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Predictive Transport Model of Bisphenol-A in Main Pampanga River

AUSTERO S. [1,2,3,*], RESURRECCION A.[1,4] , ROLLON A.[1,5], KWAN C.[6], HERRERA E.[7,8], BALLESTEROS F.[5], ALVIOR-SINOY M.C.[1], MACASIEB R.[4]

[1]Environmental Engineering Program, University of the Philippines Diliman, Philippines

[2]National University, Philippines

[3]Department of Community and Environmental Resource Planning, College of Human Ecology, University of the Philippines Los Baños, Philippines

[4]Intstitute of Civil Engineering, University of the Philippines Diliman, Philippines

[5]Chemical Engineering Department, University of the Philippines Diliman, Philippines

[6]Research and Analytical Services Laboratory, Natural Sciences Research Institute, University of the Philippines Diliman, Philippines

[7]Water Resources and Coastal Engineering Group, Institute of Civil Engineering, University of the Philippines Diliman, Philippines

[8]National Hydraulic Research Center, Institute of Civil Engineering, University of the Philippines Diliman, Philippines

*corresponding author:
e-mail: sbaustero@up.edu.ph

Abstract Phenolic endocrine disrupting compounds (EDCs) like Bisphenol-A (BPA) can interfere in the natural processes being done by the endocrine system of living organisms. To assess the effect of such contaminant in the Main Pampanga River of the Philippines, a transport model was developed using the Water Quality Analysis Simulation Program (WASP) by US EPA. The flow inputs were estimated using the Hydrologic Modeling System (HEC-HMS) by the US Army Corps of Engineers – Hydrologic Engineering Center. The following data were used to estimate the flows via HEC-HMS: IFSAR DEM, land cover, soil map, rainfall and weather data, streamflow data, and dam parameters. WASP Inputs included the following: physical and chemical properties, river cross-sectional profiles, boundary conditions, and loads. BPA concentrations from literature, population data, and waste generation data were used to estimate the BPA boundary concentrations and loads. The statistical parameters of the calibration and validation of the BPA transport model showed that the model is acceptable (NSE > 0.5) with good fit relative to observed data points (R-squared > 0.8). The PBIAS values are also between -25 and +25, thus satisfying the criteria for model accuracy.

Keywords: Endocrine disrupting compounds, Bisphenol-A, HEC-HMS, WASP, Pampanga River

1. Introduction

Endocrine disrupting compounds (EDCs) have become micropollutants of concern the past years. These chemicals can cause harmful health effects to living species through the different mechanisms performed by the endocrine system (Nohynek, Borgert, Dietrich, & Rozman, 2013). These can affect the development, reproduction, behavior, metabolism, and homeostasis of living organisms (Lv, Xiao, Zhang, Jiang, & Tang, 2016).

Among the EDCs mentioned, bisphenol-A (BPA) is chosen as the target micropollutant for this study. Bisphenol-A used in food and beverage containers has been detected in blood and placental tissue samples of pregnant women (Schonfelder, et al., 2022). In another study, BPA was said to induce the proliferation of human prostate cancer cells even at very low doses (Wetherill, Petre, Monk, Puga, & Knudsen, 2002).

To evaluate the effect of BPA to the living organisms in the area, its occurrence, fate, and transport must be investigated. Assessing the transport of emerging pollutants like BPA in vital aquatic environments like the Main Pampanga River is crucial since this is affected by the surrounding environment which could be a source of environmental hazards that could pose ecological and health risks.

This study focuses on producing a model that incorporates the hydrologic model derived from the IFSAR Digital Elevation Model from NAMRIA (2018), soil map from PhilGIS (2018), land cover from NAMRIA (2015), rainfall data from ASTI (2018), weather data from BSWM (2018), streamflow data from DPWH (2018) and micropollutant data from literature and other researchers. The area covers Pampanga River Basin (PRB) which is mostly within the boundaries of Bulacan, Pampanga, Tarlac, and Nueva Ecija (Japan International Cooperation Agency; CTI Engineering International Co., Ltd.; Nippon Koei Co., 2011).

BPA is considered as a phenolic endocrine disrupting compound, thus, this could be included in the group *Phenol and Phenolic Substances*. The acceptable concentration of phenolic substances in freshwater and marine water for Classes AA, A, and B is less than 0.001 mg/L. The acceptable limits for Class C and D waters are 0.05 mg/L and 0.5 mg/L, respectively.

Table 1 lists the BPA levels in a lake and some rivers in China, Philippines, and Spain. Based on the list, the amount of BPA in the surface water ranged from 11 ng/L (0.011 mg/L) to 800 ng/L (0.8 mg/L). The BPA level in Tenejeros River is very high and this exceeded the limits for Phenol and Phenolic Substances stated in DAO 2016-08 set by DENR.

Table 1. BPA Levels in Surface Waters

Location	**BPA Level (ng/L)**	**Reference**
Luoma Lake, China	49.38	(Liu, et al., 2017)
Manzanares River, Spain	37	(Esteban, et al., 2014)
Jarama River, Spain	106	(Esteban, et al., 2014)
Panlong River, China	46	(Wang, et al., 2016)
Pearl River Estuary, China	62.78	(Diao, et al., 2017)
Tenejeros River, Manila, Philippines	800	(Santiago & Kwan, 2007)

2. Materials and Methods

2.1. Study site and field sampling strategy

The PRB is geographically located between 14°30' to 16°15' N latitude and 120°15' to 121°30' E longitude. As shown in **Figure 1**, this is positioned within the administrative boundaries of eleven (11) provinces namely: (1) Aurora, (2) Bataan, (3) Bulacan, (4) Metropolitan Manila, (5) Pampanga, (6) Tarlac, (7) Nueva Ecija, (8) Nueva Vizcaya, (9) Pangasinan, (10) Rizal, and (11) Zambales. The Main Pampanga River runs from the Caraballo Mountains and goes to Pantabangan River which is temporarily stored in Pantabangan Dam. The river traverses the Central Plain of Luzon Island and further south, the water is discharged into Manila Bay (Japan International Cooperation Agency; CTI Engineering International Co., Ltd.; Nippon Koei Co., 2011).

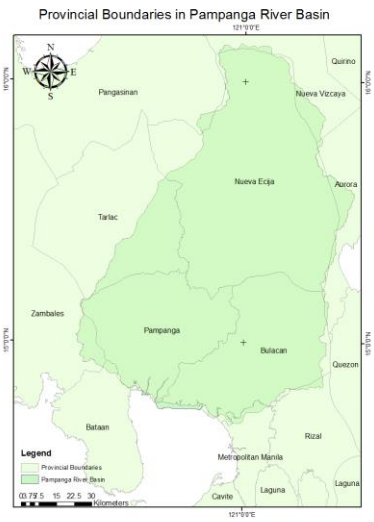


Figure 1. Provincial boundaries in Pampanga River Basin

The Field Guide for Surface Water Sample and Data Collection by USDA (2001) was used as basis in choosing sites that are "safe, accessible, and easily located". The presence of tributaries and confluences that represent the upstream and downstream conditions of the river were also taken into consideration in picking the most relevant and appropriate sites for the study.

The surface water samples were collected from 18 sampling points in 7 sampling sites along Pampanga River. The sampling sites in PRB are shown in **Figure 2**.

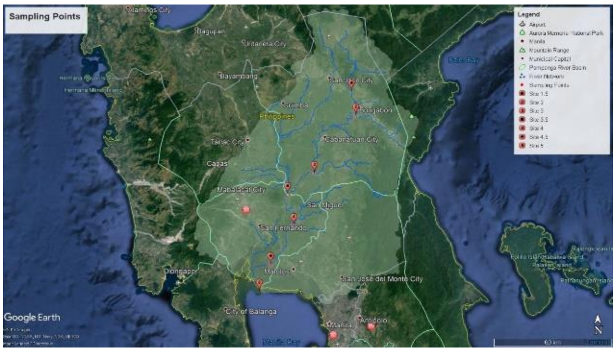


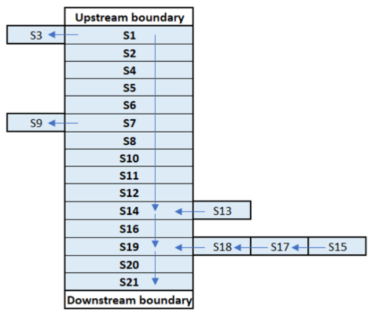
Figure 2. Sampling Locations in Pampanga River Basin

Reconnaissance and site assessment were done on October 16 – 20, 2018. The first fieldwork was conducted during a wet season on November 16 – 24, 2018 while the second fieldwork was done during a dry a season on March 4 – 11, 2019. Another field work was organized last October 29 – 31, 2021.

2.2. Modeling of BPA Transport in Main Pampanga River

ArcGIS along with HEC-GeoHMS extension was used to delineate the watershed, sub-basins, and stream network, while HEC-HMS was utilized to develop the hydrologic model. On the other hand, WASP was used in the creation of the contaminant transport model.

For this study, only the surface water was considered with the assumption of complete mixing in the vertical and lateral directions of the water column, thus, a one-dimensional (1D) model was employed. The 1D network segmentation of the WASP micropollutant model with the corresponding reach element per segment is in **Figure 3**.



Segment	Reach Element
S1	R70
S2	R70a
S3	R70b
S4	R90
S5	R110
S6	R140
S7	R160
S8	R160a
S9	R160b
S10	R310
S11	R330
S12	R400
S13	R410
S14	R510
S15	R630
S16	R550
S17	R600
S18	R640
S19	R650
S20	R740
S21	R750

Figure 3. 1D model network segmentation and corresponding reach elements

The contaminant transport model included twenty-one (21) segments which started from reach R70 and ended at

R750 which is the outlet in Manila Bay. The model represents a portion of the total number of reaches under the hydrologic domain.

During the reconnaissance phase, the study area was inspected for possible sources of BPA contamination. For the contaminant transport model, the waste treatment facilities (WTF) located near reaches R310 in Cabanatuan, Nueva Ecija and R510 in San Isidro, Nueva Ecija were incorporated in the model since these are near the segments that are included in the model. In **Figure 4**, the selected WTF and the population data is displayed.

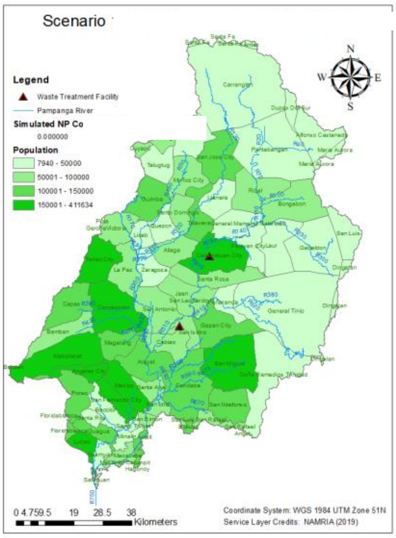


Figure 4. Selected BPA Sources with Population Data

The predictive BPA transport model was calibrated using estimated BPA loads. The BPA loads were computed based on the projected population and the approximated amount of BPA input in certain locations. The performance of the model was evaluated using the coefficient of determination or R-squared (R^2) of the simulated vs. actual values in a 45-degree or one-one plot. Other parameters taken into consideration were Nash-Sutcliffe efficiency (NSE) and percent bias (PBIAS). The outliers were determined using the Inter Quartile Range (IQR) method. The efficiency of the model was assessed through the Nash-Sutcliffe efficiency which is expressed as

Equation 1

$$NSE = 1 - \left(\frac{\sum (S_i - A_i)^2}{\sum (A_i - \bar{A}_i)^2} \right)$$

where
S = simulated value and A = actual value

An NSE value equal to one (NSE = 1) means the simulated values and actual values matched perfectly (Somura et al., 2012). For NSE values less than 0.5 (NSE < 0.5) the model is considered as unacceptable. The model is good for NSE values greater than 0.6 ($0.6 < NSE \leq 0.8$) and when NSE values are greater than 0.8 (NSE > 0.8), the model is excellent (García et al., 2008). The tendency of the model towards underestimation or overestimation is determined using percent bias (PBIAS) which is computed using the following equation:

Equation 2

$$PBIAS = \frac{\sum_{i=1}^{n} (A_i - S_i) \times 100}{\sum_{i=1}^{n} (A_i)}$$

where
S = simulated value and A = actual value

The optimal PBIAS value is zero (PBIAS = 0). When PBIAS is greater than zero (PBIAS > 0), the model tends to predict values lower than the observed data. When PBIAS is less than zero (PBIAS < 0), the model is likely to predict values higher than the observed data (Pak et al., 2015; UP-TCAGP, 2015).

3. Results and Discussion

Model calibration and validation

The calibration of the BPA transport model was done using the BPA concentration data collected in the upstream and downstream sampling locations in year 2021. The validation of the model was made using the BPA concentration data of the water samples gathered during the fieldwork in 2018. The R-squared (R^2), NSE, and PBIAS values of the calibration and validation of the BPA transport model are shown in **Table 2**.

Table 2. Statistical Parameters of the Transport Model

Year	Location	R^2	NSE	PBIAS
2021	Upstream of Main Pampanga River	0.9763	0.9047	14.19
2021	Downstream of Main Pampanga River	0.9064	0.5929	19.21
2018	Main Pampanga River	0.8489	0.7327	7.825

The NSE values of the calibration and validation of the BPA transport model are all greater than 0.5, thus, the model performance is considered as acceptable. Meanwhile, the R^2 values of the calibration and validation of the BPA transport model are greater than 0.8 which shows that it has a good fit with the observed data points. Lastly, the PBIAS values of the calibration and validation of the BPA transport model are positive which means that the simulated BPA concentration values are underestimated.

4. Conclusions

In this study the predictive BPA transport model was developed using the flows from the hydrologic model and by employing estimated BPA loads based on literature data. The statistical parameters of the calibration and validation of the BPA transport model show that the model is acceptable (NSE > 0.5) with good fit relative to observed data points (R-squared > 0.8). The PBIAS values are also between – 25 and + 25, which satisfy the criteria for model accuracy.

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