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Recalibration and cross-validation of pesticide trapping equations for vegetative filter strips (VFS) using additional experimental data

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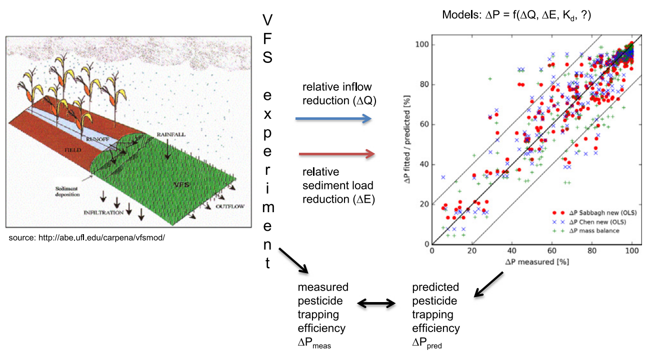
HIGHLIGHTS

- Lack of parsimonious mechanistic approaches for modelling pesticide trapping in filter strips
- Sabbagh regression equation needed broader data basis and rigorous evaluation
- Experimental data basis has been considerably widened
- Suitability of Sabbagh equation for modelling pesticide trapping in vegetative filter strips has been confirmed
- Regression-free mass balance approach is viable alternative

GRAPHICAL ABSTRACT



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ABSTRACT

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 the model VFSMOD is frequently used. While VFSMOD simulates infiltration and sedimentation mechanistically, the reduction of pesticide load in surface runoff by the VFS is calculated with the empirical Sabbagh equation. This multiple regression 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 calibration data points ($n = 47$). To corroborate and improve the predictive capability of the Sabbagh equation, additional experimental VFS data were compiled from the available literature. The enlarged dataset ($n = 244$) was used to recalibrate the Sabbagh equation, the recently proposed Chen equation and a set of "reduced" Sabbagh equations with fewer independent variables, with ordinary least squares (OLS) regression and to test an alternative, regression-free mass balance approach. The Sabbagh equation fitted the dataset slightly better than the Chen equation (coefficient of determination $R^2 = 0.82$ vs. 0.79). The purely predictive mass balance approach performed slightly worse (Nash-Sutcliffe Efficiency NSE = 0.74), but significantly better than the Sabbagh and Chen equations with their old coefficients. In a k-fold cross validation analysis to assess the predictive capability of the various regression equations, both the full Sabbagh and the reduced Sabbagh equations with two or more variables outperformed the Chen equation. Finally, a maximum-likelihood-based calibration and uncertainty analysis were conducted for the Sabbagh equation using the DREAM_ZS algorithm and two different likelihood functions. The DREAM simulations corroborated the parameter values obtained with OLS regression. The study confirmed the suitability of the Sabbagh equation for regulatory modelling of pesticide trapping in VFS. However, the regression-free mass balance approach turned out to be a viable alternative.

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1. Introduction

Modern agriculture often relies on the use of pesticides in order to maintain a high production level. However, a fraction of the pesticide amount applied to agricultural fields can reach surface waters and groundwater via a number of different pathways and can cause harmful effects to the environment (e.g. Flury, 1996). One major input pathway of pesticides into surface waters is surface runoff from agricultural fields (Wauchope, 1996). Total pesticide losses from fields via surface runoff are usually around 0.5% or less of the amount applied, although losses of up to 5% have been observed under worst-case conditions (Wauchope, 1978). There are a number of mitigation measures available to reduce transfer of pesticides to surface waters via surface runoff and erosion (Reichenberger et al., 2007; Catalogne and Le Hénaff, 2016). Of these, the most widely implemented mitigation measures are vegetative filter strips (VFS) (Brown et al., 2012). These are densely vegetated areas designed to intercept surface runoff, often located at the downslope field border (Brown et al., 2012; Muñoz-Carpena et al., 2010). The dense vegetation–soil system reduces pesticide loads in surface runoff by increasing i) infiltration that reduces total surface runoff volume (and dissolved pesticides), ii) surface roughness that reduces surface runoff velocity and produces settling of sediment and sediment-bound pesticides, and iii) contact between dissolved pollutants and soil and vegetation surfaces that enhances their removal from runoff (Muñoz-Carpena et al., 2018; Lacas et al., 2005). The effectiveness of VFS in reducing surface runoff volumes and associated eroded sediment and pesticide loads has been demonstrated in general, but also found very variable (Reichenberger et al., 2007). Both hydrological considerations (e.g. Schulz, 2004) and experimental VFS studies (e.g. Poletika et al., 2009) have shown that the most important factor influencing VFS efficiency for a given runoff event is the hydraulic load, i.e. the volume of incoming surface runoff and rainfall divided by the overflown area of the VFS. Hence, to simulate the efficiency of VFS in reducing surface runoff and pesticide inputs into surface water in a risk assessment context, fixed reduction fractions (e.g. as a function of the VFS length) are not suitable, because they will underestimate VFS efficiency for small runoff events and overestimate it for large ones. Instead, an event-based, dynamic model is needed. The most widely used dynamic, event-based model to simulate the effectiveness of VFS in reducing surface runoff volumes, eroded sediment and pesticide loads is VFSMOD (Muñoz-Carpena and Parsons, 2014). While VFSMOD simulates infiltration and sedimentation mechanistically, the reduction of pesticide load in surface runoff by the VFS (ΔP) is calculated with the empirical multiple regression equation of Sabbagh et al. (2009). This equation uses the following inputs: observed or, in case of VFSMOD, simulated reduction of total inflow (surface runoff volume + precipitation on the VFS; ΔQ) and eroded sediment load (ΔE), absolute surface runoff volume and eroded sediment load entering the VFS, linear adsorption coefficient K_d of the pesticide, and the clay content of the field soil (as a proxy for the clay content of the eroded sediment). For regulatory modelling purposes, i.e. modelling in the context of pesticide authorization, the low data requirements of the Sabbagh equation are a major advantage compared with complex, physically-based pesticide trapping models (e.g. Perez-Ovilla, 2010). However, the Sabbagh 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 experimental data points ($n = 47$) which were used for calibration. Hence, evaluation against additional experimental data is necessary in order to confirm or disprove the suitability of the Sabbagh equation for regulatory modelling of pesticide trapping in VFS. Moreover, Chen et al. (2016) proposed an alternative regression equation with a different structure based on 181 experimental data points. This equation uses fewer independent variables, but has more parameters than the Sabbagh equation due to incorporating interactions between variables. The authors claimed that their approach was superior to the Sabbagh equation both in terms of predictive power and model structure / scientific foundation.

The objective of the present 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 equation with other pesticide trapping equations, notably the Chen equation and an alternative, regression-free mass balance approach (Reichenberger et al., 2017), iii) rigorously testing its predictive capability, and iv) exploring different methods for parameter estimation.

2. Theory and calculations

In this section, the three equations mentioned above are described.

2.1. Sabbagh equation

The Sabbagh equation for pesticide trapping efficiency with the coefficients fitted by Sabbagh et al. (2009) is given as

$$\Delta P = 24.79 + 0.54\,\Delta Q + 0.52\,\Delta E - 2.42\ \ln\left(F_{ph} + 1\right) - 0.89\%C \quad (1)$$

where ΔP = relative reduction (%) of total pesticide load, ΔQ = relative reduction (%) of total water inflow, ΔE = relative reduction (%) of incoming sediment load, F_{ph} = phase distribution coefficient (ratio of dissolved and particle-bound pesticide mass in inflow), and %C = clay content (%) of field topsoil (as a proxy for the clay content of the eroded sediment). The phase distribution coefficient is given by the following equation:

$$F_{ph} = \frac{Q_i}{K_d E_i} \quad (2)$$

where Q_i = total water inflow into the VFS (run-on + rainfall + snowwmelt (L)), E_i = incoming sediment load (kg), K_d = linear sorption coefficient (L/kg).

Consequently, the Sabbagh equation has five regression parameters and six independent variables: ΔQ, ΔE, Q_i, E_i, K_d and %C. If one expresses K_d as a function of generic K_{oc} (linear adsorption coefficient normalized to organic carbon) and the organic carbon content of the field topsoil, the number of independent variables increases to seven. The Sabbagh equation is not applicable to situations with sediment-free run-on ($E_i = 0$), because then F_{ph} becomes infinity and ΔE becomes NaN (Not a Number).

2.2. Chen equation

The Chen equation with the original coefficients fitted by Chen et al. (2016) is given as:

$$\Delta P = 101 - (8.06 - 0.07\,\Delta Q + 0.02\,\Delta E + 0.05\%C - 2.17\,Cat + 0.02\,\Delta Q\,Cat - 0.0003\,\Delta Q\,\Delta E)^2 \quad (3)$$

where Cat is a categorical variable with Cat = 1 for $K_{oc} > 9000$ L/kg and Cat = 0 for $K_{oc} \le 9000$ L/kg. Note that for the Chen equation the fit is not performed against ΔP directly, but against the transformed variable $(101 - \Delta P)^{0.5}$. The main idea behind the Chen equation was to increase predictive performance by i) replacing the continuous phase distribution variable F_{ph} with a categorical adsorption variable, and ii) incorporating interactions between explanatory variables (Chen et al., 2016). The equation is not process-based, but purely statistical.

The Chen equation has seven regression parameters, but only four independent variables: ΔQ, ΔE, %C and K_{oc}. The actual mass distribution between the liquid and the solid phase of the surface runoff is not taken into account. The Chen equation is not applicable either to situations with sediment-free run-on ($E_i = 0$), because then ΔE becomes NaN. It has to be noted, though, that Chen et al. (2016) used at least three studies