Evaluation of pesticide trapping efficiency equations for vegetative filter strips (VFS) using additional experimental data

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Introduction

Vegetative filter strips (VFS) are widely used for mitigating pesticide inputs into surface waters via surface runoff and erosion. To simulate the effectiveness of VFS in reducing surface runoff volumes, eroded sediment and pesticide loads the model VFSMOD (Muñoz-Carpena and Parsons, 2014) is frequently used. While VFSMOD simulates infiltration of surface runoff water and sedimentation of eroded soil material mechanistically, pesticide load reduction (deltaP) by the VFS is calculated with the empirical multiple regression equation of Sabbagh et al. (2009). This equation uses the variables deltaQ (relative reduction of total water inflow) and deltaE (relative reduction of incoming sediment load) calculated by VFSMOD. The Sabbagh equation has not been widely accepted by regulatory authorities, on the grounds that its reliability has not been sufficiently established yet. Hence, evaluation against additional experimental data is necessary.

Chen et al. (2016) proposed an alternative regression equation, derived from the same experimental data as used by Sabbagh et al. (2009), however using a cross-validation approach.

The objective of this study was to improve the validation status of the Sabbagh equation by testing it against additional experimental data. The equation of Chen et al. (2016) and an alternative, non-regression-based approach should also be tested against the new data.

Data acquisition and suitability check

Experimental VFS datasets were compiled from available literature (peer-reviewed papers, PhD theses, study reports) and checked for their suitability. The following experimental data are necessary for testing the Sabbagh equation, on an event basis:

- precipitation volume
- volume of surface runoff water leaving the field (or a control plot)
- mass of eroded sediment leaving the field
- mass of pesticide leaving the field (measured in both in dissolved and particle-bound phase)
- volume of surface runoff leaving the VFS
- mass of eroded sediment leaving the VFS
- mass of pesticide leaving the VFS (in both phases)

Moreover, the equation requires:

- Kd of the pesticide for the field topsoil
- clay and OC content of the field topsoil

Individual data points needed to fulfil the following criteria:

- pesticide concentration in in- and outflow, dissolved and particle bound, ≥ LOQ
- 0 ≤ deltaQ < 100
- measured deltaE existing and ≥ 0
- measured deltaP existing and ≥ 0

Many datasets had to be discarded because suspended sediment loads had not been measured or pesticides were not analyzed in both phases. The collected data included two studies with snowmelt-induced runoff events, but none of the three equations could predict deltaP for such events adequately. These data points where therefore excluded from further analyses. Finally, 43 data points from 3 studies were found usable, containing 8 substances with a Koc range of 78-14000 L/kg: acetochlor, atrazine, chlorpyrifos, desethyl terbuthylazine, diflufenican, isoproturon, pendimethalin and terbuthylazine.

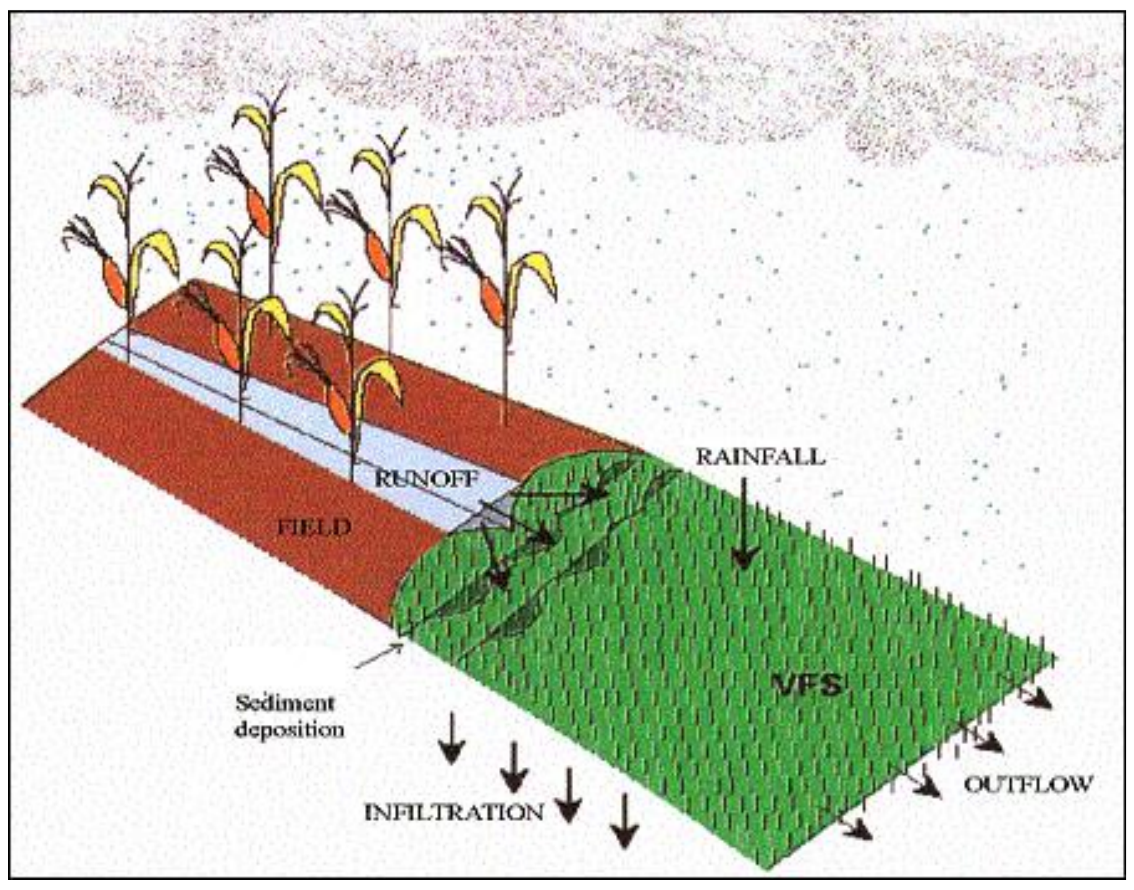

Fig. 1: Schematic representation of a VFS.
Source: http://abe.ufl.edu/carpena/vfsmod/

The three equations

A) Sabbagh et al. (2009):

deltaP = 24.79 + 0.54 deltaQ + 0.52 deltaE - 2.42 ln(Fph+1) - 0.89 %C

Fph = Qi/(Kd * Ei)

with

deltaP	relative reduction (%) of total pesticide load
deltaQ	relative reduction (%) of total water inflow Qi (L)
deltaE	relative reduction (%) of incoming sediment load Ei (kg)
Fph	phase distribution coefficient (mass ratio)
Kd	linear sorption coefficient (L/kg)
%C	clay content of field soil (as proxy for clay content of the eroded sediment; %)

B) Chen et al. (2016):

deltaP = 101 - (8.06 - 0.07 deltaQ + 0.02 deltaE + 0.05 %C - 2.17 Cat + 0.02 deltaQ/Cat - 0.0003 deltaQ/deltaE)^2

with

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

C) Approach „dilution + constant particle-bound concentration“ (inspired by Muñoz-Carpena et al., 2015):

C' = Ci * Vi / Qi	(instantaneous mixing of run-on and rainfall or snowmelt)
S' = Si = Kd * Ci	(particle-bound conc. remains constant)

mf = min(mi, Mf * S' + Vf * C')

mo = mi - mf

with

C'	dissolved pesticide conc. in surface runoff after dilution with rainfall (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)
Mf	eroded sediment mass retained in filter (kg)
Vf	volume of water retained in filter (L)
S'	particle-bound pesticide conc. in surface runoff after dilution with rainfall (mg/kg)
mf	predicted total pesticide mass retained in filter (mg)
mi	total incoming pesticide mass in run-on (mg)
mo	total pesticide mass leaving the filter in surface runoff (mg)

The approach can be recast as a single equation:

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

Results and Discussion

The main findings are:

- Sabbagh equation and dilution approach reasonably predict deltaP for the new data (cf. Fig. 2 and 3).
- Using the empirical Fph (ratio of dissolved and particle-bound incoming pesticide masses) instead of Fph calculated from a generic Koc (as used by Sabbagh et al.) led to slightly stronger overestimation of deltaP; reason: empirical Kd in runoff > Kd from generic Koc and field OC because suspended matter has higher OC content than the bulk soil
- Equation “dilution + constant particle-bound concentration”: The fit was only slightly better for the option with the empirical Kd than for the option with the Kd calculated from generic Koc.
- The equation of Chen et al. was unable to predict deltaP values < 55 % (r^2= 0.19; not shown).

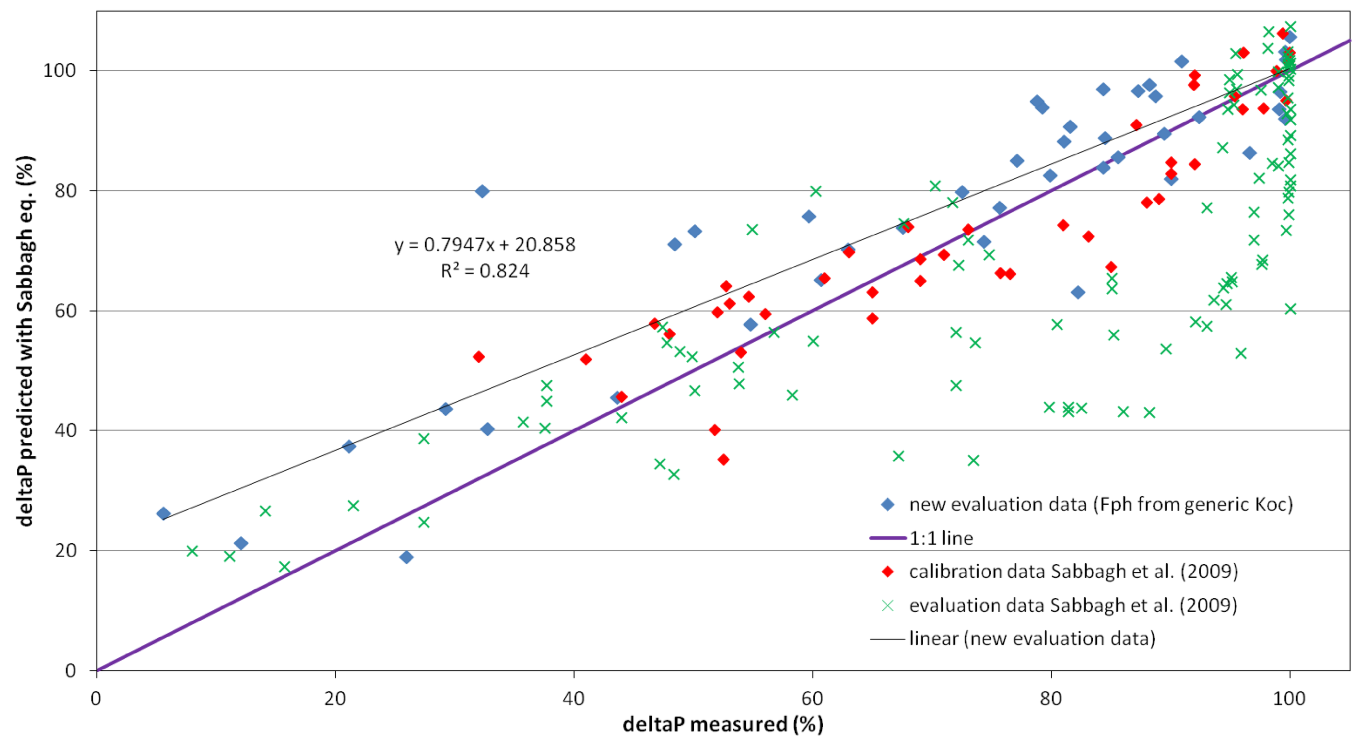

Fig. 2: Observed deltaP vs. deltaP predicted with the Sabbagh equation (Fph calculated using a generic Koc). Calibration data (n = 44; 3 invalid data points were deleted) and validation data points (n = 104; points with deltaQ = 100 % left out) of Sabbagh et al. (2009) are plotted in addition.

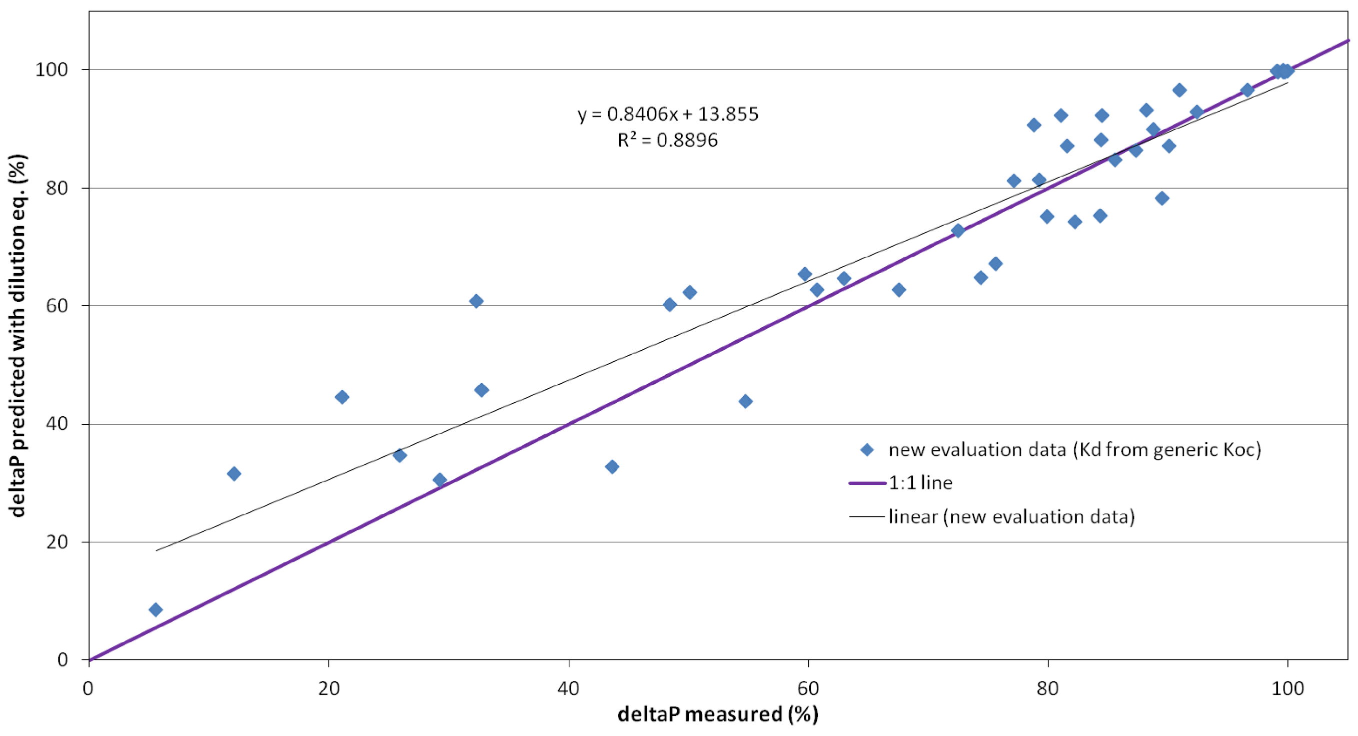

Fig. 3: Observed deltaP vs. deltaP predicted with the equation „dilution + constant particle-bound conc.“, using Kd based on generic Koc.

Conclusions and Outlook

- The regression equation of Sabbagh et al. (2009) was tested against 43 additional independent data points from 3 studies. It predicted deltaP for the newly collected data reasonably well. Further improvements are expected upon re-calibration with a larger dataset.
- The usability of the Sabbagh equation has been corroborated.
- The non-regression approach “dilution + constant particle-bound concentration” performed at least as well as the Sabbagh equation.
- The regression equation of Chen et al. (2016) yielded unsatisfactory results for the new data. The decrease of deltaP with increasing deltaE in the Chen et al. equation is not in agreement with observable reality. Moreover, the introduction of a categorical variable seems unnecessary and poorly justified.

Next steps:

- Recalibration and reevaluation of Sabbagh equation with all available data (calibration + validation data of Sabbagh + newly collected data), e.g. using cross-validation + bootstrapping
- Test the dilution approach on the data of Sabbagh et al.
- Investigate outliers

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