DEVELOPMENT OF A SOFTWARE PACKAGE FOR TREND DETECTION IN TEMPORAL SERIES: APPLICATION TO WATER AND INDUSTRIAL EFFLUENT QUALITY DATA FOR THE ST. LAWRENCE RIVER

DANIEL CLUIS

INRS-Eau, Box 7500, Ste. Foy, QC G1V 4C7, Canada

CLAUDE LANGLOIS

Environment Canada, Inland Waters and Lands Directorate, Quebec region, 1001 Pierre Dupuy, Longueuil, J4K 1A1, Canada

RAYMOND VAN COILLIE

Environment Canada, Environmental Protection Branch, Quebec region, 1179 Bleury St., Montreal, H3B 3H9, Canada

and

CLAUDE LABERGE

INRS-Eau, Box 7500, Ste. Foy, QC G1V 4C7, Canada

(Received April 1989)

Abstract. Despite the considerable amount of effort and resources involved in monitoring water quality, water quality assessment and environmental follow-up are sometimes carried out with simple statistics, the main reason being the lack of appropriate statistical methods adapted to the nature of sampled water quality data.

A survey of the classical methods used for trend detection and of their limitations is first presented, including the most recent non-parametric techniques adapted to the structure of the sampled data and to the possible types of trends occuring. This paper then presents an interactive user-friendly software package developed for microcomputers making use of these latest adapted techniques. Afterwards, some applications of the software are described pertaining to the concentrations measured at long-term stations on the St. Lawrence River and to the mass loadings discharged by regulated industries. Finally, conclusions are drawn about the assumptions, performance and limitations of the package as well as about the research needs to improve the usefulness and applicability of the software.

1. State of Knowledge

Follow-up environmental studies are an essential step in the objective assessment of the efficiency of any sanitation program. These are often neglected, despite the large amount of public money involved. Are the effluent loadings reduced? Is the quality of the target water improving? Water and effluent quality data (concentrations and loads) have characteristics which make the application of classic statistical methods difficult and therefore general statistical packages cannot be used. Most trend detection tests assume that the data are normally distributed and temporally independent, while water quality data are rarely normally distributed or independent. An

Environmental Monitoring and Assessment **12**: 429–441, 1989.

example of non-stationarity is the presence of seasonality which can be seen in many water quality data sampled at regular intervals (bi-weekly or monthly for example). Data collected at such intervals exhibit persistence or partial redundancy (non-independence). The sampling frequency often leads to difficulties in using standard time series techniques such as the Box and Jenkins type. Water quality data also have widely asymmetric distributions, often closer to log-normal than to normal. In addition, the presence of outlying, censored or missing values make analysis even more difficult.

Statistical problems related to non-normality and unequal variances are well documented (Scheffé, 1959); more recently, Montgomery and Loftis (1987) studied in addition the effects of temporal persistence, seasonal fluctuations and unevenly spaced samples on the results obtained using Student's *t* test. They showed that the test should not be used if the samples have different distributions, or if they have unequal variances or lengths. In addition, seasonal variations or temporal persistence invalidate the results. Thus, this classical parametric test cannot be used to detect water quality trends.

Recently, non-parametric methods have been used, where rank and not the shape of the distribution is important in detecting water quality trends, thus reducing the effects of outliers. Helsel (1987) has reviewed these methods and found the following advantages: (a) data transformation is not necessary, (b) unlike analysis of variance, the test results are reliable even for samples that are not normally distributed, (c) the power of the tests remains very good, even if the distribution is asymmetrical, as is common in water quality data, (d) data below the detection limits of a chemical test are not introduced as fictitious values and therefore do not bias the results.

Classical non-parametric tests (Conover, 1971), also have their problems, as other characteristics of hydrological data, such as seasonality and persistence, reduce their effectiveness in trend detection. Although classical tests such as the Mann-Whitney and Spearman tests are very useful for the detection of monotonic or stepwise trends, they do not address the problems of temporal persistence and seasonal fluctuations found in water quality data. In the last 15 years, a number of authors have attempted to adapt non-parametric tests to allow trend detection, without being influenced by other types of short-term interdependence. The method used is the reverse of the decomposition of the Box-Jenkins method in which a shot-term structure is obtained by making the series stationary and identifying the seasonal fluctuations. Two particular trend types are used in this method. The first is a stepwise trend calculated by dividing the data into two parts determined by the date of change. The mean levels before and after this date are compared using the Mann-Whitney test, or a suitable modification, to determine if they are different. The second trend type is a progressive, monotonic modification of the series level with time. Spearman's or Kendall's test (or a suitable modification) is applied, using time as the second variable.

Lettenmaier (1976) has adapted these non-parametric tests for the detection of long-term trends, taking into account the short-term dependency (persistence) of the data. While allowing for the interdependence of successive data, Lettenmaier used the effective number of observations and Information Content concepts to allow the use of the Mann-Whitney and Spearman tests.

Hirsch *et al.* (1982) have looked at the problems related to seasonal fluctuations present in the vast majority of hydrological series. Kendall's test (Lehmann, 1975) is used for each seasonal sub-series. The resulting statistics are added together and used to determine if a trend is present. Unfortunately, this test cannot be used when a series has persistence as well as seasonal fluctuations. Hirsch and Slack (1984) and Van Belle and Hughes (1984) investigated this problem, while the latter presented a new method for determining if a trend is caused by a particular season. As the advantages of these non-parametric tests became recognized, Lettenmaier *et al.* (1982) incorporated them into a program for use on mainframe computers.

Once the structure of the series is known, the appropriate test for the trend type may be chosen with the aid of a decision tree. Table I shows that with the presence of seasonal fluctuations, the seasonal Kendall and the Hirsch and Slack test are recommended even for a stepwise trend model. An appropriate modification of the Mann-Whitney test would appear more appropriate; unfortunately, these modifications are not found in the literature. It is essential that the structure of the data be properly identified so that the appropriate tests are used. Using a seasonal test on data that are not seasonal, for example, will lead to a significant loss of power.

Another essential element that must be evaluated is the type of trend exhibited by the data (monotonic or stepwise) and the approximate dates of the changes. Retrospective graphical techniques such as Double-Mass and CUSUM functions (Cluis, 1983) are used to obtain this information while the results obtained are not affected by the presence of persistence or seasonal fluctuations. Even if the Double-Mass technique has been used effectively with meteorological and hydrological series to reveal homogeneity where persistence was present (Searcy and Hardison, 1960), the software puts the emphasis on the analysis of the CUSUM graphs which prove to be more sensitive. These visual techniques are used as preliminary analytical tools in the software package described later.

TABLE I

Decision tree for the choice of test

Model	Persistence	Seasonal fluctuations	Appropriate test
Monotonic trend	Markovian	no seasons	Lettenmaier/Spearman
		with seasons	Hirsch and Slack
	none	no seasons	Spearman of Kendall
		with seasons	Seasonal Kendall
Stepwise trend	Markovian	no seasons	Lettenmaier/ Mann-Whitney
		with seasons	Hirsch and Slack
	none	no seasons	Mann-Whitney
		with seasons	Seasonal Kendall

A new set of non-parametric tests now exists that are better adapted to the real structure of water quality data. As these tests have only recently been developed, their power has been only partially established (Berryman *et al.*, 1988), and therefore Monte-Carlo simulations must be carried out to validate their performance. Bradley (1968), however, demonstrated that even under the worst conditions, the power of non-parametric procedures varied between 85% and 96% of that of parametric procedures. In fact, when tested with numerous asymmetrical distributions, their power generally exceeded that of traditional methods.

2. Software

An interactive program for the analysis of water quality data was developed for IBM compatible microcomputers using Fortran 77. The software is designed to detect and quantify a single type of change (monotonic or stepwise); in the event of multiple changes over time, successive runs are necessary, each dealing with parts of the series. The software is able to analyze on a single run up to 1500 data points spread over more than a year. Statistical as well as graphical output is supplied to the user. The program is composed of stand-alone modules which are executed in succession, using a series of intermediate data files to transfer the results downstream from the first modules.

MODULE 1: Data to be analyzed are acquired by this module:

– requests can be sent to or received from the NAQUADAT data bank (the Canadian national storage and retrieval bank for water quality data) in Ottawa via the DATAPAC network (a dedicated telephone network for data exchange).

– requests for flow measurements for the St. Lawrence River can be sent to or received from the HYDAT data bank (the Canadian national storage and retrieval bank for discharge and water levels).

– data can be entered manually at the console if necessary.

MODULE 2: This module reads the input data obtained in module 1 (concentrations or loads) and creates a file of the appropriate form to be used in subsequent modules.

MODULE 3: This module allows the user to eliminate values judged to be outliers. A first estimate of the type of trend present is made using different CUSUM and Double-Mass curves chosen from a menu. Care must be taken, however, as at this stage the shapes of the curves can be affected by any unevenly spaced observations.

MODULE 4: This module analyzes the sampling frequency and allows the elimination of any years or months which may bave been poorly sampled or not sampled at all. The equality of the means of the different seasons (composed of groups of months) is tested with an analysis of variance to identify any homogeneous seasons. Finally, the module determines if there is a relationship between concentration and flow.

MODULE 5: This module allows the work interval to be chosen, and values are generated for any interval without data. In any interval with more than one observation, the observations are grouped using their mean. Missing data are filled in using temporal interpolation, seasonal mean or a flow-concentration relationship according to the recognized structure. Work intervals, therefore, must be chosen so as to minimize the loss of information due to such regrouping or data reconstruction. Once an equidistant working series has been obtained, this module presents autocorrelation and partial autocorrelation coefficients.

MODULE 6: This module creates the inertia graphic functions (CUSUM and Double-Mass) for the chosen work interval. These graphs allow the user to determine the dates of level changes. If the analysis is being used to determine the effects of the installation of a treatment plant, this a priori information will be used by looking for a stepwise trend on either side of the date of first operation.

MODULE 7: This module provides a synthesis of the data characteristics and chosen options. Information such as the slope of the monotonic trend, date of change, and initial and final levels, is provided by a parametric interpretation of the results.

MODULE 8: This last module analyzes the way two sub-samples (defined by dates, months or flow classes) exceed the norm by comparing their intensity-duration-frequency curves.

3. Case Studies

The first case study involves the phenol loadings discharged in the effluents from two Montreal refineries. The treated loadings are discharged into the St. Lawrence River and as such are subject to the terms of federal Department of the Environment discharge permits. Flow and concentration data were collected on a three-day basis from both industries to allow the verification of their compliance with the regulations. The software package was used to perform a retrospective analysis of these data banks (results are presented in Tables II and III). Both industries showed similar results. For the first refinery, 1030 measurements were taken on a regular basis between January 1978 and December 1985, while at the second, 1168 observations were taken between January 1978 and April 1986. In both cases: (a) the first exploratory modules of the program detected no evident outlier caused either by data transcription or analytical error; (b) the hypothesis of seasonality was rejected by the ANOVA analysis; (c) a one month work interval was used for the rest of the analysis; (d) since the time series for the first industry had observations in every month, no fill-in technique was needed, while for the second industry, twelve observations (year 1981) were given the mean of the corresponding month; (e) autocorrelation of the monthly working series exhibited a Markovian persistence. The CUSUM functions exhibit different trend types. The CUSUM of the first industry (Figure 1) had an abrupt slope change at interval 20 indicating a stepwise trend for the discharged loadings, while the CUSUM of the second industry (Figure 2) was parabolic, characteristic of a monotonic trend. In both cases, the trend seems to be negative, indicating a reduction in the loadings discharged. In the first case, a Mann-Whitney test for non-seasonal persistent data was used to detect a step change

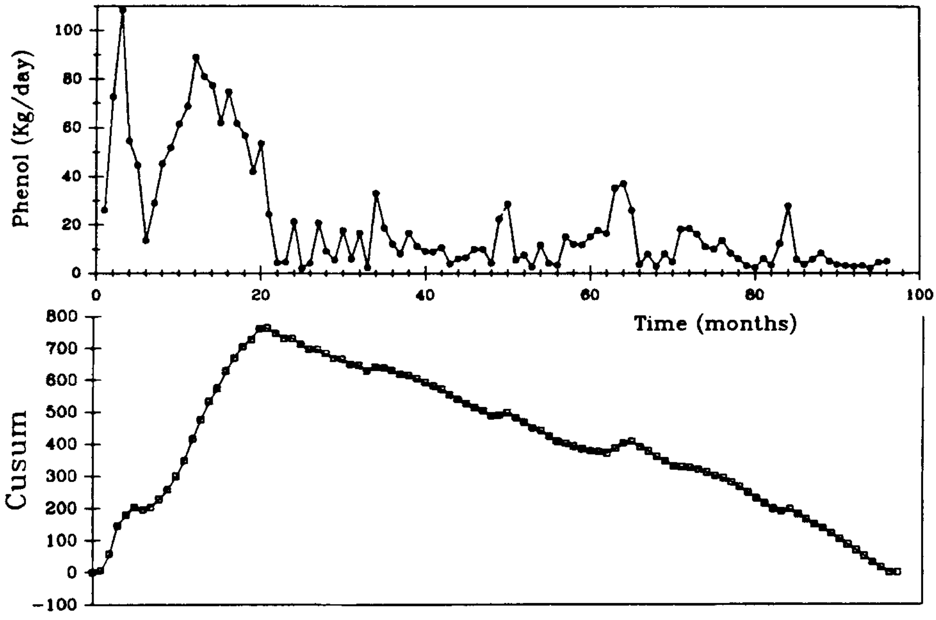

Fig. 1. Time plot and CUSUM of the Phenol effluent for the first refinery (month 1 = January 1978, month 96 = December 1985).

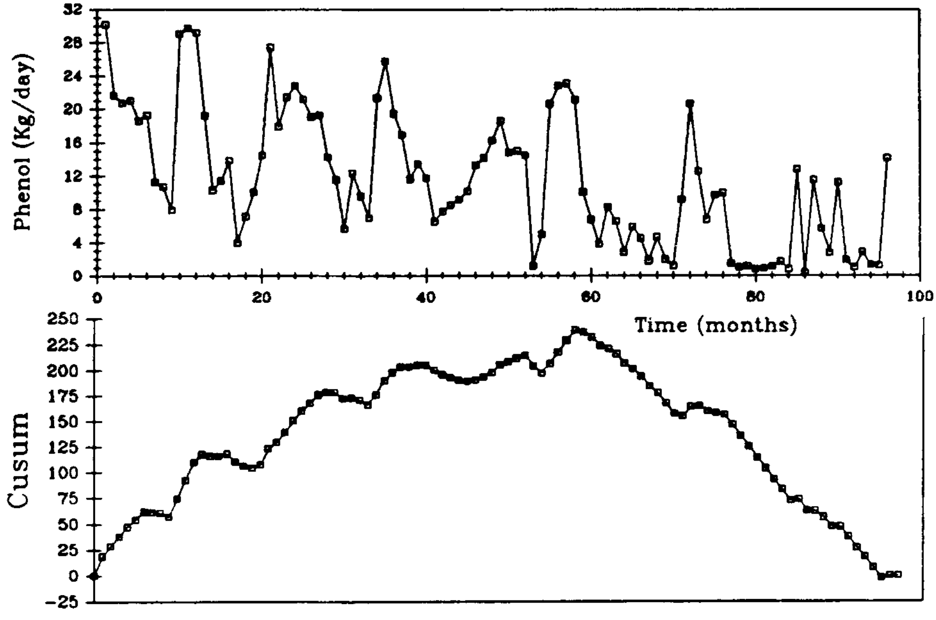

Fig. 2. Time plot and CUSUM of the Phenol effluent for the second refinery (month 1 = January 1978, month 96 = December 1985).

in the mean level of discharged loads. As the data for the second industry exhibited non-seasonality and persistence, the Spearman/Lettenmaier test was used to detect a monotonic trend.

These tests confirmed a significant negative trend for both refineries. The decrease

TABLE II

Summary of the trend analysis for the first refinery

Trend detection			
Name of data file	:	Phenol. dat	
Type of data	:	Mass discharges	
Original data			
First observation	:	1/13/78	
Last observation	:	4/30/86	
Number of observations	:	1168	
Number of low outliers	:	0	
Number of high outliers	:	0	
Low Frequency years	:	none	
Working series			
Starting month	:	1	
Interval (months)	:	1	
Number of intervals in year	:	12	
Persistence	:	Markovian	
Seasonality	:	no	
Starting date	:	1/78 (RK = 1)	
Ending date	:	4/86 (RK = 100)	
Number of data	:	100	
Test			
Suggested	:	Mann-Whitney/Lettenmaier	
Chosen	:	Mann-Whitney/Lettenmaier	
Value of statistic	:	1695	
Test value	:	1.90	
P value	:	.029	
Negative step trend detected			
Approximative date of the step	:	15/8/79	
Associated rank	:	20	
		Before step	After step
Mean	:	59.0 kg d^{-1}	10.3 kg d^{-1}
Stand. dev.	:	22.4 kg d^{-1}	9.2 kg d^{-1}
Stand. dev. mean	:	1.5 kg d^{-1}	0.5 kg d^{-1}
Adequacy of the trend model to data			
RMSE	:	12.80 kg d^{-1}	

TABLE III

Summary of the trend analysis for the second refinery

Trend detection		
Name of data file	:	Phenol2. dat
Type of data	:	Mass discharges
Original data		
First observation	:	1/01/78
Last observation	:	31/12/85
Number of observations	:	1030
Number of low outliers	:	0
Number of high outliers	:	0
Low Frequency years	:	1981
Working series		
Starting month	:	1
Interval (months)	:	1
Number of intervals in year	:	12
Persistence	:	Markovian
Saisonality	:	no
Starting date	:	1/78 (RK = 1)
Ending date	:	12/85 (RK) = 96)
Number of data	:	96
Test		
Suggested	:	Spearman/Lettenmaier
Chosen	:	Spearman/Lettenmaier
Value of statistic	:	−0.633
Test value	:	−3.443
P value	:	.001
Negative monotonic trend detected		
Slope of the trend	:	-2.2 kg d^{-1} yr^{-1}
Estimated initial level	:	20.3 kg d^{-1}
Estimated final level	:	2.9 kg d^{-1}
Adequacy of the trend model to data		
RMSE	:	6.20 kg d^{-1}

in the discharged loadings is illustrated by the parametric results. The mean level of effluent from the first refinery dropped from 59.0 kg day^{-1} before August 1979 to 10.3 kg day^{-1} after that date. The mean level for the second industry decreased gradually from 20.3 kg day^{-1} to 2.9 kg day^{-1} during the eight-year study period.

As these two industries had to comply with a monthly discharge permit 25 kg day^{-1} of phenol, an intensity-frequency-duration analysis was performed on the monthly effluent data. This analysis compares two sub-populations for each studied industry. For the first industry, the two sub-populations were defined using the previously detected date of change (August 1979). While for the second industry, two four-year sub-populations were chosen (the first four years and the last four years).

Tables IV and V indicate these two industries showed improvements in all parts of the study. The decrease in the level of effluent as demonstrated by the reduction in the distribution tails is also seen as a decrease in the frequency of permit violations from 95% to 6% for the first refinery, and from 17% to 0% for the second. Finally, the duration of consecutive monthly exceedances was significantly reduced.

TABLE IV

Intensity – Frequency – Duration analysis of the exceedances for two subsamples associated to the series of the first refinery

Exceedance of standard

Name of data file	:	Phenol. dat.
Type of data	:	Mass discharges
First observation	:	13/1/78
Last observation	:	30/4/86
Number of observations	:	1168
Discharge permit (monthly)	:	25.000 kg d^{-1}

		Sample 1		Sample 2	
Periods	:	1/1978-8/1979		9/1979-4/1986	
Months	:	all		all	
Flows	:	all		all	
Number of data	:	20		77	
Mean values	:	58.7 kg d^{-1}	(21.9)	9.9 kg d^{-1}	(8.0)
Exceedances	:	19	(95%)	5	(6%)
Mean exceed.	:	61.1 kg d^{-1}	(19.8)	31.9 kg d^{-1}	(4.3)
Mean duration	:	9.5 int	(4.5)	1.7 int	(0.9)

Sample distributions

	1.9 – 23.2	23.2 – 44.5	44.5 – 65.8	65.8 – 87.0	87.0 – 108.3 Kg d^{-1}
S 1:	5.0%	15.0%	45.0%	25.0%	10.0%
S 2:	92.2%	7.8%	0.0%	0.0%	0.0%

Exceedances distributions vs permit (P)

	– P	P – 2P	2P – 3P	3P – 4P	4P and more
S 1:	5.0%	25.0%	50.0%	15.0%	5.0%
S 2:	93.5%	6.5%	0.0%	0.0%	0.0%

Duration of exceedances (intervals)

	0 – 1	1 – 2	2 – 3	3 – 4	4 and more
S 1:	5.0%	0.0%	0.0%	0.0%	95.0%
S 2:	93.5%	2.6%	0.0%	3.9%	0.0%

TABLE V

Intensity – Frequency – Duration analysis of the exceedances for two subsamples associated to the series of the second refinery

Exceedance of standard

Name of data file	:	Phenol2. dat.	
Type of data	:	Mass discharges	
First observation	:	1/ 1/78	
Last observation	:	31/12/85	
Number of observations	:	1030	
Discharge permit (monthly)	:	25.000 kg d^{-1}	
		Sample 1	Sample 2
Periods	:	1/1978-12/1981	1/1982-12/1985
Months	:	all	all
Flows	:	all	all
Number of data	:	36	48
Mean values	:	17.1 kg d^{-1} (7.2)	7.5 kg d^{-1} (6.8)
Exceedances	:	6 (17%)	0 (0%)
Mean exceed.	:	28.6 kg d^{-1} (1.5)	—
Mean duration	:	1.5 int (0.9)	—

Sample distributions

	0.3–6.3	6.3–12.3	12.3–18.3	18.3–24.2	24.2–30.2 Kg d^{-1}
S 1:	5.6%	27.8%	13.9%	36.1%	16.7%
S 2:	54.2%	20.8%	12.5%	12.5%	0.0%

Exceedances distributions vs permit (P)

	–P	P–2P	2P–3P	3P–4P	4P and more
S 1:	83.3%	16.7%	0.0%	0.0%	0.0%
S 2:	100.0%	0.0%	0.0%	0.0%	0.0%

Duration of exceedances (intervals)

	0–1	1–2	2–3	3–4	4 and more
S 1:	83.3%	8.3%	0.0%	8.3%	0.0%
S 2:	100.0%	0.0%	0.0%	0.0%	0.0%

The second case study involved dissolved nitrogen (nitrite + nitrate) concentrations in the St. Lawrence River during the years 1980 to 1986. Six stations are considered from west to east as the river flows down: Cornwall and Beauharnois upstream and west of Montreal, Desbaillets and Varennes on the south shore of Montreal Island, Lanoraie and Trois-Rivieres downstream and east of Montreal. Table VI presents a summary of the results from a trend detection analysis using the software.

The trend pattern of the three upstream stations (Cornwall, Beauharnois and Desbaillets) differs from the pattern of the downstream stations. Figure 3 shows the

TABLE VI

Summary results of trend detection of Nitrogen concentrations (1980-1986)

Station	*n*	Test	p Value	Trend type	Parametric results
Cornwall	30	Seas. Kendall	0.0002	M+	0.07 to 0.26 $+0.03\ yr^{-1}$
Beauharnois	36	Kendall	0.0280	M+	0.08 to 0.26 $+0.03\ yr^{-1}$
Desbaillets	29	Kendall	0.0490	M+	0.11 to 0.22 $+0.02\ yr^{-1}$
Varennes	45	Hirsch-Slack	>0.05	NT	0.226 (0.09)
Lanoraie	89	Mann-Whitney	>0.05	NT	0.278 (0.11)
Trois-Rivières	29	Spearman/Lett.	>0.05	NT	0.250 (0.15)

Note: M+ means significant increasing monotonic trend, NT means no significant trend. All parametric results are in mg l^{-1}.

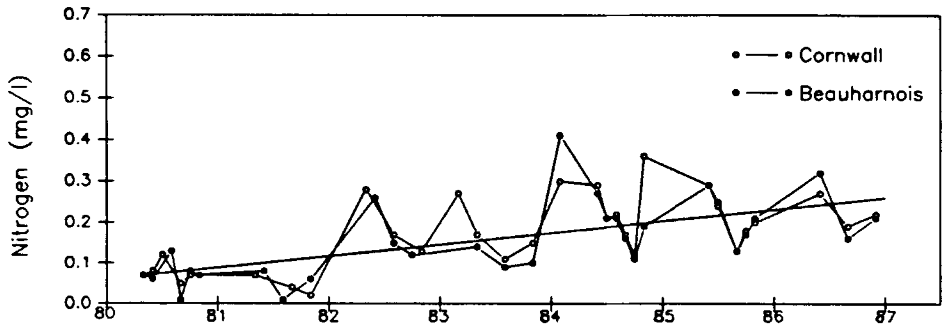

Fig. 3. Time plot (1980-1987) of dissolved nitrogen concentrations for two stations west of the Montreal Island.

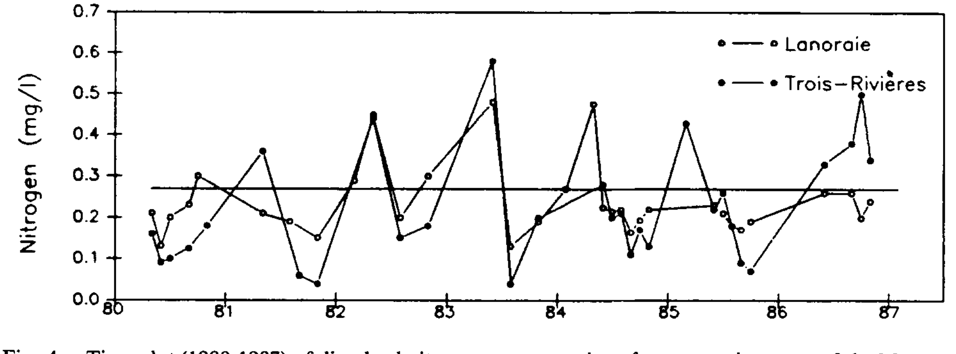

Fig. 4. Time plot (1980-1987) of dissolved nitrogen concentrations for two stations east of the Montreal Island.

series of two stations west of Montreal Island illustrating an important increasing monotonic trend. On the other end, Figure 4 presents the series from two stations east of the Island where no significant trends were detected. Finally, Table VI shows that for stations south of Montreal, lower mean nitrogen concentrations were obtained.

The increased levels of nitrates detected in upstream stations can be related to the increased use of agricultural fertilizers and to the increase in the number of feedlots for cattle and hogs. A similar increase in levels was also noted in Lake Ontario between 1969 and 1983 (Great Lakes Water Quality Board, 1985), and in the Ottawa River between 1981 and 1985 (Environment Canada, 1985). An increase in land use also took place along Quebec tributaries, but the already high levels of nitrates in the corresponding downstream stations did not change.

4. Conclusions

This software package allows the user to carry out environmental follow-up studies using data collected from monitoring networks. A complete analysis of 1500 observations takes about 20 minutes with an AT-class microcomputer. This program was developed especially for use with environmental time series, making use of the most recent developments in trend detection. The software should be updated as improved trend detection techniques appear in the literature; this objective is made easy by the open structure of the Fortran code. The proposed package opens numerous possibilities in various fields involving environmental follow-ups: for example, it could be used to detect changes in pollutants sampled in the air from large cities, to assess the effectiveness of municipal water treatment programs and to detect long-term trends of water quality changes in aquatic ecosystems. Some research remains to be done to evaluate the power of the newly developed non-parametric tests using mathematical simulations.

Acknowledgement

This software was developed for, and is available from Environment Canada, Quebec region.

References

Berryman, D., Bobee, B., Cluis, D., and Haemmerli, J.: 1988, 'Non-Parametric Tests for Trend Detection in Water Time Series', *Water Resources Bulletin* **24**(3), 545–556.

Bradley, J. V.: 1968, *Distribution-Free Statistical Tests*, Prentice-Hall.

Cluis, D.: 1983, 'Visual Techniques for the Detection of Water Quality Trends: Double-Mass Curves and CUSUM Functions', *Environmental Monitoring and Assessment* **3**, 173–184.

Conover, W. J.: 1971, *Practical Non-Parametric Statistics*, 2nd ed. John Wiley, New York.

Environment Canada: 1985, 'First Annual Report', Ottawa River Federal-Provincial Water Quality Coordinate Committee. Ottawa.

Great Lakes Water Quality Board: 1985, 'Report To the International Joint Commission', Kingston, Ontario.

Helsel, D. R.: 1987, 'Advantages of Non-Parametric Procedures for Analysis of Water Quality Data' *Journal of Hydrological Sciences* **32**, 179–190.

Hirsch, R. M., Slack, J. R., and Smith, R. A.: 1982, 'Techniques of Trend Analysis for Monthly Water Quality Data', *Water Resources Research* **18** 107–121.

Hirsch, R. M. and Slack, J. R.: 1984, 'A Non-Parametric Trend Test for Seasonal Data with Serial Dependence', *Water Resources Research* **20**, 727–732.

Lehmann, E. L.: 1975, *Non-Parametrics: Statisticals Methods Based on Ranks*, Holden-Day, San Francisco.

Lettenmaier, D. P.: 1976, 'Detection of Trends in Water Quality Data from Records with Dependent Observations', *Water Resources Research* **12**, 1037–1046.

Lettenmaier, D. P., Conquest, L. L., and Hughes, J. P.: 1982, 'Routine Streams and Rivers Water Quality Trend Monitoring Review', C. W. Harris Hydraulics Laboratory, University of Washington, report #75.

Montgomery, R. H. and Loftis, J. C.: 1987, 'Applicability of the *t*-Test for Detecting Trends in Water Quality Variables', *Water Resources Bulletin* **23**, 653–662.

Scheffé, H.: 1959, *The Analysis of Variance*, John Wiley, New York.

Searcy, J. K. and Hardison, C. H.: 1960, 'Double-Mass Curves', U.S.G.S. Water Supply Paper 1541-B, 66 pp.

Van Belle, G. and Hughes, J. P.: 1984, 'Non-Parametric Tests for Trends in Water Quality', *Water Resources Research* **20**, 127–136.