## Tested equations

The following equations were tested for deltaP\_tot, deltaP\_dissolved and deltaP\_particle\_bound:

* Sabbagh et al. (2009)
* Chen et al. (2016)
* “dilution + constant particle-bound concentration” (inspired by Muñoz-Carpena et al., 2015)

Predicted deltaP\_dissolved and deltaP\_particle\_bound were calculated in the same way from predicted deltaP\_tot as in VFSMOD (cf. Muñoz-Carpena et al., 2015), assuming sorption equilibrium in the outflow.

### Equation of Sabbagh et al. (2016)

deltaP = 24.79 + 0.54 \* deltaQ + 0.52 \* deltaE - 2.42 \* ln(FpH+1) - 0.89 \* %C (eq. 1)

FpH = Qi/(Kd\*Ei) (eq. 2)

with

deltaP relative reduction (%) of total pesticide load

deltaQ relative reduction (%) of total inflow Qi

deltaE relative reduction (%) of incoming sediment load Ei

Qi total runoff inflow (run-on + rainfall + snowmelt; L)

Ei incoming sediment load (kg)

FpH phase distribution coefficient (mass ratio)

Kd=Koc\*OC(%)/100 linear sorption coefficient (L/kg)

%OC organic carbon in sediment

%C clay content of field soil (as proxy for the clay content of the eroded sediment)

### Equation of Chen et al. (2016)

sqrt(101 - deltaP) = temp = 8.06 - 0.07 \* deltaQ + 0.02 \* deltaE + 0.05 \* clay - 2.17 \* Cat + 0.02 \* deltaQ/Cat - 0.0003 \* deltaQ/deltaE (eq. 3)

deltaP = 101 – temp2 = 101 - (8.06 - 0.07 \* deltaQ + 0.02 \* deltaE + 0.05 \* clay - 2.17 \* Cat + 0.02 \* deltaQ/Cat - 0.0003 \* deltaQ/deltaE)2 (eq. 4)

with

Cat for Koc > 9000 L/kg, Cat = 2; for Koc ≤ 9000 L/kg, Cat = 1

### Approach “dilution + constant particle-bound concentration” (from Muñoz-Carpena et al., 2015)

C’ = Ci \* Vi / Qi (instantaneous mixing of run-on and rainfall) (eq. 7)

S’ = Si = Kd \* Ci (particle-bound conc. remains constant ; Muñoz-Carpena et al., 2015) (eq. 8)

mf = min(mi, Mf \* S' + Vf \*C') (eq. 9)

mo = mi – mf (eq. 10)

with

C’ dissolved pesticide conc. in surface runoff after dilution with rainfall or snowmelt (mg/L)

Ci dissolved pesticide conc. in run-on (mg/L)

Vi run-on from the source area (L)

Qi total runoff inflow (run-on + rainfall + snowmelt; L)

Si particle-bound pesticide conc. in run-on (mg/kg)

Kd linear sorption coefficient (L/kg)

S’ particle-bound pesticide conc. in surface runoff after dilution with rainfall (mg/kg)

Vf volume of water retained in filter (L)

Mf total sediment load retained in filter (kg)

mf predicted total pesticide mass retained in filter (mg)

mi total incoming pesticide mass in run-on (mg) = Ci \* Vi + Si \* Ei

mo total pesticide mass leaving the filter in surface runoff (mg)

Formulate equation for deltaP:

deltaP is by definition given as:

deltaP = (mi - mo)/mi \* 100% = mf / mi \* 100% (eq. 11)

Express deltaP as function of deltaQ and deltaE:

deltaQ = (Qi – Qo)/Qi \* 100 % = Vf/Qi \* 100% (eq. 12)

deltaQ/100% = Vf/Qi

Vf = deltaQ/100% \* Qi

deltaE = (Ei – Eo)/Ei \* 100 % = Mf/Ei \* 100 % (eq. 13)

deltaE/100% = Mf/Ei

Mf = deltaE/100% \* Ei

with

Qo surface runoff volume leaving the buffer strip (L)

Eo eroded sediment leaving the buffer strip (kg)

Insert eq. 9 in eq. 11:

deltaP/100% = min[mi, Mf \* S' + Vf \*C']/ mi (eq. 14)

insert eqs. 12 and 13 in eq. 14:

deltaP/100% = min[mi, deltaE/100% \* Ei \* S' + deltaQ/100% \* Qi \*C'] / mi (eq. 15)

insert eqs. 7 and 8 in eq. 15:

deltaP/100% = min[mi, deltaE/100% \* Ei \* Kd \* Ci + deltaQ/100% \* Qi \*Ci \* Vi/Qi] / mi

deltaP/100% = min[mi, deltaE/100% \* Ei \* Kd \* Ci + deltaQ/100% \* Ci \* Vi] / mi (eq. 16)

With

mi = Ci \* Vi + Si \* Ei = Ci \* Vi + Ci \* Kd \* Ei = Ci \* (Vi + Kd \* Ei) (eq. 17)

one obtains

deltaP/100% = min[Ci \* (Vi + Kd \* Ei), deltaE/100% \* Ei \* Kd \* Ci + deltaQ/100% \* Ci \* Vi] / Ci \* (Vi + Kd \* Ei) (eq. 18)

Now we can cancel Ci :

deltaP/100% = min[(Vi + Kd \* Ei), deltaE/100% \* Ei \* Kd + deltaQ/100% \* Vi] / (Vi + Kd \* Ei) (eq. 19)

Eq. 19 expresses deltaP as a function of Vi, Kd, Ei, deltaE and deltaQ.

## Mathematical analysis of the three equations

Before comparing predicted and measured deltaP values, it is important to explore the mathematical behaviour of the three equations, especially at the borders of the possible range of inputs.

The equation of Sabbagh et al. depends on six input variables: deltaQ, deltaE, Qi, Ei, Kd and clay (seven if one expresses Kd as a function of Koc and OC content).

The equation of Chen et al. only depends on four variables: deltaQ, deltaE, clay and Koc.

* No dependence on the actual mass distribution.

The equation “dilution + constant particle-bound concentration” depends on five variables: deltaQ, deltaE, Vi, Kd, Ei (six if one expresses Kd as a function of Koc and OC content).

* no explicit dependence on Qi, but on Vi
* no dependence on clay content

In conclusion, the three equations have only three independent variables in common: deltaQ, deltaE and (if Kd is expressed as a function of Koc and OC content) Koc.