Final Technical Report to the Department of Energy*

Project Title

Development of Enabling Scientific Tools to Characterize the Geologic Subsurface at Hanford

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1. Executive Summary

The BER long-term measure states that sufficient scientific understanding must be provided by 2015 to allow a significant fraction of DOE sites to incorporate coupled physical, chemical, and biological processes into decision making for environmental remediation and long-term stewardship. Defensible decisions must be based on sound scientific understanding of the complex subsurface environments and processes controlling contaminant fate and transport.

Important variables in the fate and transport of subsurface contaminants include the physical and chemical properties of geologic formations in which they reside. A major challenge is to adequately describe subsurface heterogeneity in physical and chemical properties at multiple scales. Currently this challenge constrains our ability to improve conceptual models. In many cases, these problems cannot be resolved with existing knowledge and technology. It is clear that new approaches are needed and that advances in this area will likely lead to improved conceptual and predictive models, ultimately leading to better information for decision makers (N.R.C., 2000).

The development and production of nuclear weapons has left the DOE with serious subsurface environmental remediation and stewardship challenges. More than 100 sites within the DOE complex have soils, sediments or groundwater contaminated with radionuclide, metals, or organic materials. An important goal of the ERSP is to provide the DOE with field-scale site descriptions of subsurface properties, such as porosity, permeability, and mineralogy, which affect contaminant transport or transformation. While some of this information can be interpreted from analyses performed on core samples recovered from well bores, coring is expensive, core recovery is often incomplete, and analysis of recovered samples is both time-consuming and expensive. In contrast, neutron and spectral gamma logs can rapidly acquire continuous borehole data, leading to improved coverage and decreased time for analysis. However, these logs can also be expensive, and in uncharacterized environments such as the DOE sites, careful investigation must be done to select the most valuable logs to be run and to develop robust and efficient applications to properly interpret log data in terms of porosity, clay content, permeability, and water saturation. These properties are critical in developing reservoir models and in decisions regarding the selection of conceptual and predictive models and remediation efforts.

This final report to the Department of Energy provides a summary of activities conducted under our exploratory grant, funded through U.S. DOE Subsurface Biogeochemical Research Program in the category of enabling scientific tools, which covers the period from July 15, 2010 to July 14, 2013. The main goal of this exploratory project is to determine the parameters necessary to translate existing borehole log data into reservoir properties following scientifically sound petrophysical relationships. For this study, we focused on samples and Ge-based spectral gamma logging system (SGLS) data collected from wells located in the Hanford 300 Area. The main activities consisted of 1) the analysis of available core samples for a variety of mineralogical, chemical and physical; 2) evaluation of selected spectral gamma logs, environmental corrections, and calibration; 3) development of algorithms and a proposed workflow that permits translation of log responses into useful reservoir properties such as lithology, matrix density, porosity, and permeability. These techniques have been successfully employed in the petroleum industry; however, the approach is relatively new when applied to subsurface remediation.

This exploratory project has been successful in meeting its stated objectives. We have demonstrated that our approach can lead to an improved interpretation of existing well log data. The algorithms we developed can utilize available log data, in particular gamma, and spectral gamma logs, and continued optimization will improve their application to ERSP goals of understanding subsurface properties.

2. Technical Summary

2.1 Research goals objectives and accomplishments

The main goal of this exploratory project was to determine the parameters necessary to translate geophysical log data into subsurface properties following scientifically sound petrophysical relationships. We proposed to do this through the adaptation of techniques that have been successfully used in oilfield research, which include a procedure to quantify mineral composition in sedimentary formations using dual range (mid-and far-infrared) Fourier Transform Infrared (DRFT-IR) spectroscopy (Poulin et al., 2006; Snyder et al., 1983; Stark et al., 1993; Wouters et al., 1999) combined with multi-element chemical analysis and measurement of selected petrophysical properties. The chemical analysis is used to both validate mineralogy and to provide input for nuclear parameter forward modeling to build a table of chemistry, mineralogy, petrophysical properties and computed nuclear response parameters (Herron and Herron, 1997; McKeon and Scott, 1989). This information is used to develop algorithms to translate geophysical log data into properties such as lithology, matrix density, porosity and permeability.

The specific objectives of our project at its commencement were as follows:

1. Develop DRFT-IR for use at Hanford. The geologic setting at Hanford is quite different from the typical oilfield. Several minerals (in particular mafic minerals) are known to be present in the formations, but not currently present in our DRFT-IR mineral library.

2. Analyze Hanford core and outcrop samples for a suite of chemical and physical properties. This includes mineral composition, chemical composition, and matrix density. Core samples as well as additional data including laboratory bulk density, and chemical composition for a larger sample set were provided by Andy Ward (PNNL).

3. Compute the matrix geophysical response parameters related to well logging, using the analytical data from core samples and Schlumberger's Nuclear Parameter program (SNUPAR). Parameters include thermal and epithermal neutron response, and photoelectric absorption and thermal neutron capture cross section; gamma-ray response in API units will be computed from Th, U, and K concentrations.

4. Develop algorithms based on relationships between mineralogy, chemistry, physical properties, and computed nuclear response parameters to allow estimation of lithology, porosity, permeability, and water saturation from log data.

5. Evaluate available log data for the purposes of applying algorithms.

2.2 Summary of Project Activities

To date, we have analyzed 120 core samples and log data from 4 wells within the IFRC (399-3-31, 399-2-26, 399-2-31, and 399-2-30) and 4 wells more widely distributed within the 300 Area (399-3-18, 399-3-19, 399-3-20, and 399-1-23). To create a Hanford-relevant DRFT-IR mineral library, several new minerals have been identified through analysis of core samples and existing data and are now included in the mineral library. Analyses performed include dual range (mid-and far-infrared) Fourier Transform Infrared (DRFT-IR) spectroscopy to quantify mineral composition, multi-element chemical analysis, matrix density, and nuclear parameter forward modeling using SNUPAR. Additional work on objective 4 is ongoing, but we have been successful in developing algorithms to estimate matrix density and lithology, including clay and other lithological components. We currently estimate porosity based on the observed relationship between total clay and porosity. Permeability is estimated using the k-lambda model, which requires matrix density, clay, and porosity as input functions. We are currently working on a manuscript that details the translation algorithms and work flow.

We have conducted a detailed evaluation of algorithms currently used at Hanford to make environmental corrections (i.e., casing thickness and a water filled-borehole) and compute detector efficiencies. In an effort to make use of existing SGLS data for our work, we have developed new environmental correction algorithms based on least-squares regression techniques that include uncertainty in the data, and propagation of errors with respect to the predicted correction factors. Goodness- of- fit evaluation of the new algorithms yields reduced chi-square values with acceptable chi-square probabilities (>0.001) that are significantly lower than the current Hanford algorithms. When these new algorithms are applied to existing log data along with an empirical detector based efficiency correction, are applied to existing log data, a significant improvement in the accuracy and precision of the SGLS derived K, U, and Th concentrations are achieved as indicated by the reduction in uncertainties and improved agreement between core and log data.

2.3 Products

This grant provided salary, and travel support for PI Kenna. This included multiple trips to Cambridge, MA to use the SDR DRFT-IR Laboratory and meet with Co-PI Herron. Conference presentations included the Subsurface Biogeochemical Research program`s Annual PI meeting in 2010, 2011, and 2012 and the American Geophysical Union`s Fall Meeting in 2010 and 2011. PI Kenna also gave an invited talk related to the project to the Rutgers-Newark Chapter of the Geophysical Society of Exploration Geophysicists (SEG) (see Appendix for additional information). The work summarized in this Final Report will form the basis of two refereed publications. Final datasets including analytical results, revised SGLS interpretations as well as petrophysical property interpretations based on translation algorithms will be submitted through DOE`s E-Link and www.300areaifrc.org/ .

This exploratory project has been successful in meeting its stated objectives. We have demonstrated that our approach can lead to an improved interpretation of existing well log data. The algorithms we developed can utilize available log data, in particular gamma and spectral gamma logs, and continued optimization will improve their application to ERSP goals of understanding subsurface properties.

3. Financial Summary

CATEGORY	BUDGET	ACTUAL
SALARY AND WAGES	$45,613	$63,960
FRINGE BENEFIT	$14,551	$20,505
SUPPLIES AND MATERIALS	$5,685	$3,187
PUBLICATIONS	$1,000	$410
COMMUNICATIONS	$2,000	$538
SERVICES	$16,187	$2,177
DOMESTIC TRAVEL	$12,367	$7,057
F&A DEDUCTION	$52,597	$52,166
Totals:	$150,000	$150,000

The project period was 4/14/2010 – 7/14/2013. The total spending was equal to the amount awarded ($150,000). Actual vs. budgeted expenses were in reasonable alignment. Non-project resources covered a majority of outside laboratory analyses, which was budgeted in Services category, and we initially budgeted for travel to Hanford, which did not occur. These funds were re-allocated to PI salary, with permission from David Lesmes (DOE Program Director).

4. Appendix

<u>Report</u>

Kenna, T.C. 2014, Development of Enabling Scientific Tools to Characterize the Geologic Subsurface at Hanford, Final Technical Report to the Department of Energy U.S. Department of Energy Subsurface Biogeochemical Research Program Exploratory Grant, DE-SC0004625 July 15, 2010 - July 14, 2013

<u>Refereed Publications</u>

Kenna, T.C., Herron, M.M. and Ward, A.L., (in prep). Improving the accuracy and precision of K, U, and Th concentrations derived from spectral gamma log data at USDOE's Hanford site. Journal of Applied Geophysics.

Kenna, T.C., Herron, M.M. and Ward, A.L., (in prep). The translation of log responses into reservoir properties useful for input in flow and reactive transport models. For submission to Journal of Environmental & Engineering Geophysics.

<u>Invited Talks</u>

Kenna, T.C., Herron, M.M., Ward, A.L., 2012. Translation of geophysical log responses to estimate subsurface hydrogeologic properties at the Hanford 300 Area. Invited talk presented on 4/4/2012 to the Rutgers-Newark Chapter of the Geophysical Society of Exploration Geophysicists, Rutgers, NJ.

<u>Conference Proceedings</u>

Kenna, T.C., Herron, M.M. and Ward, A.L., 2010. Development of Enabling Scientific Tools to Characterize the Geologic Subsurface at Hanford, Department of Energy (DOE) Subsurface Biogeochemical Research (SBR) 5th Annual PI Meeting, March 29-31, 2010, Washington, D.C., pp. 54.

Kenna, T.C., Herron, M.M. and Ward, A.L., 2010. Development of enabling scientific tools to characterize the geologic subsurface at Hanford, Abstract H23C-1215 presented at 2010 Fall Meeting, AGU, San Francisco, Calif., 13-17 Dec.

Kenna, T.C., Herron, M.M., Ward, A.L., Development of Enabling Scientific Tools to Characterize the Geologic Subsurface at Hanford. Department of Energy (DOE) Subsurface Biogeochemical Research (SBR) 6th Annual PI Meeting, April 26–28, 2011, Washington, DC., pp 51.

Kenna, T.C., Herron, M.M., Ward, A.L., 2011. Translation of geophysical log responses to estimate subsurface hydrogeologic properties at the Hanford 300 Area. Abstract H51H-1299 presented at 2011 Fall Meeting, AGU, San Francisco, Calif., 5-9 Dec.

Kenna, T.C., Herron, M.M. and Ward, A.L., 2010. Development of enabling scientific tools to characterize the geologic subsurface at Hanford, Abstract H23C-1215 presented at 2010 Fall Meeting, AGU, San Francisco, Calif., 13-17 Dec.

5. References

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McKeon, D.C. and Scott, H.D., 1989. SNUPAR-a nuclear parameter code for nuclear geophysics applications. Nuclear Science, IEEE Transactions on, 36(1): 1215-1219.

Poulin, M., Hidore, J., Sutiyono, S., Herron, M.M., Herron, S.L., Seleznev, N., Grau, J., Horkowitz, J.P., Chabernaud, T. and Alden, M., 2006. Deepwater core comparison with answers from a real-time petrophysical evaluation. SPE Reservoir Evaluation and Engineering, 9(2): 165-171.

Snyder, R.W., Painter, P.C. and Cronauer, D.C., 1983. Development of FT-i.r. procedures for the characterisation of oil shale. Fuel, 62: 1205–1214.

Stark, P.B., Herron, M.M. and Matteson, A., 1993. Empirically minimax affine mineralogy estimates from Fourier-transform infrared spectroscopy data using a decimated wavelet basis. Applied Spectroscopy, 47: 1820-1829.

Wouters, L., Herron, M.M., Abeels, V., Hagood, M. and Strobel, J., 1999. Innovative applications of dual range Fourier transform infrared spectroscopy to analysis of Boom Clay mineralogy. Aardkundige Mededelingen, 9: 159-168.