



National Institute for Public Health
and the Environment
Ministry of Health, Welfare and Sport

Guidance for the derivation of environmental risk limits

Recalculation of standards to Dutch characteristics;
Equilibrium partitioning method

version 2.0

Colophon

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1 Notes to this version

The previous version of this guidance was published in 2015, building on an RIVM report from 2007 [1]. In 2018, the European technical guidance for derivation of environmental quality standards (EQS) under the Water Framework Directive [2] has been revised, including a larger part of the former national methodology. In addition, European defaults for characteristics of suspended matter were adopted. The present document is a revised version, removing parts which are now sufficiently covered in the WFD-guidance.

2 Standard soil and sediment

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 and Dutch standard sediment 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 and the percentage of clay (lutum). 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 [3]. Using Dutch standard conditions for all ERLs is thus a way of expressing ERLs, a systematisation 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 [4] guidance documents, default compartment characteristics of soil and sediment differ from those used in the Netherlands. Table 1 summarises the different parameters and their values.

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

Compartment	The Netherlands			REACH & WFD	
	%o.m. [-]	%o.c. [-]	%clay [-]	%o.m. [-]	%o.c. [-]
soil	10	5.88	25	3.4	2
suspended matter	see REACH & WFD				10
sediment	10	5.88	25	8.5 ^a	5

a: Values for %o.m. calculated from %o.c. using Eq. 2, since REACH guidance presents only %o.c. values.

Sources used in Table 1:

- Dutch values based on VROM [3],
- REACH values based on Table R.16-8 [4],
- WFD values on WFD EQS guidance [2]

3 Recalculation of standards to Dutch characteristics

3.1 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 and standard sediment have different values for the organic matter content, a recalculation to Dutch standard characteristics for soil and sediment is included as an additional step in the EqP method.

3.1.1 General equations needed in conversions

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

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

$$\% \text{ o.m.} = 1.7 \times \% \text{ o.c.} \quad (2)$$

3.1.2 Calculation of $K_{\text{comp-water}}$

In the EqP method outlined in REACH guidance R.16 [4], the 'dimensionless' partition coefficient $K_{\text{comp-water}}$ is used, in units of $\text{m}^3 \text{m}^{-3}$. This parameter is also called the total compartment-water partition coefficient. It is calculated, for each compartment of interest according to the equations given Appendix A.16-3. The default values for compartment-specific characteristics ($F_{\text{air-comp}}$, RHO_{solid} , etc.) from REACH [Table R.16-8] [4] should be used in these equations; their values are listed in the ERL report with variables and default values. The selection of the K_{oc} value that is used in EqP calculations, is described in the ERL report on data collection.

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

$$K_{\text{comp-water}} = \frac{C_{\text{total, comp}}}{C_{\text{porew, comp}}} \quad (4)$$

$$K_{\text{comp-water}} = F_{\text{air-comp}} \times K_{\text{air-water}} + F_{\text{water, comp}} + F_{\text{solid, comp}} \times \frac{K_{p, \text{comp}}}{1000} \times RHO_{\text{solid}} \quad (5)$$

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

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

3.1.3 EqP for soil

The calculation of the MPC_{soil} by equilibrium partitioning according to the REACH methods 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.

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

$$MPC_{soil, EU, EqP, dw} = \frac{RHO_{soil}}{F_{solid_{soil}} \times RHO_{solid}} \times MPC_{soil, EU, EqP, ww} \quad (8)$$

The values for the environmental compartment characteristics (*viz.* F_{solid_{soil}} and RHO_{soil}) have been taken from REACH guidance R.16, table R.16-8. The formulae, parameters and default characteristics necessary to calculate the density are also mentioned in Appendix A.16-3 and will not be repeated here.

3.1.4 EqP for sediment

Following WFD guidance, [2] bulk sediment characteristics are used in EqP calculations for sediment, in contrast to REACH, which uses 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 carbon 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 relevant ERL report). 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 $K_{\text{susp-water}}$ should be derived.

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

$$QS_{\text{sediment, EU, EqP, dw}} = \frac{\text{RHO}_{\text{sed}}}{\text{Fsolid}_{\text{sed}} \times \text{RHO}_{\text{solid}}} \times QS_{\text{sediment, EU, EqP, ww}} \quad (10)$$

The default values for sediment characteristics ($\text{Fsolid}_{\text{susp}}$, RHO_{susp} , etc.) have been taken from REACH guidance (A.16-3). The formulae, parameters and default characteristics necessary to calculate the density are also mentioned in REACH guidance and will not be repeated here.

3.2 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.

3.2.1 *Recalculation departing from a standard in water*

The soil or sediment standard is derived from a standard in water and is calculated using EqP (section 3.1). 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 3.1 and subsections for detail):

- the value for K_{psoil} or K_{psusp} 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 $K_{\text{soil-water}}$ 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.

$$\text{MPC}_{\text{soil, NL, EqP, ww}} = QS_{\text{fw, eco}} \times \frac{K_{\text{soil-water}}}{\text{RHO}_{\text{soil}}} \times 1000 \quad (16)$$

$$\text{MPC}_{\text{soil, NL, EqP, dw}} = \text{MPC}_{\text{soil, NL, EqP, ww}} \times \frac{\text{RHO}_{\text{soil}}}{\text{Fsolid}_{\text{soil}} \times \text{RHO}_{\text{solid}}} \quad (17)$$

$$\text{JG - MKE}_{\text{sediment, NL, EqP, ww}} = QS_{\text{fw, eco}} \times \frac{K_{\text{sed-water}}}{\text{RHO}_{\text{susp}}} \times 1000 \quad (18)$$

$$\text{JG - MKE}_{\text{sediment, NL, EqP, dw}} = \text{JG - MKE}_{\text{sediment, NL, EqP, ww}} \times \frac{\text{RHO}_{\text{sed}}}{\text{Fsolid}_{\text{sed}} \times \text{RHO}_{\text{solid}}} \quad (19)$$

3.2.2 *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 a the appropriate 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.

$$MPC_{\text{Dutch st.soil, dw}} = MPC_{\text{soil, EU, dw}} \times \frac{FOC_{\text{Dutch st.soil}}}{FOC_{\text{soil, EU}}} \quad (20)$$

$$MPC_{\text{Dutch st.sed, dw}} = MPC_{\text{sed, EU, dw}} \times \frac{FOC_{\text{Dutch st.sediment}}}{FOC_{\text{sediment, EU}}} \quad (21)$$

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 $PNEC_{\text{sediment}}$, but will be derived using characteristics for suspended matter.

References

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3. VROM. 1999. Environmental risk limits in the Netherlands. A review of environmental quality standards and their policy framework in the Netherlands. The Hague, the Netherlands. Ministry of Housing, Spatial Planning and the Environment.
4. ECHA. 2016. Guidance on information requirements and Chemical Safety Assessment. Chapter R.16: Environmental exposure assessment. Version 3.0. Helsinki, Finland. European Chemicals Agency. Report ECHA-16-G-03-EN.

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