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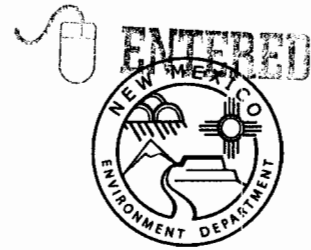
RYAN FLYNN
Cabinet Secretary
BUTCH TONGATE
Deputy Secretary

CERTIFIED MAIL - RETURN RECEIPT REQUESTED

February 19, 2015

Tim Davis
Chief, Environmental Officer
National Aeronautics and Space Administration
White Sands Test Facility
P.O. Box 20
Las Cruces, NM 88004-0020

Attention of: RE-14-038

RE: APPROVAL WITH MODIFICATIONS
SOIL BACKGROUND STUDY INVESTIGATION REPORT
NATIONAL AERONAUTICS SPACE ADMINISTRATION (NASA)
JOHNSON SPACE CENTER (JSC) WHITE SANDS TEST FACILITY (WSTF)
DOÑA ANA COUNTY, NEW MEXICO
EPA ID #NM08800019434
HWB-NASA-14-002

Dear Mr. Davis:

The New Mexico Environment Department (NMED) has received the NASA WSTF
(Permittee's) *Response to Second NMED Disapproval Comments*, dated December 17, 2014
(Response) on the NASA White Sands Test Facility (WSTF) Soil Background Study
Investigation Report. NMED has completed its review of the Response and hereby issues this
approval with the following modifications. NMED's comments on the Response are as follows.

Comment(s):
1.   **Permittee Comment-Evaluation of Software Capabilities, page 2:** "There are two primary mechanisms by which statistical software can be evaluated: (1.) making the source code available for evaluation, and (2.) providing a mechanism to conduct simulations with the software. ProUCL is developed for profit under contract with Lockheed Martin, and provides neither of these mechanisms for evaluation. The authors make numerous references to the simulations that were conducted with their source code but there is no way for others to verify their simulations since simulations are not built into the software and the source code is not made available. This also makes it difficult to compare other software products to ProUCL."

NMED Response: The methods incorporated in ProUCL Version 5.0.00 (ProUCL 5) have been tested and verified extensively by the developers as well as other researchers, scientists, and users (see ProUCL Version 5.0.00 Technical Guide, Acknowledgements, pg., ix). The results obtained by ProUCL are reported to be in agreement with the results obtained from other statistical software packages including Minitab, SAS, and programs written in R Script (see ProUCL Version 5.0.00 Technical Guide, Executive Summary, pg., ix).

2.   **Permittee Comment-Evaluation of Software Capabilities, page 3:** "The fact that the EPA contracted to have the ProUCL software developed should not make it a *de facto* standard since the potential to evaluate the ProUCL software is extremely limited, especially compared to more of the packages available for the R environment."

NMED Response: NMED promotes consistency by recommending that ProUCL be used at all Resource Conservation and Recovery Act (RCRA) sites requiring statistical analysis of environmental data sets (Soil Screening Guidance, December 2014 and previous versions). NMED reached this decision based on the flexibility and capability of ProUCL to compute statistics used in making informed decisions for a wide variety of environmental conditions in a cost-effective and protective (of human health and the environment) manner. The United States Environmental Protection Agency (USEPA) has designed ProUCL to compute decisions statistics using several parametric and nonparametric methods covering a wide range of data variability, distributions, skewness, and sample sizes. While NMED is aware that other statistical methods and approaches are available outside of ProUCL, the NMED currently recommends that approaches which differ from those available to the regulated community and regulatory agencies through ProUCL 5 be identified, described, and demonstrated as a more appropriate approach at a specific site than the ProUCL methods.

Since its initial development, ProUCL has been upgraded and enhanced to include many graphical tools and statistical methods described in various USEPA guidance documents including *Supplemental Guidance to RAGS: Calculating the Concentration Term* dated May 1992; *Calculating Upper Confidence Limits for Exposure Point Concentrations at Hazardous Waste Sites* dated December 2002; *Guidance for Comparing Background and Chemical Concentrations in Soil for CERCLA Sites* dated September 2002; *Data Quality Assessment: Statistical Methods for Practitioners* (EPA QA/G-9S) dated 2006; and *Statistical Analysis of Groundwater Monitoring Data at RCRA Facilities – Unified Guidance* dated 2009 among others. Several statistically rigorous methods (e.g., for data sets with non-detects [NDs]) not readily

available in existing regulatory documents or the environmental literature are found in ProUCL 5.

3.   Permittee Comment-ProUCL Comparison UTLs, page 7: "For comparison, calculations were performed for 95%-confidence-95%coverage UTLs using ProUCL. These are presented in Table 5. Depending on whether there are non-detects in the sample, ProUCL produces several different UTL calculations. ProUCL's calculations based on the WH and HW methods are excluded when there are non-detects. These (WH and HW in Table 5) are very close to the calculations in my 24-Mar-2014 report but are generally slightly larger due to their simplification of not using sufficient statistics. When non-detects occur in the sample, ProUCL calculates gamma-based UTLs using a GROS method that completely ignores the non-detects in estimating the gamma parameters. [..]. Also calculated by ProUCL when non-detects occur are the Kaplan-Meier (KM) estimates which estimate means and standard deviations using the nonparametric KM formulas but then substitute them into formulas for parametric UTL calculations. Regardless of the presence or absence of non-detects, ProUCL will produce a UTL estimate based on the maximum order statistic. It does not, however, provide the specified confidence and/or coverage and, in fact, is often substantially below that which is specified (such as the 46% confidence presented above when the confidence specified in the ProUCL dialog box is 95%).

NMED Response: NMED recommends methods discussed in Chapter 3 of the ProUCL Version 5.0.00 Technical Guide for data sets that do not contain NDs (i.e., uncensored data). Final selection of the type of upper limit to be calculated for uncensored data should be based on the data distribution (e.g., Gamma), the sample size(s), the subsequent use(s) of the background values, and the user's understanding of the information provided in the ProUCL Users and Technical Guides.

For data sets containing NDs, ProUCL uses several estimation methods including Kaplan-Meier (KM) methods and regression on order statistics (ROS) methods. These methods compute upper limits which adjust for data skewness. For example, ProUCL 5 can compute upper-tolerance limits (UTLs) using KM estimates of the mean and standard deviation (calculated using both the detected and non-detected results in a data set) in gamma UTL equations, provided the detected observations in the left-censored data set follow a gamma distribution. For skewed data sets, parametric methods (see the example above) or nonparametric methods which account for data skewness can be used (when sample sizes are sufficient) to compute background threshold values (BTVs).

The Permittee indicates that when NDs occur in the sample, UTLs based on the gamma regression on order statistics (GROS) methods were calculated using ProUCL. However, the KM methods (i.e., calculation of means and standard deviations using nonparametric KM formulas substituted into parametric UTL formulae) available in ProUCL were also used to predict UTLs for data sets that contained NDs.

Tables 5a through 5o in the Response show that for data sets that do not contain NDs, the UTLs calculated by ProUCL using KM methods with the Wilson-Hilferty (WH) and Hawkins-Wixley

(HW) models, are similar to those calculated by the Permittee. In fact, the UTLs calculated by the Permittee are typically lower, with some exceptions, than those predicted by ProUCL 5.

For data sets with NDs, the Permittee should use UTLs obtained from the KM methods described in Chapter 5 of the ProUCL Version 5.0.00 Technical Guide rather than ProUCL methods based on regression on order statistics.

Based on the information provided by the Permittee, it appears that the UTLs calculated represent viable and conservative estimates of the UTL for all data sets that do not contain NDs. It also appears that the most conservative UTL estimates for data sets with NDs come from using the results of the KM method(s) in ProUCL 5. Revise the Soil Background Report to indicate these two types of UTLs will be used as the soil background concentrations at WSTF. However, the Permittee must ensure that the Soil Background Report clearly identifies and discusses all deviations from the methods recommended in the ProUCL Version 5.0.00 Technical Guide and demonstrates that the deviations result in appropriate and conservative values for conditions specific to WSTF.

4. NMED General Comment:

The Permittee includes discussions of several technical issues associated with the use of ProUCL 5. Some of these concerns are addressed in the ProUCL Version 5.0.00 Technical Guide (e.g., Section 3.4.4 and the associated subsections discuss the issue of nonparametric tolerance limits). Others are not (e.g., potential need to improve the GROS method); however, NMED is aware that USEPA is interested in strengthening this method in forthcoming revisions of the ProUCL software. Because NMED does not have a formal mechanism for influencing or effecting revisions to the ProUCL software, the Permittee is encouraged to contact USEPA with comments, concerns, and questions related to ProUCL through:

Felicia Barnett (STL)
US EPA, Region 4
61 Forsyth Street, S.W.
Atlanta, GA   30303-8960
barnett.felicia@epa.gov
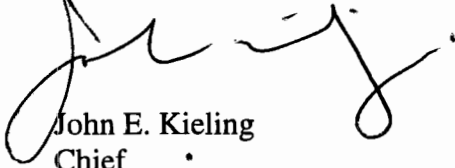(404) 562-8659   phone
(404) 562-8439   fax

In addition, the Permittee may be able to obtain additional information on the development and peer-review of ProUCL software from Ms. Barnett

The Permittee must address all comments in a response letter no later than **May 29, 2015**.

If you have any questions regarding this letter, please contact Vicky Baca at (505) 476-6059.

Sincerely,

John E. Kieling
Chief
Hazardous Waste Bureau

cc: N. Dhawan, NMED HWB
       D. Cobrain, NMED HWB
       K. VanHorn, NMED HWB
       L. King, EPA 6PD-N
       M. Zigmond, NASA WSTF

File: NASA WSTF, 2015, AWM_Soil_Background_Study_IR
       HWB-NASA-14-002