Revisions to LOADEST, April 2013

1. Introduction

This document describes several changes to LOADEST, a load estimation program distributed by the U.S. Geological Survey (http://water.usgs.gov/software/loadest/). The following sections of this document describe changes that have been made to the underlying software program since its initial release in December, 2004. The information contained herein generally supersedes that presented in the original software documentation (*Runkel and others*, 2004).

2. Bias Diagnostics and Residual Analysis

Recent research illustrates the potential for LOADEST to produce biased load estimates when the selected regression model is a poor representation of the relationship between load and the explanatory variables. *Stenback and others* (2011), for example, document a positive bias (over estimation) of estimated nitrate loads in several Iowa rivers. Fortunately, problems with load bias may be identified through careful analyses of model residuals and a comparison of the observed and estimated loads. LOADEST has therefore been modified to include several features that facilitate residual analysis and bias identification, as described in the subsections below. These features are illustrated using the nitrate loading analysis presented by Stenback and others (2011) for the Thompson Fork of the Grand River at Davis City, Iowa. This application is now included as one of seven example applications distributed with the LOADEST software (for a description of the first six applications, see *Runkel and others*, 2004).

2.1 Bias Diagnostics

Part Ia of the *constituent output file* has been modified to report several statistics that may be used to diagnose load bias. These statistics are based on a comparison of observed and estimated loads for all dates/times within the calibration data set. Although this comparison does not directly address bias in load estimation for unsampled dates/times, large discrepancies between observed and estimated loads are indicative of a poor model fit. Note that this comparison of observed and estimated loads uses one-half the detection limit as the concentration when an observation is censored. The statistics are therefore slightly inaccurate for censored data sets. Although not discussed herein, the statistics presented below for load are also determined for the concentration model, as reported in Part Ib of the *constituent output file.*

The first bias diagnostic reported in the constituent output file is a table of summary statistics (minimum, maximum, median, and various percentiles) for the estimated and observed loads corresponding to the calibration data set. In addition, summary statistics are reported for the ratio of estimated and observed loads. For the case of the Thompson Fork, these ratios are generally greater than 1.0, suggesting a positive load bias (estimated > observed; Table 1).

Table 1 Summary Statistics, Estimated and Observed Loads for Calibration Data Set

	Min.	25th	Med.	75th	90th	95th	99th	Max.
Est.	4.34E-02	7.93E+00	6.39E+01	2.24E+03	1.37E+04	3.70E+04	1.33E+05	1.34E+05
Obs.	2.91E-01	1.57E+00	2.48E+01	1.28E+03	4.58E+03	8.51E+03	1.81E+04	1.82E+04
Est/Obs	0.15	5.04	2.57	1.75	2.99	4.35	7.34	7.35

Estimated and observed loads corresponding to the calibration data set are also used to calculate the Partial Load Ratio, the Load Bias in Percent, and the Nash-Sutcliffe Efficiency Index. The Partial Load Ratio (*PLR*; *Stenback and others*, 2011) is equal to the sum of the estimated loads divided by the sum of the observed loads:

$$PLR = \frac{\sum_{k=1}^{N} \hat{L}}{\sum_{k=1}^{N} L} \qquad (1)$$

where L is the observed load, $\hat{L}$ is the estimated load, and N is the number of observations in the calibration data set. Equation (1) can be reformulated to calculate the Load Bias in Percent (B_p):

$$B_p = 100\left(\frac{\sum_{k=1}^{N} (\hat{L} - L)}{\sum_{k=1}^{N} L}\right) \qquad (2)$$

where the various quantities are as defined above. The Nash-Sutcliffe Efficiency Index (E; *Nash and Sutcliffe*, 1970) is given by:

$$E = 1 - \frac{\sum_{k=1}^{N} (L - \hat{L})^2}{\sum_{k=1}^{N} (L - \bar{L})^2} \tag{3}$$

where $\bar{L}$ is the mean of the obser5ed loads.

Although interpretation of *PLR*, B_p, and *E* is application specific, some general guidelines are presented here and implemented within the LOADEST software. As with the summary statistics presented table 1, values of *PLR* in excess of 1.0 are indicative of positive load bias in which estimated loads exceed observed loads (over estimation), while values of *PLR* less than 1.0 indicate negative load bias (under estimation, in which estimated loads are less than observed loads). The over and under estimation quantified by *PLR* may also be expressed in terms of B_p, the Load Bias in Percent[1]. Positive values of B_p indicate positive load bias (over estimation); similarly, negative values of B_p indicate negative load bias (under estimation). The Nash-Sutcliffe Efficiency Index extends the comparison of observed and estimated loads using the mean of the observed loads (equation 3). Values of *E* range from negative infinity to 1.0, with a value of 1.0 indicating a perfect fit and a value of 0.0 indicating that the load estimates are only as accurate as the mean. Values of $E < 0$ indicate that the observed mean is a better estimate of load than the selected regression model.

For the case of Thompson Fork, values of *PLR* and B_p are 4.4 and 345%, respectively, indicating a positive bias and the potential over estimation of loads. A negative value of *E* (-31.1), meanwhile, suggests that the mean of the observed data would be a better estimate of load than the selected regression model. The high value for the load bias (B_p = 345%) triggers a warning message that is written to the *constituent output file* whenever the absolute value of B_p exceeds 25%[2]. Similarly, the calculated value of *E* triggers a warning message that is written whenever *E* is negative. These warning messages clearly state that the calibrated model should not be used for load estimation.

[1] In general $PLR = (B_p + 100) / 100$

[2] Due to similarities between *PLR* and B_p (footnote 1), a similar cutoff and warning has not been implemented for *PLR*.

2.2 Residual Output File

A note has been added to the *constituent output file* stating that additional information related to model calibration is contained in the *residual output file* and that users should conduct a thorough residual analysis using the data contained therein. To facilitate this analysis, additional quantities are now included in the *residual output file* (Appendix 1). Additions to the *residual output file* include observed and estimated loads in real space (expressed as load rather than *ln*[load]), observed and estimated concentrations in real space, the estimate of *ln*[concentration], and a flag indicating whether or not a given observation is censored[3]. As with the bias diagnostics (Section 2.1), observed concentrations and loads are calculated using one-half the detection limit as the concentration when an observation is censored. These additions allow for the development of plots comparing observed and estimated loads in real space, providing a means to visually detect load bias. Columns 3, 9, and 10 of the residual output file (Appendix 1), for example, may be used to plot the time series of observed and estimated loads. For the case of the Thompson Fork, this plot clearly shows a positive bias in the estimated loads corresponding to the calibration data set (estimated loads > observed loads, Figure 1). Other examples of plots prepared using the residual output file are shown in Figures 7, 8, 9, and 17 of the LOADEST documentation (*Runkel and others*, 2004).

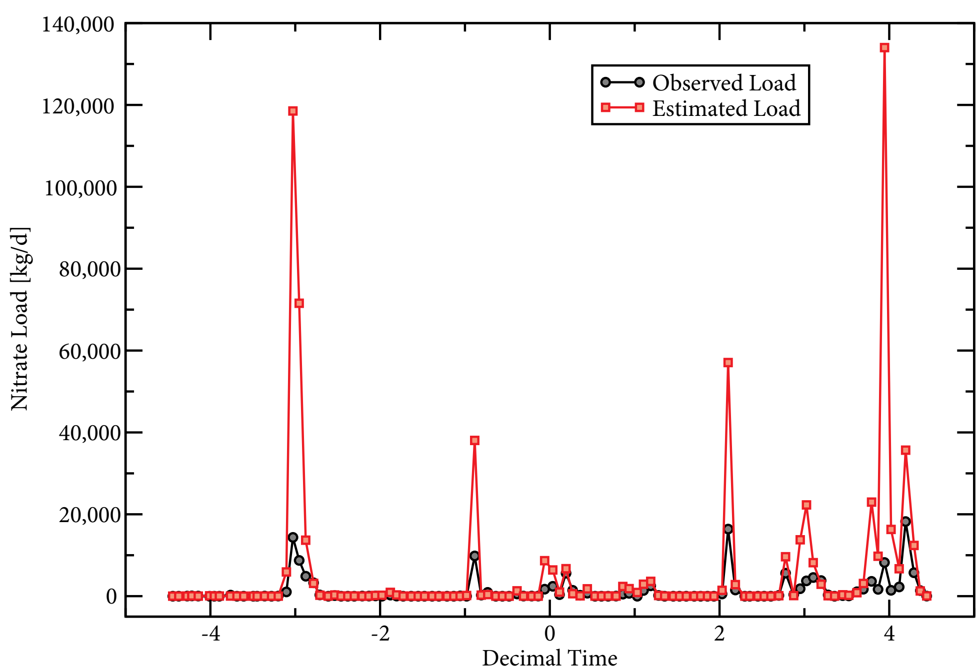

Figure 1: Comparison of observed and estimated loads corresponding to the calibration data set.

[3]For a description of other quantities within the *residual output file*, see Section 3.4.3 and Figure 2 of the LOADEST documentation (Runkel and others, 2004).

2.3 Probability Plot Correlation Coefficient and the Turnbull-Weiss Statistic

The initial release of LOADEST included calculations of the Probability Plot Correlation Coefficient (PPCC) and the Turnbull-Weiss Statistic that allowed LOADEST users to test the normality of model residuals. Calculation of the Turnbull-Weiss statistic has been eliminated in the updated version of LOADEST due to difficulties associated with interpretation of the statistic. Calculations for the PPCC in the initial release of LOADEST utilized expected values of concentrations whenever a given observation was censored. This use of the expected values resulted in PPCC values that were closer to 1.0 than methods that employ one-half the detection limit for censored data. The PPCC calculation within LOADEST has therefore been revised using the algorithm of Royston (1993) that has been extended to multiply censored data by Millard in the Environmental Stats for S+ library. PPCC values from the updated software should be nearly identical to those from the initial software release for uncensored data sets, and slightly less for censored data sets.

3. Dynamic Array Allocation

The initial release of LOADEST was written using FORTRAN-77 and fixed-size arrays that placed limitations on the size of the user's application. The number of observations in the *calibration file*, for example, was limited to 2,400. The updated version of LOADEST uses FORTRAN-95 and dynamic array allocation, such that most of these limitations are no longer in place (the limitations on number of constituents, observations in the calibration file, observations in the estimation interval, and number of user-defined seasons shown in Table 25 of the LOADEST documentation no longer apply).

4. References

Nash, J.E. and Sutcliffe, J.V., 1970, River flow forecasting through conceptual models part I—A discussion of principles: Journal of Hydrology, v. 10, no. 3, p 282-290.

Royston, P., 1993, A toolkit for testing for non-normality in complete and censored samples: J. of the Royal Statistical Society. Series D (The Statistician), v. 42, No. 1, p. 37-43.

Runkel, R.L., Crawford, C.G., and Cohn, T.A., 2004, Load Estimator (LOADEST): A FORTRAN Program for Estimating Constituent Loads in Streams and Rivers: U.S. Geological Survey Techniques and Methods Book 4, Chapter A5, 69 p.

Stenback, G.A., Crumpton, W.G., Schilling, K.E., and Helmers, M.J., 2011, Rating curve estimation of nutrient loads in Iowa rivers: Journal of Hydrology v. 396, p. 158-169.

— Robert L. Runkel
U.S. Geological Survey
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Appendix 1 — Example Residual Output File


```
#
#  Residual output file
#
#  notes
#  -----
#  DTIME     decimal time minus "center" of decimal time
#  LN(CFLOW) natural log of (uncentered) streamflow
#  F         flag indicating observation is censored (C) or uncensored (U)
#  CCONC     observed concentration for F=U; 1/2 of the observed concentration for F=C
#  CCONCAML  estimated concentration
#  YHATC     estimated natural log of concentration
#  CLOAD     observed load for F=U; 1/2 of the observed load for F=C (units dependent on ULFLAG)
#  CLOADAML  estimated load (units dependent on ULFLAG)
#  YHAT      estimated natural log of load (where load is in kg/d)
#  RESID     difference between observed and estimated values of log load (or log concentration)
#  Z         z-score for residual
#
#
#DATE    TIME  DTIME        LN(CFLOW)    F CCONC       CCONCAML     YHATC        CLOAD        CLOADAML     YHAT         RESID        Z
#
19991014 1200 -4.44392E+00  2.38784E+00 C 5.00000E-02 9.19607E-02 -3.57950E+00 1.33216E+00 2.45013E+00 -2.96969E-01 -6.30814E-01 -3.39440E-01
19991109 1200 -4.37269E+00  2.55490E+00 C 5.00000E-02 1.74251E-01 -2.95316E+00 1.57437E+00 5.48670E+00  4.96431E-01 -9.38381E-01 -5.96717E-01
19991215 1200 -4.27406E+00  2.76254E+00 U 2.00000E-01 4.34299E-01 -2.04972E+00 7.75075E+00 1.68307E+01  1.60751E+00  4.40282E-01  4.64197E-01
20000104 1200 -4.21929E+00  3.28579E+00 U 7.00000E-01 1.09170E+00 -1.11905E+00 4.57779E+01 7.13937E+01  3.06142E+00  7.62379E-01  6.24451E-01
20000201 1200 -4.14279E+00  2.38784E+00 U 8.00000E-01 4.99590E-01 -1.91332E+00 2.13146E+01 1.33107E+01  1.36921E+00  1.69018E+00  1.09114E+00
20000321 1200 -4.00891E+00  3.20883E+00 C 5.00000E-02 1.38183E+00 -8.90910E-01 3.02764E+00 8.36737E+01  3.21260E+00 -2.33355E+00 -1.59812E+00
20000410 1200 -3.95426E+00  2.55490E+00 C 5.00000E-02 5.07566E-01 -1.88019E+00 1.57437E+00 1.59820E+01  1.56940E+00 -1.60295E+00 -1.05031E+00
20000502 1200 -3.89415E+00  3.03447E+00 C 5.00000E-02 6.80199E-01 -1.60069E+00 2.54322E+00 3.45979E+01  2.32847E+00 -1.79967E+00 -1.27652E+00
20000619 1200 -3.76300E+00  3.32215E+00 U 3.70000E+00 4.23055E-01 -2.09765E+00 2.50931E+02 2.86912E+01  2.11919E+00  3.40598E+00  2.08956E+00
20000717 1200 -3.68650E+00  3.57347E+00 C 5.00000E-02 3.76939E-01 -2.22380E+00 4.35980E+00 3.28675E+01  2.24436E+00 -1.37340E+00 -9.73506E-01
20000815 1200 -3.60727E+00  2.29253E+00 C 5.00000E-02 6.47570E-02 -3.97760E+00 1.21105E+00 1.56848E+00 -7.90378E-01 -4.70517E-01 -1.72993E-01
20000925 1200 -3.49524E+00  2.88032E+00 C 5.00000E-02 1.59636E-01 -3.10004E+00 2.17990E+00 6.95983E+00  6.74975E-01 -8.60423E-01 -5.16098E-01
20001012 1200 -3.44880E+00  1.42503E+00 C 5.00000E-02 2.31065E-02 -4.96863E+00 5.08643E-01 2.35059E-01 -2.64891E+00 -1.91880E-01 -8.03755E-02
20001113 1200 -3.36136E+00  3.08099E+00 U 3.00000E-01 4.02619E-01 -2.17700E+00 1.59859E+01 2.14541E+01  1.79869E+00  9.73023E-01  6.81430E-01
20001213 1200 -3.27940E+00  1.21373E+00 U 4.00000E-01 4.57892E-02 -4.28381E+00 3.29407E+00 3.77082E-01 -2.17540E+00  3.36752E+00  1.91894E+00
20010111 1200 -3.20008E+00  2.29253E+00 U 7.00000E-01 3.99052E-01 -2.20271E+00 1.69548E+01 9.66548E+00  9.84512E-01  1.84604E+00  1.22618E+00
20010215 1200 -3.10419E+00  5.47059E+00 U 1.80000E+00 1.01705E+01  1.08560E+00 1.04635E+03 5.91215E+03  7.45087E+00 -4.97810E-01 -1.96363E-01
20010315 1200 -3.02748E+00  8.27142E+00 U 1.50000E+00 1.23882E+01  1.43852E+00 1.43510E+04 1.18522E+05  1.06046E+01 -1.03305E+00 -7.10760E-01
20010411 1200 -2.95351E+00  7.84549E+00 U 1.40000E+00 1.14497E+01  1.27558E+00 8.74866E+03 7.15498E+04  1.00158E+01 -9.39103E-01 -6.24451E-01
20010509 1200 -2.87680E+00  6.56920E+00 U 2.80000E+00 7.84154E+00  8.01276E-01 4.88297E+03 1.36750E+04  8.26517E+00  2.28344E-01  1.49723E-01
20010612 1200 -2.78365E+00  5.88985E+00 U 3.70000E+00 3.53544E+00 -3.69455E-03 3.27106E+03 3.12557E+03  6.78084E+00  1.31203E+00  8.02727E-01
20010709 1200 -2.70967E+00  4.51174E+00 U 1.30000E+00 1.04724E+00 -1.23034E+00 2.89684E+02 2.33360E+02  4.17608E+00  1.49271E+00  9.73506E-01
20010814 1200 -2.61104E+00  3.08099E+00 C 5.00000E-02 1.93828E-01 -2.93036E+00 2.66432E+00 1.03284E+01  1.04532E+00 -9.50788E-01 -6.52675E-01
20010911 1200 -2.53433E+00  4.82623E+00 U 4.00000E-01 9.35962E-01 -1.30318E+00 1.22074E+02 2.85642E+02  4.41774E+00  3.86894E-01  3.88595E-01
20011008 1200 -2.46036E+00  3.39115E+00 C 5.00000E-02 3.45352E-01 -2.34100E+00 3.63316E+00 2.50944E+01  1.94484E+00 -1.29848E+00 -8.67992E-01
20011106 1200 -2.38091E+00  3.08099E+00 C 5.00000E-02 3.77388E-01 -2.26090E+00 2.66432E+00 2.01096E+01  1.71478E+00 -1.34948E+00 -9.37178E-01
20011204 1200 -2.30419E+00  3.08099E+00 C 5.00000E-02 6.21245E-01 -1.76616E+00 2.66432E+00 3.31039E+01  2.20952E+00 -1.68218E+00 -1.13387E+00
20020107 1200 -2.21104E+00  1.96403E+00 U 8.00000E-01 2.47249E-01 -2.68468E+00 1.39514E+01 4.31182E+00  1.74042E-01  2.46153E+00  1.68665E+00
20020205 1200 -2.13159E+00  2.55490E+00 U 9.00000E-01 7.56270E-01 -1.57684E+00 2.83387E+01 2.38130E+01  1.87275E+00  1.47148E+00  9.02046E-01
20020305 1200 -2.05488E+00  3.42394E+00 U 8.00000E-01 2.22067E+00 -4.91387E-01 6.00683E+01 1.66740E+02  3.82724E+00  2.68243E-01  2.19844E-01
20020402 1200 -1.97817E+00  3.65351E+00 C 5.00000E-02 2.34746E+00 -4.32417E-01 4.72311E+00 2.21746E+02  4.11578E+00 -2.70009E+00 -2.08956E+00
20020508 1200 -1.87954E+00  4.69043E+00 U 1.00000E+00 3.47898E+00 -3.75531E-02 2.66432E+02 9.26912E+02  5.54757E+00  3.75531E-02  1.03427E-01
20020604 1200 -1.80556E+00  4.32068E+00 C 5.00000E-02 1.63304E+00 -7.97929E-01 9.20402E+00 3.00610E+02  4.41744E+00 -2.40665E+00 -1.68665E+00
20020702 1200 -1.72885E+00  3.08099E+00 C 5.00000E-02 3.01139E-01 -2.48919E+00 2.66432E+00 1.60466E+01  1.48649E+00 -1.20637E+00 -8.34915E-01
20020806 1200 -1.63296E+00  3.03447E+00 C 5.00000E-02 1.96726E-01 -2.91840E+00 2.54322E+00 1.00064E+01  1.01076E+00 -9.57328E-01 -6.81430E-01
20020905 1200 -1.55077E+00  1.29828E+00 C 5.00000E-02 1.42766E-02 -5.41390E+00 4.48090E-01 1.27944E-01 -3.22092E+00 -1.17245E-01 -3.44067E-02
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20021104 1200 -1.38639E+00  2.17600E+00 C 5.00000E-02 1.16713E-01 -3.43342E+00 1.07784E+00 2.51595E+00 -3.62728E-01 -6.96627E-01 -4.13527E-01
20021203 1200 -1.30693E+00  1.79824E+00 C 5.00000E-02 1.10437E-01 -3.47443E+00 7.38743E-01 1.63170E+00 -7.81504E-01 -6.77777E-01 -3.88595E-01
20030107 1200 -1.21104E+00  1.74781E+00 C 5.00000E-02 1.78560E-01 -2.98810E+00 7.02412E-01 2.50846E+00 -3.45599E-01 -9.19525E-01 -5.69436E-01
20030205 1200 -1.13159E+00  1.55857E+00 U 2.00000E-01 1.71781E-01 -2.99134E+00 2.32523E+00 1.99714E+00 -5.38089E-01  1.38191E+00  8.34915E-01
20030304 1200 -1.05762E+00  2.69800E+00 U 1.40000E+00 9.66174E-01 -1.31924E+00 5.08643E+01 3.51027E+01  2.27345E+00  1.65571E+00  1.05031E+00
20030401 1200 -9.80906E-01  3.48646E+00 C 5.00000E-02 2.02248E+00 -5.78915E-01 3.99648E+00 1.61656E+02  3.80223E+00 -2.58137E+00 -1.91894E+00
20030506 1200 -8.85015E-01  7.46302E+00 U 2.30000E+00 8.92540E+00  9.82330E-01 9.80470E+03 3.80482E+04  9.34004E+00 -1.49421E-01 -5.73729E-02
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