maximum permissible addition
MPC	maximum permissible concentration
NOEC	no observed effect concentration
o.c.	organic carbon
o.m.	organic matter
QS	quality standard
QSAR	quantitative structure activity relationship
REACH	Registration, Evaluation, Authorisation and Restriction of Chemical substances.
RIVM	National Institute for Public Health and the Environment
SI	International System of Units
VROM	former Ministry of Spatial Planning, Housing and Environmental Protection, now Ministry of Infrastructure and the Environment
WFD	Water Framework Directive