Recalibration and cross-validation of pesticide trapping 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 and sedimentation mechanistically, the reduction of pesticide load by the VFS (ΔP) is calculated with the empirical multiple regression equation of Sabbagh et al. (2009). This equation has not been widely accepted by regulatory authorities, because its reliability has not been sufficiently demonstrated yet. A major drawback is the small number of underlying data points (n = 47). Hence, evaluation against additional experimental data is necessary. Moreover, Chen et al. (2016) proposed an alternative regression equation based on 181 experimental data points.

The objective of this study was to corroborate and improve the predictive capability of the Sabbagh equation by i) broadening the underlying experimental database, ii) comparing the performance of the Sabbagh eq. with other pesticide trapping equations, iii) rigorously testing its predictive capability, and iv) exploring different methods for parameter estimation.

Materials and Methods

- Additional experimental VFS data were compiled from the available literature.
- The enlarged dataset (n = 244) was used to recalibrate the Sabbagh and Chen equations, as well as a set of "reduced" Sabbagh eqs. with ordinary least squares (OLS) regression and to test a mechanistic, regression-free mass balance approach (Reichenberger et al., 2017).
- A k-fold cross validation analysis was performed to assess the predictive capability of the Sabbagh and Chen equations and the "reduced" Sabbagh eqs.
- Finally, a maximum-likelihood-based calibration and uncertainty analysis were performed for the Sabbagh equation using the DREAM_ZS algorithm (Vrugt, 2016) and two different likelihood functions: a simple log-likelihood function (LL) assuming homoscedasticity (homogeneity of variance) of total model residuals, and a generalized likelihood function (GL) explicitly accounting for heteroscedasticity (Schoups and Vrugt, 2010).

Equations

A) Refitted Sabbagh equation (OLS regression)

ΔP = -11.5142 + 0.5949 ΔQ + 0.4892 ΔE - 0.3753 ln(Fph + 1) + 0.2039 %C

B) Reduced Sabbagh equations (OLS)

ΔP = -12.6211 + 0.5763 ΔQ + 0.4862 ΔE + 0.2305 %C
ΔP = -6.2680 + 0.5728 ΔQ + 0.5071 ΔE - 0.4611 ln(Fph + 1)
ΔP = -6.8053 + 0.5456 ΔQ + 0.5063 ΔE
ΔP = 17.0577 + 0.8046 ΔQ

C) Refitted Chen equation (OLS)

$\Delta P = 101 - (10.441 - 0.0165\,\Delta Q - 0.0062\,\Delta E - 0.0179\,\%C - 1.7045\,Cat + 0.0184\,\Delta Q\,Cat - 0.0006\,\Delta Q\,\Delta E)^2$

D) Mass balance approach (Reichenberger et al., 2017)

ΔP/100% = min[(Vi + Kd * Ei), (ΔE/100% * Ei * Kd + ΔQ/100% * Vi)] / (Vi + Kd * Ei)

with

ΔP	relative reduction (%) of total pesticide load
ΔQ	relative reduction (%) of total water inflow Qi (L)
ΔE	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; %)
Cat	for Koc > 9000 L/kg, Cat = 1; for Koc ≤ 9000 L/kg, Cat = 0
Vi	incoming run-on from the source area (L)

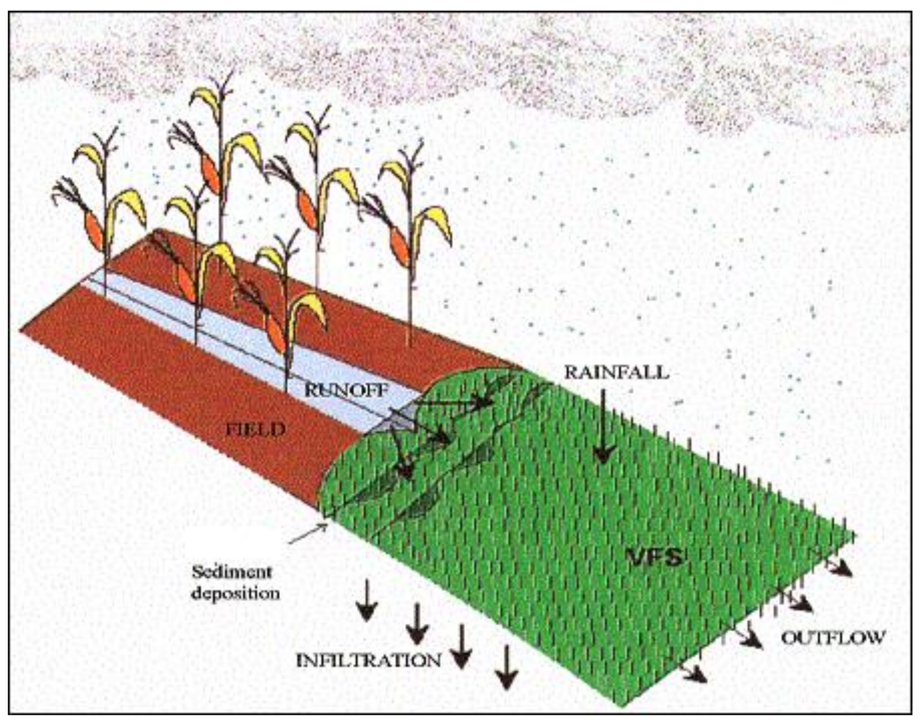

Fig. 1: Schematic representation of a VFS.
Source: http://abe.ufl.edu/carpena/vfsmod/

Goodness of fit / predictive accuracy

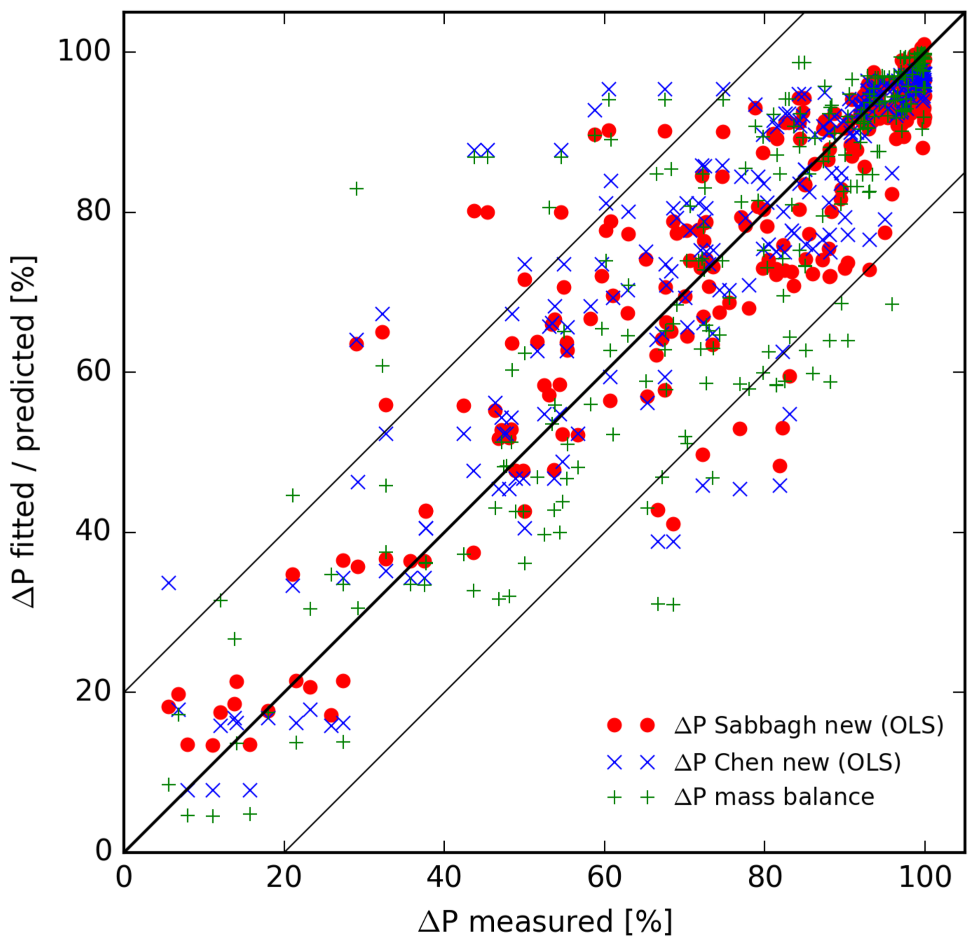

Fig. 2: Measured ΔP vs. ΔP fitted with the Sabbagh and Chen eqs. (OLS) and ΔP predicted with the mass balance approach for the full test data set (n = 244)

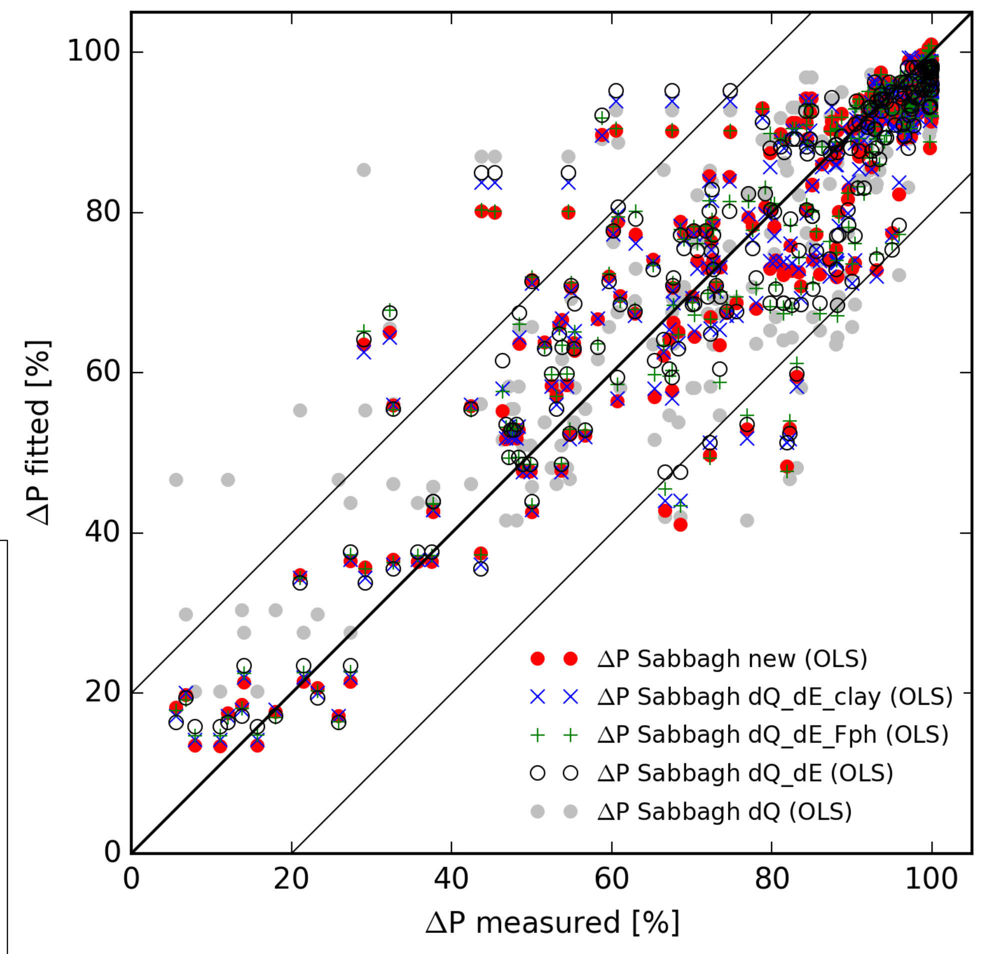

Fig. 3: Measured ΔP vs. ΔP fitted with the full and the four reduced Sabbagh equations (OLS) (n = 244)

- Despite heteroscedasticity, the Sabbagh equation fitted the whole dataset slightly better (Coefficient of Determination R^2 = 0.819) than the Chen equation (R^2 = 0.793) and was less outlier-prone (cf. Fig. 2).
- For the reduced Sabbagh eqs. (Fig. 3) with > 1 independent variables, R^2 lay between the values for the full Sabbagh and the Chen equation.
- The mass balance approach performed slightly worse (Nash-Sutcliffe Efficiency NSE = 0.741) than the refitted Sabbagh and Chen equations (cf. Fig. 2).
- However, all three equations performed acceptably well and significantly better than the original Sabbagh and Chen equations (NSE = 0.53 and 0.56, respectively).

Cross-validation analysis

Table 1: Performance indicators averaged over the 2100 [1)] individual cross-validation tests

Indicator	Sabbagh equation		Chen equation		difference Sabbagh - Chen	
	mean	Median	mean	median	mean	median
			Calibration			
Pearson r^2	0.820	0.820	0.792 [2)]	0.792 [2)]	0.027	0.028
adjusted r^2	0.816	0.816	0.786 [2)]	0.785 [2)]	0.030	0.030
			Prediction			
Q^2 [3)]	0.806	0.813	0.766 [4)]	0.777 [4)]	0.040	0.032
Pearson r^2	0.799	0.815	0.771 [4)]	0.788 [4)]	0.029	0.024
RMSEP	10.286	10.307	11.212 [4)]	11.289 [4)]	-0.926	-0.851

1) 6 different levels of k (k = 2, 4, 6, 8, 10, 12); 50 iterations per level of k
2) These measures were calculated during the linear regression and therefore refer to the transformed variable $(101 - \Delta P)^{0.5}$
3) Predictive squared correlation coefficient (Consonni et al., 2010)
4) The predictive accuracy indicators for the Chen equation were calculated after back-transforming $(101 - \Delta P)^{0.5}$ to ΔP.

- For all equations, mean and median regression coefficients over the 2100 tests were very similar to those obtained for the full dataset.
- The Sabbagh equation performed consistently better than the Chen equation in both calibration and validation (Table 1).
- All reduced Sabbagh eqs. with > 1 independent variables performed better in both calibration and prediction than the Chen eq. → Even with only ΔQ and ΔE as independent variables one can achieve good predictive accuracy.

Calibration and uncertainty analysis with DREAM_ZS

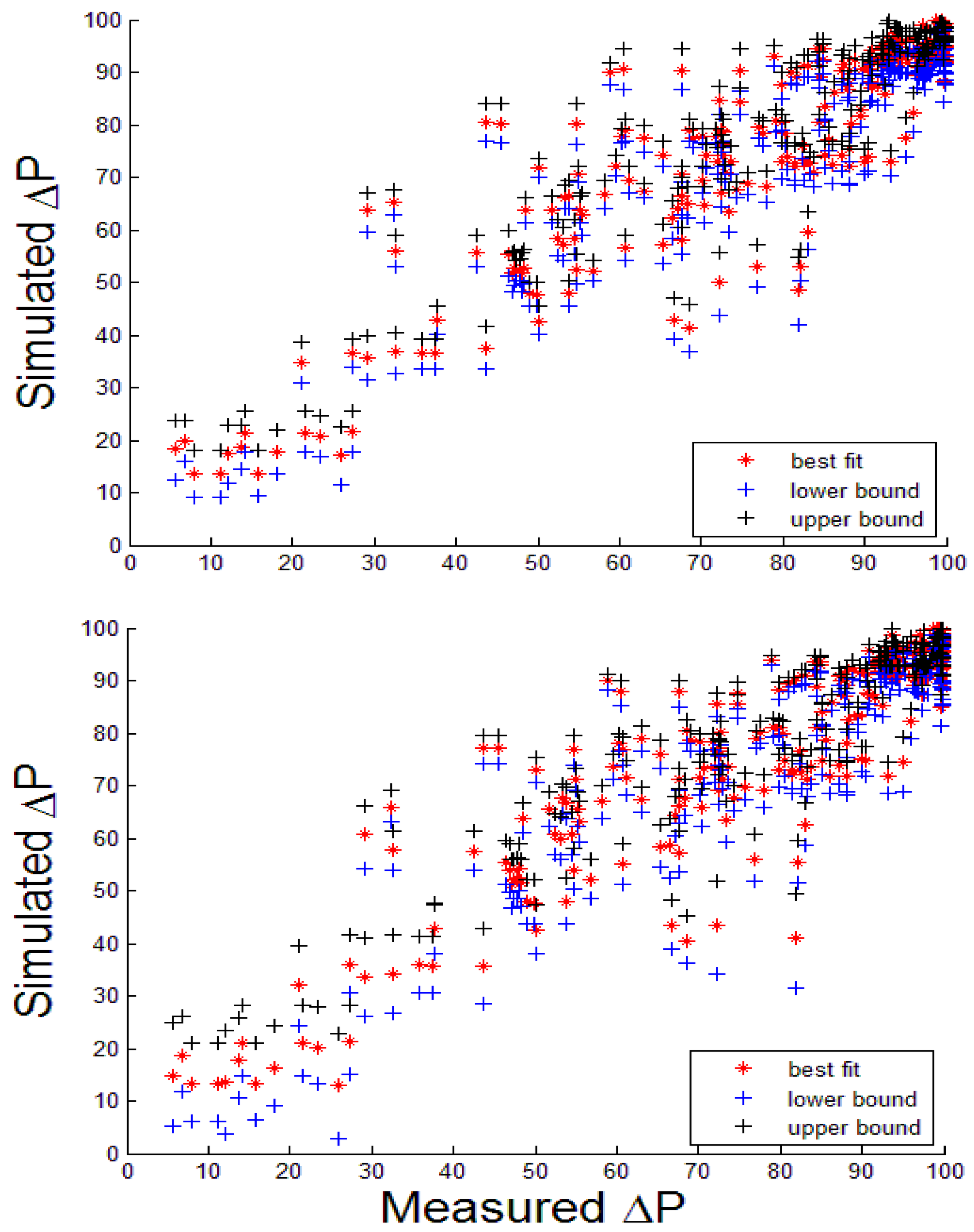

Fig. 4: Total predictive uncertainty intervals estimated with DREAM (left: log-likelihood function (LL); right: generalized likelihood function (GL) according to Schoups and Vrugt (2010)). Total predictive uncertainty intervals are given by the 2.5th and 97.5th percentiles of the posterior distribution of simulated ΔP for each data point. Results are given for the run with the highest likelihood of the best parameter set out of ten trials.

- The DREAM_ZS simulations with the LL option corroborated the Sabbagh parameter values obtained with OLS.
- The simulations with the GL option yielded a slightly worse fit (R^2 = 0.815) than LL and OLS and showed signs of nonuniqueness (posterior correlation coefficient between heteroscedasticity parameters σ_0 and σ_1 was r = -0.998).
- Predictive uncertainty intervals tended to be larger for GL than for LL, notably for small measured ΔP and negative outliers (Fig. 4). However, there were also some data points for which GL yielded smaller uncertainty intervals than LL.
- Potential explanation: The linear error model used in GL is not applicable to ΔP: The measurement error of ΔP should be smallest at the extremes of ΔP and largest in the middle range. → Better not account for heteroscedasticity than do it wrongly.

Conclusions and Outlook

- This study confirmed the suitability of the Sabbagh equation for modelling pesticide trapping in VFS. The new parameter set obtained with OLS regression has been corroborated by both the cross-validation analysis and the DREAM_ZS simulations and can therefore be recommended for use in regulatory modelling with VFSMOD.
- Of course, once the experimental database is extended with new studies, refitting the Sabbagh or any other regression equation will again yield different coefficients. Consequently, fitted/predicted ΔP values for the same data points will change, which is undesirable from a regulatory point of view. However, the larger the underlying database gets, the smaller the changes resulting from including additional data will be.
- In contrast to the empirical Sabbagh and Chen eqs., the mass balance approach of Reichenberger et al. (2017) does not need calibration. Hence, it will always yield the same results for a given experimental data point provided that the same Kd value is used. However, this also means that predicted ΔP values do not improve when new data become available.
- Because of its advantage of being mechanistic and its overall good predictive performance, the mass balance approach can be recommended as a viable alternative to the Sabbagh equation for regulatory modelling. There is also scope for improvement: Possibly further relevant processes, such as sorption of dissolved pesticide to soil or plant material in the VFS, can be included in the mass balance approach in a simple, yet process-based manner.

References

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