Trace metal transport modeling using OpenMI: a case study of Zenne river, Brussels Belgium

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Introduction:

In 2000, the European Water Framework Directive was developed, requiring a good ecological status for all surface waters in all member states by 2015 (EC, 2000). In order to achieve this, Environmental Quality Standards (EQS) for several substances and pollutants have been laid down (EC, 2008). Since then, large investments were made for the management of the wastewaters of Brussels. This improved the water quality flowing into the river Zenne (Garnier et al., 2012). Despite these investments, the river still receives high loads of pollutants, especially considering the low discharge of the river and the water quality downstream from Brussels does not comply with the requirements set by the EU-WFD. It is in this context that an interuniversity, multidisciplinary research project ‘Good Ecological Status of the river Zenne (GESZ)’ was launched to evaluate the effects of the wastewater management plans in the river basin on the ecological functioning of the river. With this project, different water quantity and quality processes need to be considered: the hydrology in the river basin, the hydraulics in the river, in the canal and in the sewers, erosion and sediment transport, the carbon-nitrogen-phosphorus (C-N-P) cycle, the transport of trace metals and the transport and decay of faecal indicator bacteria. In such a framework, dynamics of trace metals needs to be considered. In the 2011 report of the Flemish Environment Agency (VMM), several metals, such as zinc, arsenic and cadmium had high concentrations in water surfaces under their jurisdiction. Nevertheless, average concentrations of metals except for arsenic have decreased by more or less 50% in the last 10 years (Steertegem, 2011).

Since many of the processes interact with each other, an integrated model considering all the processes is needed. The Open Modelling Interface or OpenMI (Gregersen et al., 2007; Moore and Tindall, 2005) was used in integrating the different models simulating these processes. This paper presents an OpenMI-based integrated trace metal transport model consisting of five models.

Materials and methods:

Simulators: Five models were used to form an integrated trace metal dynamics model linked dynamically through OpenMI.
US EPA Storm Water Management Model (SWMM), a physically-based dynamic rainfall-runoff simulator (Rossman, 2010), is used to simulate the hydraulic properties. Soil Water Assessment Tool, known as SWAT (Arnold et al., 1998) is used to simulate runoff and sediment loads from rural catchments. A temperature simulator, which is based on a non-linear air-stream regression as suggested by Mohtseni et al. (1998), provides the stream water temperature values. A sediment simulator (Shrestha et al., accepted) simulates the deposition/resuspension of solid materials. This simulator is based on the Shield’s diagram (Shields, 1936) for scour and deposition while the carrying capacity is limited by using Velikanov’s energy equations as proposed and implemented by Zug et al. (1998). A Carbon-Nitrogen-Phosphorus (C-N-P) simulator based on the River Water Quality No.1 (Reichert, 2001) simulates the C-N-P cycle.

The trace metal transport simulator calculates the dissolved and particulate metal concentrations through a partitioning coefficient: $K_D$. The partitioning coefficient $K_D$ describes metal speciation over adsorbed and dissolved states. In the literature, two approaches are being used to determine the $K_D$ and hence metal speciation: a constant $K_D$ and a variable $K_D$ approach. Recently, there is growing realization that $K_D$ depends on various ancillary environmental parameters and should thus be considered as variable (US EPA, 2005; Wu et al., 2005). Hence, a variable $K_D$ approach was used. To relate $K_D$ to the environmental variables, a multivariate linear regression (MLR) method was used. For this, independent physicochemical parameters such as dissolved oxygen, conductivity, pH, suspended particulate matters and temperature were considered. Four species of trace metal were selected: Copper (Cu), Cadmium (Cd), Zinc (Zn) and Lead (Pb).

The MLR model calibration and validation: The MLR was used in deriving an equation relating $\log K_D$ with measured physicochemical variables during several GESZ sampling campaigns. The $\log K_D$ values were determined by taking the ratio of the particulate to dissolved metal concentrations. In developing the model, interaction terms, (which are products of two independent parameters) were considered to make the equation more robust. Terms with high correlation, determined using VIF statistics (O’Brien, 2007) were removed from the equation. In selecting the appropriate model, the Bayesian Information Criteria (BIC) was used in order to optimize the fit and prediction of the equation. The goodness of fit was evaluated using $R^2$ and the prediction power is given by PRESS statistic (Allen, 1974).

Build up of the integrated model: As already depicted, five models have been used to form an integrated trace metal (Figure 1). A hydraulic model of the river system between the border of the Walloon Region and the mouth of the river was built up using SWMM. The upstream catchments of the river in the Walloon Region were modelled with SWAT, as well as the major rural catchments in the Flemish Region. These SWAT models provide the upstream boundary conditions for the SWMM model. In a first step, the SWAT model was built, calibrated, and validated autonomously. In a second step, the SWMM model was linked to SWAT on the OpenMI platform and, consequently, calibrated and validated. Then, the temperature, the sediment models and the C-N-P model were linked to the validated SWMM model. In doing so, the parameters of the temperature model were calibrated autonomously while the parameters were validated in an integrated model. The parameters of the sediment and C-N-P model were validated in different integrated models as well. Finally, the trace metal model was linked to these four models. Figure 1 shows the component models of the integrated trace metal model with the quantities exchanged between the models.
Figure 1. Component models of the integrated heavy metal transport model, and relevant exchange of data between components through OpenMI.

Validation of the integrated model: The integrated model was used to simulate the heavy metal dynamics in the river Zenne for a time span of 2007-2010. The metal concentrations (total, dissolved and particulate) were validated using VMM measurements at three important locations, Lot (ca. 15 km upstream of Brussels), Vilvoorde (just downstream of Brussels), and Eppegem (ca. 10 km downstream of Brussels).

Results:

The summary of equations used in determining the predicted log $K_d$ is shown in Table 1. These equations were chosen based on the lowest BIC and low VIF statistic. With this, a balance between fit and prediction is achieved.

Table 1. Summary of logKd equations derived using MLR

<table>
<thead>
<tr>
<th>Independent Variables</th>
<th>$R^2$</th>
<th>PRESS</th>
</tr>
</thead>
<tbody>
<tr>
<td>Log Kd-Cd 5 (MeT$_{Cd}$, Cond, O$_2$, SPM)</td>
<td>0.55</td>
<td>19.21</td>
</tr>
<tr>
<td>Log Kd-Cu 6 (MeT$_{Cu}$, O$_2$, pH, SPM)</td>
<td>0.52</td>
<td>14.19</td>
</tr>
<tr>
<td>Log Kd-Pb 4 (MeT$_{Pb}$, pH, SPM)</td>
<td>0.49</td>
<td>15.40</td>
</tr>
<tr>
<td>Log Kd-Zn 2 (Cond, Temp)</td>
<td>0.19</td>
<td>26.62</td>
</tr>
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</table>
Figure 2 shows how the parametric partitioning coefficient values fair when compared with the observed log $K_D$ equation. The equations are able to mimic the observed values. There are some overestimations with the values of log $K_D$ of cadmium. All other log $K_D$ values are well within the prediction interval of 1 standard deviation, which is actually 68% confidence interval as log $K_D$ values are normally distributed.

![Log $K_D$ - Cd](image1)

![Log $K_D$ - Cu](image2)

![Log $K_D$ - Pb](image3)

![Log $K_D$ - Zn](image4)

Figure 2. Observed vs calculated log $K_D$ values. The calculated log $K_D$ values are based on a parametric log $K_D$ model developed using MLR. Broken lines indicate 1-standard deviation prediction interval. Solid line corresponds to bisector line.

Total, dissolved and particulate metal concentrations of cadmium, copper, lead and zinc along the Zenne river for years 2007 to 2008 were simulated. In general, the model was able to simulate the metal concentrations. The values of the metals were well within the range of the observed values from GESZ measurement campaigns. However, overestimations were observed for total and dissolved zinc for all stations. Total copper was also underestimated for Lot and Vilvoorde. Particulate concentrations for all metals were overestimated for station Eppegem. Figure 3 shows a sample simulation results for total and dissolved zinc at station Vilvoorde for the span of years 2007 to 2008.
Figure 3. Simulated and observed total and dissolved zinc concentrations for station Vilvoorde for period January 1, 2007 to December 31, 2008. Solid lines indicate simulation values, circular markers are observed values. Broken lines show the range of GESZ measured values at station Haren Buda.

Conclusions:
This paper was able to show the possibility of creating an integrated trace metal transport model in OpenMI for Zenne river. It was shown that the model was able to calculate for total metal concentrations with modest errors graphically. Also, dissolved and particulate metal concentration could be determined. The availability of more observed values would make the discrepancies in the simulations more quantifiable.

References:


