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Mathematical Modeling of Nitrate and Salinity along the Rosetta Branch in the Nile Delta

النمذجة الرياضية للنترات والملوحة على طول فرع رشيد في دلتا النيل

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Abstract: A physico-chemical water quality model has been developed and tested for the Rosetta Branch in the Nile Delta. This paper discusses the set up of this model, the investigation on sufficient availability of water quality sampling and pollution data to enable such Modeling exercise, the extensive model verification by statistical techniques, as well as the model refinement and scenario analyses carried out by the model. The model has been set up making use of the MIKE11 river Modeling software. The physico-chemical water quality (WQ) model is linked with a detailed full hydrodynamic (HD) model developed for the same Rosetta branch, and also implemented in the MIKE11 Modeling system. All significant pollution sources along the Rosetta branch were considered. Pollution along the Rosetta Branch mainly originates from the drains. Three drains (El-Moheet, Sabal, and Tala) are monitored with different water quality variables measured on monthly basis. The measured concentrations for the Modeled variables and the discharges along the drains and at the model boundaries are used as model inputs. In between the different instantaneous values for these observations, linear interpolations are made. The model was calibrated and validated based on the available sampling data along the Branch. Given the data limitations for calculation of the model input and for model calibration, the simulation results can be considered good. The paper focuses on the model results for NO_3-N and TDS, and links the results towards their use in water management applying the combined HD-WQ model as integrated decision support tool. This was illustrated in the paper by prior simulation of scenarios in the model.

Keywords: *Water quality modeling, nitrate, salinity, Mike11 Modeling system.*

المستخلص: تم تطوير نموذج فيزيائي-كيميائي لمحاكاة واختبار نوعية المياه في فرع رشيد في دلتا نهر النيل. أعتمد هذا النموذج على نتائج نمذجة حركة المياه الهيدروديناميكية في الفرع والسابق بناؤه باستخدام برنامج MIKE11. يناقش هذا البحث كيفية إعداد نموذج رياضى لمحاكاة حركة وتركيز النيترات والاملاح الكلية الذائبة لفرع رشيد بدلتا نهر النيل. وقد تم إعداد النموذج بإستخدام برنامج MIKE11. في هذا البحث تم عرض كيفية إعداد النموذج ومعايرته وذلك بإستخدام طرق إحصائية لتحليل النتائج. وتم استخدام نتائج النموذج الهيدروليكى للفرع الذى تم اعداده ومعايرته فى دراسة سابقة كأساس لنموذج إدارة نوعية المياة. تم أخذ مصادر التلوث المختلفة من ثلاثة مصارف زراعية في الاعتبار وهى (مصرف المحيط- مصرف سبل – مصرف تلا). بعد معايرة النموذج وتحسينه ومقارنة النتائج بالقياسات الفعلية، أظهرت النتائج دقه عالية. لذا توصى الدراسة بإمكانية إستخدام النموذج المعد فى دراسات لإدارة نوعية المياة في نهر النيل بالإضافة إلى إعتباره وسيلة مفيدة لمساعدة متخذى القرار لإدارة نوعية المياه. أيضاً يمكن استخدامه للتنبؤ بحالة نوعية المياه المستقبلية وتحليل سيناريوهات مختلفة لتقييم تأثير تطبيقها على تحسين نوعية المياة.

كلمات مدخلية: *نمذجة نوعية المياه، النترات، الملوحة، نظام نمذجة Mike11.*

INTRODUCTION

A physico-chemical water quality model has been developed and tested for the Rosetta Branch in the Nile Delta. This paper discusses the set up of this model, the investigation on sufficient availability of water quality sampling and pollution data to enable such Modeling exercise, extensive model verification by statistical techniques, model refinement and scenario analyses carried out by the model. The model has been set up making use of the MIKE11 river Modeling software of DHI Water & Environment (DHI, 2002). The physico-chemical water quality (WQ) model is linked with a detailed full hydrodynamic (HD) model developed for the same Rosetta branch, and also implemented in the MIKE11 Modeling system. The description of this hydrodynamic model is given in the paper of Willems *et al*. (2005).

Delineation of the model area

The Rosetta Branch is being Modeled from downstream the Delta Barrage (the split with the Damietta Branch, as upstream boundary) up to the Mediterranean Sea (as downstream boundary), see Figure 1.

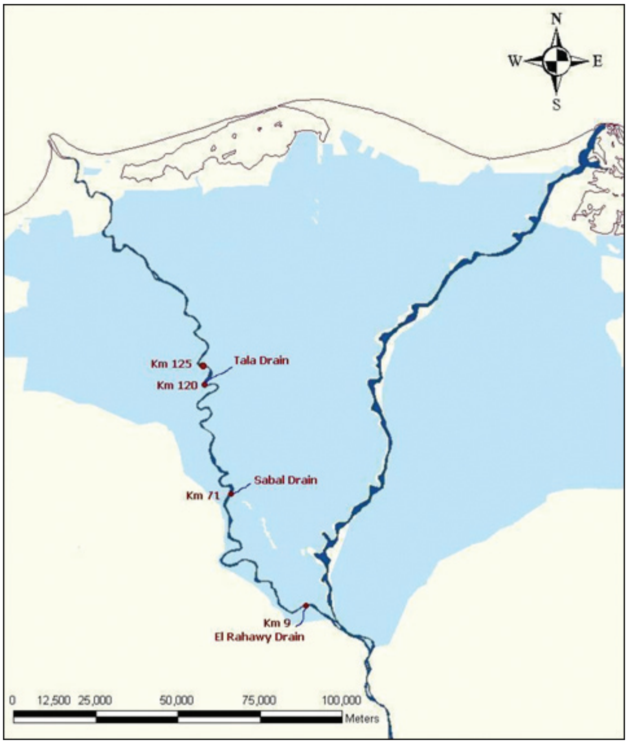

Fig. 1. Rosetta Branch within the Nile Delta.

Pollution sources

Pollution along the Rosetta branch mainly originates from the drains. Three drains (El-Moheet, Sabal, and Tala) are monitored with different water quality variables measured on a monthly basis within the framework of the National Water Quality and Availability Management Program (NAWQAM). The measured concentrations for the Modeled variables and the discharges are used as inputs for the model for the period 1997-2003. In between the different instantaneous values for these observations, linear interpolations are made. There are also 2 other drains (El-Tahrir and Zawiet El-Bahr) and 2 industrial drains (El Malya and Salt & Soda) along the Rosetta Branch. For these drains no monitoring data within the NAWQAM project is available, but the available data from the Nile Research Institute for the years 1997 and 1998 were used.

Selection of water quality processes to be Modeled

The water quality model considered and implemented in MIKE11 is a coupled model of an advection-dispersion (AD) submodel and a WQ submodel. The latter submodel deals with transforming processes of compounds in the river and the AD submodel is used to simulate the simultaneous transport process. The WQ submodel solves the system-coupled differential equations describing the physical, chemical and biological interactions in the river. The river water quality can be dealt with at different levels of detail. In this paper, the results of the NO_3-N and TDS are presented.

The processes are described with process velocities of 1st order (dC/dt-C), the dependence on temperature with Arrhenius-terms (ln(dC/dt)~T, with T the temperature of the river water and the process deceleration at low concentrations of certain parameters with Monod-terms (dC/dt~K/(K+C)). This way of presenting the processes is called macroscopic, because it tries to represent the way they are observed macroscopically with equations. The different processes on a microscopic scale that form the basis of the macroscopic observation are thus not considered.

Nutrients

The nutrients considered are the inorganic forms of nitrogen. Degradation of dead organic matter leads to a release of the organic bound nitrogen in the form of ammonia (ammonification). The degrading bacteria, however, utilise some of the nitrogen for their own growth. The rest of the ammonia released by ammonification or discharged from pollution sources can be taken up by plants or nitrifying bacteria to nitrate. The nitrate is eventually transformed into free nitrogen by a denitrification process (DHI, 2002; El-Sadek, 2002; El-Sadek *et al.*, 2002). The principles of this cycle are illustrated in Figure 2.

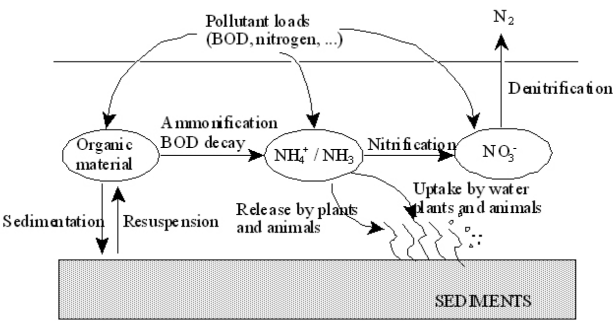

Fig. 2. Rosetta Branch within the Nile Delta.

The degradation, ammonification and nitrification are all processes taking place in the aerated zones of the water. Denitrification is anaerobic process requiring anoxic conditions. These onditions can be found in the sediment and in bacteria films on plants.

Nitrate Process

The reactions influencing the nitrate concentration are given by:

$$\frac{dNO_3-N}{dt} = +K_{nitr} * NH_4 - N * \theta_{nitr}^{(T-20)} \quad \text{(nitrification)}$$
$$-K_{denitr} * NO_3 - N * \theta_{denitr}^{(T-20)} \quad \text{(denitrification)} \qquad (1)$$

where:

K_{denitr} : denitrification rate (1/day or $(g/m^3)^{1/2}$/day)

θ_{denitr} : Arrhenius temperature coefficient for the denitrification process

K_{nitr} : the nitrification rate at 20°C (mg/l)

θ_{nitr} : the Arrhenius temperature coefficients of the nitrification process

T : water temperature (°C)

t : time

Total dissolved solids (TDS)

TDS is assumed to be a conservative pollutant; only advection and dispersion processes are considered. It is a measure of the salinity of the water.

Model parameters

For the model parameters of all physico-chemical processes mentioned above, default values were selected based on standard values found in literature (DHI, 2002).

Water quality input data and model boundaries

At the different drains water quality loads have to be specified (the pollution load, split up in discharge and concentration) for the period 1997-2003. This has been done for the three monitored drains. For the modeled water quality variables, concentration time series were created. Along each drain also the observed discharge series is specified. In the model, the discharges and the concentrations are multiplied to calculate the water pollution load as input to the model during the period 1997-2003. In between the time moments where the water quality samples have been taken, linear interpolations are assumed.

Water quality model validation

At the different locations along the Rosetta Branch where water quality samples are available, the full simulated hourly time series for the period 1997-2003 was compared with a limited number of water quality sampling results during the same period. The locations are: km 0 (at Delta Barrage), km 122, km 124, km 170, km 183, and km 203. At these locations, eleven measurement campaigns were carried out within the framework of the National Water Quality and Availability Management Program (NAWQAM). Only the first 6 periods were considered for model validation as the last ones are outside the model simulation period (hydrodynamic simulation till end of 2003). These periods were:

- 17-18/10/2000 September 2000 (NRI, 2000),
- 19-20/3/2001 February 2001 (NRI, 2001),
- 13-15/3/2002 March 2002 (NRI, 2002a),
- 26-27/8/2002 August 2002 (NRI, 2002b),
- 22-24/3/2003 February 2003 (NRI, 2003a),
- 24-25/9/2003 August 2003 (NRI, 2003b).

The more precise dates for the campaigns in 2000, 2001, 2003 are within the next month of the campaign start month, this can be because the campaign started from the most upstream location at the Aswan High Dam and reached Rosetta Branch within 30-35 days. Results are calibrated by the following types of plots:

- Time series for final simulation results
- Longitudinal profiles: variation of the concentration or load versus the distance along the Rosetta Branch: comparison of model derived profiles with observed data at the 6 locations of the measurement campaigns;
- Scatterplot of Modeled versus observed concentrations and loads for all 6 measurement campaigns and all 6 locations;
- Modeled and observed concentrations or loads versus discharge;
- Difference in load from up-to downstream along the different reaches (in between locations where water quality measurements are available).

All these plots were prepared and evaluated and according to the evaluation results, model parameters were modified to improve the model. Then model results are presented hereafter for the concentrations and loads of NO_3-N and TDS. Only a selection of the validation plots is given in this paper for discussion. Time series for final simulation results are show in Figure 3 and Figure 4 for NO_3-N and TDS respectively.

In Figures 5 and 6, the longitudinal profile is given for the NO_3-N and TDS loads respectively. The ‘observed loads’ in these figures are calculated by means of the observed concentrations multiplied by the modeled discharges at the same location. The dates of the measurements are only known within a time span of a few days. This leads to uncertainty in the discharge values to be selected from the hydrodynamic model results. The uncertainty is indicated by the error bands for the observed data in the figures, and by the lower and upper limits for the model results. The bands and limits indicate the highest and lowest values in the known periods for the measurement campaigns.

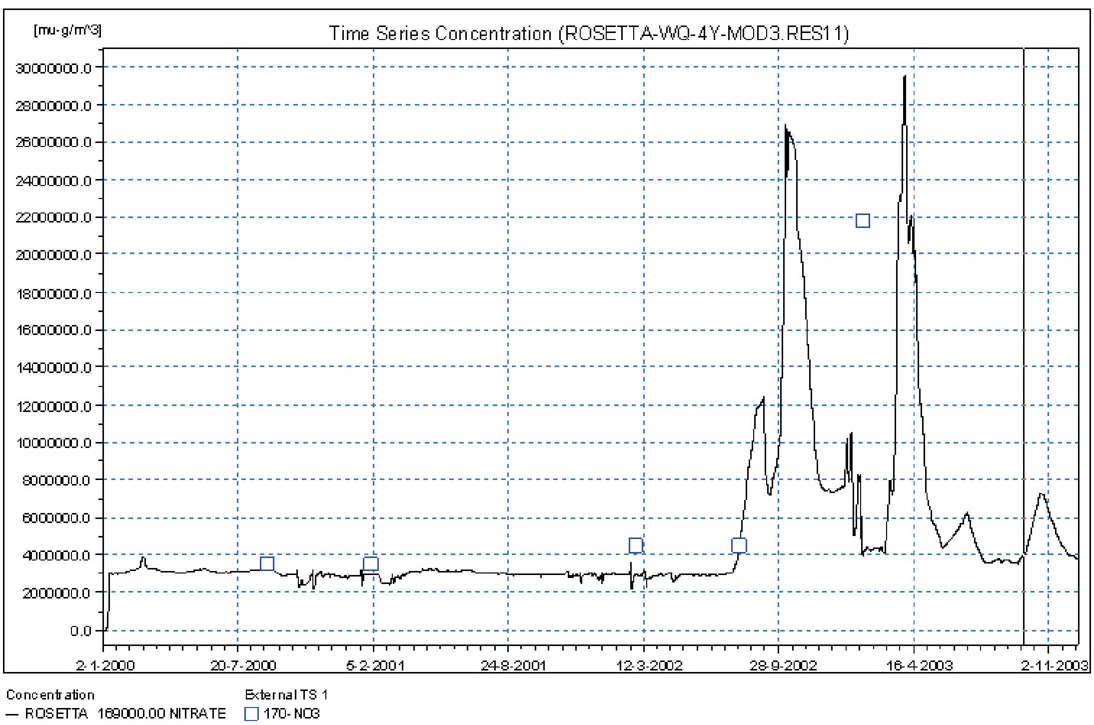

Fig. 3. Modeled versus observed concentrations for NO_3-N.

Further analysis of the results have been carried out to verify the relationship between the observed and Modeled concentrations, discharges and loads at the different locations along Rosetta branch and at the sampling locations. In Figure 7 and Figure 8, the relationship between the concentrations and loads was analysed on the one hand, and the discharges, on the other hand. It is clear from the figures that the load increases with discharge, while this is less the case for the concentrations. The model results and measurements show under and over estimation at low and higher concentrations respectively. This can be explained by measured data limitation. Moreover, TDS was better predicted by the model.

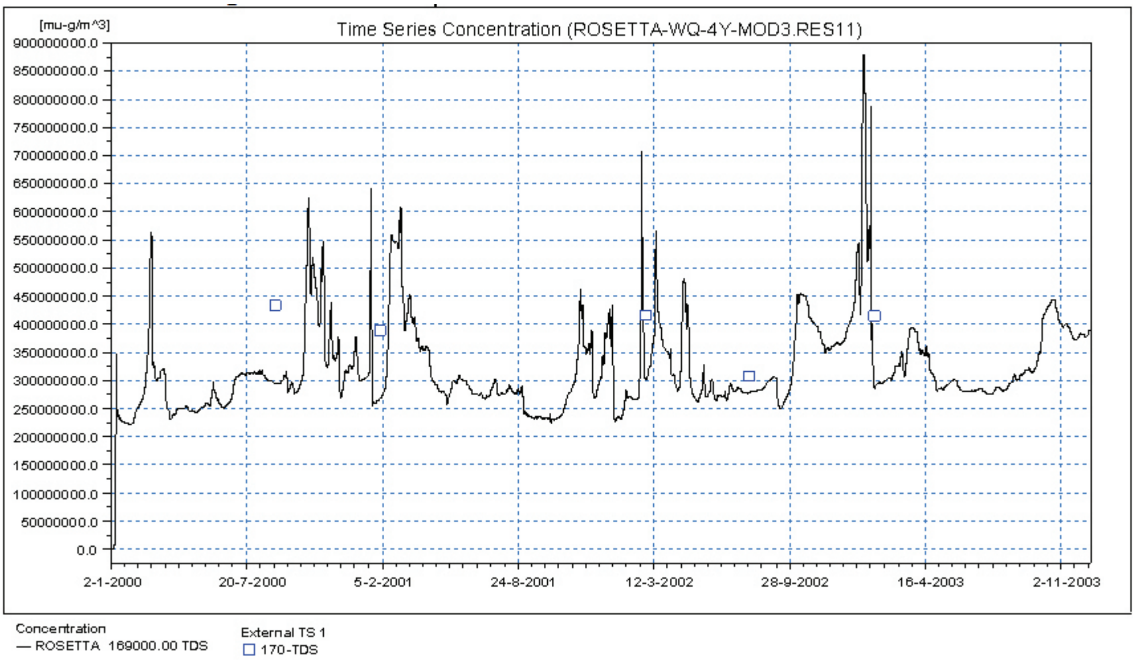

Fig. 4. Modeled versus observed concentrations for TDS.

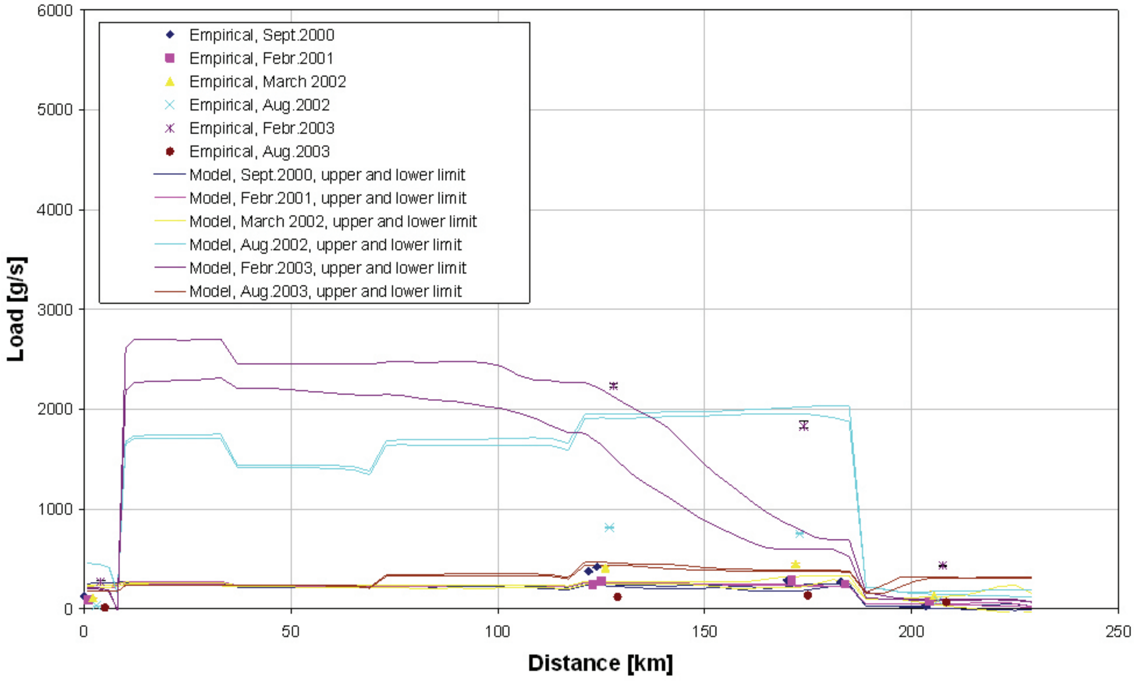

Fig. 5. Longitudinal profile of NO_3 load.

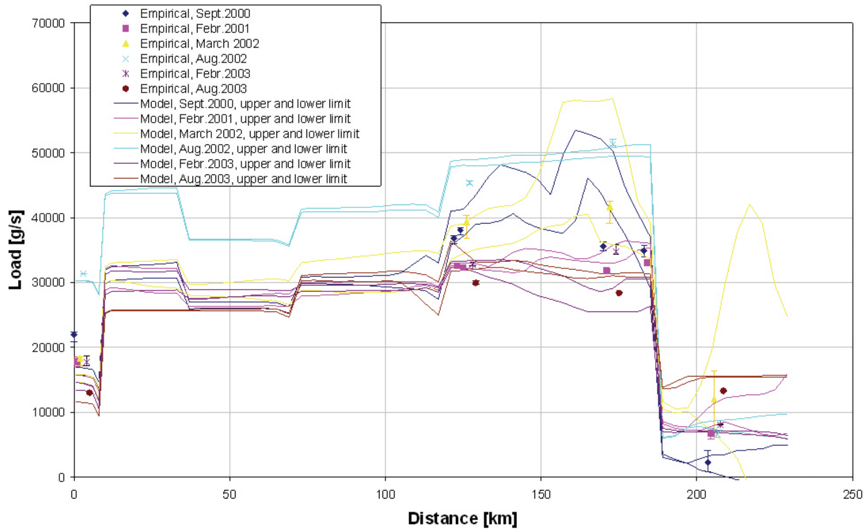

Fig. 6. Longitudinal profile of TDS load.

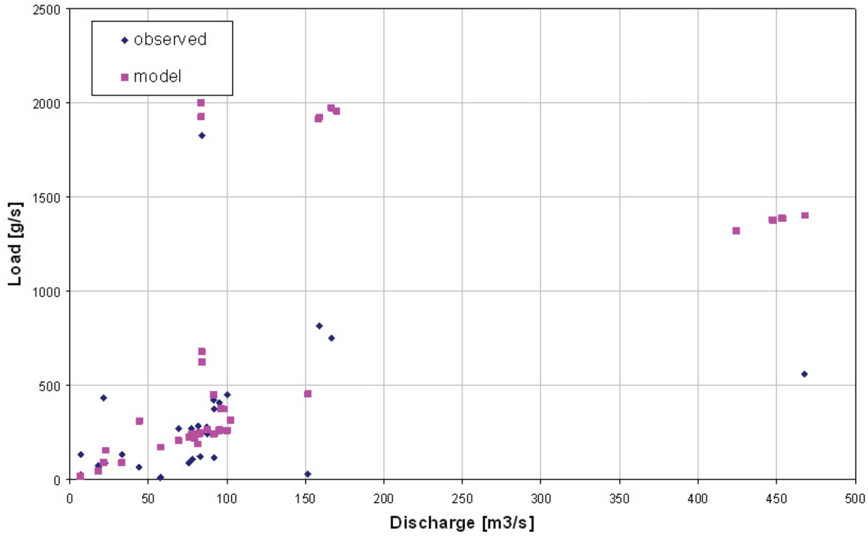

Fig. 7. Load versus discharge for NO3-N.

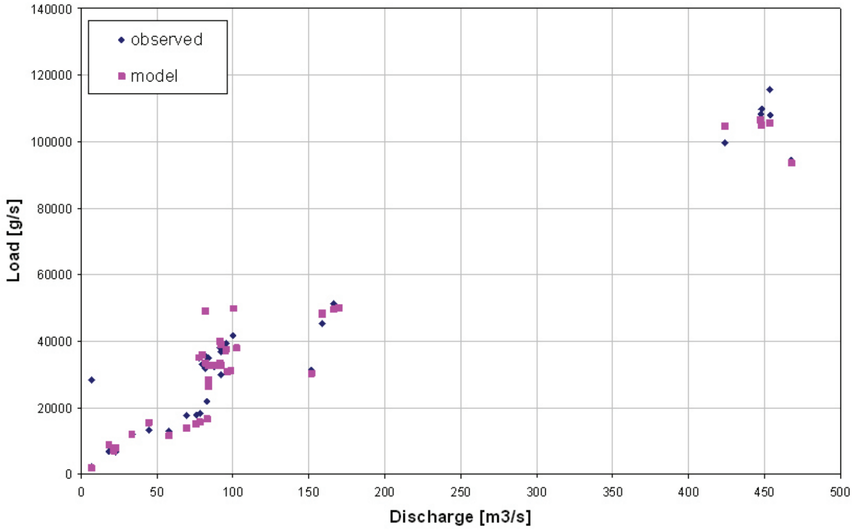

Fig. 8. Load versus discharge for TDS.

The observed and Modeled concentrations and loads were also plotted against the bisector, as presented in Figure 9 and Figure 10. By means of these scatterplots, systematic over-and/or underestimation of the model results can be checked for given ranges of concentrations or loads. When model evaluations are made based on these plots, one has to take into account the uncertainties on both the Modeled and observed concentrations and loads. As explained before, these uncertainties originate from the lack of information on the precise dates of the measurement campaign periods. The upper and lower values during these periods are indicated in the scatterplots by the error bounds on the points. In the scatterplots, indication is also made of the mean error and the standard deviation of the model residual errors (the differences between the model results and the observations). The mean error reflects the systematic deviation of the model, while the standard deviation is a measure of the random uncertainty in the model results. The standard deviation is slightly higher than the real standard deviation of the error on the model results due to uncertainties in the dates of the measurement campaigns. The mean error is not affected by these uncertainties, and can be correctly used to evaluate the systematic error of the model. From Figure 9 and Figure 10, it can be seen that the calibrated models do not show systematic differences for the NO_3-N and TDS concentrations.

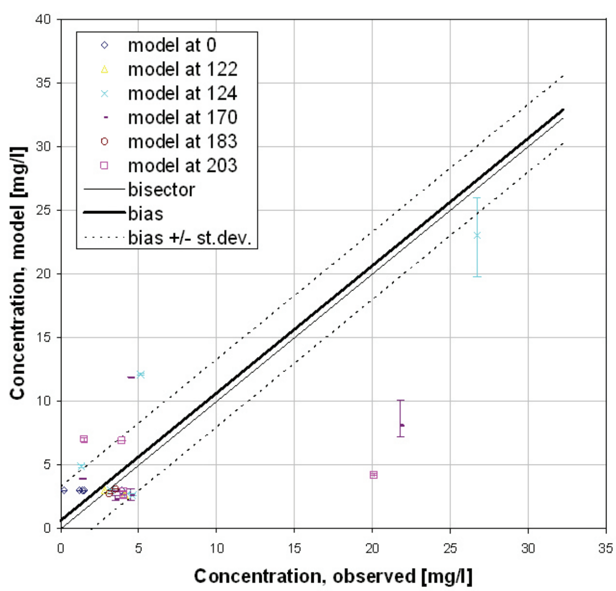

Fig. 9. Scatterplot of Modeled versus observed concentrations for NO3-N.

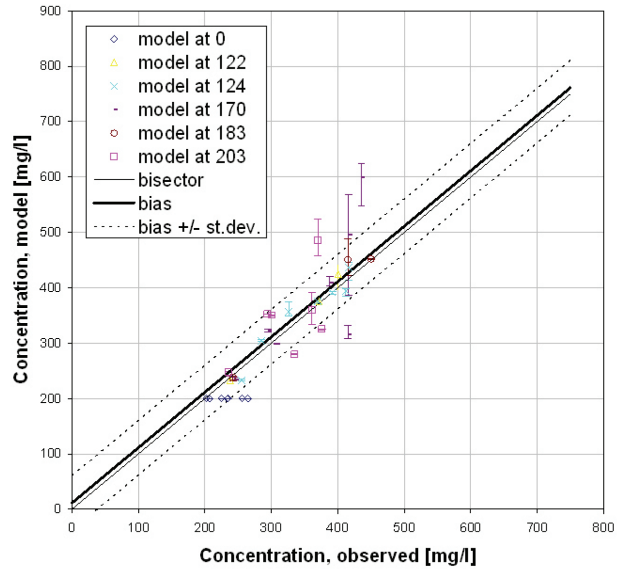

Fig. 10. Scatterplot of Modeled versus observed concentrations for TDS.

Statistical analysis

The qualitative judgement of when the model performance is good is a subjective matter. Therefore statistical criteria are used for the quantitative judgement. Statistical based criteria provide a more objective method for evaluation of the performance of the models (El-Sadek *et al*, 2008; El-Sadek, 2010). In this study the following statistical criteria were used to evaluate the performance of the models:

Mean Absolute Error (MAE)

$$MAE = \frac{\sum_{i=1}^{n} \left| (O_i - P_i) \right|}{n} \quad (2)$$

where O_i is the observation at time i, P_i is the prediction at time i. The MAE has a minimum value of 0.0.

Relative Root Mean Square Error (RRMSE)

$$RRMSE = \frac{\sqrt{\frac{1}{n}\sum_{i=1}^{n}(P_i - O_i)^2}}{\bar{O}} \quad (3)$$

where $\bar{O}$ is the mean of the observed values over the time period (1 to n). The RRMSE has a minimum value of 0.0, with a better agreement close to 0.0.

Model Efficiency (EF)

$$EF = \frac{\sum_{i=1}^{n}(O_i - \bar{O})^2 - \sum_{i=1}^{n}(P_i - O_i)^2}{\sum_{i=1}^{n}(O_i - \bar{O})^2} \qquad (4)$$

EF ranges from minus infinity to 1.0, with higher values indicating better agreement. If EF is negative, the model prediction is worse than the mean observation.

Coefficient of Residual Mass (CRM)

$$CRM = \frac{\sum_{i=1}^{n} O_i - \sum_{i=1}^{n} P_i}{\sum_{i=1}^{n} O_i} \qquad (5)$$

The CRM has a maximum value of 1.0. If CRM is negative the model overestimates and vice versa.

Coefficient of Determination (CD)

$$CD = \frac{\sum_{i=1}^{n}(O_i - \bar{O})^2}{\sum_{i=1}^{n}(P_i - \bar{O})^2} \qquad (6)$$

The CD describes the ratio of the scatter of the simulated values and the observed values around the average of the observations. A CD value of one indicates to what extent the simulated and observed values match perfectly. It is positive defined without upper limit and with zero as a minimum.

Goodness of Fit (R2)

$$R^2 = \left[\frac{\sum_{i=1}^{n}(O_i - \bar{O})(P_i - \bar{P})}{\sqrt{\sum_{i=1}^{n}(O_i - \bar{O})^2}\sqrt{\sum_{i=1}^{n}(P_i - \bar{P})^2}} \right]^2 \qquad (7)$$

where P is the mean of the predicted values over the time period (1 to n). R2 is ranging from 0.0 to 1.0 indicating a better agreement for values close to 1.0 and it is known as the goodness of fit (Shahin *et al*., 1993; Legates and McCabe, 1999; El-Sadek, 2007). The characteristic of the different statistical criteria is given in Table 1 and statistical performance analysers calculated between observed and simulated values for NO3-N and TDS at km 122 and km183 are shown in Table 2.

Table 1. The characteristic of the different statistical criteria.

RRMSE		**MAE**		**CD**	
RRMSE=0	model is perfect	MAE=0	model is perfect	CD=0	no prediction capability
RRMSE=min	optimal	MAE=min	optimal	0<CD	some at least prediction capability
		0<MAE	model is less perfect		
				CD=max	optimal

FE		**CRM**		**R²**	
EF=1	model is perfect	CRM=1	no prediction capability	R2=1	perfect
EF=max	optimal	CRM<1	some at least prediction capability	R2=max	optimal
EF<1	less perfect			R2=0	no prediction capability
EF= $-\infty$	no prediction capability	CRM closes to 0	optimal		

Table 2. Statistical performance analysers calculated between observed and simulated values for NO3-N and TDS at km 122 and 183.

Year	**MAE**	**RRMSE**	**CD**	**EF**	**CRM**	**R²**
NO3-N (km 122)	1.119	0.562	0.910	0.708	-0.086	0.650
NO3-N (km 183)	1.296	0.682	0.860	0.572	-0.446	0.700
TDS (km 122)	0.945	0.529	0.800	0.742	-0.269	0.814
TDS (km 183)	0.985	0.508	0.780	0.689	-0.210	0.790

CONCLUSIONS AND RECOMMENDATIONS

A model has been set up for the physico-chemical water quality of the Rosetta Branch in the Nile Delta. For the water quality submodel and given the data limitations for calculation of the model input and for model validation, the simulation results can be considered good. The water quality model can be considered useful as decision support tool in water management. Decisions can be based on prior simulation of scenarios in the model. Apart from this interesting application to support decisions in water management, the model can also be used for:

- Interpolation (in time) of the physico-chemical water quality sample data, to fill up the gaps of the time periods in between the measurement campaigns and the time gaps between the samples taken during each of the measurement campaigns;
- Extrapolation to predict future evolutions in the water quality concentrations;
- Scenario analysis to predict the impact of changes in external driving forces such as land use changes and climate change;
- To analyse correlations between the different water quality variables to optimise and reduce the list of variables to be considered for future measurement campaigns;
- To analyse correlations in time of water quality variables to optimise the measurement frequency (again for future measurement campaigns).
- The model can be further improved, validated and the accuracy increased if more water quality data become available in the future. The following recommendations are proposed based on the experience and expertise built up during the project:
- More detailed measurement campaigns along the Rosetta branch need to be carried out, with more frequent measurements (e.g. same frequency as for the drains, and by preference on the same days) and at more locations along the branch (at least up- and downstream of the drains). This would allow better calibration and validation of the model to be done;
- Estimation needs to be made on the diffuse pollution (pollution different from the drains) along the branch.

Due to the limitations in the availability of water quality sampling data (low spatial as well as temporal resolution), the use of satellite imagery (remote sensing) to estimate water quality variables could be tested as well in the future. As final recommendation a model might be set up to have a more accurate estimation of the domestic and agricultural pollution from the drains. The data needed for the Modeling of the agricultural input into the drain, such as information on the fertilization, the subsurface drainage geometry, and the crop information need to be collected for this purpose. Agricultural pollution prediction models are needed to predict changes in agricultural management practises on the pollution loads along the drains.

REFERENCES

DHI (2002) *MIKE11 Reference & User Manual, DHI Water & Environment*, Denmark.

El-Sadek, A (2002) Modeling of NO_3-N leaching to shallow groundwater during the fall-winter season. *TheScientificWorldJournal*, 2: 1006-1016.

El-Sadek, A (2007) Upscaling field scale hydrology and water quality Modeling to catchment scale. *Water Resources Management*, 21: 149-169.

El-Sadek, A (2010) Monte Carlo approach to developing a water quality process-factor. *International Journal of Water Resources and Environmental Management*, 1: 97-104.

El-Sadek, A, ElKahloun, M, and Meire, P (2008) Ecohydrology for integrated water resources management in the Nile basin. *Ecohydology & Hydrobiology*,237- :(2-4)8 244.

El-Sadek, A, Feyen, J, Skaggs, W, and **Berlamont, J** (2002) Economics of nitrate losses from drained agricultural land. *Environmental Engineering*, **128**(4): 376-383.

Legates, D, and McCabe, G (1999) Evaluating the use of 'goodness-of-fit' measures in hydrological and hydroclimatic model validation. Water Resources Research **35** (1): 233-241.

NRI (2000) *Water quality data report for NAWQAM project in September 2000*. Nile Research Institute, National Water Research Center, Delta barrage, Egypt.

NRI (2001) *Water quality data report for NAWQAM project in February 2001*. Nile

Research Institute, National Water Research Center, Delta barrage, Egypt.

NRI (2002a) *Water quality data report for NAWQAM project in March 2002*. Nile Research Institute, National Water Research Center, Delta barrage, Egypt.

NRI (2002b) *Water quality data report for NAWQAM project in August 2002*. Nile Research Institute, National Water Research Center, Delta barrage, Egypt.

NRI (2003a) *Water quality data report for NAWQAM project in February 2003*. Nile Research Institute, National Water Research Center, Delta barrage, Egypt.

NRI (2003b) *Water quality data report for NAWQAM project in August 2003*. Nile Research Institute, National Water Research Center, Delta barrage, Egypt.

Shahin, M., Van Oorschot H, and De Lange, S (1993) Statistical analysis in water resources engineering. A. A. Balkema Publishers, The Netherlands. 394 pp.

Willems, P, Radwan, M, El-Sadek, A, and **Abdel-Gawad, S** (2005) Hydrodynamic Modeling of the Rosetta branch in the Nile Delta. International Conference of UNESCO Flanders FIT FRIEND/Nile Project – "Towards a better cooperation", Sharm El-Sheikh, Egypt, 20-23 November 2005.

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