seawaveQ—An R Package Providing a Model and Utilities for Analyzing Trends in Chemical Concentrations in Streams with a Seasonal Wave (seawave) and Adjustment for Streamflow (Q) and Other Ancillary Variables
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By Karen R. Ryberg and Aldo V. Vecchia

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Conversion Factors

Inch/Pound to SI

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<th>Multiply</th>
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<th>To obtain</th>
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<td>cubic meter per second (m³/s)</td>
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SI to Inch/Pound

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<td>cubic foot per second (ft³/s)</td>
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Acknowledgments

The authors thank the time and effort of the U.S. Geological Survey personnel that reviewed this report, tested the R package and vignette, and contributed suggestions to improve the package. The U.S. Geological Survey testers and reviewers were Bill Damschen, North Dakota Water Science Center and Patrick Phillips, New York Science Center.

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seawaveQ—An R Package Providing a Model and Utilities for Analyzing Trends in Chemical Concentrations in Streams with a Seasonal Wave (seawave) and Adjustment for Streamflow (Q) and Other Ancillary Variables

By Karen R. Ryberg and Aldo V. Vecchia

Abstract

The seawaveQ R package fits a parametric regression model (seawaveQ) to pesticide concentration data from streamwater samples to assess variability and trends. The model incorporates the strong seasonality and high degree of censoring common in pesticide data and users can incorporate numerous ancillary variables, such as streamflow anomalies. The model is fitted to pesticide data using maximum likelihood methods for censored data and is robust in terms of pesticide, stream location, and degree of censoring of the concentration data. This R package standardizes this methodology for trend analysis, documents the code, and provides help and tutorial information, as well as providing additional utility functions for plotting pesticide and other chemical concentration data.

Introduction

Vecchia and others (2008) first introduced the concept of using a periodic solution to a conceptual storage equation with pulse input function to model seasonality in pesticide concentrations in streamwater. The resulting seasonal model (referred to in later publications as the “seawave” model) was shown to provide much better representation of seasonality in pesticide data than the standard sine and cosine functions used to model seasonality in other water-quality constituents such as nutrients and major ions. Vecchia and others (2008) also demonstrated the usefulness of using “streamflow anomalies” (described later in this report) as predictor variables for pesticide concentration. Sullivan and others (2009) compared several methods for analyzing trends in pesticide concentrations for 31 sites and 11 pesticides. The methods compared included the seasonal Kendall (SEAKEN) test for nonflow-adjusted concentrations [a modified version of the nonparametric seasonal Kendall test described by Hirsch and Slack (1984)], a parametric regression model incorporating the seasonal model from Vecchia and others (2008) and referred to in Sullivan and others (2009) as the “seawave” model, and the seawave model with the addition of streamflow anomalies, called “seawave-Q”. The best approach in terms of maximizing the number of sites and pesticides that could be assessed and accounting for variable streamflow conditions when comparing trends for multiple sites and pesticides was determined to be the seawaveQ model. Thus, the seawaveQ model was selected as the statistical tool for analyzing pesticide trends for cornbelt streams (Sullivan and others, 2009), analyzing pesticide trends for urban streams (Ryberg and others, 2010), and for use in ongoing pesticide assessments. In response to requests from outside agencies for a software package to allow them to apply the seawaveQ model to their datasets, the R package, seawaveQ, was developed.

The model was developed to “handle a number of difficulties often found in pesticide data, such as strong seasonality in response to use patterns, high numbers of concentrations below laboratory reporting levels (RLs), complex relations between streamflow and concentration, and intermittent or changing sampling frequencies (both inter-annually and intra-annually)” (Vecchia and others, 2008). The model is fitted to pesticide data using maximum likelihood methods for censored data and is robust in terms of pesticide, stream location, and degree of censoring of the concentration data (Vecchia and others, 2008).

The R package seawaveQ was developed to provide a standardized methodology for fitting the seawaveQ model and to make the trend analysis method widely available for public use. In addition, several enhancements to the seawaveQ model have been included, as well as utility functions for working with chemical concentration data. These enhancements and utilities include procedures for preparing and summarizing input data, added flexibility to include other explanatory variables besides streamflow, graphical methods for assessing model fit, and plotting routines that may be used for pesticide and other chemical concentration data.
The body of this report provides a brief overview of the seawaveQ package, including the statistical methods used. A complete example using seawaveQ for trend analysis is provided in the vignette, or tutorial, in appendix 1. Additional detail for each function, including the arguments and returned values, is provided in appendix 2. Visual examples of the seasonal wave part of the model are provided in appendix 3 to help users understand how the seasonal wave fits into the model.

**Description Of The SeawaveQ Package**

The seawaveQ package is a collection of functions written for R (http://www.r-project.org/; R Core Team, 2012a), an open source language and a general environment for statistical computing and graphics that runs on a variety of operating systems including Linux®, Mac OS®, UNIX®, and Windows®.

The main purpose of this package is to fit the seawaveQ model to pesticide concentration data. The main function, fitswavecav, internally calls other functions to prepare the data, fit the model, and plot model results and regression diagnostics. The internal functions need not be called by the user, but they are documented in the R help. In addition, optional functions are provided to plot water-quality data and to combine the water-quality with ancillary data. A flowchart showing how the input data, main function, optional functions, internal functions, and output work together to create the seawaveQ package is shown in figure 1. Table 1 lists the functions in seawaveQ and provides a brief description of each.

More details on seawaveQ functions and tutorial examples of preparing datasets for analysis are available in appendix 1 (vignette) and appendix 2 (help documentation). Vignettes are PDF documents that contain examples of R code and results of running the code, as well as descriptive text (R Core Team, 2012c). Vignettes can be used as tutorials for the package and the vignette for seawaveQ is included in this document to familiarize users with the functions in seawaveQ. In addition to the vignette, the package has detailed help documentation files for each function (appendix 2). After installing the package, the help documentation may be accessed in the same manner as the help for other R functions. Help features within R are further described in the manual An Introduction to R (Venables and others, 2013). Additional information on the installation and administration of R and packages that extend it are available in the manual R Installation and No

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**Figure 1.** Flowchart showing the input, functions, and output that are part of seawaveQ.
Input Data

In addition to the functions, seawaveQ provides some sample datasets that are used to illustrate the format of the datasets used by the package functions and the datasets are used in the vignette. The sample datasets are listed in table 2. To use seawaveQ, an analyst is required to have concentration data and continuous ancillary data. The sample datasets IllRivValleyCty and qwMoRivOmaha provide examples of the necessary data format. It is assumed that the unit of concentration is micrograms per liter. Continuous ancillary data can be dimensionless streamflow or sediment anomalies, as in the example dataset cqwMoRivOmaha, computed using the R package waterData (Ryberg and Vecchia, 2012), or they can be anomalies based on other continuously monitored data, such as specific conductance or temperature. See Vecchia and others (2008) for more information on anomalies. Users that need additional help getting their own data into R should consult the R manual titled “R Data Import/Export” (R Core Team, 2013a).

Statistical Methodology

The seawaveQ model is a parametric regression model specifically designed for analyzing seasonal- and flow-related variability and trends in pesticide concentrations. The model is expressed as follows,

$$\log C(t) = \beta_0 + \beta_1 W(t) + \beta_2 LTFA(t) + \beta_3 MTEA(t) + \beta_4 STFA(t) + \beta_5 t + \eta(t)$$  (1)

where

- $\log$ denotes the base-10 logarithm;
- $t$ is decimal time, in years, with respect to an arbitrary time origin;
- $C$ is pesticide concentration, in micrograms per liter;
- $W$ is a seasonal wave representing intra-annual variability in concentration;
- $LTFA, MTEA, and STFA$ are long-term, mid-term, and short-term, respectively, dimensionless flow anomalies computed from daily streamflow (described later in this section);
- $\beta_0, \beta_1, \ldots, \beta_5$ are regression coefficients; and
- $\eta(t)$ is the model error.

The seasonal wave is a dimensionless, periodic function of time with an annual cycle, similar to a mixture of sine and
cosine functions often used to model seasonality in concentration data. However, the seasonal wave is better suited for modeling seasonal behavior of pesticide data than a mixture of sines and cosines. The seasonal wave is a periodic (with a period of 1 year) solution to the following differential equation (Vecchia and others, 2008):

\[
\frac{d}{dt} W(t) = \lambda(t + s*) - \phi W(t)
\]  

(2)

where

- \( \lambda(.) \) is a pulse input function with \( \lambda(.) > 0 \) during specified application season(s) and \( \lambda(.) = 0 \) otherwise;
- \( s* \) is a seasonal shift that determines the time at which \( W \) reaches its maximum; and
- \( \phi \) is a decay rate corresponding with an approximate half-life of \( 12/\phi \) months.

As in Sullivan and others (2009, Appendix 2), the pulse input function is selected from a menu of 14 choices with either 1 or 2 distinct application seasons (when pesticides may be transported to the stream) of lengths from 1 to 6 months and the half-life is selected from 4 choices (1, 2, 3, or 4 months). The half-life is referred to as a model half-life when discussing model results to distinguish it from the chemical half-life of pesticides. Thus, 56 (14x4) choices for the wave function are available. As described in Sullivan and others (2009, appendix 2), the observed concentration data were used to select the best wave function and to estimate the seasonal shift (\( s* \)) through a combination of graphical and maximum likelihood techniques. Appendix 3 shows the 56 different seasonal waves with two different seasonal shifts, specified as \( cmax_t=0.3 \) and \( cmax_t=0.6 \).

The dimensionless flow anomalies in equation 1 are orthogonal (uncorrelated) time series computed using daily flow records from a streamgage at the site of the pesticide sampling. The anomalies represent different scales of streamflow variability, long-term (LTFA), mid-term (MTFA), and short-term (STFA) and the specific scales selected can vary depending on the site or pesticide being analyzed. In Sullivan and others (2009), which focused on agricultural pesticides and included many large basins, LTFA represented annual streamflow variability, MTFA represented monthly variability within years, and STFA represented daily variability within months. In Ryberg and others (2010), which focused on urban pesticides for small basins, LTFA represented streamflow variability for 100-day intervals, MTFA represented monthly variability within years, and STFA represented daily variability within 10-day intervals. The anomalies can be computed using the R package waterData (Ryberg and Vecchia, 2012), which has several options for the time scales used. In addition, dimensionless anomalies similar to the
streamflow anomalies but calculated from other continuously monitored parameters such as temperature, specific conductance, or turbidity can be calculated and used as ancillary variables in the seawaveQ model (and can be computed in the waterData package).

The seawaveQ model (equation 1) is fitted to pesticide data using maximum likelihood methods for censored data, as described in Sullivan and others (2009), using this package.

The vignette, appendix 1, guides the user through an example that uses anomalies based on streamflow and anomalies based on sediment.

Summary

The seawaveQ model fits a parametric regression model to concentration data from streamwater samples to assess variability and trends. The model incorporates the strong seasonality (through a pulse input function and a model half-life) and the high degree of censoring (through survival regression) common in pesticide data and users can incorporate numerous ancillary variables, such as streamflow anomalies. The model is fitted to pesticide data using maximum likelihood methods for censored data and is robust in terms of pesticide, stream location, and degree of censoring of the concentration data. The model was incorporated into an R package to standardize the methodology for trend analysis, to document the code, and to provide help and tutorial information.

In addition to the functionality of the original seawaveQ model, several enhancements have been included such as procedures for preparing and summarizing input data; flexibility to include explanatory variables besides streamflow; graphical methods for assessing model fit; and procedures for managing model output.

The package is available in the free, public Comprehensive R Archive Network, http://cran.r-project.org/ (R Core Team, 2013b) The appendixes of this document provide an example of how to use the R package and document the functions.

Disclaimer

This package was written by U.S. Federal government employees in the course of their employment and is therefore in the public domain (in the United States), which means it is not copyrighted and use is unlimited. However, some of the functions depend on other R packages, which, although free and open source, are released under licenses. Those packages are survival [LGPL (Lesser General Public License) ≥ (greater than or equal to version) 2], NADA [GPL (General Public License) ≥ 2], and lubridate (GPL). R itself is released under the free software license GNU GPL, either version 2, June 1991, or version 3, June 2007. Additional information on licensing is available at http://www.r-project.org/Licenses/ and http://www.gnu.org/licenses/license-list.html#SoftwareLicenses.

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References Cited


Appendixes 1–3
Appendix 1. Vignette

Vignettes are the established R community method for providing examples of how to use the package.

The pdf file can be accessed at http://pubs.usgs.gov/of/2013/1255/Downloads/Appendix_1.pdf

Appendix 2. R Documentation

The official R documentation for this package can be accessed at http://pubs.usgs.gov/of/2013/1255/Downloads/Appendix_2.pdf
Appendix 3. Visualizations of the Seasonal Wave

The pulse input function, jmod, is selected from a menu of 14 choices with either 1 or 2 distinct application seasons (when pesticides may be transported to the stream) of lengths from 1 to 6 months and the half-life (hlife) is selected from 4 choices (1, 2, 3, or 4 months). The half-life is referred to as a model half-life when discussing model results to distinguish it from the chemical half-life of pesticides. Thus, 56 (14x4) choices for the wave function are available. The observed concentration data are used to select the best wave function and to estimate the seasonal shift, the decimal season of maximum chemical concentration, cmaxt, through a combination of graphical and maximum likelihood techniques. The following plots show the 56 different seasonal waves with 2 different seasonal shifts, 0.3 and 0.6. The plotted seasonal waves were generated by setting the arguments of the function compwaveconv to 0.3 and 0.6 for cmaxt, 1 through 14 for jmod, 1 to 4 for hlife, and generating a plot for each combination of options, for example:

```r
swave <- compwaveconv(cmaxt=0.3, jmod=1, hlife=1, mclass=1)
plot(seq(0, 1, 1/360), swave, typ="l", xaxs="i", yaxs="i", ylim=c(-0.6, 0.6), cex.axis=0.6, cex.lab=0.6, ylab="Seasonal wave", xlab="Decimal seasons")
```
Figure 3–1.  Visualization of seasonal waves with seasonal shift of the decimal season of maximum chemical concentration \(c_{\text{max}}\) equal to 0.3.  \(j_{\text{mod}}\) is the pulse input function, \(h_{\text{life}}\) is model half-life in months, and decimal season is the fraction of the calendar year represented by a specific month and day.
Figure 3–1. Visualization of seasonal waves with seasonal shift of the decimal season of maximum chemical concentration ($c_{max}$) equal to 0.3. $jmod$ is the pulse input function, $hlife$ is model half-life in months, and decimal season is the fraction of the calendar year represented by a specific month and day.—Continued
Figure 3–2. Visualization of seasonal waves with seasonal shift of the decimal season of maximum chemical concentration (cmaxt) equal to 0.6. jmod is the pulse input function, hlife is model half-life in months, and decimal season is the fraction of the calendar year represented by a specific month and day.
Figure 3–2. Visualization of seasonal waves with seasonal shift of the decimal season of maximum chemical concentration (cmaxt) equal to 0.6. jmod is the pulse input function, hlife is model half-life in months, and decimal season is the fraction of the calendar year represented by a specific month and day.—Continued