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IMPROVEMENTS NECESSARY FOR A RIVER POLLUTANT TRANSPORT MODEL TO OBTAIN A BETTER PERFORMANCE

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ABSTRACT. A wealth of field facts, including the high human pressure on rivers, the eutrophication danger and the complexity of in-river phenomena (causing difficulties in water quality modelling) revealed the need to offer reliable tools for the pollutant transport modelling and for the understanding and estimation of the complex in-river pollutant behaviour. This paper presents an application of ADModel (a detailed advection dispersion pollutant transport model) for the case of River Swale (UK), in order to show why an improved representation (a) of the hydrodynamic river characteristics and (b) of the pollutant transformations; is very important for the advection-dispersion models, as it generates a major gain in the modelling skills (e.g. prediction improvement) and on the understanding of in-river phenomena. ADModel obtained good results during calibration against field measurements of concentration, showing that an improved version (using detailed representation of the river stretch and pollutant transformations) facilitates a better model performance and a wider applicability, including the identification of additional phenomena along the river stretch, of importance in ordinary situations and also during un-controlled pollution situations.

Keywords: *ADModel, in-river pollutant transport model, river water quality, phosphorus prediction, rating equations.*

INTRODUCTION

Fresh water is a vital resource under constant pressure due to pollution and climate change. Even if significant counteraction is being conducted these latest decades, there is a need for continuous and careful

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water resources management in order to slow down their future deterioration [1, 2]. Models for the transport of pollutants along rivers are very useful in this endeavour, especially when applied for the key determinants of river water quality, such as phosphorus (P) compounds. There is a large number of studies on the modelling of P compounds, because they are significant driving forces for the eutrophication [3]. In this respect it is important to mention the main tendency to focus on catchment and multi-catchment scale models [3, 4], while detailed models (at high time and space resolution, such as ADModel) are the subject of less studies, e.g. [5 to 8], probably due to the need for large amount of experimental data and a high workload spent for their development. It is known that measuring P species at high time and space resolution is expensive and not commonplace, therefore there are situations where monitoring is not available or where extensive data sets are unreliable [8]. Modelling is still very much needed for those un-monitored situations and also in cases where data are scarce. Details on how to treat such challenging cases by means of knowledge management and other process systems engineering techniques are extensively discussed and illustrated elsewhere [10], while a recent example of integrating already existing models for a river basin lacking detailed measurements is also available [8].

In addition, the importance of ecosystem processes, together with the ecosystem status, as indicators of ecological health is increasingly being recognised [11]; and there is much scope for detailed modelling studies to add to this growing body of research.

This work is related to aspects of the detailed modelling of the advective dispersive pollutant transport in rivers such as: the proper representation of river parameters (*e.g.,* river bed shape), the description of pollution sources discharging effluent into the river, and the identification of an adequate pollutant transformations model. Generally, the greatest attention is given to the latter aspect, as the good understanding of pollutant dynamics (needed for the further pollutant transport modelling task) involves on one side information on the river channel parameters, discharge and concentrations monitoring data, and on the other side details on kinetics and rate-determining controls on the processes comprised in the transformations model (emphasized also in [12]). It is also important to remark that all the effort should be rewarded by the results of detailed models via (1) the improved capacity with respect to details offered within the simulation results; (2) the opportunity to explore in-river phenomena at high time and space resolution with the help of simulations; and (3) the possibility to include such models in software to control the reduction of pollutants concentration right during their discharge in the river, [13, 14]. ADModel, presented in this research, offers these opportunities and proved to open possibilities further research. ADModel has been first presented in 2010 [5] and calibrated with respect to nitrogen compounds, [7].

This paper is part of the recent research (including [15]), aiming at an improved version of ADModel with respect to phosphorous compounds, in order to facilitate better prediction accuracy and a wider use of the model. On the other hand, the additional improvements related to the representation of hydrodynamic aspects along the river stretch facilitate increased prediction accuracy of ADModel in general (for all considered nutrient species, not only P components), facilitating the further application of ADModel to other pollutant species.

RESULTS AND DISCUSSION

The present section points the ADModel's improvements and presents a discussion on the results.

A. Improvements in representing the river stretch

Rating equations are employed in the water quality models for the modelling of water depth as function of the water flow along the river channel. The reason for using such models is that monitoring of water flow is carried out along rivers with higher frequency (e.g. intensive automatic measurements may be implemented in some locations) compared to the water depth (e.g. measured on a monthly basis or occasionally during intensive campaigns).

Two approaches for the rating equations at monitoring sites have been proposed. The simple approach (denominated "old rating" and represented using blue stars in **Figure 1** and **Figure 2**) considers a single rating equation at each monitoring site, employed to express the non-linear dependency of water depth on discharge for all flow ranges. The detailed approach (denominated "new rating" and represented using black crosses in **Figure 1** and **Figure 2**) considers the adjustment of rating equations at each site, in order to provide different values of the rating equation's coefficients for low flows and high flows.

The demarche is based on the available discharge and water depth field data, which has been split into two independent data sets: a development set and an evaluation set. The evaluation of the old and new rating coefficients against experimental data reveals better estimation performance for the new approach, when different sets of coefficients are employed for the low discharge and high discharge respectively (see **Figure 1** and **Figure 2**).

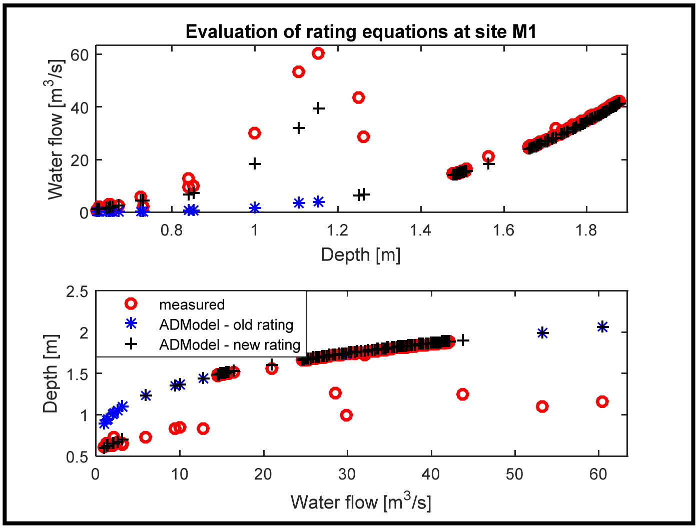

Figure 1. *Rating equations improvement at the upstream (site M1) end of the river stretch*

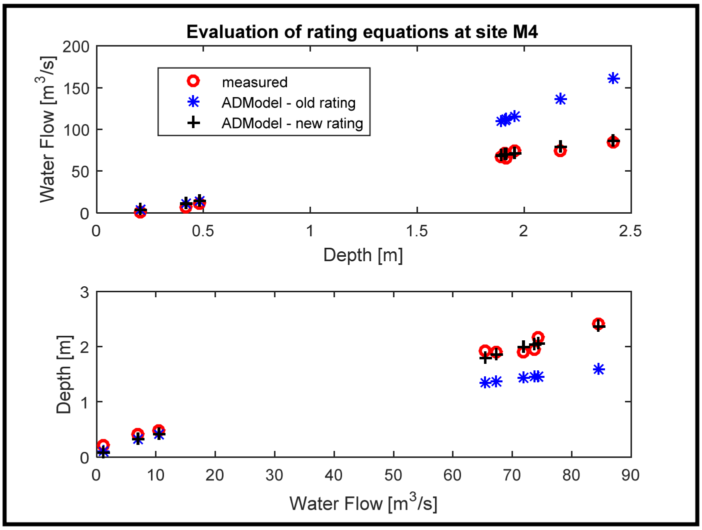

Figure 2. *Rating equations improvement at the downstream (M4 in 1b) end of the river stretch*

B. Improvements in representing the SRP and OP transformations

ADModel results including concentration time series (conservative and non-conservative simulations) are presented against the concentrations measurements in Figure 3 (corresponding to the three transformations model) and Figure 4 (corresponding to the five vs. three transformations model).

Predictions of the initial non-conservative ADModel (Figure 3) follow the shape of the conservative model predictions for the most of the points, while they should be closer to the measurements. These results reveal the need to include additional transformations in the model and/or improve the dynamic representation of the existing ones. SRP concentrations are overestimated during the most of the time, showing evidence that SRP sinks (not considered at all in this ADModel version) should be included in the model, as they have significant contribution to the SRP variability. Therefore, the adsorption and the uptake of SRP are included in the five transformations version of ADModel. OP is, in the most occasions underestimated for the higher range of concentrations (over 0.4 mg/L), while it is overestimated for the lower range of concentrations. In this case there is a need of representing better the transformation rates of sedimentation and re-suspension in order to cater for the variability of these phenomena in relation with the water flow and seasonality.

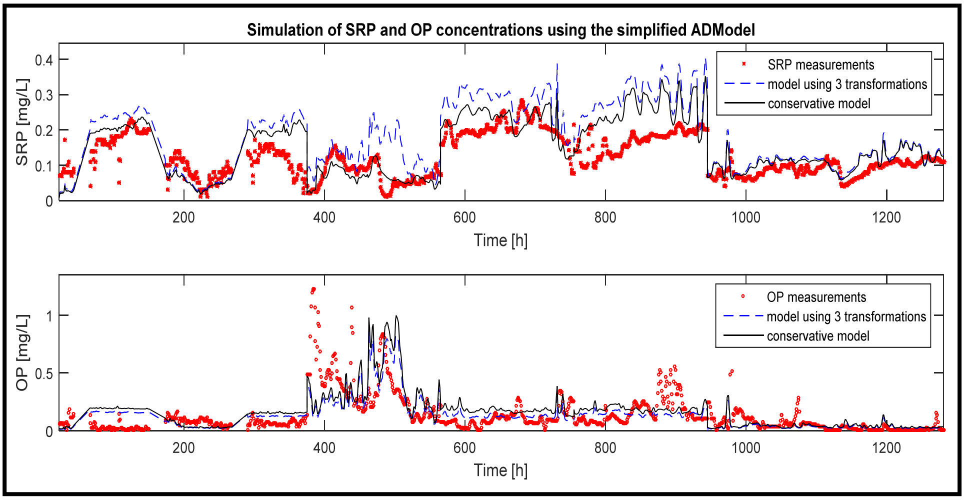

Figure 3. Results of ADModel for the simulation of SRP (upper plot) and OP (lower plot) against field data. ADModel is using the initial, simpler approach for the transformation rates.

The results of ADModel employing the more complex five transformations approach show improvement in predictions (see Figure 4), especially with respect to SRP, for which the NS criteria value is 0.48 (compared to 0.07 and -1.05 corresponding to the conservative ADModel and to the simpler 3 transformations ADModel, respectively, as shown in Figure 4). There is no evident tendency of significant underestimating or overestimating correlated to specific ranges of SRP concentrations. On the other hand, there is little improvement in the prediction of OP concentrations, for which the NS criteria value is 0.20 (compared to 0.05 and 0.18 corresponding to the conservative ADModel and to the simpler 3 transformations ADModel respectively). The OP larger concentrations are underestimated, while the OP lower concentrations are overestimated.

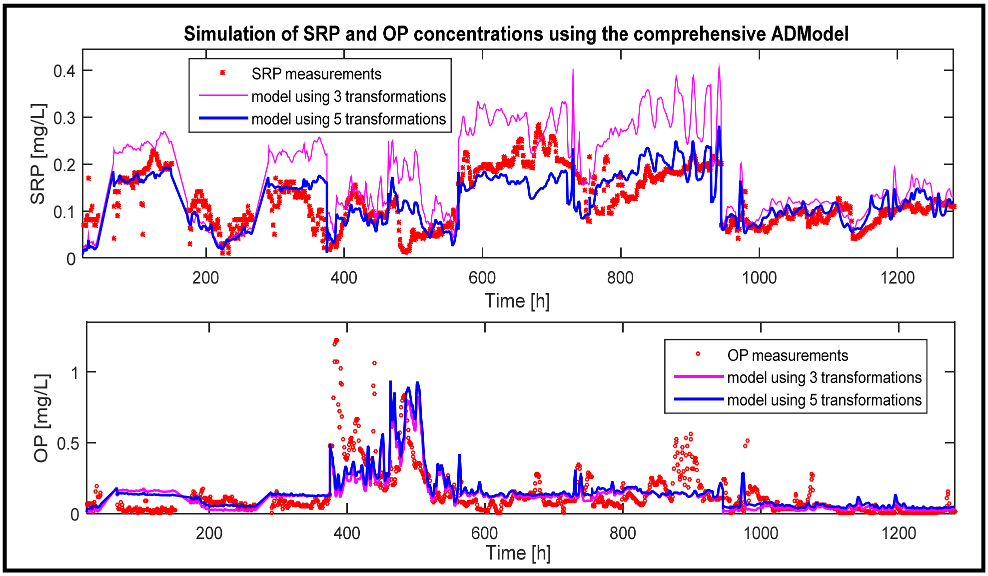

Figure 4. Results of ADModel for the simulation of SRP (upper plot) and OP (lower plot) against field data. ADModel is using the improved approach for the transformation rates.

A representation of all NS coefficient values for ADModel runs is available in Figure 5.

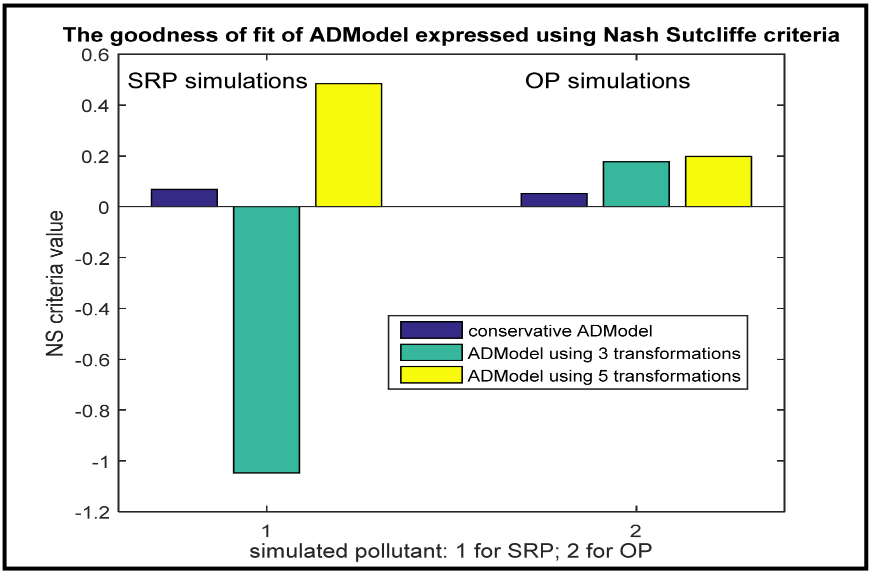

Figure 5. Nash Sutcliffe coefficient values for the simulations of SRP and OP against field data.

A further analysis on the model results has been conducted in order to search for answers in the correlations of the experimental data and simulated data to the controlling factors of the transformation rates. Its visual representation is available in Figure 6. Its findings show that that for the lower SRP concentrations the overestimations can be mainly related with (1) the largest valued of the water flow; and (2) the highest values of the seasonality factor (corresponding to late spring), which may indicate the need to improve the representation of the SRP uptake by plants, as in that period this activity is higher compared to other periods. The underestimation of higher SRP concentrations is correlated with (1) flows lower than 50 m^3/s; (2) seasonality factor around 0.5 (corresponding to the mid-spring); and (3) temperatures above 15 °C and also between 7 and 10 °C, which may indicate a need of higher mineralization rates during those periods. Such increased rates could be obtained with the help of a better estimated OP concentration, which is also generally underestimated during those periods. Though, for the OP the larger underestimations occur at flows between 50 m^3/s and 100 m^3/s; lower to mid values of the seasonality factor (under 0.5, corresponding to the beginning of winter to the early mid-spring), and temperatures above 7 °C.

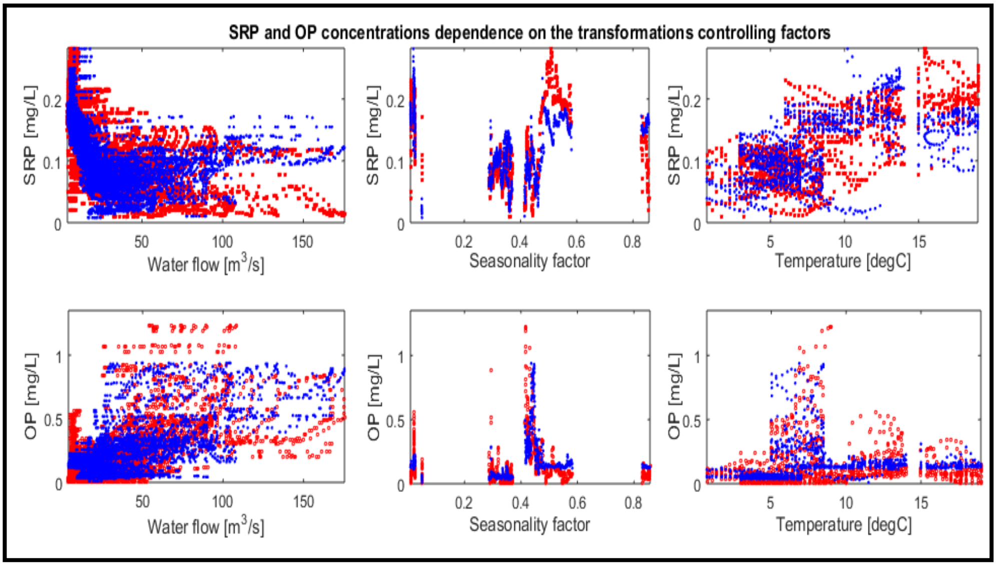

Figure 6. The concentrations of SRP and OP depending on the water flow, seasonality and temperature: simulated with the improved ADModel (blue markers) and measured (red markers).

The multiple forms of phosphorus undergo multiple transformations during in-river transport, including a continuous internal “recycling” process which involves transformations of one form into another. These inter-dependencies between components, the transfers between phases and the other transformations are complex and play a key role in formulating water quality models. Results show that for this case study a more detailed model for the P transformations enables ADModel to make better prediction of P components during their transport along the reach of River Swale, compared to the simpler approaches, especially for the SRP.

Further investigations with respect to OP transformations need to be conducted in order to improve the representation of already included transformations and also to include additional transformations, such as the excretion by living organisms and the respiration of living organisms. It is worth mentioning that additional field data is also needed for the implementation of such further improvements.

CONCLUSIONS

The present paper discussed the case study of ADModel, a powerful advection-dispersion model for the detailed prediction of OP and SRP along a stretch of River Swale (UK). Transformations are the main key factors influencing the SRP and OP transport along the river, especially for the present case study. Therefore, five empirical models (correlating transformation rates to temperature, water flow and seasonality) have been offered for a more comprehensive representation of the phenomena. ADModel including these five transformations has been compared against simpler approaches: (1) a conservative ADModel and (2) ADModel including three transformations.

Simulation results show that an improved representation of transformations leads to better results of ADModel. There are small improvements of the prediction performance associated to OP (NS criteria increased from 0.18 to 0.20) and significant improvements of the prediction performance associated to SRP (NS criteria increased from -1.05 to 0.48). The results of this research enable to conduct further work using ADModel [18], namely the investigation of additional in-stream phenomena: unidentified transformations or unknown additional in-stream sources and sinks of OP and SRP.

A main benefit of ADModel consists of its practical use in multiple directions: (a) prediction of SRP and OP concentrations along the river stretch in normal and abnormal (e.g. accidental release) of pollutant discharge in the river; (b) prospections related to the river stretch response in case of the modification of pollution load due to multiple types of phosphorus sources in the river catchment (e.g. dynamics of agricultural activities or animal farms, increased population, changes in the waste water treatment plants); and (c) the opportunity to include ADModel in pollution counteraction tools (e.g. software based on model predictive control).

EXPERIMENTAL SECTION

A. The river stretch and field data

Among the widely investigated forms pf Phosphorous there are three measurable components (SRP - Soluble Reactive Phosphorus, TDP - Total Dissolved Phosphorus and TP - Total Phosphorus), while two others can be derived from the first three (PP - Particulate Phosphorus and DHP - Dissolved Hydrolysable Phosphorus, consisting of Dissolved Organic P, Polymeric P and Colloid). The Organic Phosphorus (OP) consists of PP and Dissolved Organic P. The three forms of measurable P are available for the River Swale in the form of time series and the species included in ADModel are OP and SRP.

The findings have been validated with the help of field data including measurements of river bed characteristics, water flow time series, water depth time series and concentration time series for the P compounds at up to four sites (noted with M1, corresponding to the upstream end of the stretch, to M4, corresponding to the downstream end of the stretch) along the river stretch (54km long), collected at a resolution from 15 minutes (for the water flow) to 3 hours (for concentrations).

Employed field data is available online, [16].

B. The method: ADModel description

ADModel is a detailed advection-dispersion mathematical model for the pollutant transport along rivers, based on the analytical solution (equations 1 and 2) of the general one-dimensional advection-dispersion equation identified for the continuous discharge of pollutants [17] in the case of the initial and boundary conditions specified in equations 3, 4 and 5:

$$c(x,t) = c_0 + \frac{(c_S - c_0)}{2}\left[erfc\left(\frac{x - V_x t}{\sqrt{4D_x t}}\right) + \exp\left(-\frac{xV_x}{D_x}\right) erfc\left(\frac{x + V_x t}{\sqrt{4D_x t}}\right)\right] \tag{1}$$

$$erfc(x) = 1 - erf(x) = 1 - \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{x} e^{-t^2/2}dx \tag{2}$$

$$\begin{aligned} c_0 &= c(x,0) & x > 0;\quad t = 0 \\ c_{S0} &= c(x_S,0) & x = x_S;\quad t = 0 \\ c_S &= c(x_S,t) & x = x_S;\quad t > 0 \end{aligned} \tag{3, 4, 5}$$

where c [mg/L] is the concentration along the river stretch (x [m]) in time (t [s]); c_0 [mg/L] is the initial concentration along the stretch assuming nonzero initial condition throughout the river; c_S [mg/L] is the concentration at source during the release; c_{S0} [mg/L] is the initial concentration at the source (x_S [m]); and; V_x [m/s] is the mean water flow velocity along the river; D_x [m/s] is the longitudinal dispersion coefficient; *erf* is the error function; *erfc* is the complementary error function.

Pollutant species transformations have been added to the equation. Initially ADModel has considered three transformations involving SRP and OP (mineralization, sedimentation and re-suspension, presented in Table 1), as they are employed in QUESTOR [5]. QUESTOR is a water quality modelling framework for river networks, capable to simulate also SRP and OP at daily step, previously calibrated also for the monitoring M1 and M4, which are involved in the present research. The unassertive ADModel results when employing the three transformations approach, discussed later on during this paper, motivated the improvement of transformations representation, in order to (1) include two additional types of processes (uptake and adsorption) and (2) identify a different formulation of transformation rates in order to ensure their dynamics according to the change of controlling factors (see Table 1).

The controlling factors considered by the three transformations model are the water flow and water temperature, as the flow influences sedimentation and re-suspension while temperature influences mineralization. An additional controlling factor (seasonality) has been added, because phosphorous transformations vary among the times of the year (e.g. living organisms lifecycle involving phosphorus compounds is affected by the seasons of the year). The seasonality influence on the transformation rates is expressed via the seasonality factor, a continuous function, taking values between 0 (early winter) and 1 (early summer).

Further on during the calibration of ADModel empirical transformation models have been proposed for the estimation of each transformation rate, in order to make ADModel applicable for a wide range of field situations.

Table 1. ADModel configurations with respect to SRP and OP transformations model.

Transformations	Simple three transformations ADModel, [5]	Comprehensive five transformations ADModel, [15]
Mineralization	Transformation of OP to SRP First order with respect to OP Depending on temperature	Transformation of OP to SRP First order with respect to OP Depending on water temperature
Sedimentation	Consumption of OP Zero order with respect to SRP. Constant rate	Consumption of OP First order with respect to SRP Depending on water flow
Re-suspension	Source of OP Zero order with respect to OP Constant rate	Source of OP Zero order with respect to OP Depending on water flow and seasonality
Uptake	Not included	Consumption of SRP Zero order with respect to SRP Depending on water flow and seasonality
Net adsorption	Not included	Including adsorption as consumption of SRP and desorption as source of SRP First order with respect to SRP Depending on temperature

The Nash Sutcliffe (NS) coefficient, [5], has been employed as criteria for the assessment of the model's goodness of fit during all simulations, comparing estimated concentrations with measurements. The possible range of the NS coefficient is between minus infinity and one. The closer the NS value is to 1 the better the agreement between the estimates and field data is and the model is more performant.

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