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Operationalizing real-time monitoring data in simulation models using the public domain HECDSSVue platform

Vi Tran
Life and Environmental Sciences Department, University of California, Merced, CA 95343, USA.
HydroEcological Engineering Advanced Decision Support (HEADS), Lawrence Berkeley National
Laboratory, Berkeley, CA 94720, USA. vitran@lbl.gov

Stefanie Helmrich
Environmental Systems Graduate Program, University of California, Merced, CA 95434 USA
shelmrich@ucmerced.edu

Nigel W.T. Quinn
HydroEcological Engineering Advanced Decision Support (HEADS), Lawrence Berkeley National
Laboratory, Berkeley, CA 94720, USA. nwquinn@lbl.gov
Sierra Nevada Research Institute, University of California, Merced, CA 95343, USA.
nquinn@ucmerced.edu

Peggy A. O'Day
Life and Environmental Sciences Department, University of California, Merced, CA 95343 USA.
poday@ucmerced.edu

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Abstract

This technical note describes a public domain, semi-automated data screening and quality assurance processing tool useful for both discrete and continuous data serving both a field research project assessing salinity and methylmercury drainage load control options and the use of a public domain watershed-based water quality forecasting model that is being used to provide decision support for short-term salinity control strategies in the San Joaquin River Basin of California. The US Army Corps of Engineers HEC-DSSVue data management and visualization platform was enhanced in the former application with Python scripts that performed the basic data quality assurance functions. Analogous tools were developed for use on the HOSTGATOR cloud server using the same Python scripts and algorithms to migrate quality controlled data directly to a server for use by the WARMF water quality forecasting model. The Python scripts for both applications are easily adaptable by other potential users who do not currently have the resources to implement an enterprise- level hydrological data management and real-time quality assurance software system.

1.0 Introduction

Improvements in the accuracy and reliability of environmental sensors and cellular telemetry and falling costs have increased their deployment for hydrologic and water quality monitoring (Bhardwaj

2009; Randhawa et al., 2016; Opalinski1, et al., 2016) These deployments support the continuous operation of water quality simulation and forecasting models (Quinn and Hanna, 2002. Quinn, 2006).

Tasks associated with continuous operation include: (a) downloading continuous sensor data from dataloggers; (b) performing quality assurance and quality control on the downloaded data; (c) error-correcting data and interpolating missing data time-series measurements; and (d) uploading and archiving datasets at the appropriate time interval for use in numerical watershed simulation and forecasting models. Real-time data quality assurance is the most challenging of these common tasks or workflows. Although there are several popular commercial environmental hydrologic data management systems (such as WISKI, HYDSTRA and AQUARIUS) that have been used to successfully complete this data quality assurance workflow, the high cost and complexity of these commercial software products that sometimes require trained, dedicated staff has limited their use. Small public and private water agencies, non-profits and private entities performing monitoring, can benefit from easy-to-implement and accessible data screening and management platforms in the public domain.

This technical note provides an overview of a system that has been developed in support of real-time water quality management in the western San Joaquin Valley, California (USA) focused on agricultural and wetland salt loading to the San Joaquin River. Environmental sensor networks have been established and operational for more than a decade in this area (Quinn and Hanna, 2002; Quinn, 2006). The system makes use of state-of-the-art cellular telemetry and fully automated web-based data reporting. Cost is a big factor given that the wetland entities such as private duck clubs and wildlife refuges do not generate income in the traditional sense – most of the 140,000 acres (64,000 ha) of the contiguous Grasslands Ecological Area (GEA) is dedicated to sustaining migratory waterfowl on the Pacific Flyway (Quinn and Hanna, 2006). Small agricultural water district budgets are also insufficient to employ staff dedicated to hydrologic and water quality data quality assurance.

2.0 Study objectives

This technical note provides an overview of the workflows and software developed to achieve two main project goals. The first uses the public domain database and data visualization software HEC-DSSVue (USCOE, 2009) to share data resources among scientists and wetland managers after performing customized real-time data screening and data quality control procedures. The second is to utilize the same customized quality assurance algorithms on a cloud platform (HOSTGATOR) to operationalize the Watershed Analysis Risk Management Framework (WARMF) model, a water quality simulation model (Herr et al., 2001) used to forecast San Joaquin River salt load assimilative capacity. The intent of this technical note is to share the data-handling and data quality control workflows algorithms developed for these applications in the public domain and make them accessible to analysts and water managers tasked with similar compliance monitoring and decision support challenges. Although this system focuses on salinity and the management of salt loads it has equal applicability to other constituents and pollutants.

3.0 Application setting

Grassland Water District (GWD) is a private entity that manages federal wetland water supply deliveries to 165 duck clubs and land and cattle operations in the Grassland Ecological Area (GEA). The San Joaquin Valley Drainage Authority (SJVDA) oversees and coordinates agricultural drainage monitoring and compliance with San Joaquin River (SJR) water quality objectives. Both entities have developed telemetered real-time sensor networks that measure flow and salinity of canal water supply diversions and drainage export to the SJR. The sensor networks deployed in GWD and the SJVDA service area utilize a variety of water quality sondes manufactured by YSI(Xylem) Inc., In-SITU Inc. and Sutron Inc. to measure electrical conductivity (EC), temperature and pressure head at 15-minute intervals. Flow is measured certain monitoring sites using SONTEK acoustic Doppler transducers that utilize stage and velocity measurements to estimate current flow conditions. Both entities use Sutron X-Link 500 dataloggers to store the data and transmit the data via GSM and CDMA telemetry to both the HYDROMETCLOUD server, supported by SUTRON Inc. as a paid service. The SJVDA transmits the same data to HOSTGATOR, a cloud-based server that allows ftp uploads, storage and ftp export of processed data.

4.0 Project data and data management requirements

Continuous sensor data presents a challenge due to the large amount of information that needs to be downloaded and post-processed. Continuous sensor data can contain erroneous and/or missing data values due to telemetry issues, dead batteries, sensor drift due to biological fouling or sediment build-up on sensor electrodes, wiper malfunction, a sensor response time set too low, or unknown reasons (Plana et al., 2019; Horsburgh et al., 2015; Copp et al., 2010; Wagner et al., 2006). Erroneous and/or missing data needs to be detected and removed or replaced. Discrete data collected for data quality assurance purposes typically contains fewer data points compared to continuous sensor data and can require different input formats (e.g. replicates, blanks). Discrete data often contains meta data associated with each analyte and datapoint for quality assurance purposes that includes method information, detection limits, and standard deviations of the data between replicates.

5.0 HEC-DSSVue software

129   Software requirements for the project were to develop a public domain software solution for real-
130   time data quality assurance that was easy to teach to university students involved in field research,
131   and water district and agency project partners, that could be readily replicated on project and
132   cooperator computer platforms. The Java-based visual utilities program HEC-DSSVue was selected
133   as the software platform that met most project requirements. The Hydrologic Engineering Center
134   (HEC) of the US Army Corps of Engineers has developed water resources systems software for over
135   50 years focused on watershed hydrology, river hydraulics, and hydrologic data management. The
136   DSS database is the core data management system for all HEC models and is especially efficient and
137   flexible for time series data storage and analysis. HEC-DSSVue is a visualization add-on that allows
138   users to plot, tabulate, edit, and manipulate data in a HEC-DSS database file. There is a large
139   number of customized libraries accessible to programmers that provide enhanced functionality
140   using Java, C, and C# (.net) programming languages. This functionality has been exploited on the
141   project to develop a real-time data quality assurance capability. The same Java language scripts,
142   used to perform quality assurance functions including data interpolation, out-of-range data
143   censoring, and rate-of-change error trapping, have been exported for use as CRON (Unix-based
144   **chron**ological time-based job scheduler) jobs on the HostGator platform. HEC-DSSVue also provides
145   utility functions allowing easy import and manipulation of data sets into the HEC-DSS database. The
146   HEC-DSSVue database parses the data in a format that can be automatically uploaded into the
147   Watershed Analysis Risk Management Framework (WARMF) model. This model is used for
148   watershed drainage simulation and forecasting at key water quality compliance monitoring stations
149   along the San Joaquin River.

151   **6.0 Real-time data processing and quality assurance**

152   **6.1 Workflow with developed HEC-DSSVue scripts**

153   The data management and data quality assurance workflow that was automated in HEC-DSSVue
154   include tasks for data import, data screening, and correction of erroneous values (Figure 1). These
155   workflow subtasks are described in more detail below.

156   6.1.1. Data importing

157   HEC-DSSVue offers 2 methods for importing a dataset: either through the user interface or through
158   Jython scripting (HECDSS-Vue offers Jython (Java-based Python) scripting and HEC libraries to
159   automate/ customize tasks with programming). Generally, it is preferable to use the available data
160   importing feature in the user interface due to its ability to detect errors in the imported data. If the
161   number of individual datasets is large, importing through Jython scripting is preferable. For water
162   quality data, the basic structure of a dataset is a Time Series Container object, which contains
163   information about the watershed, location, parameter, time interval, and a series of timestamps
164   and recorded values. To import new data to a DSS file, the script reads the raw data and creates a
165   Time Series Container for each dataset, which is then saved to a DSS file under a unique pathname.

166   6.1.2 Data screening
167   Data screening detects anomalies and replaces missing and rejected data with either a value based
168   on linear interpolation, an average value, or a user-selected value. The customized user interface
169   (Figure 2), developed using the Java Swing library, allows users to visually acknowledge each
170   modification of the data and have more control over the data screening process. A
171   screening/replacing method is selected, and the updated data plotted to visualize the modification.
172   An overview of the interface and functions is provided in Appendix A and is available on GitHub at:
173   (https://github.com/nwm-54/hecdss/blob/master/README.md) The python scripting is shown in

174 Appendix B and the code available for download from the following GitHub url:
175 https://github.com/nwm-54/hecdss/blob/master/dashboard.py

176 The script for automated screening of data for erroneous values is a two-step process as
177 shown in the workflow in Figure 1. The first da ta screening step in the workflow is a range
178 check (maximum, minimum). Data values that fall outside a typical range for a particular
179 site are removed (i.e., errors in data transmission result in large negative numbers that can
180 be readily detected). The second step in the workflow is the adjacent value rate of change
181 (absolute value or percentage). Rate of change is particularly useful for parameters with
182 seasonal variations, e. g., temperature. The script allows to customize the rate of change by
183 selecting the number of data points that are compared to each other. More sophisticated
184 methods such as statistical analysis and machine learning (Moatar et al., 2001; Talagala et
185 al., 2019) were beyond the scope of this project and likely too complex for the intended
186 project users. Finally, the missing data gaps are filled via interpolation. The Python scripts
187 were also tasked with other methods of filling in missing values via averaging or with user-
188 specified data values.
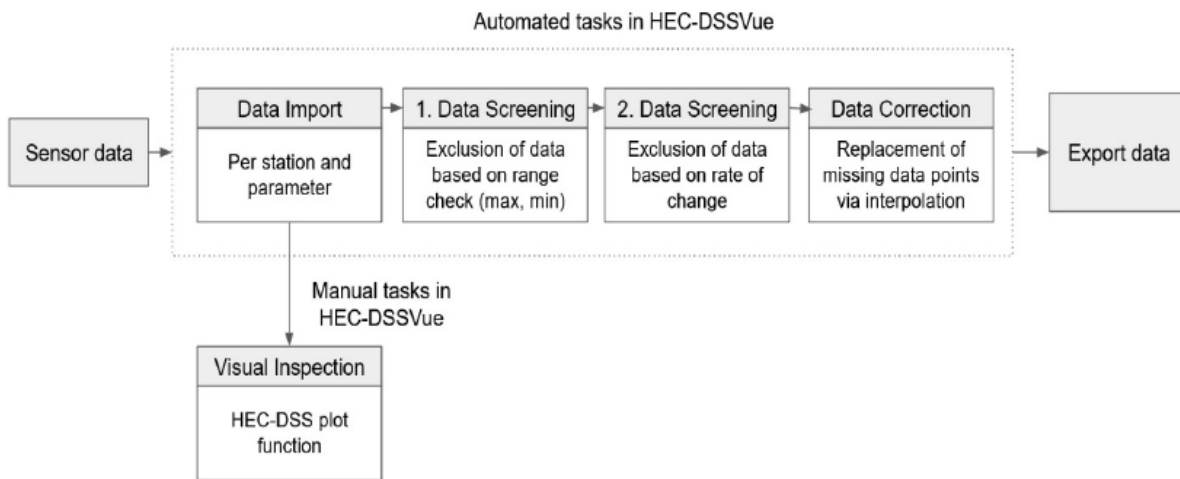
189

190 Figure 1. Flowchart showing workflow for data management of continues sensor data with
191 HEC- DSSVue.

192

193 **6.2 Data screening dashboard functions** A simple dashboard (Figure 2) was developed to
194 set data screening parameters for upper and lower data limits and rate of change criteria
195 that would be indicative of sensor drift or failure. The definition of the various options
196 shown in the dashboard is shown in the box below. The dashboard dialog also allows plots
197 to be made of the data time series to display the resulting time series once

Dashboard interface options
- *Button: Reset:* Erases the newly screened dataset and the table will return to the original dataset
- *Button: Plot:* Plots the dataset after screening/replacing.
- *Button: Save As Copy:* The program will save the screened dataset (with rejected value erased).
  - The pathname is auto generated based on the time the screening was made to make sure that it is unique. The pathname can be changed in the main window.
- *Button: Overwrite:* The program will overwrite the original dataset with the screened dataset (with rejected value erased).
- *Input: Ordinate:* In a dataset, each ordinate matches with a timestamp. By picking a Start and End Ordinate, we can define a time window on which the screening conditions are applied.
- *Input: Conditions:* Pick screening conditions by ticking the boxes and choose a value for each criterion.
  - The background for the input box is color coded: light gray = default value; dark gray = unused conditions; white = others.
  - If all four criteria are selected, a point x_t is accepted only when:
    - Min value $<= x_t <=$ Max value
    - With moving average over k, and $A_t = A_{t-k} + A_{t-k+1} + ... + A_{tk}$:
      - For Absolute Difference: $A_{t-1} - A_t <=$ Change Limit
      - For %: $\frac{A_{t-1}-A_t}{A_{t-1}}.100 <=$ Change Limit

198 the data substitution and data overwrite operations have been completed.

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200
201
202
203

ORDINATE	DATETIME	ORIGINAL	REPLACE
1	1 March 2018, 24:00	1500.00	1500.00
2	2 March 2018, 24:00	1523.00	1523.00
3	3 March 2018, 24:00	1546.00	1546.00
4	4 March 2018, 24:00	1515.00	1515.00
5	5 March 2018, 24:00	1519.00	1519.00
6	6 March 2018, 24:00	1589.00	1589.00
7	7 March 2018, 24:00	1592.00	1592.00
8	8 March 2018, 24:00	1600.00	1600.00
9	9 March 2018, 24:00	1602.00	1602.00
10	10 March 2018, 24:00	1601.00	1601.00
11	11 March 2018, 24:00	1616.00	1616.00
12	12 March 2018, 24:00	1630.00	1630.00
13	13 March 2018, 24:00	1645.00	1645.00
14	14 March 2018, 24:00	1670.00	1670.00
15	15 March 2018, 24:00	1671.00	1671.00
16	16 March 2018, 24:00	1689.00	1689.00
17	17 March 2018, 24:00	1700.00	1700.00
18	18 March 2018, 24:00	1733.00	1733.00
19	19 March 2018, 24:00	1800.00	1800.00
20	20 March 2018, 24:00	1840.00	1840.00
21	21 March 2018, 24:00	1801.00	1801.00
22	22 March 2018, 24:00	1803.00	1803.00
23	23 March 2018, 24:00	1809.00	1809.00
24	24 March 2018, 24:00	1818.00	1818.00
25	25 March 2018, 24:00	1834.00	1834.00

Ordinate
Start 10
End 24

Conditions
Min Value: ☑ 150 uS/m
Max Value: ☐ 99,999,999 uS/m
Change Limit: ☑ 4,850 ◉ Abs Difference ◯ %
Moving average over: ☑ 5 point(s)

Invalid value will be marked as R (rejected)
Compute

Missing 175/1037   Rejected 0/1037   Replaced 175/1037

Reset   Plot   parameter   Save As Copy   Overwrite

Figure 2. The data screening and data quality assurance user interface (dashboard) showing the original and final data columns and the dialog boxes for setting minimum and maximum data value thresholds and data value rate of change criteria that flags drift or sensor failure.

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6.2.1 Data substitution options

214 A separate dialog box is provided to define the data range for application of the data screening
215 criteria. This dialog box also allows the user to choose between automated linear interpolation, the
216 use of average values or the acceptance of a user specified value. The specific field circumstance
217 will determine which one of these options is most appropriate.

- *Input: Ordinate*: In a dataset, each ordinate matches with a timestamp. By picking a Start and End Ordinate, we can define a time window on which the screening conditions are applied.
- *Input: Flag:* pick types of flagging to replace
- *Input: Method:*
  - Linear Interpolation: Interpolate between two valid data points. If there are no valid data points to interpolate from or to, that value would be replaced by the average of valid data points in the dataset.
  - Average Value: Replace data points with the average of valid data in the dataset.
  - Custom Value: Replace data with a user-picked value
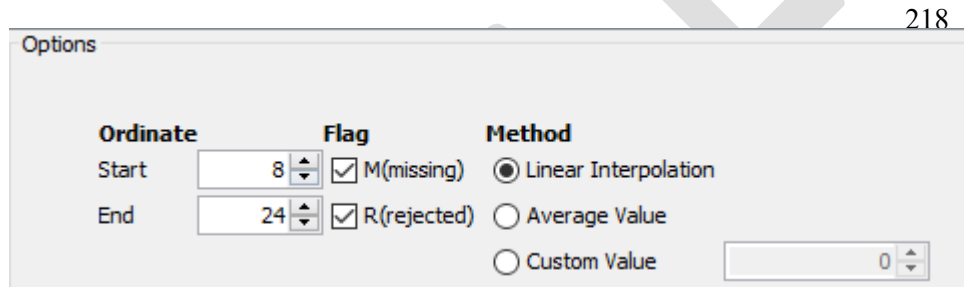
218

223 '

224 Figure 3. Dialog box for choosing data substitution options.

225

6.2.2 Additional options for customizing QA workflow

227 A number of visualization options have been added to allow color coding of various data elements
228 to make the final time series table easier to interpret.

Customizing the QA procedures
- To customize the default value for each parameter (the min/max value that appear in gray background on the screening tab) -> modify the *defaultScreenValue_CONST* variable following the given format
  - Example: *defaultScreenValue_CONST* = { 'PH':[6.0,9.0,'pH'], 'SPCOND':[150.0, 5000.0, 'uS/m']
- To change the color for Replaced cell (currently green) -> modify the *Color_SCREEN* variable to the desired RGB value following the given format
  - Example: *Color_SCREEN* = Color(205,0,0)
- To change the color for Replaced cell (currently red) -> modify the *Color_REPLACE* variable
  - Example: *Color_REPLACE* = Color(0,205,0)

7.0 Data quality assurance and WARMF model updating on the HOSTGATOR cloud server

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230 To aid data screening and automation of WARMF model updates for model-based forecasting, a
231 data quality assurance workflow analogous to the workflow presented above for HEC-DSSVue was
232 developed. HOSTGATOR is a commercial, subscription-based data cloud storage platform that is
233 customizable using Python and other similar scripting tools. The HOSTGATOR platform allows real-
234 time data processing to convert 15-minute raw data to error-corrected daily mean values suitable
235 for upload to the WARMF model. The WARMF water quality forecasting model requires a very large
236 amount of 15-minute, hourly and daily mean data to run and erroneous data can cause model
237 crashes that can be time-consuming and expensive to recover from – sometimes requiring intensive
238 troubleshooting. Although salt load assimilative capacity forecasts are currently made weekly – the
239 goal is to develop a robust data quality assurance program that will allow daily forecast model runs.
240 The same data processing Python scripts and algorithms were used in the HOSTGATOR
241 implementation of the real-time data screening and quality assurance workflow. This ensures
242 archival of the same data values whether processed and stored in the HEC-DSSVue database or in
243 the WARMF model input data files downloaded from HOSTGATOR.

244 GWD drainage data could be processed by HOSTGATOR for uploading to the WARMF model but
245 would require that the CDMA (version modems) be replaced with CDM (AT&T) modems since the
246 CDMA ftp messaging is incompatible with the HOSTGATOR incoming ftp server software. The added
247 cost and potential disruption to current operations have delayed this transition.
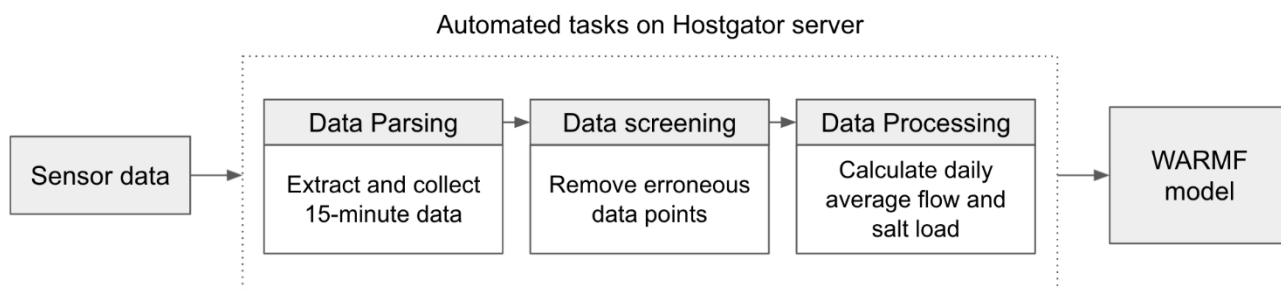
248 Figure 4. HOSTGATOR workflow to automate real-time sensor data migration and quality assurance
249 as input to the WARMF model.

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251 Raw sensor measurements from each SJVDA monitoring station are transmitted via cellular
252 telemetry every 15 minutes for drainage canal stage, water temperature, and EC in .csv file format.
253 A naming convention specifying the date and time of data collection, the parameter name and the
254 value of the parameter was used. On the HOSTGATOR server the 15-minute data is first scanned to
255 check the validity of the data. Valid data has a numeric value that falls within a predefined range of
256 reasonable values. Any invalid data is not be included in the calculation of daily average flow, EC,
257 and salt load. If no valid data are shown for any day, the average flow and salt load are left blank.
258 This process is repeated for all monitoring stations.

259 $$Flow = 3.33*Weir\ width\ *(stage - offset)^{1.5}\ (equation\ 1)$$
260 $$Salt\ load = Electrical\ Conductivity*0.64\ (equation\ 2)$$

261 For those stations where acoustic Doppler transducers are deployed the transducers compute flow
262 internally from velocity and stage measurements and report these directly to the SUTRON
263 datalogger and HOSTGATOR server. In this workflow the daily salt load is calculated from valid flow
264 and EC data for each 15-minute measurement period.

265 On the HOSTGATOR server, the Python code and algorithms for data averaging and calculation of
266 salt load are located in the CRON folder and executed daily. A CRON routine is a time-based job
267 scheduler software program written as a UNIX script. The HOSTGATOR server provides its own
268 Graphical User Interface for specifying each CRON job, allowing the application to run each data
269 error-checking task and data averaging task automatically at a specified date and time. Processed
270 HOSTGATOR average daily flow, EC, and salt load output are loaded to an outgoing ftp directory
271 after parsing into a .csv format suitable for uploading to the WARMF model directory as a WARMF
272 model input file. The WARMF model web server schedules these ftp data downloads and updates
273 the model input files automatically. On HOSTGATOR data must be migrated from the Outgoing ftp
274 folder to the Outgoing html folder to overcome known incompatibilities with the external WARMF
275 model server.

276

7.1 HOSTGATOR data processing output

278 An example of output from the HOSTGATOR server for the Hospital Creek monitoring site overseen
279 by the SJVDA is shown in Figure 5 below. Although this site is not a large source of salt load to the
280 SJR, uncorrected positive and negative data spikes can compromise the ability of the WARMF model
281 to accurately forecast salt load assimilative capacity at compliance monitoring stations. Simple,
282 easy-to-implement quality assurance is a cost-effective way to improve forecast model performance
283 and provide effective decision support for environmental water quality management.

284 Figure 5. Example of data screening to remove outliers and erroneous data points. The area
285 between the lower and upper bounds represent the valid data range, and data outside of this range
286 are outliers. Hospital Creek EC and stage (flow) data outliers are removed before calculating the
287 mean.

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8.0 Summary and Conclusions

This technical note has described a public domain, interactive and semi-automated data screening and quality assurance processing tool useful for both discrete and continuous data using the HEC-DSSVue data management and visualization platform. Analogous tools were developed for use on the HOSTGATOR cloud server using the same Python scripts and algorithms to migrate quality-controlled data directly to a server for use by the WARMF water quality forecasting model. The former application serves a research project directed at assessing salt and methylmercury drainage load control options. The latter application provides real-time data updates to the WARMF water quality forecasting model that is being used to provide decision support for short-term salinity control strategies. The Python scripts for both applications are easily adaptable by other potential users who do not currently have the resources to implement an enterprise- level hydrological data management and real-time quality assurance software system.

9.0 Data Availability

The intended purpose of this Technical Note was to address a deficiency in many field research projects and water district applications that utilize continuous data – which is the lack of appropriate tools for performing data quality assurance in real-time. There is commercial software available to perform these functions- however it is costly both in its acquisition and the need for dedicated personnel to use and maintain it. This is beyond the resources of researchers and many small water districts. The Python scripts and a user manual are available at the following urls.

(a) Readme file showing dashboard interface in HEC-DSSVue for performing real-time data quality screening and error corrections on monitoring stations data. (https://github.com/nwm-54/hecdss/blob/master/README.md)

(b) Annotated Python code for performing data quality control checks including data interpolation, removal of data spikes and data correction. Python code is consistent for both HEC-DSSVue and HOSTGATOR CRON job applications. https://github.com/nwm-54/hecdss/blob/master/dashboard.py

10.0 Acknowledgments

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