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December 9, 2010

Mr. Randall T. Hicks
R.T. Hicks Consultants, Ltd.
901 Rio Grande Blvd. NW
Albuquerque, NM 87104

Attention: David Hamilton

Dear Mr. Hicks:

Subject: FY10 NMSBA report on the AMIGO project

In August 2010, as part of the New Mexico Small Business Assistance (NMSBA) Program, Sandia National Laboratories (SNL) agreed to provide consulting services to your firm on the AMIGO software tool. I served as the Principal Investigator, and two other Sandians provided project guidance: Jim Brainard, a senior hydrogeologist in the Geoscience Research & Applications group, and Mark Rigali, the manager of the Geochemistry department. The project objectives were: (1) to examine the capabilities of AMIGO; (2) to potentially collaborate with state agencies to help focus the pathway for future testing and review; and (3) to provide your firm with a written summary of our findings and recommendations for future testing and review. This letter report summarizes our findings and recommendations.

AMIGO examination. Examination of the AMIGO software tool began with identification of principal equations, parameters, databases, assumptions, and limitations. Most of this information is available in the AMIGO manual, API Publication 4734 (“Modeling Study of Produced Water Release Scenarios”), and the HYDRUS-1D manual. A brief summary of findings are provided below. For a more detailed summary, see the PowerPoint presentation included as an attachment to this letter.

AMIGO is a combination of a simplified vadose zone model and saturated zone model. For the vadose zone model, simulated by the HYDRUS-1D numerical code, a modified Richard’s equation is used for water flow. The modification to this equation is simply an added sink term for the water uptake at the root level. Solute transport is simulated using a traditional 1-D solute transport equation, simplified from equation 3.1 of the HYDRUS-1D manual. Because chloride has high concentrations in brine spills and is expected to have the earliest and, likely, greatest effect on saturated zone groundwater quality, AMIGO focuses solely on chloride transport. AMIGO has the properties of five soil types (medium sand, clay, caliche, silt, loam) and nine soil profiles built into the code. The documentation of (or ability to view) these parameters in the tool is not readily available.

The vadose zone model includes a number of simplifying assumptions. Many of these assumptions are conservative with respect to potential impacts at a nearby groundwater monitoring well, implying that the model will tend to predict that chloride will travel faster than it would in the field. The major assumptions include:

1. No upward flow
2. No lateral dispersion (i.e., no lateral flow)
3. No vapor transport
4. No thermal gradients
5. Porosity of 0.25 for all soil profiles
6. No dual porosity
7. No hysteresis
8. No deliquescence
9. No density or viscosity effects

Certainly, the first three assumptions listed are conservative. The other assumptions listed may or may not be conservative depending on the application or they may have negligible effects.

The saturated zone is represented by a mixing cell located directly beneath the modeled vadose zone. This cell mixes the water and chloride entering from above with groundwater flowing horizontally. The fluxes of water and chloride through the cell are constrained by conservation of mass, as explained in Section 10.2 of the AMIGO manual. The major assumptions of the saturated zone calculations include:

1. A mixing cell thickness equal to the thickness of the aquifer or screen length of a monitoring well, whichever is smaller
2. A mixing cell length equal to the length of the spill area
3. Groundwater flow in the same direction as the length of the spill
4. Placement of a monitoring well immediately down gradient of the mixing cell
5. Instant mixing of chloride within the cell
6. Groundwater in the well is monitored for chloride but not pumped
7. No dispersion, except within the cell and except when modeling transport beyond the mixing cell to an optional distant well (user-defined)

The third, fourth, sixth, and seventh assumptions are generally conservative. The third and fourth assumptions maximize capture of chloride at the monitoring well while the sixth and seventh minimize dilution. The other three assumptions involve mixing. Instant mixing within the cell is a reasonable simplifying assumption because groundwater samples collected for regulatory purposes are fairly large volume measurements as a result of monitoring well screen lengths and well purging procedures that cause mixing over the screen length during sampling. (The guidelines of the New Mexico Environment Department for the construction of monitoring wells call for a 20-ft screen with the top placed 5 feet above the water table.)

Based on the findings of this examination, AMIGO appears to be an appropriate tool for conservatively estimating the effects of brine spills or chloride-rich surface materials on groundwater chloride concentrations. For confirmation, verification and validation through testing are needed, as discussed below.

Testing and Review. Typically, a suite of verification and validation exercises is undertaken to quantify the predictive accuracy and uncertainty of numerical codes. Verification and validation exercises of the AMIGO code are primarily documented in API Publication 4734. However, because AMIGO is based on the HYDRUS-1D code, certain validation exercises documented in the HYDRUS-1D manual are also applicable to AMIGO. Validation of the vadose zone model of AMIGO is provided in examples 1 and 2 of the HYDRUS-1D manual. Verification, however, that AMIGO provides the same results as HYDRUS-1D is undocumented.

In chapter 12 of API Publication 4734, AMIGO is shown to reproduce vadose zone chloride transport observations originating from actual brine releases. One set of data pertains to two controlled brine releases at anode beds, and the other pertains to historical brine releases beneath two junction boxes. In both cases, the results match the observations well; however, some fitting was permitted. For the two controlled releases beneath the anode beds, longitudinal dispersivity was adjusted to fit the observations. For the releases beneath the junction boxes, dispersivity, spill size, spill dimensions, and initial chloride concentrations were fitted.

AMIGO's saturated zone mixing model is validated in chapter 3 of API Publication 4734 through comparisons of AMIGO simulation results to that of MODFLOW. Results are compared for two applications, one in Shreveport, Louisiana, and one in Hobbs, New Mexico. Breakthrough curves at the monitoring wells show good general agreement and slightly faster (conservative) transport for the mixing model.

Additional testing would enhance confidence in AMIGO's predictive capabilities. First, using AMIGO to simulate examples 1 and 2 of the HYDRUS-1D manual should confirm that HYDRUS-1D is implemented correctly in AMIGO. Second, testing AMIGO's predictions, without fitting, to field observations or to the results of more sophisticated models would indicate whether AMIGO could serve as a good screening tool in the field. Specific recommendations regarding further testing are provided in the recommendations section below.

Feedback from state regulators. To help focus the needs for additional testing and review of AMIGO, regulators from around the state were contacted. This section summarizes their feedback. The first three people below I was able to contact by phone. The remaining responses are taken from voice mail or email messages. I was unable to get a response from Edward Hansen of the New Mexico Oil Conservation Division (NMOCD) of the NM Energy, Minerals and Natural Resources Department.

Randy Rust, an environmental protection specialist for the Bureau of Land Management (BLM) in Carlsbad, has used AMIGO in the past and thinks it is useful as a reality check when assessing the rate of chloride transport. The BLM is primarily concerned with surface contamination and whether remediation is necessary. If deemed necessary, the concern becomes how soon, which is related to how fast salts leach downward. Randy's biggest challenge using AMIGO is determining depth to groundwater and other parameters needed to predict the groundwater flux. Using AMIGO, he has never predicted fast enough transport through the vadose zone in the Carlsbad vicinity to affect groundwater.

Myra Harrison, district resource manager of the State Land Office (SLO) in Hobbs, has not used AMIGO but is familiar with it. She believes AMIGO could be quite useful in helping formulate recommendations for action (or no action) at brine spill sites. In her district, a brine spill is a fairly frequent occurrence. Currently, the environmental staff members at the office are new and would require training on the software. Myra would welcome further testing of AMIGO and may be interested in participating at some level.

Mike Bratcher, an environmental specialist at the Artesia office of the NMOCD, has not used AMIGO but has heard of it. He believes its use would be beneficial when trying to predict the downward migration of salt and the potential impacts to groundwater. He notes that NMOCD is also concerned about the effects of brine spills and surface salts on plants and animals in contact with salts near the surface. I noted that AMIGO predicts salt concentrations over time for the entire soil column in addition to salt concentrations in the saturated zone. The importance of salt concentrations near the surface implies that a conservative approach for predicting salt concentrations in a monitoring well when field data are uncertain could be nonconservative for predicting salt concentrations at the surface.

Bill Olson, chief of the ground water quality bureau of the NM Environment Department (NMED), explained that his department does not review or endorse software but it will evaluate how software is used when it is applied at a particular site such as a soil cleanup site.

Jami Bailey, director of the Oil, Gas, and Minerals Division at the SLO writes that her division "really does not have a need for a software tool such as you describe."

Larry Hill, district NMOCD supervisor in Hobbs, writes, "I am sorry that I cannot express all my concerns on the AMIGO software issue. The probability of flawed or misrepresented data input does not leave me with a fuzzy feeling. All our submittals using this program are sent directly to our Environmental Bureau in Santa Fe. Please contact Mr. Glenn VonGonten for any further comments you may need."

Glenn von Gonten, senior hydrologist at NMOCD in Santa Fe writes, "OCD has looked at Amigo - it is a package that API put together back in 2008, I believe. Like any model, it could be useful. However, OCD does not use Amigo or other models because OCD requires Operators to investigate, delineate, and remediate ground water contamination. OCD does not allow an Operator to model away ground water impacts. OCD does not review models that consultants or the industry bring to our attention."

Recommendations. Based on examination of the AMIGO software tool and input from state regulators, the following recommendations are offered for consideration:

- *Improve the documention of equations and parameter values*. Include in the AMIGO manual the flow and transport equations, the van Genuchten parameters for each soil type, and plots of the matric potential and hydraulic conductivity vs. water content for each soil type. Also include other minor missing information noted in the attached Powerpoint presentation. Without this information, the software cannot be fully examined and understood.

- *Verify and document correct HYDRUS-1D implementation in AMIGO*. Demonstrate that the tool can reproduce the results of examples 1 and 2 in the HYDRUS-1D manual and include the input files for these examples in the software package.
- *Develop a conservative field method for applying AMIGO as a screening tool*. In the absence of site data, which is common according to Randy Rust, potential users must estimate parameter values. To do this, appropriate guidance could ensure that predictions of groundwater impacts are conservative for the concern being evaluated. For most parameters, the current AMIGO manual recommends obtaining data as accurate as possible but generally does not suggest what to do when data are unavailable. Defining a conservative field method for applying AMIGO in the absence of site data would have two primary purposes. First, it would help users choose conservative inputs so that insignificant releases could be screened out. Second, if the initial results indicate that a release might be potentially significant, the field method would help users perform sensitivity analyses for uncertain parameters. Sensitivity analyses are useful in determining which parameters must be determined more accurately (perhaps by direct measurement) in order to improve AMIGO predictions. A conservative field method for groundwater impacts, however, would likely be nonconservative for predicting salt concentrations near the surface, so this method and its focus should be clear. The development of a conservative field method could make AMIGO more useful and user-friendly as a screening tool.
- *Testing AMIGO and the conservative field method*. AMIGO and the conservative field method could be tested in several ways. First, simple demonstrations of the effects of altering the values of individual parameters would indicate which values for a given parameter are more conservative than others and which parameters have the greatest effects on chloride transport. Much of this type of analysis is included in API Publication 4734. Second, the results of more sophisticated flow and transport models could be used as benchmarks for testing AMIGO. Because AMIGO is a simplified model that uses conservative assumptions, it would be expected that AMIGO would predict faster chloride transport than a more sophisticated model. One potential benchmark is example 11 in the HYDRUS-1D manual. It includes the effects of upward vapor transport and heat transport. Another benchmark might come from a HYDRUS-2D example that includes the effects of lateral dispersion. Third, AMIGO predictions using the conservative field method could be applied to past spills or future field experiments to test the feasibility of the method as a conservative screening tool. A literature search for reports of chloride tracer tests may also provide useful test data. Documentation of each of these tests should build confidence in the use of AMIGO as a reliable screening tool for predicting potential groundwater effects.
- *Develop rules of thumb.* If AMIGO is established through additional testing as a reliable screening tool, it could potentially be used to define or support simple rules of thumb for quickly deciding what actions to take for new brine spills or new salt-rich surface deposits. This work would likely build on the work presented in API Publication 4758, “Strategies for Addressing Salt Impacts of Produced Water Releases to Plants, Soils, and Groundwater,” where a similar approach is developed.

A future NM Small Business Assistance project with SNL could potentially address many or all of these recommendations. Proposals for larger leveraged projects, involving a group of NM small businesses, are reviewed once a year. For more information, contact Genaro Montoya at (505) 284-0625.

Sincerely,

Paul E. Mariner
Sandia National Laboratories

PM/pm

Enclosure:
Hardcopy of Microsoft PowerPoint presentation, "An Examination of the AMIGO Software Tool," by P.E. Mariner, December 2010

Copy to:
James Brainard, SNL
Mark Rigali, SNL

An Examination of the AMIGO Software Tool

December 2010

P.E. Mariner
Technical Staff

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Purpose of Presentation

- To provide
  - An assessment of AMIGO software capabilities and limitations
  - Recommendations with regard to additional testing and review activities that could help establish AMIGO as a useful tool for assessing environmental impacts of brine spills

Tasks

1. Examine the capabilities/limitations of AMIGO
   a) Identify equations, parameters, databases
   b) Identify assumptions, limitations, conservatisms
2. Examine current documentation of AMIGO testing and review
3. Summarize findings and recommendations with regard to further testing and review

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Introduction

- What is AMIGO?
  - AMIGO is a screening tool designed to quickly and conservatively estimate the downward transport over time of unreactive solutes (e.g., chloride) from a brine spill (or from a chloride-rich material on the surface) through the vadose zone to a hypothetical groundwater observation well immediately down gradient of the spill area or beyond.
  - AMIGO combines:
    - HYDRUS-1D (Šimůnek et. al, 1998) to simulate downward transport of water and solutes through the vadose zone
    - A flow-through mixing-cell model in the saturated zone directly beneath the spill area

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Introduction (cont.)

- Relevant New Mexico regulations and guidelines
  - 19.15.29 NMAC, Release notification
    - Minor release, >5 to as much as 25 barrels
      - Requires timely written notice
    - Major release, >25 barrels or "volume that may with reasonable probability be detrimental to water or exceed the standards in [19.15.30.9]"
      - Requires immediate verbal notice and timely written notice
  - 19.15.30 NMAC, Remediation
    - "The responsible person shall abate the vadose zone so that water contaminants in the vadose zone will not with reasonable probability contaminate ground water or surface water, in excess of the standards…"
  - 20.6.2.3103, Groundwater standards
    - Chloride, 250 mg/L
  - Monitoring Well Construction and Abandonment Guidelines, New Mexico Environment Department
    - Relevant to AMIGO's saturated zone mixing cell thickness
    - 20-foot section of screen
    - Top of screen shall be 5 feet above water table to allow for seasonal fluctuations

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Task 1a: Model Equations

- Vadose zone: 1-D downward water flow (modified Richard's equation)

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left[K(\theta)\left(\frac{\partial h}{\partial z} + 1\right)\right] - S$$

  - θ is water content
  - t is time
  - z is depth
  - $K(\theta)$ is unsaturated hydraulic conductivity (from HYDRUS-1D libraries but not provided) $[LT^{-1}]$
  - h is pressure head [L]
  - S is sink term at root level for water uptake $[L^3L^{-3}T^{-1}]$ to simulate transpiration (S comes from daily weather data and is prevented when Cl at root level exceeds 10% or 1% of source concentration)
  - from Equation 2.1 of Šimůnek et al. (2008) *(equation not in manual)*

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Task 1a: Model Equations

- Vadose zone: 1-D solute transport

$$\frac{\partial \theta c}{\partial t} = \frac{\partial}{\partial z}\left(\theta D \frac{\partial c}{\partial z}\right) - \frac{\partial qc}{\partial z}$$

- θ is water content determined from flow equation
- c is aqueous concentration [ML^{-3}]
- t is time
- z is depth
- D is dispersion coefficient [L^2T^{-1}] (dispersion length set at undefined conservative value (AMIGO manual, Section 10))
- q is volumetric flux density [LT^{-1}] determined from flow equation
- Equation simplified from Equation 3.1 of Šimůnek et al. (2008) to fit extent of AMIGO use *(equation not in manual)*

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Task 1a: Model Equations

- Saturated zone – Conservation of mass for flow-through mixing cell

$$\frac{dC}{dt} = \frac{q_{in}C_{in}H + q_v C_v D - (q_{in}H + q_v D)C}{HDn}$$

- C is Cl concentration within and exiting mixing cell [ML^{-3}]
- C_{in} is background Cl concentration in the aquifer [ML^{-3}]
- C_v is incoming Cl concentration from vadose zone [ML^{-3}]
- q_{in} is horizontal water flux [LT^{-1}]
- q_v is water flux from the vadose zone [LT^{-1}]
- H is thickness of aquifer or length of well screen
- D is length of mixing cell
- t is time
- n is porosity of mixing cell
- Equation from Section 10.2 of AMIGO manual

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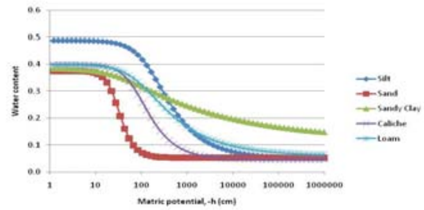
Task 1a: Model Parameters and Databases

- Vadose zone
  - Soil profile
    - Materials ($K_{h,sat}$)
      - Medium sand (642.98)
      - Clay (11.35)
      - Caliche (1.0)
      - Silt (43.74)
      - Loam (12.04)
      - *$K_{h,sat}$ values and dimensions not in documentation*
    - Nine profiles (Appendix A of manual)
    - Properties of each soil type
      - Van Genuchten parameters *(not in documentation)*
        - Resulting characteristic curves, K(θ) *(curves not shown in documentation)*
      - Dispersion length set at 10% of soil profile length
        - *not clearly stated in documentation*



These curves were calculated from van Genuchten parameters provided by R.T. Hicks Consultants, Ltd.

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Task 1a: Model Parameters and Databases

- Saturated zone properties
  - Hydraulic conductivity [LT^{-1}]
  - Slope of water table
  - Aquifer thickness (or length of well screen)
  - Background Cl concentration in aquifer
  - Aquifer porosity
  - Depth of water table
- Climate data
  - Historical daily temperature and precipitation measurements
  - Potential evapotranspiration (PET)
    - May be calculated using method of Samani and Pessarakli (1986)
      - This is what was done for Hobbs example *(not explained in documentation)*

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Task 1b: Assumptions and Conservatisms

- Vadose Zone
  - Conservative assumptions
    - No upward flow
    - No lateral dispersion
    - No vapor transport (only ET sink in root zone)
    - No chloride uptake by roots
  - Other simplifying assumptions
    - No thermal gradients
    - Porosity of 0.25 for all soil profiles
    - No dual porosity
    - No hysteresis
    - No deliquescence
    - No density or viscosity effects

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Task 1b: Assumptions and Conservatisms

- Saturated zone
  - Conservative assumptions (with respect to groundwater impacts)
    - Observation well is immediately down gradient of where the plume enters the saturated zone
    - Groundwater flow is in the same direction as the length of the spill
    - Groundwater is not pumped from the well
    - No dispersion, except within the cell and except when modeling transport beyond the mixing cell to an optional distant well (user-defined)
  - Other simplifying assumptions
    - Instant mixing of Cl across the thickness of the aquifer (or length of the well screen)

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Task 2: AMIGO Testing and Review Status

- Development of AMIGO model
  - API Publication 4734 (Hendrickx et al. 2005)
- HYDRUS-1D testing and review
  - AMIGO uses HYDRUS-1D module
    - HYDRUS-1D testing documented in manual

Task 2: AMIGO Testing and Review Status

- API Publication 4734 (Hendrickx et al. 2005)
  - Original development and testing of AMIGO
  - Testing documented
    - Field tests (Section 12)
      - Two controlled releases of brine at anode beds (fitted dispersivity)
      - Brine releases at junction boxes (fitted dispersivity, spill sizes and dimensions, initial chloride concentrations)
    - Mathematical verification
      - Comparison to MODFLOW for saturated zone (Hendrickx et al. 2005, Chapter 3)
      - AMIGO sensitivity analyses
  - Testing results indicate AMIGO can reproduce observations. Because these tests involve various degrees of fitting, they do not directly address AMIGO's predictive ability in the field and the likelihood of its predictions erring on the cautious side.

Task 2: AMIGO Testing and Review Status

- HYDRUS-1D testing relevant to AMIGO (Šimůnek et al. 2008)
  - Mathematical verification
    - Examples 1 (column infiltration test) and 2 (water flow in a field soil profile under grass, variable precipitation for 270 days) match results from UNSAT2 and SWATRE
    - Example 3 (solute transport with nitrification chain) match results of CHAIN
  - Observation and mathematical verification
    - Example 4 (solute transport with nonlinear cation adsorption) matches results of MONOC
    - Example 5 (solute transport with nonequilibrium adsorption) matches results of CFITIM
  - Observation
    - Example 6 (fitting analysis of outflow experiment)
    - Example 7 (fitting analysis of multistep outflow experiment)

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Task 3: Findings

- AMIGO assessment
  - Uses appropriate equations
  - Conservative assumptions built into AMIGO (noted above) help provide confidence that the tool will tend to produce conservative predictions of groundwater effects
  - Needs improved documentation (as noted)
- AMIGO testing and review status
  - Mathematically verified for saturated zone
  - No documentation of testing against examples in HYDRUS-1D manual
  - Reproduces field observations, but some parameters fitted
  - Little testing of predictive ability

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Task 3: Recommendations

- Improve documentation
  - Add missing equations and parameter values (e.g., identified in gray italics above)
  - Include the following diagrams for each soil type
    - K(θ) vs. θ
    - matric potential vs. θ
  - Develop and document a conservative field method for applying AMIGO to a new spill
    - Step-by-step approach with rules of thumb to ensure conservative predictions (e.g., when selecting soil profiles and parameter values)
    - Include a method for developing simple sensitivity analyses to evaluate effects of parameter uncertainty

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Task 3: Recommendations (cont.)

- Further testing and review
  - Document verification that AMIGO produces the same results as HYDRUS-1D for examples 1 and 2 of the HYDRUS-1D manual
  - Evaluate effects of AMIGO conservatisms by testing against results of more sophisticated models
    - HYDRUS-1D example 11 includes upward vapor transport and heat transport
    - HYDRUS-2D includes effects of lateral dispersion
  - Test AMIGO results from the "conservative method" against multiple sets of data
    - No fitting
    - Must show that using the "conservative method" for AMIGO does not produce nonconservative results
    - Literature search for Cl tracer tests might provide good data sets for testing AMIGO

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References

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