An Inverse Calibrator For VFSMOD-W Using The Global Multilevel Coordinate Search/ Nelder-Mead Simplex Algorithm

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Abstract. *When designing vegetative filter strips (VFS) for trapping sediments, the modeler faces the challenge of identifying the appropriate model parameters for the specific application conditions. When possible, local runoff/sediment inflow/outflow through the VFS and precipitation data should be collected to support the modeling predictions. Although manual model calibration is often used, this procedure generally lacks objectivity and the outcome is linked to the expertise of the user. An automated inverse optimization procedure can be used as an objective and robust model calibration alternative. The graphical user interface of VFSMOD-W, a vegetative filter strip design system, was extended to allow for the inverse optimization of the hydraulic and sediment components of the model. A robust and efficient optimization technique, the Global Multilevel Coordinate Search algorithm in sequential combination with the local Nelder-Mead Simplex algorithm (GMCS-NMS), was selected for this purpose. This is a good alternative to other existing optimization procedures, because it is adapted for solving complex nonlinear problems accurately and efficiently, does not require powerful computing resources, and initial values of the parameters to be optimized are not needed. Several examples are presented to demonstrate the benefits of the GMCS-NMS strategy compared to manual calibration when identifying the VFSMOD-W most sensitive parameters.*

Keywords. Inverse modeling, parameter optimization, vegetative filter strips.

Introduction

Modeling water, solute, and/or sediment transport is nowadays widely used for assessing the impact of human activities on water resources and for designing best management practices to reduce these impacts. Particularly, the vegetative filter strip model system (VFSMOD-W) allows for predicting water and contaminant transport through vegetated filters. VFSMOD-W, developed by Muñoz-Carpena and Parsons (1999; 2005), simulates water and sediment transport in vegetated filters based on overland flow hydraulics and infiltration into the soil matrix. The success in modeling such processes heavily depends on the quality of the model parameters, i.e. they are representative of the hydraulic properties of the soil and the vegetated filter. A popular method for parameter estimation is manual calibration by a "trial and error" procedure comparing simulated values of runoff/sediment outflow from the vegetative filter with those experimentally measured. However, this method is time consuming; subjective, since the modeler does not know when to stop the calibration process; it is difficult to judge in which direction the parameters should be modified; and quantification of the uncertainty on the obtained parameters cannot be performed in a rigorous way. Therefore, the manual calibration method cannot ensure that the best parameter set is found. A more elaborated, complex and increasingly attractive form of parameter estimation is inverse modeling. This procedure provides effective parameters in the range of the particular model applications and overcomes the drawbacks of manual calibration (Ritter et al., 2003). Basically the process searches for the best set of parameters in an iterative way, by varying the parameters and comparing the numerical solution given by the model with the observations of a certain state variable (Lambot et al., 2002; Ritter et al., 2003; 2004). By coupling the computer model with an optimization algorithm, the parameter search consists of finding the global minimum of an objective function defined by the error between measured and simulated values. Different techniques have been developed in the past to numerically solve inverse problems. Among others, we may consider methods such as the Steepest Descendent, Newton's, Gauss, Levenberg-Marquardt, Simplex, and Global Optimization Techniques (Hopmans and Simunek, 1999). Each of these have their own advantages and drawbacks, and the success of finding the global minimum depends generally on the presence of multiple local minima in the objective function. In addition to these algorithms, the GMCS-NMS (Global Multilevel Coordinate Search combined with a Nelder Mead Simplex) is a powerful available alternative (Lambot et al., 2002; Ritter et al., 2003). This consists in the sequential combination, as described by Lambot et al., (2002), of the global optimization algorithm developed by Huyer and Neumaier (1999) and the classical Nelder-Mead Simplex (Nelder and Mead, 1965).

In this work, we have integrated the GMCS-NMS within the VFSMOD-W and its graphical user interface to allow the model users to perform automatic inverse optimization of the hydraulic and sediment transport parameters of VFSMOD-W when experimental data are available.

Materials and methods

Inverse modeling calibration procedure

The inverse simulation of the flow or sediment transport parameters is carried out by minimizing an objective function, $OF(\vec{b})$, that represents the error between measured and simulated values, such that it can be defined as a nonlinear least squares problem by:

$$OF(\vec{b}) = \sum_{i=1}^{N} w_i \left[Y_o(t_i) - Y_s(t_i, \vec{b}) \right]^2 \qquad (1)$$

where the right-hand side represents the deviations between observed (Y_o) and predicted (Y_s) time series (hydrographs or sedimentographs) using the parameter vector $\vec{b}$; t is the time; N is the number of measurements available; and w_i is the weight of a particular measurement, which denotes the measurement error and is set equal to s^{-2}, where s is the standard deviation of the measured data (Lambot et al., 2002).

To perform the inverse calibration of the parameter vector $\vec{b}$, VFSMOD is coupled with the Global Multilevel Coordinate Search, GMCS, algorithm (Huyer and Neumaier, 1999). This algorithm combines global and local search capabilities with a multilevel approach. The GMCS is a good alternative to other existing optimization algorithms, because it can deal with objective functions with complex topography, it does not require powerful computing resources, and initial values of the parameters to be optimized are not needed. To refine the minimization of the objective function, the GMCS is combined sequentially with the Nelder-Mead Simplex (NMS) algorithm (Nelder and Mead, 1965) (Fig. 1). Further details about application of GMCS-NMS to inverse modeling of soil hydraulic properties are given in Lambot et al. (2002) and Ritter et al. (2003). Furthermore, model adequacy, uncertainty and correlation associated with the estimated parameters is determined according to Hollenbeck et al. (2000) and Ritter et al. (2004).
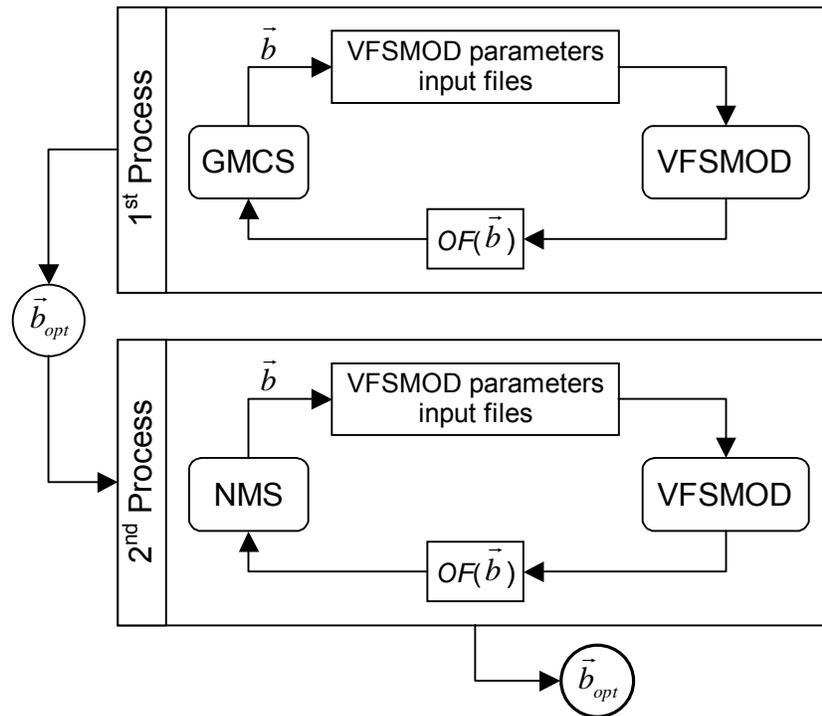

Figure 1. Scheme for the inverse modeling procedure to calibrate the VFSMOD parameters

When calibrating parameters, some criteria must be defined to evaluate the goodness-of-fit of the model simulation using the optimized parameters. Several authors point out that to assess the performance of the model calibration, the use of a single statistic might be misleading and

more should be used along with graphical representations (Berthouex and Brown, 2002; James and Burgues, 1982; Tufte, 1983; Legates and McCabe, 1999). The goodness of fit of the simulations with the optimized parameters was evaluated in terms of the coefficient of efficiency (Nash and Sutcliffe, 1970) and the root mean square error. The coefficient of efficiency (C_{eff}) has been widely used to evaluate the performance of hydrologic models. It compares the variance about the 1:1 line (perfect agreement) to the variance of the observed data and it ranges from $-\infty$ to 1. Thereby C_{eff} = 1 implies that the plot of predicted vs. observed values matches the 1:1 line (Legates and McCabe, 1999). The root mean square error (also called residual variation or standard error of estimate), RMSE, is a useful single measure of the prediction capability of a model since it indicates the precision with which the model estimates the value of the dependent variable (Berthouex and Brown, 2002).

Table 1. Statistics used in assessing the model performance with the optimized parameters.

Statistic	Equation	Best fit
Coefficient of efficiency	$C_{eff} = 1 - \dfrac{\sum_{i=1}^{N}\left(Y_{o_i} - Y_{s_i}\right)^2}{\sum_{i=1}^{N}\left(Y_{o_i} - \bar{Y}_o\right)^2}$	1.0
Root Mean Square Error	$RMSE = \sqrt{\dfrac{\sum_{i=1}^{N}\left(Y_{o_i} - Y_{s_i}\right)^2}{n}}$	0.0

VFSMOD-W and User Interface Program

The vegetative filter strip model, VFSMOD, is a field scale, mechanistic, storm-based model developed to route incoming hydrographs and sedimentographs from an adjacent field through a vegetated filter strip (Muñoz-Carpena and Parsons, 1999). The model handles time dependent hyetographs and runoff hydrographs, space distributed filter parameters (vegetation roughness or density, slope, infiltration characteristics) and varying particle sizes of incoming sediment. Model outputs include infiltration and surface runoff hydrographs and sedimentographs from the vegetated filter, and its sediment trapping efficiency. The modeling system provides an integrated environment for users that consists of a front-end graphical user interface program, VFSMOD-W, the source area program, UH, and the vegetative filter strip model, VFSMOD (Muñoz-Carpena and Parsons, 2004). The UH program was developed to generate the input datasets for VFSMOD by estimating runoff hydrographs and sediment losses from upslope source areas for a storm event. Thus, the user may generate a synthetic rainfall hyetograph based on NRCS methods (Haan et al., 1994); a runoff hydrograph based on land use and topography of the source area using the NRCS curve number and the unit hydrograph method (USDA NRCS, 1986); and sediment losses from the upslope source area using the Modified Soil Loss Equation (Wischmeier and Smith, 1978; Williams, 1975).

In addition to a design component, the graphical user interface includes also both sensitivity and uncertainty analysis in the vegetative filter strip design system (Parsons and Muñoz-Carpena, 2001). Inverse optimization of the vegetated filter properties has now been added through an additional menu option in the graphical user interface of VFSMOD-W v4.x. The calibration option in the program menu allows for estimating separately selected flow and/or sediment transport parameters. Since sediments are transported by flow, the parameters of the model flow component must be optimized first, followed by the inverse simulation of the sediment transport parameters. In VFSMOD-W v4.x, the user may indicate the project name (Muñoz-Carpena and Parsons, 2005), the files containing the measured hydrograph or sedimentograph,

and the parameter space, which is defined by those parameters to be optimized within a specified interval limited by a lower and an upper bound (Fig. 2a and 2b).

a)

b)
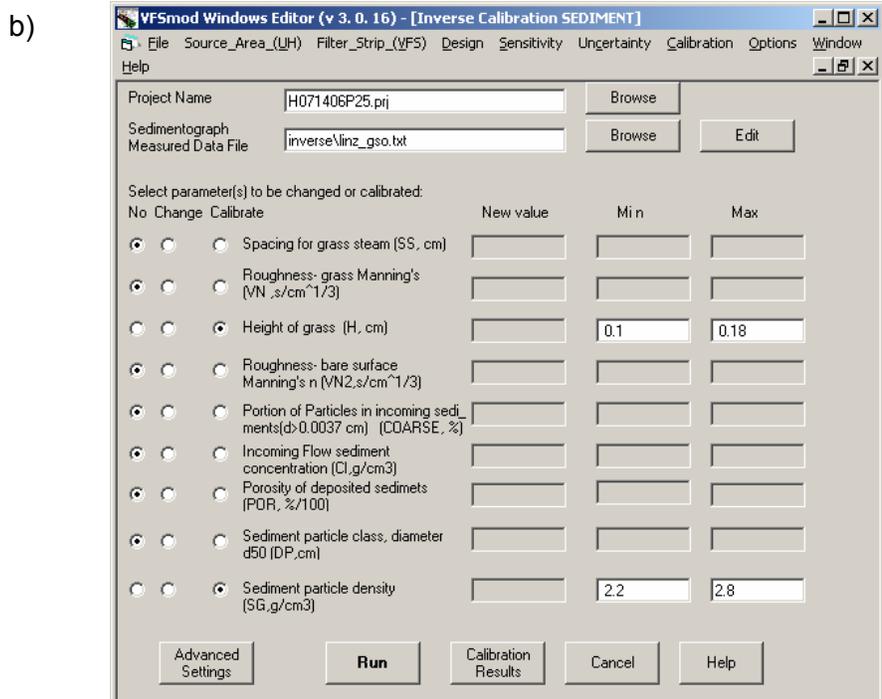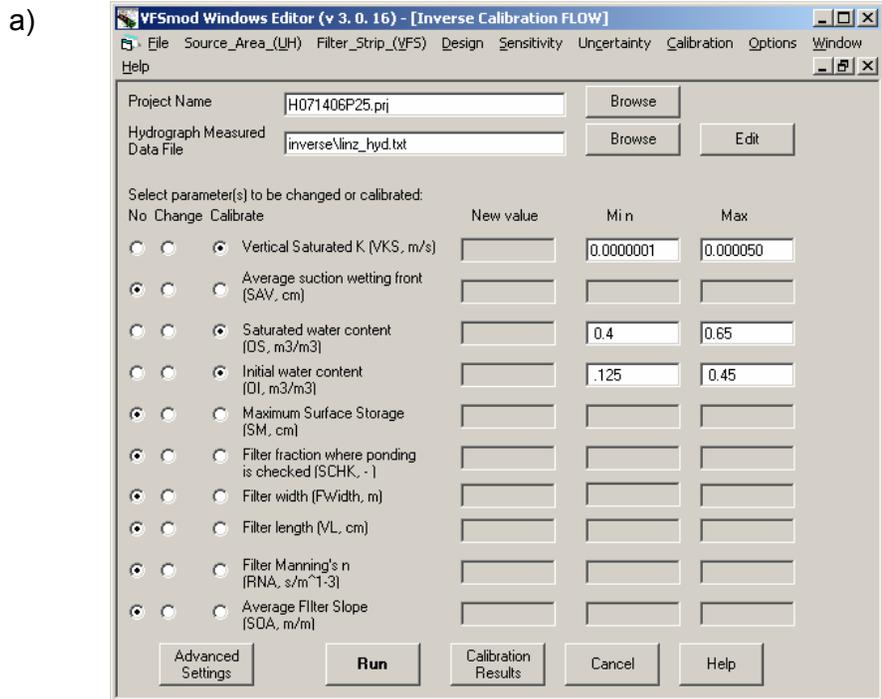
Figure 2. Examples of screens for editing parameters for optimization of the model a) flow component and b) sediment component.

Additionally, advanced settings include the numbers of iteration of the optimization process, the filename were output is stored, and the option to activate the graphical output for visual inspection during the calibration process (Fig. 3).
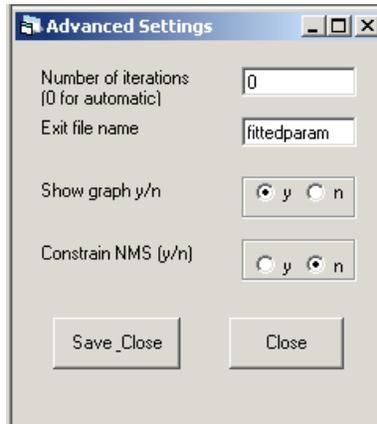
Figure 3. Example of screen for advanced settings.

The results from the inverse modeling procedure can be viewed consisting of a numerical and a graphical output (Fig. 4). The latter shows the match between the observed hydrograph or sedimentograph with that generated by VFSMOD with the optimized parameters.
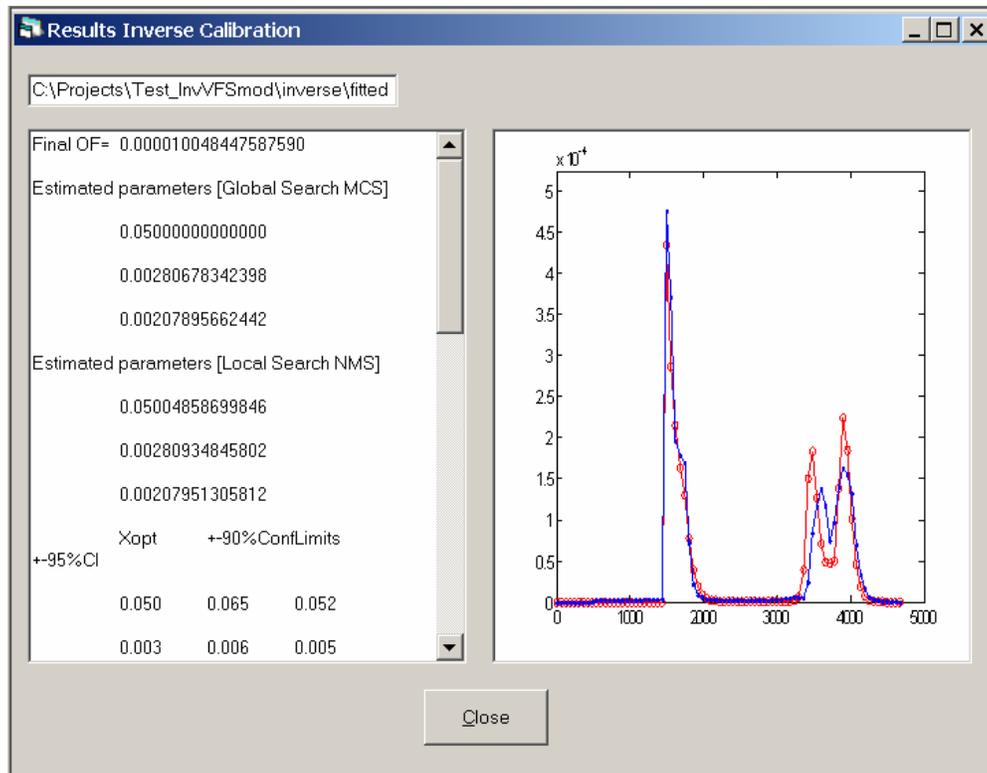
Figure 4. Example of screen with optimization results.

The numerical output includes the parameter set with confidence limits estimated by the GMCS and the NMS. Further information related to the optimization is also available: covariance and correlation matrices, model adequacy, *RMSE*, C_{eff}, number of iterations of model execution, and total duration of the whole process.

Additional Considerations

Concurrent Inverse optimization of all possible parameters (Fig. 1-2) is not recommended to avoid problems of identifiability and non-uniqueness, i.e. when more than one parameter set lead to the same model response, the parameters are unidentifiable and the solution is non-unique and leads to equifinality (Beven and Freer, 2001). Instead, the optimization should focus on those parameters that the model is most sensitive to. Thus, it is recommended to choose the parameter to optimize based on an initial sensitivity analysis (Muñoz-Carpena et al., 2007). Parameter correlation should also be considered. Availability of prior information about the parameter ranges is also important (Abbaspour et al., 1997; Russo et al, 1991).

Application example

The inverse simulation procedure was tested with a natural runoff event in a 8.7 m long vegetative filter strip measured in Central Florida on July 2006. Details on the experimental setup are described in Kuo et al. (2005). Parameters of the flow component of VFSMOD selected for optimization were: the saturated hydraulic conductivity, VKS (m/s); the Manning's roughness coefficient, RNA; and the filter width, $FWIDTH$ (m). Only the median particle size of the incoming sediment, d_{50} (cm) was chosen for the VFSMOD sediment trapping component. The search parameter space was determined with the following intervals based on Muñoz-Carpena et al. (1999; 2007): VKS (m s^{-1}) [0.000001 – 0.003]; RNA [0.02 – 0.6]; and $FWIDTH$ (cm) [1.0 – 3.0]. Once the flow component was optimized, calibration of the sediment output was carried out by optimizing d_{50} (cm) within the interval [0.0003 – 0.0029].

Firstly, a manual model calibration of these parameters was carried out in order to compare the traditional calibration method with the new inverse optimization procedure. This consisted of iteratively changing the selected parameters and running the corresponding simulation with VFSMOD until an adequate, but subjective, fit was achieved (C_{eff}, $RMSE$ and the visual inspection of the match between observed and predicted values). The same parameter search space was used for both the automatic inverse optimization and the manual procedure.

The inverse optimization of the three flow parameters was carried out in 23 minutes (1085 iterations), and the sediment component was calibrated in 3.5 minutes (136 iterations). The time spent in the manual calibration was subjectively estimated as 210 and 94 minutes for both components, respectively. Results demonstrate the better performance of inverse modeling for the parameter estimation. Table 2 and 3 show the calibrated parameters obtained with both procedures. Notice the improvement in the goodness-of-fit criteria (higher C_{eff}, and lower $RMSE$) when performing inverse simulation instead of manual calibration. In addition the identification of the 90% confidence interval in the automatic procedure indicates the uncertainty of the calibration procedure where no such measure is available for the manual calibration.

Figures 5 and 6 allow for visual comparison of the performance of VFSMOD-W using the calibrated parameters in Tables 2 and 3, for simulating outflow rate (Fig. 5) and sediment outflow (Fig. 6).

Tabla 2. Calibrated selected parameters of the VFSMOD flow component, with 90% confidence intervals (for inverse optimization only).

Material	VKS (m s^{-1})·10^{-5}	RNA	$FWIDTH$	C_{eff}	$RMSE$ (m^{3}s^{-1})
Manual calibration	5.20	0.60	1.4414	0.940	0.319·10^{-4}
Inverse optimization	4.44 ±0.16	0.440 ±0.005	1.879 ±0.037	0.980	0.185·10^{-4}

Tabla 3. Calibrated selected parameters of the VFSMOD sediment component, with 90% confidence intervals (for inverse optimization only)

| Material	d_{50} (cm)·10^{-4}	C_{eff}	RMSE (g cm^{-1})
Manual calibration	8.19	0.936	0.248·10^{-4}
Inverse optimization	9.01 ±0.21	0.970	0.170·10^{-4}
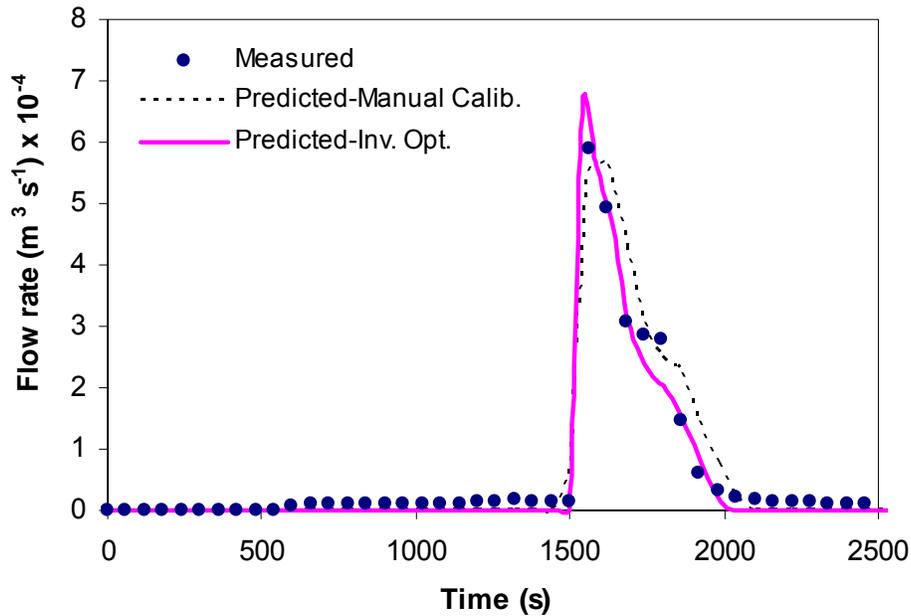
Figure 5. Example of VFSMOD-W performance using the flow component parameters obtained by inverse modeling and by manual calibration.
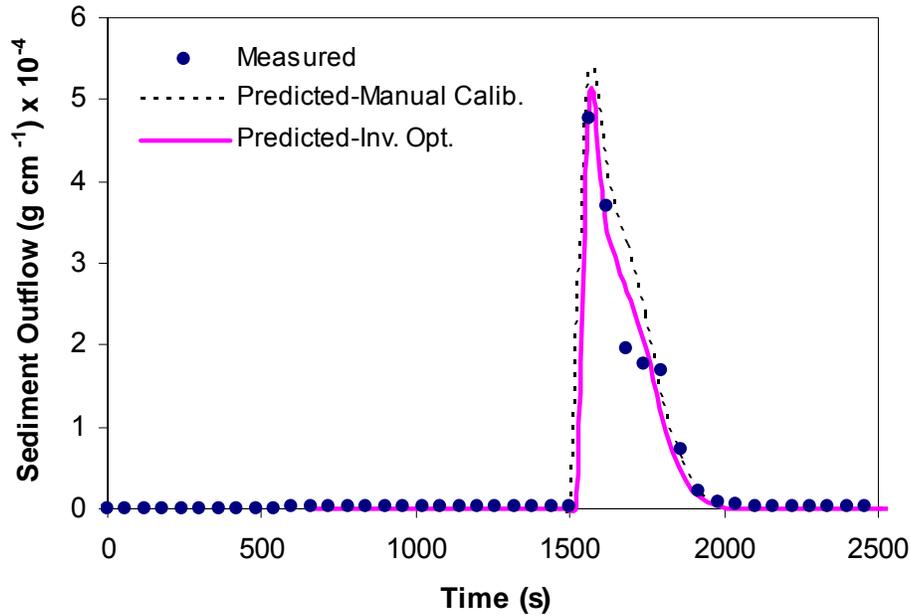

Figure 6. Example of VFSMOD-W performance using the sediment component parameters obtained by inverse modeling and by manual calibration.

Conclusion

Inverse modeling capability was implemented in the vegetated filter strip modeling system, VFSMOD-W using the Global Multilevel Coordinate Search algorithm in sequential combination with the local Nelder-Mead Simplex algorithm (GMCS-NMS). Consequently, the graphical user interface of VFSMOD-W was extended to allow for the automatic inverse optimization of the hydrologic and sediment components of the model. The GMCS-NMS is a good alternative to other existing optimization algorithms, because initial values of the parameters to be optimized are not needed and it does not require powerful computing resources.

The application example presented shows the robustness and efficiency of this parameter estimation procedure with respect to the traditional manual calibration. The implementation of an easy-of-use and automatic calibrator for VFSMOD-W and its integration into the programs GUI will likely benefit modelers designing vegetative filter strips when experimental data are available. The new procedure aims to reduce the uncertainty and subjectivity typically associated to water quality model calibration tasks.

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