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GROUND WATER
QUALITY BUREAU

Date: September 13, 2021
Refer To: N3B-2021-0289

Steve Pullen
Ground Water Quality Bureau
New Mexico Environment Department
1190 S. St. Francis Drive
P.O. Box 5469
Santa Fe, NM 87502-5469

Subject: Submittal of the Work Plan for Groundwater Modeling for Contaminant Migration from Wells R-42 and R-28, Revision 1

Dear Mr. Pullen:

Enclosed please find the "Work Plan for Groundwater Modeling for Contaminant Migration from Wells R-42 and R-28, Revision 1." On June 25, 2021, the U.S. Department of Energy Environmental Management Los Alamos Field Office (EM-LA) submitted the initial version of this work plan in response to the New Mexico Environment Department (NMED) letter, "Notice of Non-Compliance, Los Alamos National Laboratory (LANL), Regional Aquifer Wells R-28 and R-42," dated May 27, 2021. On July 15, 2021, NMED provided a response, including a series of comments, and required that a revised work plan be submitted within 30 days of the letter. Subsequently, on August 3, 2021, NMED granted an extension for the revised work plan to 60 days from the July 15 letter. In addition to the revised work plan, EM-LA is submitting a response to the 11 comments in NMED's July 15 letter (Enclosure 2).

If you have questions, please contact Christian Maupin at (505) 695-4281 (christian.maupin@em-la.doe.gov) or Cheryl Rodriguez at (505) 414-0450 (cheryl.rodriguez@em.doe.gov).

Sincerely,

Troy Thomson

Troy Thomson
Acting Program Manager
Environmental Remediation
N3B-Los Alamos

Sincerely,

M Lee Bishop for

Digitally signed by M Lee Bishop for
Date: 2021.09.09 13:19:46 -06'00'

Arturo Q. Duran
Compliance and Permitting Manager
U.S. Department of Energy
Environmental Management
Los Alamos Field Office

Enclosure(s): One hard copy with electronic files:

1. Work Plan for Groundwater Modeling for Contaminant Migration from Wells R-42 and R-28, Revision 1 (EM2021-0570)
2. Response to Comments in New Mexico Environment Department Letter, "Los Alamos National Laboratory, Work Plan for Groundwater Modeling for Contaminant Migration from Wells R-42 and R-28, NMED Response," Dated July 15, 2021 (EM2021-0473)

cc (letter and enclosure[s] emailed):
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WORK PLAN FOR GROUNDWATER MODELING FOR CONTAMINANT MIGRATION FROM WELLS R-42 AND R-28, REVISION 1

1.0 INTRODUCTION

The U.S. Department of Energy (DOE) Environmental Management Los Alamos Field Office (EM-LA) submitted an initial version of this work plan (N3B 2021a) in response to the New Mexico Environment Department's (NMED's) letter dated May 27, 2021, "Notice of Non-Compliance, Los Alamos National Laboratory (LANL), Regional Aquifer Wells R-28 And R-42" (NMED 2021a). As requested, the work plan detailed "DOE's proposed initial modeling, both conceptual and computer simulation, of the contaminant migration." The contaminants referred to in NMED's May 27, 2021, letter are naturally occurring iron and manganese that have been liberated from the aquifer sediments near the wells (R-42 and R-28) where a pilot-scale study is underway to evaluate the technical feasibility of using amendments (sodium dithionite and molasses, respectively) added directly into areas within the hexavalent chromium plume as part of a potential groundwater remediation strategy (Figure 1.0-1). The geochemically reducing conditions around R-42 and R-28 were intentionally induced in a small, pilot-scale, footprint within the regional aquifer. The pilot-scale study described above is being implemented in accordance with the "Pilot-Scale Amendments Testing Work Plan for Chromium in Groundwater beneath Mortandad Canyon" (Pilot-Scale WP; LANL 2017a), which was submitted to NMED on July 11, 2017, and subsequently approved by NMED on July 31, 2017 (NMED 2017). A supplement to the pilot-scale study titled "Supplemental Work Plan for Pilot-Scale Amendments Testing for Chromium in Groundwater beneath Mortandad Canyon" (N3B 2019a) was submitted to NMED on September 24, 2019, and subsequently approved by NMED on July 29, 2020 (NMED 2020).

Upon submittal of the initial version of the work plan, NMED provided a letter with a series of comments on technical aspects of the work plan and they stated that EM-LA "should provide NMED with a revised Work Plan within 30 days of this letter addressing NMED's concerns…" (NMED 2021b). Subsequently, NMED granted EM-LA an extension to 60 days. This work plan fulfills the request for a revised work plan, laying out the technical steps required to complete the modeling analysis.

2.0 BACKGROUND

As noted above, the pilot-scale study involved the deployment of a sodium dithionite solution into R-42 and a molasses solution into R-28 in the fall of 2017. EM-LA submitted two notices of intent to discharge (NOIs), one for each proposed amendment deployment, to the NMED Ground Water Quality Bureau (GWQB) on May 22, 2017 (LANL 2017b,c). The amendments were subsequently deployed into these two wells in accordance with no-permit-required determinations made by the NMED-GWQB and received on June 27, 2017, for R-28 and July 18, 2017, for R-42. The Pilot-Scale WP and the NOIs noted the possibility of iron, manganese, and other constituents being liberated from aquifer sediments as a result of the conditions induced by deployment of the amendments. Accordingly, monitoring at R-42 and R-28 has included these and other constituents since deployment of the amendments in the fall of 2017.

The results of the sampling conducted at R-42 and R-28 as part of the pilot-scale study have been included in a series of periodic reports submitted to NMED over several years (LANL 2018a; LANL 2018b; N3B 2018a; N3B 2018b; N3B 2019b; N3B 2019c; N3B 2019d; N3B 2020a). These reports provide the data in the context of tracking the progress of the study and evaluating the principle geochemical indicators that provide insights into how conditions around these wells are evolving since amendment deployment.

Additionally, modifications were made to EM-LA’s discharge permit 1835 (DP-1835) to include monitoring for iron and manganese for compliance monitoring of the effluent from the ion-exchange treatment system. The monitoring occurs weekly and is included in quarterly reports submitted as a requirement under DP-1835 (e.g., N3B 2021b). Sampling and analysis are also being conducted at extraction wells and nearby monitoring wells on a monthly basis for a wide range of constituents, including iron and manganese. Those data indicate no apparent increases in iron or manganese at those locations with the exception of extraction well CrEX-3, which shows elevated manganese. However, the data remain inconclusive with regards to whether the elevated manganese at CrEX-3 is directly related to the elevated manganese at R-28. This work plan discusses additional investigations that will be performed to address the potential for an R-28 amendment signature at CrEX-3.

3.0 PROPOSED MODELING APPROACH

The Notice of Non-Compliance (NMED 2021a) directed DOE to develop a work plan for the development of both conceptual and numerical models for the fate and transport of iron and manganese. The following two subsections outline DOE’s proposed approach for the conceptual (section 3.1) and numerical (section 3.2) models.

3.1 Conceptual Model

The conceptual model for fate and transport of iron and manganese as a result of amendments deployment in R-42 and R-28 will be developed to enable representation of the behavior of these constituents from the time of amendments deployment, to the present-day condition, to potential future behavior. The components of the conceptual model include the behavior of the amendments during deployment and the subsequent hydrogeochemical processes acting on the amendments, breakdown products, and the reduced iron and manganese species.

The hydrologic elements of the conceptual model consist of the following phases: (1) pre-amendment-test behavior of the groundwater flow field, as influenced by natural gradients and gradients induced by interim measure (IM) operations; (2) local displacement of native groundwater with amendment solutions, and in the case of dithionite at R-42, the subsequent rapid withdrawal of a much larger volume than the amendment solution volume, which imparted relatively short-lived changes to the flow conditions near the amendment injection wells; and (3) re-establishment of flow conditions as influenced by IM operations. Induced gradients caused by supply well pumping appear to be very small to non-existent for most supply wells. Nevertheless, this potential influence will be included in the modeling analysis as well.

Numerous geochemical processes will also be included in the conceptual model, including

- reduction-oxidation processes,
- fate of the sodium dithionite and molasses and their breakdown products upon injection into the formation,
- solubility and speciation of iron and manganese as a function of geochemical conditions,
- sorption of reduced iron and manganese aqueous species via cation exchange processes, and
- potential re-oxidation of iron and manganese species as they migrate into oxidizing groundwater.

The conceptual model will be described using a combination of field observations at the site and general hydrogeochemical principles. Assumptions and system-scale simplifications will be identified and justified, and the accompanying numerical modeling will be based on these assumptions and simplifications.

A primary feature of the conceptual model concerning the source of reduced iron and manganese is that rather than being introduced into the aquifer (with the exception of a small amount of iron and manganese introduced with the molasses), these species are generated through liberation from the aquifer sediments under amendment-induced reducing conditions. For well R-28, these reducing conditions are caused by the stimulation of microbial growth from molasses consumption and the consumption of some of the organic breakdown products of molasses. Therefore, elevated total organic carbon (TOC) levels are a pre-condition to the generation of iron and manganese, and it follows that iron and manganese generation will occur only in locations where TOC has migrated and remained elevated enough in concentration to stimulate significant microbial growth. Conversely, to a first approximation, elevated iron and manganese should not have been generated at any location that remains at background levels of TOC. Thus, bounding calculations of the extent of reduced iron and manganese generation will be conducted through simulations of the “TOC footprint,” the extent of migration of the dissolved organic compounds introduced to the aquifer. Some iron and manganese migration slightly beyond this footprint can be expected, although this migration will be retarded by cation exchange. Manganese is likely to transport somewhat further beyond the TOC footprint than iron because it oxidizes much more slowly than iron in the presence of dissolved oxygen (oxidation will effectively permanently immobilize both iron and manganese).

For R-42, the well that received the sodium dithionite amendment, a similar concept can be applied except in this case the iron and manganese were generated from aquifer sediments as a result of direct chemical reduction by dithionite, a process that is much faster than the biostimulation-induced reduction at R-28. Another important difference at R-42 is that the vast majority of the amendment solution was withdrawn from R-42 in the 7 weeks after the amendment was deployed by pumping nearly 8 times the volume of the amendment solution from the well over the 7-week period. An estimated 90–95% of the amendment solution was withdrawn (based on the recovery of the co-injected bromide tracer), and with it a significant amount of iron and manganese was also withdrawn from the aquifer. Any remaining dithionite solution would have rapidly induced sediment reduction very near R-42 and ceased to retain its ability to promote further reduction as it drifted downgradient. Thus, unlike at R-28, where iron and manganese generation could occur within a relatively large TOC footprint that was not withdrawn from the aquifer and drifted downgradient, iron and manganese generation at R-42 should have been limited to a footprint that was little or no larger than the volume of aquifer into which the dithionite solution was injected (i.e., within at most about 10 m of R-42). Iron and manganese would be expected to migrate downgradient from this small footprint, experiencing retardation by cation exchange and oxidation to insoluble species after encountering dissolved oxygen.

3.2 Numerical Modeling

This work plan discusses two numerical modeling approaches for providing estimations of the fate and transport of reduced iron and manganese in the regional aquifer liberated from aquifer sediments during the pilot-scale study. The two approaches, three-dimensional modeling and geochemical modeling, will be described first, followed by a brief discussion of the way in which these approaches will be used synergistically to investigate the extent of iron and manganese concentrations in the aquifer.

Three-dimensional modeling: This study will leverage the development of the three-dimensional flow and transport model currently being updated for the Chromium project. Previous versions of this model have been reported in various reports over the past several years (e.g., LANL 2018c,d). The model, implemented using the Finite Element Heat and Mass (FEHM) computer code, has been used most recently to study the influence of IM operations at the chromium site on plume behavior, including simulation of plume control due to extraction of chromium-contaminated water in the interior of the plume and injection of water of very low chromium concentration at the leading edge of the plume. In the references provided above, the model has been used to optimize IM operation, examine the impact of converting an infrastructure well originally envisioned to be an injection well to an extraction well, and, more generally, to provide insights into aquifer behavior. The model as currently constructed simulates regional aquifer groundwater flow and hexavalent chromium transport. Inputs to the model include hydrologic parameters such as permeability, porosity, and transport properties such as dispersivity and sorption coefficients. Details regarding how these parameters are set and adjusted during model calibration are provided in “Fate and Transport Modeling and Risk Assessment Report for RDX Contamination in Deep Groundwater” (N3B 2020b).

The “Compendium of Technical Reports Conducted Under the Work Plan for Chromium Plume Center Characterization ”(LANL 2018c) also presented a set of calculations demonstrating a capability to simulate chemical or biological remediation. At the time these calculations were performed, there was no specific information on how the amendment was deployed, so the calculations presented were useful to conceptualize system behavior but are not predictions of the amendments pilot tests themselves. Today, a great deal of data are available, including nearly 4 years of geochemical observations at R-42 and R-28, as well as observations or lack thereof, in downgradient wells. The modeling study described herein will advance the modeling using the available data and modeling tools currently in place to investigate chromium system behavior, and in this case, the extent of iron and manganese in the aquifer as a result of the pilot-scale amendments tests.

Water is introduced into or exits the simulated region via the application of head or flux-based boundary conditions, the latter used for simulating time-varying inputs and outputs of groundwater due to IM operations. Chromium is input to the model via implementation of zones at the water table in which chromium is input, to simulate the presence of “drip points” from the vadose zone. Chromium can leave at any point of fluid exit in this model, which occurs at extraction wells, although if chromium-contaminated water were to reach model boundaries or water supply wells, it would leave at those locations as well.

The model is calibrated to observed heads under ambient conditions, as well as transient head responses at wells in the vicinity of IM injection and extraction as the IM wells are turned on and off. Time-varying chromium concentrations at monitoring and extraction wells also provide a rich calibration data set that is particularly relevant to the iron and manganese modeling study. Demonstrating that the model, once calibrated, can represent the levels of chromium contamination and changes with time in the study area should provide confidence that the model can also be used confidently to simulate other constituents, such as TOC, iron, and manganese. Uncertainty in model predictions is quantified using advanced uncertainty quantification methods described in “Fate and Transport Modeling and Risk Assessment Report for RDX Contamination in Deep Groundwater” (N3B 2020b).

The chromium groundwater flow and transport model is updated periodically in order to incorporate recent data collection from existing wells and new wells. Currently, the model is being updated through calibration to initial data from well R-70 and new data from across the site area at other wells. The initial calibrated model is expected to be available by the end of September 2021, after which time the model will be validated against data not used in the calibration. The latter process will take an additional 2 months, at which time the model can be deployed in the present study.

The calibrated three-dimensional model will be used, with simplifying assumptions, to investigate the extent of iron and manganese generation and transport. This will be accomplished first in a bounding fashion and potentially later through inclusion of additional geochemical complexity. The model will simulate the input flow rates and concentrations of chemical and biological amendments, after which the transport of the chemical constituents in the aquifer will be simulated under conditions that include ambient groundwater flow and local flows impacted by IM operations. Because of the previous calibration exercise, the actual IM operating conditions will have already been incorporated in the model. For R-28, DOE and Newport News Nuclear BWXT-Los Alamos, LLC (N3B) envision an initial “bounding” simulation consisting of molasses injection and transport of molasses and its breakdown products. To ensure the calculation is bounding, TOC will initially be treated as a conservative, non-sorbing, dissolved species in groundwater. Under the assumption that the TOC footprint defines the maximum extent of reducing conditions (see conceptual model discussion above), this footprint can be used as a proxy for identifying the maximum extent of reduced iron and manganese generation in the aquifer. This three-dimensional result, including potential TOC migration above or below the injection elevation, is bounding because reduced iron and manganese can only be generated anywhere that TOC became elevated above background concentrations (it is possible that reducing conditions might exist where TOC is no longer elevated because biofilms promoted by previously elevated TOC levels can have a residual reducing effect). By treating TOC as a conservative species that does not decay, the predicted TOC footprint will be larger than the actual TOC footprint, and thus the predicted TOC footprint should provide a reasonable bounding estimate of the maximum extent of iron and manganese in excess of the 1.0- and 0.2-mg/kg limits (allowing for the possibility that reduced iron and manganese might transport somewhat beyond the actual TOC footprint in which they were generated). Simulations initiated at the time of amendment injection and extending to the present day will provide bounds on the current extent of elevated iron and manganese. Projections of future behavior can also be made under an appropriate assumed IM operating scenario.

For R-42, the sodium dithionite amendment test well, a similar calculation approach will be employed to bound present-day and future locations of the reduced zone in which elevated concentrations of reduced iron and manganese can exist. In this case, the extent of the reduced zone is likely to be much smaller than at R-28 because of the withdrawal of the vast majority of the sodium dithionite solution in the 7 weeks after it was injected (see Conceptual Model section), and also because of the very rapid reaction of sodium dithionite with sediments, which should have resulted in the sodium dithionite being rapidly consumed before it could have moved any significant distance downgradient. Recognizing that there was a considerable amount of iron and manganese that continued to be generated and was observed in R-42 long after the 7-week withdrawal period, simulations will be conducted to predict where the water residing within the original footprint of the injected sodium dithionite solution (before withdrawal) migrated downgradient. Because iron and manganese will be retarded by cation exchange and immobilized by oxidation (after they encounter dissolved oxygen), simulations of the conservative transport of the water from within the original sodium dithionite footprint should provide a conservative bound on the predicted footprint of iron and manganese in exceedance of the 1.0- and 0.2-mg/kg limits.

An additional focus of the three-dimensional modeling study will be to investigate the potential for impacts of molasses injection at R-28 to be experienced at CrEX-3. Circumstantial evidence for this potential is the close proximity of CrEX-3 to R-28 (54 m laterally), observations of biological growth in the well (including methanotrophs not seen in other CrEX wells that could be related to methanogens identified in R-28), the presence of elevated manganese (iron concentrations have remained low), and a very-near-detection-limit arrival at CrEX-3 of a naphthalene sulfonate tracer injected into R-28 in 2016, a year before the molasses injection. Alternatively, biological growth in CrEX-3 may be an inherent condition of the well since it was drilled, rather than being caused by the R-28 biological amendment. The latter alternative is supported by the lack of elevated TOC or any other constituents injected with the molasses solution, including iron, at CrEX-3. A component of the modeling work will be to examine the hydraulic conditions in the vicinity of CrEX-3 and to bring in additional data, including any data related to CrEX-3 biological activity (Willis et al. 2021), to attempt to draw more definitive conclusions about what, if any, influence the R-28 amendments test has had on CrEX-3.

An important observation to consider is the fact that no elevated concentration of iron or manganese has been detected at any monitoring well, although the closest well downstream of R-28 is R-45, which is about 400 m away. Also, CrIN-1 and CrIN-2’s injection locations are situated in between the amendments locations and R-45, the downstream monitoring well that would be expected to be the first to receive elevated TOC, iron, and manganese. Current operations involve injection of clean water into these wells in between R-28 and R-45, which may provide a barrier to migration of these constituents to R-45. Importantly, CrIN-1 and CrIN-2 showed no indications of a molasses geochemical signature or of any tracers previously injected into R-28 (deuterated water and 1,6-naphthalene disulfonate injected in 2016) before they came online as injection wells. These factors leave little information to affirm or refute the validity of the numerical model using iron, manganese, or other chemical tracers. If simulations agree with the hypothesis that the elevated TOC front ends somewhere between R-28 and CrIN-1 and CrIN-2, then the extent will have been confirmed at that level. Further modeling analyses will then be performed to identify potential locations for monitoring to delineate the extent of elevated concentrations. This data gap analysis may include the use of extraction wells in that portion of the chromium plume area that would, in the course of extracting chromium, also remove excess TOC, iron, and manganese as an ancillary benefit.

One-dimensional geochemical transport modeling: In parallel with the three-dimensional model development, geochemical modeling will be conducted and one-dimensional reactive transport simulations will be performed. There are several geochemical modeling codes that could be deployed for this portion of the study. By mutual agreement between EM-LA/N3B and NMED, the PHREEQC (PH [pH] REEQ [redox equilibrium] C [in C language]) code will be used in this study (https://www.usgs.gov/software/phreeqc-version-3). The objectives of this part of the modeling study are to (1) gain insight into the conditions necessary for generation of elevated iron and manganese and its subsequent transport and (2) provide analyses that enable the development of appropriate simplifications/abstractions in the three-dimensional model.

The creation of reducing conditions devoid of dissolved oxygen is necessary for the generation of dissolved iron (II) [Fe(II)] and manganese II [Mn(II)] in solution. The geochemical reactions associated with molasses and sodium dithionite fate and transport within the aquifer will be developed and simulated. For R-28, the molasses and its breakdown or biotransformation products will each be assumed to decay according to first-order reaction kinetics; organic compounds will be assumed to transport without sorption to aquifer sediments. The decay of the molasses and other organic compounds will be linked to the generation of Fe(II) and Mn(II) from sediments using fractional conversion factors to determine the amount of Fe(II) and Mn(II) generated per mole of organic compound degraded or biotransformed (using literature data and expert judgement). For R-42, laboratory data will be used to place bounds on the amounts of Fe(II) and Mn(II) generated per mole of dithionite injected, and the reactions generating the Fe(II) and Mn(II) will be assumed to occur very rapidly. Thus, Fe(II) and Mn(II) generation will be short lived and quite local to R-42. However, much of the Fe(II) and Mn(II) generated near R-42 will be predicted to precipitate as sulfide phases (dithionite reactions generate a large amount of sulfide and other reduced sulfur species), which will serve as a prolonged source term for Fe(II) and Mn(II) as the reduced sulfur slowly oxidizes and releases co-precipitated Fe(II) and Mn(II). Once generated at either R-28 or R-42, Fe(II) and Mn(II) will interact with sediments through cation exchange reactions. Other geochemical reactions, including precipitation of supersaturated phases and/or dissolution of undersaturated phases, will be implicitly included in the one-dimensional PHREEQC modeling. If conditions revert back to oxidizing and/or the Fe(II) and Mn(II) migrate into oxidizing zones, the oxidation and subsequent precipitation of the iron and manganese will be modeled using a kinetic model, with parameters assigned based on literature values or expert judgement. It will be important to assign uncertainties to all these parameters and to perform an uncertainty analysis for the results.

By simulating these geochemical reactions at a more fundamental level, insights will be gained about the mobility and ultimate fate of iron and manganese.

Merging of three-dimensional modeling and geochemical modeling: The previous modeling exercises should provide initial insights into the likely extent of reducing conditions and elevated iron and manganese concentrations and they will elucidate the important geochemical reactions and their effect on mobility of the reduced iron and manganese. If necessary, a final step in the analysis will be the incorporation of additional geochemical complexity into the three-dimensional model. For iron and manganese, this would likely take the form of the abstraction of complex interactions between dissolved species and sediments to a simplified sorption model that can be readily handled in FEHM. For TOC, a first-order kinetic reaction could be used to represent breakdown and biotransformation processes of the organic compounds, and the three-dimensional simulations could be run with these simplifications. At this stage, the exact form that these additional simulations would take is not known. Furthermore, if the initial hydrologic and geochemical modeling suggests large, irreducible uncertainties, these uncertainties may drive a decision to forego this final step, as it would add little to the previous analyses.

4.0 REFERENCES

LANL (Los Alamos National Laboratory), July 2017. “Pilot-Scale Amendments Testing Work Plan for Chromium in Groundwater beneath Mortandad Canyon,” Los Alamos National Laboratory document LA-UR-17-25406, Los Alamos, New Mexico. (LANL 2017a)

LANL (Los Alamos National Laboratory), May 2017. “Notice of Intent to Conduct a Pilot-Scale Amendment Study at Los Alamos National Laboratory Regional Aquifer Monitoring Well R-42,” Los Alamos National Laboratory letter number EPC-DO: 17-188, Los Alamos, New Mexico. (LANL 2017b)

LANL (Los Alamos National Laboratory), May 2017. “Notice of Intent to Conduct a Pilot-Scale Amendment Study at Los Alamos National Laboratory Regional Aquifer Monitoring Well R-28,” Los Alamos National Laboratory letter number EPC-DO: 17-190, Los Alamos, New Mexico. (LANL 2017c)

LANL (Los Alamos National Laboratory), January 2018. “Quarterly Report on Pilot-Scale Amendments Testing for Chromium in Groundwater beneath Mortandad Canyon,” Los Alamos National Laboratory document LA-UR-18-20467, Los Alamos, New Mexico. (LANL 2018a)

LANL (Los Alamos National Laboratory), April 2018. “Second Quarterly Report on Pilot-Scale Amendments Testing for Chromium in Groundwater Beneath Mortandad Canyon,” Los Alamos National Laboratory document LA-UR-18-23418, Los Alamos, New Mexico. (LANL 2018b)

LANL (Los Alamos National Laboratory), March 2018. “Compendium of Technical Reports Conducted Under the Work Plan for Chromium Plume Center Characterization,” Los Alamos National Laboratory document LA-UR-18-21450, Los Alamos, New Mexico. (LANL 2018c)

LANL (Los Alamos National Laboratory), April 2018. “Evaluation of Chromium Plume Control Interim Measure Operational Alternatives for Injection Well CrIN-6,” Los Alamos National Laboratory document LA-UR-18-23385, Los Alamos, New Mexico. (LANL 2018d)

N3B (Newport News Nuclear BWXT-Los Alamos, LLC), July 2018. “Third Quarterly Report on Pilot-Scale Amendments Testing for Chromium in Groundwater Beneath Mortandad Canyon,” Newport News Nuclear BWXT-Los Alamos, LLC, document EM2018-0019, Los Alamos, New Mexico. (N3B 2018a)

N3B (Newport News Nuclear BWXT-Los Alamos, LLC), October 2018. “Fourth Quarterly Report on Pilot-Scale Amendments Testing for Chromium in Groundwater Beneath Mortandad Canyon,” Newport News Nuclear BWXT-Los Alamos, LLC, document EM2018-0069, Los Alamos, New Mexico. (N3B 2018b)

N3B (Newport News Nuclear BWXT-Los Alamos, LLC), December 2019. “Supplemental Work Plan for Pilot-Scale Amendments Testing for Chromium in Groundwater beneath Mortandad Canyon, Revision 1,” Newport News Nuclear BWXT-Los Alamos, LLC, document EM2019-0455, Los Alamos, New Mexico. (N3B 2019a)

N3B (Newport News Nuclear BWXT-Los Alamos, LLC), January 2019. “Fifth Quarterly Report on Pilot-Scale Amendments Testing for Chromium in Groundwater Beneath Mortandad Canyon,” Newport News Nuclear BWXT-Los Alamos, LLC, document EM2019-0011, Los Alamos, New Mexico. (N3B 2019b)

N3B (Newport News Nuclear BWXT-Los Alamos, LLC), April 2019. “Sixth Quarterly Report on Pilot-Scale Amendments Testing for Chromium in Groundwater Beneath Mortandad Canyon,” Newport News Nuclear BWXT-Los Alamos, LLC, document EM2019-0133, Los Alamos, New Mexico. (N3B 2019c)

N3B (Newport News Nuclear BWXT-Los Alamos, LLC), December 2019. “Seventh Report on Pilot-Scale Amendments Testing for Chromium in Groundwater Beneath Mortandad Canyon, April to September 2019” Newport News Nuclear BWXT-Los Alamos, LLC, document EM2019-0427, Los Alamos, New Mexico. (N3B 2019d)

N3B (Newport News Nuclear BWXT-Los Alamos, LLC), June 2020. “Eighth Report on Pilot-Scale Amendments Testing for Chromium in Groundwater Beneath Mortandad Canyon, October 2019 to March 2020” Newport News Nuclear BWXT-Los Alamos, LLC, document EM2020-0253, Los Alamos, New Mexico. (N3B 2020a)

N3B (Newport News Nuclear BWXT-Los Alamos, LLC), May, 2020. “Fate and Transport Modeling and Risk Assessment Report for RDX Contamination in Deep Groundwater” Newport News Nuclear BWXT-Los Alamos, LLC, document EM2020-0135, Los Alamos, New Mexico (N3B 2020b).

N3B (Newport News Nuclear BWXT-Los Alamos, LLC), June 2021. “Work Plan for Groundwater Modeling for Contaminant Migration from Wells R-42 and R-28” Newport News Nuclear BWXT-Los Alamos, LLC, document EM2021-0348, Los Alamos, New Mexico. (N3B 2021a).

N3B (Newport News Nuclear BWXT-Los Alamos, LLC), June 2021. “Quarterly Report for the Discharge of Treated Groundwater to the Regional Aquifer under Discharge Permit 1835, Calendar Year 2021 Quarter 1” Newport News Nuclear BWXT-Los Alamos, LLC, document EM2021-0264, Los Alamos, New Mexico. (N3B 2021b)

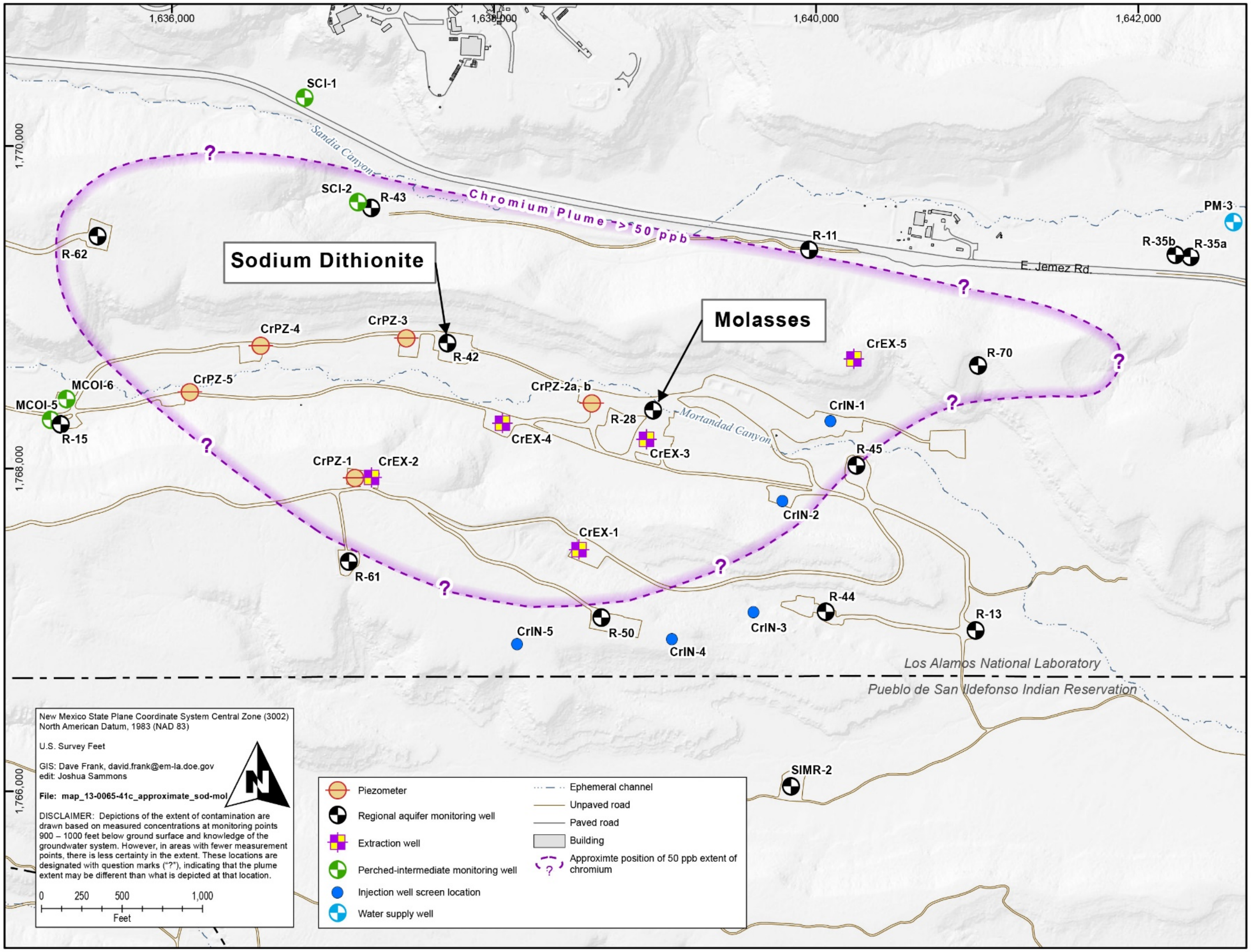
NMED (New Mexico Environment Department), July 31, 2017. “Approval, Pilot-Scale Amendments Testing Work Plan for Chromium in Groundwater beneath Mortandad Canyon,” New Mexico Environment Department letter to D. Hintze (DOE-EM) and B. Robinson (LANL) from J.E. Kieling (NMED-HWB), Santa Fe, New Mexico. (NMED 2017)

NMED (New Mexico Environment Department), January 14, 2020. “Approval with Modification, Supplemental Work Plan for Pilot-Scale Amendments Testing for Chromium in Groundwater Beneath Mortandad Canyon Revision 1,” New Mexico Environment Department letter to D. Hintze (EM-LA) from K. Pierard (NMED-HWB), Santa Fe, New Mexico. (NMED 2020)

NMED (New Mexico Environment Department) 2021. “Notice of Non-Compliance, Los Alamos National Laboratory (LANL), Regional Aquifer Wells R-28 And R-42,” New Mexico Environment Department letter to A. Duran (EM-LA) from M. Hunter (NMED-GWQB), Santa Fe, New Mexico, dated May 27, 2021. (NMED 2021a)

NMED (New Mexico Environment Department) 2021. “Los Alamos National Laboratory, Work Plan for Groundwater Modeling for Contaminant Migration from Wells R-42 and R-28, NMED Response,” New Mexico Environment Department letter to T. Thomson (N3B) and A. Duran (EM-LA) from S. Pullen (NMED-GWQB), Santa Fe, New Mexico, dated July 15, 2021. (NMED 2021b).

Willis, B., G. WoldeGabriel, D. Katzman, and P. Reimus, March 2021. “Biofouling in a Chromium Plume-Control Interim Measure Extraction Well at Los Alamos National Laboratory – 21269” WM2021 Conference, March 8–12, 2021, Phoenix, Arizona, USA. (Willis et al. 2021)



New Mexico State Plane Coordinate System Central Zone (3002)
North American Datum, 1983 (NAD 83)

U.S. Survey Feet

GIS: Dave Frank, david.frank@em-la.doe.gov
edit: Joshua Sammons

File: map_13-0065-41c_approximate_sod-mol

DISCLAIMER: Depictions of the extent of contamination are drawn based on measured concentrations at monitoring points 900 – 1000 feet below ground surface and knowledge of the groundwater system. However, in areas with fewer measurement points, there is less certainty in the extent. These locations are designated with question marks ("?"), indicating that the plume extent may be different than what is depicted at that location.

Figure 1.0-1 Chromium plume area and the locations where the sodium dithionite and molasses pilot-scale study is being conducted

Response to Comments in New Mexico Environment Department Letter, "Los Alamos National Laboratory, Work Plan for Groundwater Modeling for Contaminant Migration from Wells R-42 and R-28, NMED Response," Dated July 15, 2021

INTRODUCTION

To facilitate review of this response, the New Mexico Environment Department's (NMED's) comments are included verbatim. The U.S. Department of Energy (DOE) Environmental Management Los Alamos Field Office responses follow each NMED comment.

NMED Comment

1. *The Work Plan is very general and details of model objectives, selection of input parameters, and model uncertainties need to be established and identified.*

DOE Response

1. The revised work plan has addressed this comment by providing additional detail on many items, including approaches to estimating the fate and transport of amendments and descriptions of the three-dimensional and geochemical modeling approaches.

NMED Comment

2. *The Work Plan should be written for the comprehension of the general public, presumably with the appropriate technical terminology with accompanying explanations.*

DOE Response

2. DOE and Newport News Nuclear BWXT-Los Alamos, LLC (N3B) believe that the additional detail provided runs counter to the goal of making the work plan understandable to the general public but have made an effort to write the work plan using clear, concise language and to avoid jargon.

NMED Comment

3. *The Work Plan references the "fate and transport of iron and manganese" as the sole goal of the effort. The Work Plan should be augmented to include the Notice's stated goals of estimating "the locations of the dissolved 1.0 mg/L Fe and 0.2 mg/L Mn contours in three dimensions within the aquifer" and "identifying data gaps in the existing monitoring well network." Examples of data gaps should include insufficient monitoring wells in the vicinity of R-28 and R-42 and insufficient monitoring wells with screened intervals capable of determining vertical transport of elevated dissolved concentrations of Fe and Mn within the aquifer.*

DOE Response

3. The revised work plan emphasizes the tracking of the "TOC [total organic carbon] footprint" in a three-dimensional model would bound the location of the dissolved 1.0-mg/L iron and 0.2-mg/L manganese contours. Additional detail from the geochemical studies will enable refinement of this

bound. The revised work plan also mentions that data gaps will be identified and reported as part of the modeling effort.

NMED Comment

4. *The Work Plan states that Fe and Mn are not noted in "nearby monitoring wells," but fails to mention that the nearest downgradient monitoring wells are approximately 1300 feet away. The Notice specifically requests a data gap analysis be conducted as part of the Work Plan in order to evaluate siting of monitoring wells to delineate the Fe and Mn plumes around R-28 and R-42.*

DOE Response

4. The revised work plan includes this detail on the downgradient monitoring wells and also mentions that data gaps, in the form of absence of data at key locations or uncertainties in parameter values, will be identified and reported as part of the modeling effort.

NMED Comment

5. *The Work Plan should reference the Notice's specifically referenced considerations, i.e., migration based on the prevailing hydraulic gradient of the regional aquifer, the current hydraulic impact of the on-going injection and extraction within the chromium plume, the influence of County production wells, and the current measured impact to extraction well CrEX-3. The Work Plan should provide other potential sources of the elevated Mn at CrEX-3.*

DOE Response

5. The revised work plan provides additional discussion on the importance of addressing CrEX-3 observations and the potential influence of the R-28 molasses injection on this extraction well. The revised work plan also emphasizes that the three-dimensional model will investigate whether pumping at CrEX-3 is predicted to cause impacts at CrEX-3 from the molasses injection at R-28.

NMED Comment

6. *The Work Plan references elevated Mn at CrEX-3 and states that "the data remain inconclusive with regard to whether the elevated manganese at CrEX-3 is directly related to the elevated Mn at R-28. NMED considers the question of a related impact at CrEX-3 to be a fundamental goal of the Notice and that this goal should be stated in the Work Plan.*

DOE Response

6. DOE/N3B acknowledge the comment. Please refer to the response to Comment 5 for the strategy for investigating the CrEX-3 issue.

NMED Comment

7. *The Work Plan does not reference previous efforts to model contaminant fate and transport within the regional aquifer, e.g., LANL's Groundwater Modeling Status Report dated March 2018 (2018 Report). Nor does the Work Plan mention the model being continually updated regarding the chromium plume as indicated in LANL's comment response to a recent status report on the chromium interim*

measures performance, "DOE continues to incorporate numerous data streams into the numerical modeling being conducted for the chromium plume." The Work Plan should be augmented to identify these efforts, to reference the general findings of those efforts and any subsequent conclusions, to reference any previously identified data gaps, and to evaluate the relevance of those efforts to the fate and transport of dissolved Fe and Mn. The 2018 Report, figure 2.3-1 illustrates the simulation of the injection of molasses and a biological inhibitor at R-28 and shows the concentration of Cr(VI) removed as a result of remediation 10 months after injection, albeit only at the very top of the regional aquifer. The Work Plan should commit to similarly illustrating the concentrations of dissolved Fe and Mn downgradient of R-28 and R-42.

DOE Response

7. The previous work cited in this comment is summarized in the work plan in order to discuss its relevance and limitations. In the revised work plan, DOE/N3B commit to using the three-dimensional model of the chromium plume area to simulate iron and manganese.

NMED Comment

8. *The Work Plan fails to address the Notice requirement to "timely report to NMED [the] results of the initial modeling …."*

DOE Response

8. DOE/N3B commit to staying in close communication with the NMED Groundwater Quality Bureau (GWQB) on this effort and look forward to continuing the close technical collaboration that has already been established between N3B and NMED-GWQB on this topic.

NMED Comment

9. *The Work Plan describes two modeling approaches. Modeling approach 1 involves development of a three-dimensional reactive transport model, including the full effects of the hydraulic and geochemical behavior of the system through the various operational phases. Modeling approach 2 would utilize a one-dimensional geochemical transport model, with inputs such as flow direction and velocity informed by the three-dimensional model. Though the Work Plan identifies the need for "inputs such as flow direction and velocity informed by the three-dimensional model" (approach 1), the Plan recommends using approach 2 because the level of uncertainty in the geochemical processes is expected to dominate the analysis of this system, making a full three dimensional representation presented as approach 1 less useful than approach 2, which would fully evaluate the redox, solubility, and sorption processes. NMED requests LANL perform both approaches 1 and 2 and disregard the stated concern regarding "model development time."*

DOE Response

9. The revised work plan presents an approach that incorporates both three-dimensional modeling (approach 1) and geochemical modeling (approach 2), thereby satisfying the NMED request in this comment.

NMED Comment

10. *The Work Plan references an option in performing the one-dimensional transport process (approach 1) of utilizing either the Finite Element Heat and Mass (FEHM) code or the PHREEQC code. NMED request LANL utilize the PHREEQC code as the agency is considerably more familiar with the PHREEQC code and believes the code will provide more informative results. NMED requests a technical meeting with LANL before the PHREEQC simulations are conducted that focus on PHREEQC modeling with the objective of quantifying aqueous speciation, oxidation and reduction, mineral equilibrium and kinetics, adsorption for batch equilibrium and reactive transport simulations. NMED technical staff shall work closely with LANL technical staff during all aspects of conceptual model development and numerical model simulations quantifying hydraulic and geochemical processes controlling the movement, fate, and transport of dissolved Fe and Mn.*

DOE Response

10. DOE/N3B agrees to use PHREEQC (PH [pH] REEQ [redox equilibrium] C [in C language]), and has begun technical interactions with NMED-GWQB on the topics listed in this comment.

NMED Comment

11. *NMED is concerned that LANL intends for the groundwater flow direction and velocity to be "informed by the three-dimensional model." NMED considers this inappropriate. The model must be calibrated to actual field hydraulic data and is not suitable to obtain these parameters through model simulations. The model must simulate observed field conditions that include, at a minimum, measured (synoptic) groundwater levels from each chromium group well and piezometer, the hydraulic gradient, and groundwater flow velocity and direction through calculations based on the measured groundwater levels from both the shallow and deeper screened intervals. LANL must derive these model calibration parameters from properly prepared potentiometric surface contour maps of the regional aquifer by triangulating the three-point problem of synoptic water levels recorded at each well at the time of injection. This will provide the basis for the three-dimensional hydrogeologic conceptual model. The model must then be calibrated to such data, at a minimum, and can also be calibrated to the concentration changes of specific contaminants.*

DOE Response

11. As described in the revised work plan, DOE/N3B commit to perform a model calibration to available hydraulic and geochemical data, including concentration changes of specific contaminants. Regarding the portion of the comment related to measured groundwater levels, N3B stands by its methodology for determining water-level targets for model calibration. This is the method used in the Royal Demolition Explosive (RDX) model calibration in "Fate and Transport Modeling and Risk Assessment Report for RDX Contamination in Deep Groundwater" (N3B 2020). DOE/N3B request that a focused discussion take place to discuss this specific issue.

REFERENCE

N3B (Newport News Nuclear BWXT-Los Alamos, LLC), May, 2020. "Fate and Transport Modeling and Risk Assessment Report for RDX Contamination in Deep Groundwater" Newport News Nuclear BWXT-Los Alamos, LLC, document EM2020-0135, Los Alamos, New Mexico (N3B 2020).