Dear Mr. Tarlton:

This letter provides our general thoughts about the recently-reported DOE mathematical simulation of the Rulison site (1). We were retained to review the DOE report by the Danielson Law Firm, and our intent is to provide some feedback about how the results of the DOE simulation should be used in the task of regulating gas well drilling in the vicinity of the site. We have reviewed the document and the references included within it where we were able to locate them. We have also reviewed a number of other documents, several of which we will cite in this letter.

General Comments and Executive Summary

Computer mathematical modeling is an increasingly commonly-used tool in the arsenal of tools available for managing and regulating environmental matters (2). Most of us working in this field have seen the value of properly using such models. However, they have also at times been used in ways that result in inappropriate and sometimes disastrous decisions (3).

We strongly believe in the appropriate use of models in the context of regulatory and environmental management. At the same time, we also believe that misuse of models poses a serious potential problem, sometimes confusing the key issues, consequently working against good decision-making. It is important to recognize that the results of a mathematical model are strongly dependent on factors that are uncertain, and that this uncertainty must be dealt with explicitly and carefully.

In this connection, we wish to emphasize the following points:

1. The DOE study is not based on the use of actual monitoring data, despite the fact that considerable scientific funds have been spent on the model development.
It is not clear what type of monitoring data the reviewer believes should be used. Models for contaminated sites may include monitoring data, but it is also common for models to be based principally on site characterization data (as done here) rather than monitoring results. The current monitoring program at Rulison includes radiochemical analysis of surface water, shallow groundwater, and natural gas, all of which are outside of the calculation area of the model. The model results are consistent with these data in that no contamination is predicted to the model boundaries and none has been observed beyond the model boundaries at the monitoring points.

2. As a consequence, the DOE modeling results are not calibrated or confirmed by experiment.

Many groundwater models are calibrated by checking simulated hydraulic head values and concentrations against measurements, then adjusting boundary conditions, permeability, porosity, storage, etc. until the match between prediction and observation is close. Such head data (pressure measurements) and concentrations are not currently available at Rulison and it may not be in the best interest of site integrity to drill multiple boreholes close to the emplacement well to collect such data. For a typical groundwater model this would be a more significant problem than it is in this case for the following reasons: natural movement of gas and liquid in the reservoir is clearly restricted or gas accumulations would not be present, and the pressure impact of a gas production well (as hypothesized in the model) would dominate over any natural pressure gradient. A sensitivity test regarding the impact of pressure gradients was performed and presented in the report. Note that traditional calibrations are non-unique solutions; calibration data can be matched by multiple combinations of parameter values. The Rulison model matches observed residual liquid saturation values in the reservoir and pressures observed in the test well. The permeabilities were not adjusted by calibration but are well constrained by measurements in the reservoir, which matched the more limited data at the site itself.

3. Real, not theoretical, deep monitoring wells and analytical data from samples taken from them would be necessary to evaluate the extent and nature of contamination at Rulison and to therefore calibrate the model with actual data.

Drilling close to the emplacement well could compromise the integrity of the existing 8000 ft of competent rock between the nuclear chimney and the land surface and create a pathway for contaminant migration. Note that the hypothetical well in the model simulations was a hypothetical production well, used to simulate the impact of nearby gas development, not simulate data for use in the model. Samples have been collected from the gas wells closest to the site and no contaminants have been detected. It is our understanding that plans call for continuing to sample wells as they are drilled in the area, providing the data requested by the reviewer.

4. The modeling should be used to generate qualitative results and used with experiment to increase understanding of the geohydrologic systems, not taken as a substitute for actual measurements.
Models are recognized as valuable tools for understanding geohydrologic systems (Anderson, M.P., and W.W. Woessner 1992, *Applied Groundwater Modeling: Simulation of Flow and Advection Transport*, Academic Press, San Diego.) The model results are not considered as a substitute for monitoring because there are significant uncertainties in any model of subsurface processes, where we can observe only a small portion of the domain of interest. The results presented in the model report would suggest no need for any further action, but DOE is committed to long-term stewardship of the site, including monitoring, as stated in the COGCC informational meeting.

The authors of this study appear to us to be aware of the potential concerns, and state the following in their executive summary:

*Models are limited by the data used in them, as well as assumptions in their implementation. The results of this study are highly dependent on a combination of uncertain spatial features.*

The authors go on to develop a number of arguments for their particular choice of input parameters and discuss the uncertainty that they believe is inherent in each. They use a random selection of what they believe to be the most uncertain parameters that fall in assumed probability distributions to conduct many calculations. From the results, they develop “statistics” of the model predictions. This is called the “Monte-Carlo” approach. It is important to recognize that these statistics only apply to the internal variability of the model predictions with the assumptions made. There are no site measurements or observations to compare model predictions with, consequently no way to verify that these model “statistics” have any relevance to what might be observed were such measurements available. Not only that, but there are no comparisons provided in the document with any experimental observations using this modeling approach at any similar site anywhere. Quite simply, without experimental verification of the predicted nature and extent of contamination there is no way to determine if the model has any relationship to the realities at the site.

The parameter distributions for permeability and porosity were not assumed, they were developed from hundreds of measurements. Although assumptions were required for some aspects during model development (as is common practice when modeling complex systems), the model is based on an understanding of site geology, observed physical and chemical processes, and parameter measurements. A model based on, and consistent with, site-specific information has a “relationship to the realities at the site.”

Verification of stochastic models ideally relies on a multitude of tests of various input and output distributions of the model, as described by the reviewer’s reference No. 4. In other words, the parameter ranges used as input can be verified, and model output in terms of pressures or concentrations can be verified. As drilling progresses in the area, the sandstone lens geometry, permeabilities, and porosities can be compared to those used in the model to determine if the distributions are acceptable. Similarly, gas and water will be sampled to verify the predicted contaminant migration.
In deciding whether to allow drilling closer to the source at Rulison, we believe that an objective, independent evaluation of the reliability of model predictions is essential. As everyone knows, the issue is the subject of considerable polemic and conflict. Where the public is expected to accept technical perspectives as a basis for policy making, the public must be convinced that those perspectives are accepted by independent experts who do not have a personal or institutional interest in the outcome.

The model provides a number of predictions that might be very useful in developing plans to further characterize the subsurface at Rulison. The model provides a starting theoretical basis for further development, and comparison of experiment with model results could help increase the understanding of the site considerably. We therefore believe that the model is an important contribution to the process, but that it cannot be relied upon by itself.

As noted previously and as stated in the COGCC information hearing, DOE is committed to long-term stewardship of the site, including monitoring. There is no intention to rely only on the model results.

We think that to make regulatory decisions from the output of this model without supporting experimental data would be roughly akin to using analytical results obtained by untested analytical instrumentation that had never been calibrated. In today’s environmental regulatory system, such an approach would never be considered – yet the use of an uncalibrated mathematical model, which is even less likely to produce results that are representative of physical reality, is apparently being proposed as a real possibility. We find this appalling, and we hope that CDPHE will support a more rigorous approach to decision-making at this site.

The governing mathematical equations upon which the TOUGH2 code is developed are not akin to untested instrumentation. These equations, such as the mass balance law, do not require calibration or validation in any sense; they are universal rules based on mathematical and physical theory that are consistent with observed physical reality. The performance of TOUGH2 itself has been tested by comparing the numerical solution to analytical solutions (e.g., see the Pruess et al. 1999 reference in the model report). That said, there are significant uncertainties in the problem, stemming in large part from the naturally heterogeneous system and our limitations regarding observations. Additional observations can be used to reduce that uncertainty, as described in a previous response.

We believe that the uncertainties are too large, and the potential negative impacts of drilling are too great, to allow drilling closer than the original 3-mile limit on the basis of the model study.

In 1997 COGCC staff agreed to notify DOE of drilling activity within 3 miles of the site. The only restriction on drilling is within Lot 11, below a depth of 6000 ft. There is a requirement for permits within 0.5 miles of the Rulison test to be brought before a commission hearing prior to approval.
Specific Concerns

We do not have sufficient detailed knowledge of the model to allow us to pronounce it as “valid” or “invalid”, even if such a judgment were possible (4). However, we have reviewed the DOE report in sufficient detail to isolate specific areas of concern that we believe need to be addressed. Because the model is very complex, there are potentially many other issues hidden within those complexities that could impact the results. Consequently, even if our specific concerns can be addressed, it is still critical to make careful comparisons of model predictions with experimental results. There is just no substitute for data.

Model Assumptions

We are concerned with a number of assumptions that have been made with varying degrees of available experimental evidence. Some of our concerns include the following:

5. The assumption that tritium is the only radionuclide of concern. This assumption is made despite the known presence of potentially mobile, longer-lived radionuclides, such as $^{14}$C, $^{36}$Cl, $^{99}$Tc, and $^{129}$I (5, 6).

Contaminants in the gas phase will migrate much more rapidly than those that travel in the liquid phase (the aqueous phase is essentially immobile). Tritium, $^{85}$Kr, and $^{14}$C are the significant gas-phase contaminants produced by the test. As described in the report, measurements of radionuclides removed from the subsurface during gas production after the Rulison test indicate that the majority of $^{85}$Kr and $^{14}$C were removed but that a significant amount of tritium remained. This is the reason for the focus on tritium. If gas-phase radionuclides were found to migrate a considerable distance, liquid-phase contaminants could be included in the analysis. The migration of a liquid-phase solute with the properties of $^{99}$Tc was analyzed for one realization at the 95th percentile and showed no movement beyond the nuclear-fracture zone.

6. The estimates of initial tritium concentration and total amount.

Concentration was not assumed, only the amount. The amount of tritium produced by the test was calculated by previous workers familiar with test design. In a report considering estimates of radionuclide production for the tests on the Nevada Test Site, the following is reported “The estimates of residual tritium have a wide range of uncertainties: from 1-300%.” (Bowen, S. et al., 2001, *Nevada Test Site Radionuclide Inventory, 1951–1992*, Los Alamos National Laboratory report LA-13859-MS). This uncertainty is small relative to the orders of magnitude of uncertainty in other parameters. For example, multiplying the mass fraction by 3 (300 percent) would not visibly change the breakthrough curves in Figure 5-7. The amount of tritium removed during the gas production phase was measured on site and subject to even less uncertainty.
7. The assumption that groundwater flow is not significant.

This conclusion is based on observation at the site, as well as experience throughout the natural gas reservoir. The U.S. Geological Survey reported that Quaternary-age deposits provide the only groundwater resources in the Rulison area (these surficial deposits are over 7000 ft above the top of the model domain) and that the underlying bedrock formations are generally impermeable, yielding little or no water (Voegeli and West 1970, referenced in the report). They state, “The pressures recorded during the drill-stem tests of the different zones indicated negligible or no fluid entry to the hole. No fluid was recovered on any of the swab tests performed during drill-stem tests.” They summarize as follows: “The tests show negligible or no fluid entry to the hole, which indicates that ground-water flow in the vicinity of the Rulison site is nil.” Their conclusions are consistent with the extremely low permeabilities measured at the site and in the Williams Fork in general, compounded by the partially saturated state of the formation, reducing the effective permeability even further. A simple analytical calculation of groundwater velocity at these permeabilities would demonstrate the low importance of groundwater flow to the problem, relative to gas-phase movement.

8. The specific assumptions about the initial extent of contamination (where contaminants were initially deposited by the explosion).

It is unclear what specific assumptions are of concern. Tritium was initially distributed evenly throughout the 88 grid blocks representing the nuclear chimney. As described in the report, prompt injection has been identified at some nuclear tests where a small amount of radionuclide mass may be distributed away from the chimney, within a few cavity radii. The prolonged production testing at Rulison, with its induced gradient toward the chimney, would counteract that effect. The diffusion is rapid through the nuclear-fracture zone, such that migration is rapid out another 60 m from the chimney edge anyway.

9. The specific distributions assumed for fracture length, hydrofracture length, effective permeabilities, and anisotropy. There is great uncertainty concerning the presence, orientation and extent of fractures, or fracture-controlled permeability. If only a few (or even one) significant permeable fractures are present, contaminants can be transported to distances further than porous-media transport modeling would predict, regardless of the theoretical assumptions used in the modeling (7).

There is uncertainty in permeability, hydrofracture length, and degree of anisotropy, which is why distributions were used. It is unclear what the reviewer’s concern is with those distributions. Please note that no distributions were used for “fracture length,” “presence, orientation and extent of fractures, or fracture-controlled permeability.” All sandstone units in the model were assumed naturally fractured, with their permeability in the predominant fracture direction assumed 10 to 100 times higher than the transverse direction. We agree that an equivalent porous medium is an approximation for a fracture flow system, but discrete fracture models are fraught with additional uncertainty.
10. The assumption that the variables that are used for the Monte-Carlo calculations are uncorrelated. If the variables used for the Monte-Carlo statistical treatment (such as fracture length and effective permeability) are in fact correlated, then the statistics will be skewed. The failure to show relationships between specific variables and tritium transport distance would then be open to question, as would the specific meaning of the percentiles calculated (8, 9).

The usual positive correlation is between porosity and permeability. If we correlate high porosity with high permeability (as usual), this would serve to limit the upper tail of the distribution such that contaminant velocity would be reduced. In other words, the effect of high permeability would be significantly reduced by the lower velocity associated with high porosity. We assume the reviewer’s example means correlating the hydrofracture length with permeability (again, as noted above, all the sandstone is assumed fractured such that fracture length is not a parameter). We agree that this would promote transport, but would be counteracted by the correlation between permeability and porosity.

Specific Calculations Made

We are also concerned with the fact that certain scenarios have not been fully addressed, and in some cases have not been addressed at all in the calculations. These include the following:

11. Enhanced groundwater flow compared with assumptions.

At the permeabilities measured in the Williams Fork and at the partially saturated conditions, groundwater flow would be extremely slow, if it moves at all. As noted above, the U.S. Geological Survey concluded there was no mobile groundwater in the formation after none was found in formation tests at the site. The proposed scenario would require neglecting the site-specific data regarding permeability and saturation.

12. Initial temperature of the nuclear chimney.

An alternative scenario regarding nonisothermal conditions (the heat of the chimney) was presented in the report. More investigation could be done, but the simulations are very time consuming, so it would be helpful to know specifically what additional conditions are of interest.

13. Presence of multiple wells.

Again, several alternative scenarios regarding various multiple well configurations were presented in the report. All of these are, of course, hypothetical, and we are open to examining other scenarios of interest, though we cannot determine from the comment how the reviewer would like it to differ from what is already presented.

Again, an alternative scenario for the impact of an increase in gas production rate was presented in the report. As this is part of the hypothetical scenario, we are open to examining other scenarios of interest, though we cannot determine from the comment how the reviewer would like it to differ from what is in the report.

15. Impacts of well blowouts.

Presumably this would be a short-term increase in production rate? As with the item above, we are open to this if we can determine what is desired. Given that a blowout would occupy a very small part of a well’s lifetime of operation, the impact on radionuclide migration is expected to be minor.

16. Initial distribution of radionuclides in the subsurface.

This issue was addressed in a previous comment.

17. Impact of “turning off” tritium decay on conclusions (relevant to the case where other volatile radionuclides might be significant) – particularly for long-term calculations > 200 years from detonation (10).

Tritium decay was “turned off” in the referenced report in order to confirm that the contaminant transport behavior of the flow field was as expected because transport was so slow that decay removed the tritium before it moved significantly. It was only a check on the numerical calculations. It is physically unreasonable to track tritium without considering decay. If other radionuclides are of interest, they should be analyzed separately, using their contaminant mass and decay rate. As noted in a previous comment, the only other gas-phase radionuclides are $^{14}$C and $^{85}$Kr, the majority of which were removed during production testing. $^{85}$Kr, also decays at about the same rate as tritium. $^{14}$C has a much longer half-life and would indeed be of more concern for long-term site management, but it was produced in a much smaller amount than tritium, and the bulk was removed during testing.

18. Impact of uncertainties in the assumed initial tritium concentration and total amount of tritium on model results.

This uncertainty could be included, but as described in a previous response, it is much smaller (factor of three at most) than other uncertainties that span orders of magnitude.

Recommendations

The model should be used heuristically, in a combined effort with experimental work to elucidate the actual site characteristics, the extent of contamination, and the rate of movement of contaminants. In this approach, the inherent uncertainties of the model become tools for further investigation. However, in our view, these major sources of uncertainty disqualify the model for use as the sole decision-making tool.
In our view it is not reasonable to make a decision to allow more aggressive gas development of the Rulison site given the uncertainties and potential negative impacts of error. In effect, then, the model provides the best evidence to date that such actions should not be taken with the present state of knowledge, because it qualitatively highlights the potential impact of uncertainties.

We think that empirical data elucidating the nature and extent of contamination and subsurface conditions are critical to developing an understanding of the site with a level of confidence sufficient to allow good decisions about future development. We have heard discussions of whether there are additional pertinent data which for one reason or another (such as that they may be classified) are not in the public domain. It is probably not our role to try to resolve those issues. We simply note that the more data are available, and the more confident we are that information is not being withheld, the more confident everyone can be in the regulatory decisions made.

There are approximately 6 domestic wells within a 6 mile radius of the Rulison blast site. Hence, local ground water is obviously being used. We are concerned that any approach to decision making at this site should adequately value the ground water resource, and we are not completely convinced this has been the case in the past. There are certainly a number of examples as the population of the West has grown and the land settled where groundwater resources that were once considered of negligible value are much more highly valued today. One can imagine that, as local populations continue to increase, the ground water will become progressively more valuable -assuming it is uncontaminated. It seems imperative that regulators consider the FUTURE demands for ground waters suitable for a wide range of uses.
References

29. We appreciate your time and attention to these important issues, and we hope that our thoughts will be useful to you in your work.