18th World IMACS / MODSIM Congress, Cairns, Australia 13-17 July 2009
http://mssanz.org.au/modsim09

Investigation of monitoring designs for water quality assessment

Erechtchoukova, M.G.[1] and P.A. Khaiter[1]

[1] *Atkinson Faculty of Liberal and Professional Studies, York University, Canada*
Email: marina@yorku.ca

Abstract: The concept of water availability refers not only to the quantity of this vital natural resource but also to its quality, which makes the resource available for a certain use. It implies the necessity to evaluate the quality of water in natural sources. Traditionally, water quality is described by a set of parameters – measurable variables reflecting physical, chemical, and biological characteristics of the aquatic environment. The values of these parameters are obtained through direct observations, analysis or computations. The main source of observation data is various monitoring systems supplying raw data for water quality assessment at different levels ranging from local to global and for a diverse set of scientific or management objectives.

The effectiveness of a monitoring system must reflect the extent to which the data supplied by the system meet monitoring objectives, i.e. provide reliable estimates of selected water quality indicators. Statistically, the reliability of the estimator refers to the level of uncertainty in the estimate expressed as a ratio of its variance. The latter depends on mathematical properties of the formula or model used and a data set available for the estimation. Samples have to be collected in accordance with a monitoring design. The design has to reflect potential data uses as well as to provide reliable data for decision making.

The two types of water quality indicators, the annual average concentration and the total annual chemical load, are considered in the paper for weighing different temporal designs. The two sampling strategies – simple random sampling and stratified random sampling are applied to developing monitoring designs. Since a sampling strategy assumes the selection of both an estimator and a design which makes the estimator efficient, the selected water quality indicators have been evaluated using the simple estimators of the mean and the total and the stratified mean and the stratified total of the investigated data.

The monitoring designs were developed to evaluate the annual average concentrations and the total annual loads of chloride and hydrocarbonate ions in the cross-section Vyatskiye Polyany, the Vyatka River. Chloride and hydrocarbonate ions were chosen as water quality parameters of interest mainly due to the availability of long series of daily water discharges and relatively detailed sets of concentrations. The selected series of water discharges, concentrations and instantaneous loads exhibit different variability. Although water flow affects the dynamics of the constituents to a great extent, there are also other processes contributing notably to the constituent levels in the water column.

The analysis of data presented in the paper provides insights into enhancements of existing monitoring systems and utilization of the data supplied by these systems. In many monitoring sites, samples are collected with the frequencies insufficient for water quality estimates with a declared 10% target of the errors. Stratified random strategies generate designs with fewer total numbers of observations, but the recommendations for sampling derived from these designs may be hard to follow. The stratification is important when the specified level of uncertainty is low. The difference in the numbers produced by stratified and non-stratified strategies becomes negligible when the uncertainty level goes up to 20%. If the high uncertainty of the estimates is acceptable, the simple random sampling strategy can be recommended.

Keywords: *Water quality, monitoring design, water quality indicator*

1. INTRODUCTION

Water sustainability and the extent to which water management is sustainable have become an essential factor of the societal development. The American Society of Civil Engineering has suggested to evaluate sustainability of water resource management through the notions of current and future welfare outcomes (Loucks and Gladwell, 1999). A decision is sustainable if it assures the non-negative dynamics of welfare guaranteeing no long-term decrease in the welfare level of future generations. An evaluation of the welfare function, including marketed and non-marketed goods and services generated by the aquatic environment, suggests the application of the environmental accounting approach.

Traditionally, the water accounting method was used to analyze and present information about volumes of water in the environment related to economic aspects of water supply and consumption. Estimations of available water quantity employed hydrological characteristics of a water body. These hydrological data coupled with relevant economic estimates support an integrated approach to a range of environmental and societal issues (ABS, 2000). However, water availability depends not only on its quantity, but also on the quality of the resource. Only water of a certain quality is suitable for a designated use. Water quality is described by a set of parameters reflecting physical, chemical and biological characteristics of a water body. Values of these parameters along with estimated volumes of water must be taken into account in measuring environmental performance exceeding regulating standards (Yakhou and Dorweiler, 2004).

Values of water quality parameters can be obtained by direct observations or measurements implemented under a certain program. The long-term standardized measurements, observations, evaluation, and reporting of the aquatic environment in order to define status and trends of a water body are called monitoring. Monitoring systems have a complex infrastructure supporting all of their sampling and data processing activities. Monitoring systems comprise several components related to different aspects of their functioning. These components include the collection and analysis of physical, chemical, and biological data, as well as quality assurance and control programs which ensure that the data are scientifically valid. A key component of a monitoring system is its network of sampling sites where water quality observations and measurements are conducted. Monitoring activities are always limited by financial and logistics constraints. At the same time, the systems must provide sufficient data for a wide range of scientifically valid conclusions. Thus, the issues of possible improvements, increased efficiency and/or optimization of a monitoring system in general, and a monitoring design, in particular, are urgent.

The paper considers temporal monitoring designs for water quality assessment and their ability to support estimates of interest with a desired level of uncertainty.

2. APPROACHES TO MONITORING DESIGN

The design of a monitoring system significantly depends on monitoring objectives identified for a given area of a watershed. In general, the objectives include such common tasks as determination of water quality standards to be attained, attainment of the standards, identification of impaired waters, as well as causes and sources of water quality impairments and detection of long-term trends (USEPA, 2003). Data collection must be conducted in accordance with a proposed monitoring design. The monitoring design has to reflect these objectives as well as to provide reliable data for decision making. The extent, to which collected data represent the real state of the aquatic environment, depends on a chosen spatial and temporal monitoring resolution determined by the sampling program. That is why its selection is important for many tasks of environmental assessment.

There are four important design considerations enclosed with the development of an efficient monitoring network which can meet the required monitoring objectives. The issues include detecting what needs to be measured or observed, how it should be implemented, where it needs to be measured or observed, and when (i.e., how often) observations and measurements have to be performed. The answer to the first question identifies a list of water quality parameters which will be tracked by the system. The second question helps to select appropriate measurement tools and analytical methods. The last two questions determine the spatial and temporal location of the observation points.

There are several approaches to a monitoring design. A fixed station approach assumes that the same sites are repeatedly sampled at regular time intervals over a long period of time. Short-term monitoring is a specific study which investigates particular water quality problems and creates a ‘snapshot’ of the conditions in a given area. A rotating-basin approach is based on intensive short-term surveys conducted periodically. It may identify changes in water quality conditions over time. In a probability-based approach, sites are selected randomly from the total set of sites on water bodies in a selected area. An exhaustive approach requires sampling or surveying of all water bodies in the area. A tiered approach (USEPA, 2003) is adopted in many monitoring systems. The approach requires identification of a core set of water quality parameters which reflect designated uses and can be monitored routinely to assess attainment with applicable water quality standards. In addition to the core set of parameters of the aquatic environment, it is also necessary to identify supplemental parameters dictated by the site or project specific needs. In general the selection of variables to be measured depends on monitoring objectives, site specific water quality issues and designated uses of interest which may result in significant variations of core sets for different sites across an investigated region. A consensus on core sets of parameters is strongly desirable since it creates compatible and sharable data sets for a large scale analysis and data generalization (WQTG, 2006). Water quality parameters from the core and supplemental sets are observed with different frequencies at the same site. Moreover, core parameters can be observed with different frequencies at different cross-sections of the same section of the natural stream because of the importance of a particular location. Strictly speaking, no single approach is sufficient to provide the data for all information needs. To meet the objectives, monitoring systems integrate several designs or programs of observations. Thus, fixed station approach along with tiered monitoring design coupled with sampling programs reflecting environmental heterogeneity is useful for the long-term trend detection, for assessment of critical reaches of large streams, and at the same time it provides site-specific water-quality data.

For many tasks of water quality assessment, relatively long series of values for water quality parameters are required. Due to budgetary constraints, existing recommendations prescribe as few as 4 – 6 observations at some monitoring sites or 6 – 12 samples over a three-year period (Statistics Canada, 2008). At the same time, the systems are expected to provide sufficient data for a wide range of scientifically valid conclusions with the level of errors not exceeding 10%.

3. DEVELOPING A TEMPORAL MONITORING DESIGN

Monitoring systems operate under limited budgets. Groot and Schilperoort (1983) suggested to express the effectiveness of a monitoring design as a function of frequencies of observations, the number and location of sampling sites, and the number and kind of observed constituents. The same variables affect the cost of the monitoring program. Thus, an efficient monitoring design can be found by weighing the effectiveness against its cost. The cost of a monitoring design is assumed to increase monotonically with the number of samples collected at the monitoring sites and the number of sites. Hence, the efficiency of a monitoring design relates to the required number of samples. Focusing on temporal monitoring designs at a given site, the current study uses the number of samples collected at a given site as a measure of the design cost.

The effectiveness of a monitoring system must reflect the extent, to which the data supplied by the system meet monitoring objectives, i.e. provide reliable estimates of selected water quality indicators. Statistically, the reliability of the estimator refers to the level of uncertainty in the estimate. There are several sources of the uncertainty in the estimates obtained from monitoring data. They can be classified into data uncertainty and model uncertainty (Erechtchoukova and Khaiter, 2008). Data uncertainty comprises observational artifact and uncertainty due to a discretization. Observational artifact is caused by measurement tools and analytical methods used in the laboratories in order to obtain values of environmental indicators. Although some improvements in the results are possible, this type of errors is always present in monitoring data (Harmel et al., 2006). Monitoring data present a discrete approximation of continuous fields of values of water quality parameters. The fields are described by aggregate characteristics over a certain neighbourhood of observation points in space and time obtained through the calculations on discrete data. Model uncertainty is added at the stage of data processing. Traditionally, monitoring data are processed based on statistical estimators whose uncertainty is measured as a ratio of its variance. The latter depends on mathematical properties of the formula or model used and a data set available for the estimation. It is known, that the larger the data set used the lesser the variance of the estimates. At the same time, the distribution of observation points over an investigated period is also a factor affecting the reliability of the estimate. Hence, a design incorporates both a number of required observations and their distribution over a specified period of time.

Processing of monitoring data focuses mainly on relationships among water quality parameters, comparisons with standards and setting the confidence bounds on values of aggregate indicators describing status of water bodies before and after an anthropogenic impact. For a comprehensive analysis, a monitoring design has to ensure that collected samples unambiguously represent real water system characteristics (Overton and Stehman, 1995). Two types of water quality indicators, the annual average concentration and total annual chemical load, are further considered in the paper for weighing different temporal designs. Stream chemical load is the total mass of a chemical constituent passing through the stream cross section over a given period of time. Load amounts can be calculated by employing different approaches. The overview of these approaches and their classification are available (e.g., Aulenbach and Hooper, 2006).

Ideally, a monitoring design should be constructed for a particular objective which implies the selection of indicators and their estimators. The estimators should be built on the same mathematical assumptions as those that determine an appropriate monitoring design. However, numerous examples indicate that objectives change between the time a monitoring design is developed and the time it is applied for data collection. Moreover, data collected for one set of objectives can be used for an analysis which was not even considered at the planning stage. Following Overton and Stehman (1995), utilization of monitoring data for various types of data analysis requires simple sampling designs.

For many natural streams and reservoirs, seasonal variations in hydrological and hydrochemical regimes are typical. The variations allow to delineate distinct hydrological seasons and to suggest the application of stratified monitoring designs. A stratified estimator of a water quality indicator outperforms a non-stratified one, if the variance of the selected indicator within the strata is less than its variance between the strata (Cochran, 1963). The two sampling strategies – the simple random sampling and the stratified random sampling have been used to derive monitoring designs supporting reliable estimates of the selected water quality indicators. Since a sampling strategy assumes the selection of both an estimator and a design which makes the estimator efficient, the chosen water quality indicators have been evaluated using the estimators of the non-stratified mean and the non-stratified total and the stratified mean and the stratified total of the investigated populations.

The uncertainty of an estimator *X* can be expressed as an allowable deviation of its value calculated on available data from the actual value of the investigated water quality indicator *I*:

$$\Pr\{|x - I| \le d\} = 1 - \alpha , \tag{1}$$

where x is the estimate of I from the collected data, d is the allowable deviation, α is the level of confidence. Following Cochran (1963), under the assumption that x is normally distributed, the deviation d can also be expressed in terms of the variance of the estimator of X:

$$d = U_{1-\alpha}\sigma_X , \tag{2}$$

where σ_X^2 is the variance of x, and $U_{1-\alpha}$ is the normal deviate corresponding allowable probability $1-\alpha$ that the error won't exceed the desired margin. The formula for the variance of the estimator depends on the statistical properties of X. Combination of formulae (1) and (2) with the expression for the variance of X gives the formula for the number of observations required to achieve the desired value of d which can be interpreted as established level of uncertainty.

4. CASE STUDY

The monitoring designs were developed for the evaluation of annual average concentrations and total annual loads of chloride and hydrocarbonate ions in the cross-section Vyatskiye Polyany, the Vyatka River. It is worth to note that testing the designs requires very detailed data which are very difficult to obtain. The Vyatka River is a large Eastern-European river located in the Kirov Oblast (Region) and the Republic of Tatarstan in the Russian Federation. Its length is about 1,370 km and the watershed area is 129,000 km^2. The average water discharge is as high as 700 m^3/s. The hydrological regime is characterized by distinct seasonal variations with high flow events in spring and fall and lower water seasons in summer and in winter. Chloride and hydrocarbonate ions were chosen as water quality parameters of interest mainly due to the availability of long series of daily water discharges and relatively detailed sets of concentrations. Observed concentrations

Table 1. The required monitoring designs for the annual average concentration (*C*) and the total annual load (*L*) based on non-stratified random strategy

Constituent	Indicator	Total number of observations to keep the uncertainty of the estimate below			
		5%	10%	15%	20%
Cl	C	120	40	19	11
	L	274	157	92	58
HCO3	C	85	26	12	7
	L	244	122	67	41

varied in different samples from 0.5 to almost 8.0 mg/l for chloride ions and from 47.0 to 224.0 mg/l for hydrocarbonate ions. In order to obtain the accurate value of the annual load, concentrations measured with at least daily frequency are required. Missing values of concentrations were surrogated by monotonic interpolation between two consequent observations. At the investigated cross-section, the annual average concentration of chloride ions has been estimated as 4.21 mg/l with the annual load of this water constituent of 63,907 t. Hydrocarbonate ions are characterized by the average concentration of 161.6 mg/l and the annual load of 2,465,922 t.

The selected series of water discharges, concentrations and instantaneous loads exhibit different variability. The most variable parameter is the water discharge with the coefficient of variation of 1.31 compared to 0.34 for the concentrations and 0.85 for the instantaneous loads of chloride ions and to 0.27 for the concentrations and 0.69 for the instantaneous loads of hydrocarbonate ions. Although water flow affects the dynamics of the constituents to a great extent, there are other processes contributing notably to the constituent levels in water column.

The total numbers of observations over a year for simple random sampling strategy were determined for different levels of uncertainty in the estimates of average concentrations and chemical loads (see Table 1).

Seasonal variations in water discharges and concentrations of investigated water quality parameters suggested the application of stratified estimates. The temporal stratification was implemented manually according to the water discharger (scheme A), concentrations of the chloride ions (schemes B_1) and hydrocarbonate ions (scheme B_2), and instantaneous chemical loads of chloride ions (schemes C_1) and hydrocarbonate ions (scheme C_2). It is worth to note, that only the stratification implemented based on the hydrograph was common for both constituents. This scheme consists of four strata corresponding to the main hydrological seasons. The series of concentrations and instantaneous loads were also split into four strata with boundaries determined from the values of the parameters. These strata are both constituent and indicator specific. The stratifications used for calculations are reasonably good, but are not optimal, since the main goal was to obtain preliminary estimates of the numbers of samples required to get reliable conclusions. The summary of the designs is presented in Tables 2 and 3.

Table 2. The required monitoring designs for the annual average concentration (*C*) and the total annual load (*L*) of the hyrocarbonate ions based on stratified random sampling strategy

Con-stitu-ent	Uncer-tainty	Strata				Total
		I	II	III	IV	
Scheme A						
Duration, days		306	8	32	19	365
C	5%	25	3	25	10	63
	10%	7	1	15	4	27
	15%	3	1	9	2	15
	20%	2	0	6	1	9
L	5%	89	6	26	14	108
	10%	29	4	17	8	58
	15%	13	2	11	5	31
	20%	8	2	7	3	20
Scheme B_2						
Duration, days		205	64	47	49	365
C	5%	10	13	28	1	52
	10%	3	4	13	1	21
	15%	1	2	7	1	11
	20%	1	1	4	0	6
L	5%	40	49	27	38	154
	10%	12	29	12	23	76
	15%	5	17	6	14	42
	20%	3	11	4	9	27
Scheme C_2						
Duration, days		304	14	20	27	365
C	5%	26	14	17	17	74
	10%	7	12	13	7	39
	15%	3	11	9	4	27
	20%	2	9	6	2	19
L	5%	72	9	7	7	96
	10%	22	4	2	2	30
	15%	10	2	1	1	14
	20%	6	1	1	1	9

5. DISCUSSION

All the monitoring designs presented in Tables 1, 2 and 3 are sufficient for the estimation of the selected water quality indicators with the specified level of uncertainty. The designs prescribe the total numbers of required observation which deviate significantly. The deviations can be explained by main factors affecting the designs: variability of an investigated water quality parameter, the selected indicator and its estimator.

As it was expected, the largest numbers of observations are required for estimation of the chemical loads of chloride ions, since it is the most varying indicator in the study. Overall, the total numbers of observations required for evaluation of chemical loads surpass those sufficient for accurate calculation of the annual average concentrations by almost two and a half times. This result is consistent with the higher variability of the stream load of an constituent compared to its concentration, since both the concentration and water discharge contribute to changes in load values. Strictly speaking, a further reduction of the total numbers of observations required for the stream load calculations is possible by employing other statistics which outperform sample mean, such as regression curves or ratio estimates (Erechtchoukova and Khaiter, 2007), but the numbers still remain high.

Temporal stratification can significantly reduce the total numbers of observations required for the estimates of the selected indicators with a given level of uncertainty. At the same time, temporal stratified designs create additional obstacles in data collection since they require switching the frequencies of sample collection over an investigated period. The stratum boundaries must be determined *a priori*, whereas dates of typical hydrological and hydochemical events vary from year to year making the stratification very inaccurate and corresponding recommendations hard to follow due to a human factor. Another issue relates to multiple stratification criteria. For a single water quality parameter and its two indicators, three factors can be considered which generates three schemes with different stratum boundaries. Given that concentrations of several water constituents are usually determined from the same water sample, a few stratification schemes must be compromised into one with the increased number of required observations for some of the constituents. Although investigation of several stratification schemes for a monitoring design may suggest a more efficient scheme, temporal stratification based on hydrograph seems reasonable for natural streams with distinct hydrological seasons. In such streams, hydrological processes significantly affect the dynamics of concentrations of constituents in a water column, and changes in hydrological seasons can be easily noticed.

Table 3. The comparison of the monitoring designs for the annual average concentration (*C*) and the total annual load (*L*) of the selected water constituents

Constituent	Stratification scheme	Indicator	Total number of observations to keep the uncertainty of the estimate below			
			5%	10%	15%	20%
Cl	A	*C*	96	36	19	11
	B_1	*C*	86	34	18	11
	C_1	*C*	138	68	41	28
	A	*L*	108	58	31	20
	B_1	*L*	200	113	72	52
	C_1	*L*	106	39	20	13
HCO_3	A	*C*	63	27	15	9
	B_2	*C*	52	21	11	6
	C_2	*C*	74	39	27	19
	A	*L*	108	40	22	13
	B_2	*L*	154	76	42	27
	C2	*L*	96	30	14	9

As it is shown in Tables 1 and 2, the stratification is important when the specified level of uncertainty is low. The difference in the numbers produced by stratified and non-stratified strategies becomes negligible when the uncertainty level goes up to 20%. Such level of uncertainty requires as few as 9 - 11 observations per year for both stratified and non-stratified designs. The latter ones are much easier for practical applications. Since many monitoring systems cannot perform extensive sampling due to budgetary and logistics constraints, the non-stratified strategies become preferable.

In all considered stratification schemes, the uncertainty of the estimates can be reduced to 10% only by intensive data collection of 20 or more samples per year, which corresponds to a twice a month frequency of observations. Data collected according to programs with lower frequencies cannot support a high level of reliability of the estimates.

The designs presented in the Tables 1, 2, and 3 suggest the numbers of observations obtained *a posteriori*. The designs will guarantee the specified level of uncertainty only for the years when investigated indicators will exhibit similar variability. Usually, the series of water discharges and concentrations are not known in advance. That is why data should be collected with frequencies higher than those shown in the Tables 1, 2, and 3.

6. CONCLUSIONS

Water accounting requires a thorough and consistent approach to identifying, measuring, recording and reporting water related information. Understanding the reliability of data and the quality of the estimates they may produce is important for sustainable water resource management. In many cases, water quality monitoring is the main source of data for water related decisions. The analysis of data presented in the paper provides insights into enhancements of existing monitoring systems and utilization of the data supplied by these systems.

In many monitoring sites, samples are collected with the frequencies insufficient for water quality estimates with a declared 10% target of the errors. To achieve the target, more intensive sampling is required. The improvement of the estimates by applying advanced statistical techniques is hardly possible since the techniques require data set with specific properties. Although monitoring designs guaranteeing a certain level of uncertainty can be developed for such estimators, additional constraints on data sets may restrict the data utilization for other objectives.

Stratified random strategies result in designs with fewer total numbers of observations, but the recommendations for sampling derived from these designs may be hard to follow. When such strategies are considered for natural streams, a satisficing temporal stratification can be achieved using water discharge values. If the uncertainty of the estimates of 20% or higher is acceptable, the simple random sampling strategy can be recommended. This strategy generates the data set suitable for a wide range of objectives and is flexible in implementation.

ACKNOWLEDGMENTS

The authors are grateful to anonymous reviewers for their thoughtful suggestions and helpful comments on the manuscript. The study was conducted based on the data sets prepared in Hydrochemical Institute, the Russian Federation.

REFERENCES

ABS (Australian Bureau of Statistics) (2000), Water Account for Australia, 1993-94 to 1996-97. ABS Cat. No.4610.0.

Aulenbach, B.T. and Hooper, R.P. (2006), The composite method: An improved method for stream-water solute load estimation. *Hydrological Processes*, 20, 3029-3047.

Cochran, W.G. (1963), Sampling Techniques, 2nd ed., John Wiley, 413 pp., New York.

Erechtchoukova, M.G. and Khaiter P.A. (2007), Uncertainty reduction in modelling of chemical load in streams. In: Oxley, L. and Kulasiri, D. (eds.) MODSIM 2007 International Congress on Modelling and Simulation. Modelling and Simulation Society of Australia and New Zealand, December 2007, 2445 - 2451.

Erechtchoukova, M.G. and Khaiter, P.A. (2008), Role of models for building an efficient monitoring design. In: Miquel Sànchez-Marrè, Javier Béjar, Joaquim Comas, Andrea E. Rizzoli, Giorgio Guariso (eds.) Proc. of the iEMSs Fourth Biennial Meeting: International Congress on Environmental Modelling and Software (iEMSs 2008). International Environmental Modelling and Software Society, Barcelona, Catalonia, July 2008, 528-535.

Groot, S. and Schilperoort, T. (1983), Optimization of water quality monitoring networks. *Water Science and Technology*, 16, 275-287.

Harmel, R.D., Cooper, R.J., Slade, R.M., Haney, R.L., and Arnold, J.G. (2006), Cumulative uncertainty in measured streamflow and water quality data for small watersheds, *Transactions of the ASABE*, 49(3), 689-701.

Loucks, D.P. and Gladwell, J.S., (eds.) (1999), Sustainability criteria for water resource systems, Cambridge University Press, 139 pp., Cambridge, UK.

Overton, W.S. and Stehman, S.V. (1995), Design implications of anticipated data uses for comprehensive environmental monitoring programmes. *Environmental and Ecological Statistics*, 2, 287-303.

Statistics Canada (2008), Canadian environmental sustainability indicators 2007: Freshwater quality indicator. Data sources and methods. (Cat. N 16-256-X), online URL: http://www.statcan.gc.ca/pub/16-256-x/16-256-x2008000-eng.pdf.

US Environmental Protection Agency (USEPA) (2003), Elements of a state water monitoring and assessment program (EPA 841-B-03-003), online URL: http://www.epa.gov/owow/monitoring/elements/index.html.

Water Quality Task Group (WQTG) (2006), A Canada-wide framework for water quality monitoring. PN 1369, online URL: http://www.ccme.ca/assets/pdf/wqm_framework_1.0_e_web.pdf.

Yakhou, M. and Dorweiler, V.P. (2004), Environmental accounting: an essential component of business strategy. *Business Strategy and Environment*, 13, 65–77.