

GWERD Quality Assurance Project Plan for

Numerical Simulation for Groundwater Flow and Contaminants Transport at the Hydraulic Fracturing Retrospective Case Study Site, Killdeer, North Dakota

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Disclaimer

EPA does not consider this internal planning document an official Agency dissemination of information under the Agency's Information Quality Guidelines, because it is not being used to formulate or support a regulation or guidance; or to represent a final Agency decision or position. This planning document describes the overall quality assurance approach that will be used during the research study. Mention of trade names or commercial products in this planning document does not constitute endorsement or recommendation for use.

The EPA Quality System and the HF Research Study

EPA requires that all data collected for the characterization of environmental processes and conditions are of the appropriate type and quality for their intended use. This is accomplished through an Agency-wide quality system for environmental data. Components of the EPA quality system can be found at <http://www.epa.gov/quality/>. EPA policy is based on the national consensus standard ANSI/ASQ E4-2004 *Quality Systems for Environmental Data and Technology Programs: Requirements with Guidance for Use*. This standard recommends a tiered approach that includes the development and use of Quality Management Plans (QMPs). The organizational units in EPA that generate and/or use environmental data are required to have Agency-approved QMPs. Programmatic QMPs are also written when program managers and their QA staff decide a program is of sufficient complexity to benefit from a QMP, as was done for the study of the potential impacts of hydraulic fracturing (HF) on drinking water resources. The HF QMP describes the program's organizational structure, defines and assigns quality assurance (QA) and quality control (QC) responsibilities, and describes the processes and procedures used to plan, implement and assess the effectiveness of the quality system. The HF QMP is then supported by project-specific QA project plans (QAPPs). The QAPPs provide the technical details and associated QA/QC procedures for the research projects that address questions posed by EPA about the HF water cycle and as described in the *Plan to Study the Potential Impacts of Hydraulic Fracturing on Drinking Water Resources* (EPA/600/R-11/122/November 2011/[www.epa.gov/hydraulic fracturing](http://www.epa.gov/hydraulic%20fracturing)). The results of the research projects will provide the foundation for EPA's 2014 study report.

This QAPP provides information concerning the Chemical Mixing and Well Injection stages of the HF water cycle as found in Figure 1 of the HF QMP and as described in the HF Study Plan. Appendix A of the HF QMP includes the links between the HF Study Plan questions and those QAPPs available at the time the HF QMP was published.

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Distribution List

The following individuals will be provided copies of the approved QA Project Plan.

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Gregory Oberley, EPA Region VIII

Project / Task Organization

Kelly Smith, GWERD. Ms. Smith is the GWERD Research Lead for case studies, replacing Dr. David Jewett. She is also assisting in the coordination of the Hydraulic Fracturing Case Studies with EPA NRMRL management and other parts of EPA ORD and EPA Offices. In addition, Ms. Smith is responsible for review and approval of QAPP, and review of draft deliverables.

Steve Vandegrift, GWERD, Quality Assurance Manager, responsible for QA review and approval of QAPP and final report, QA guidance, and management of QA audits.

Douglas Beak, GWERD, Principal Investigator, responsible for ensuring completion of all aspects of the Hydraulic Fracturing Retrospective Case study in the Bakken Shale, Killdeer, ND. Dr. Beak will lead the collection, analysis, and interpretation of groundwater and surface water samples. In addition, he will lead the GWERD efforts to synthesize and incorporate all aspects of the project into the final report.

Junqi Huang, GWERD, Principal Investigator for the modeling aspects of the Hydraulic Fracturing Retrospective Case study in the Bakken Shale at the Killdeer, ND location, Dr. Huang will be responsible for models creation, site data preparation, implementation of model simulation and analysis of flow and transport and explanation of modeling results.

Steve Acree, GWERD. Mr. Acree is responsible for the testing, survey and acquisition of site hydrogeological information at the Killdeer site.

Randall Ross, GWERD. Dr. Ross is responsible for the testing, survey and acquisition of site hydrogeological information at the Killdeer site.

Gregory Oberley, U.S. Environmental Protection Agency – Region VIII, Denver, CO. Mr. Oberley is responsible for coordinating technical discussion and activities between NRMRL-Ada and EPA Region VIII and Region VIII Analytical Lab, as well as coordinating data collection activities with the state officials in North Dakota. He will also assist in ground water sampling. His HAZWOPER certification is current.

Problem Definition and Background

Hydrocarbon production from tight reservoirs has grown rapidly over the last few years. Enhanced oil/gas recovery processes require well and reservoir stimulation because the formation permeability is too low to support flow under conventional production conditions. Such enhancement/stimulation is provided by a number of hydraulic fracturing (HF) methods, all of which are designed to develop a new system of artificial fractures that increase the mobility of reservoir fluids. This substantial increase in oil/gas production from HF has been accompanied by concerns that the fracturing process could create or extend fractures linking the producing zone to an overlying aquifer. This in turn could provide a pathway for gas or fracturing fluids to migrate into these aquifers. The potential for contaminant migration could result in pollution of potable groundwater resources.

The retrospective case studies investigating the potential impacts of HF on groundwater resources were implemented at five selected sites. One of these sites is in the Bakken Shale in Dunn County, near Killdeer, ND. The study area is situated near the center of Williston Basin (Murphy, 2001) (Figure 1). The area surrounding Killdeer is currently experiencing renewed oil and natural gas exploration using horizontal drilling technology and hydraulic fracturing is being employed to stimulate oil/gas production.

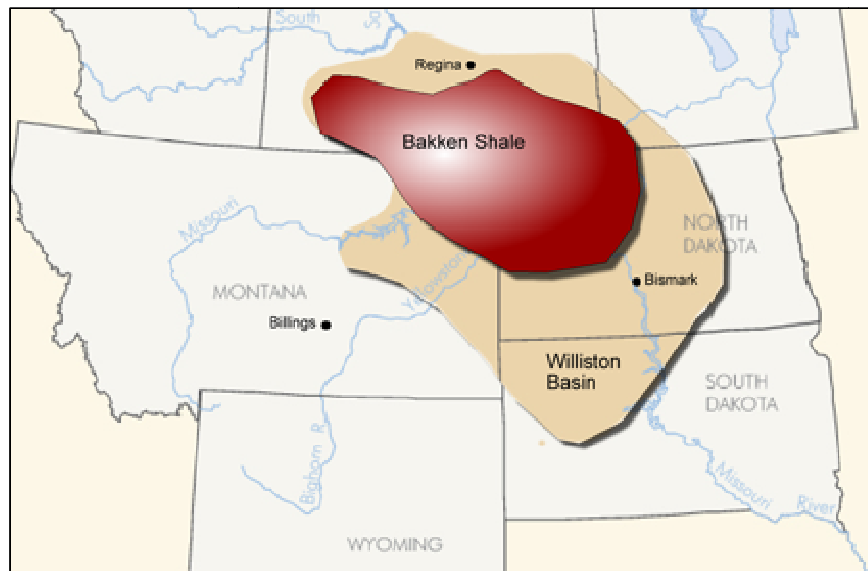


Figure 1, Williston Basin and Bakken shale distribution (From USGS)

A hydraulic fracturing incident occurred near Killdeer on September, 2010, where the oil well (Franchuk 44-20SWH, operated by Denbury) (Figures 2) experienced an uncontrolled blow out during the 5th stage of a 23 stage fracturing operation when the seven inch intermediate casing burst. This resulted in the spilling of approximately 2553 barrels (107,276 gallons) of hydraulic fracturing fluids and oil on to the surface. At this time it is suspected that hydraulic fracturing fluids and oil were released into the subsurface because the surface casing was compromised at

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38.5 ft below land surface and there is still a question about whether the conductor casing was compromised at 60 ft below land surface. During the clean up process approximately 2300 (96,600 gallons) barrels of water and 253 barrels (10626 gallons) of oil were recovered. To date it is unknown if groundwater contamination occurred and what the extent of the groundwater contamination might have been. The Franchuk well is just outside the City of Killdeers Municipal Water Supply Wells, well head protection zone (~2.5 miles). In addition, there are several farm wells in the vicinity of the Franchuk well and supply wells for drilling and hydraulic fracturing activities is approximately 0.5 miles down gradient of the Franchuk well (Figure 2).



Figure 2, Aerial view of the Franchuk 44-20SWH well and surrounding area (From Doug Beak et al, Quality Assurance Project Plan for Hydraulic Fracturing Retrospective Case Study, Bakken Shale, Killdeer and Dunn County, ND, 2011).

The objective of this modeling study is listed below.

Primary Objective: Carry out numerical simulation to investigate the flow pattern of groundwater and evaluate the fate and transport of contaminants in the study area. The modeling will be conducted in conjunction with the retrospective case study in this area.

The specific tasks of the modeling study include:

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Task 1: Establish the stratigraphic model. -

Task 2: Delineate spatial distribution of the shallow aquifer system including the Killdeer Aquifer - and the Sentinel Butte Aquifer in the study area.

Task 3: Create groundwater flow model.

Task 4: Investigate flow pattern of groundwater in the aquifer system.

Task 5: Create the fate and transport model.

Task 6: Simulate the fate and transport of the contaminants under the mass loading conditions associated with the incident of the hydraulic fracturing activities.

Project/Task Description and Schedule

To accomplish the primary objective, the work is organized into five tasks as follows:

Task 1: Establish the stratigraphic model.

The model domain is selected to cover a geological unit for which the hydrogeological boundaries could be adequately determined. The model domain is bounded on the north by the Little Missouri River, on the east by an artificial boundary, on the south by the Knife River, and on the west by the Killdeer Mountains Range; totally encompass an area of 493 square miles (1277 square kilometers), as shown in figure 3.

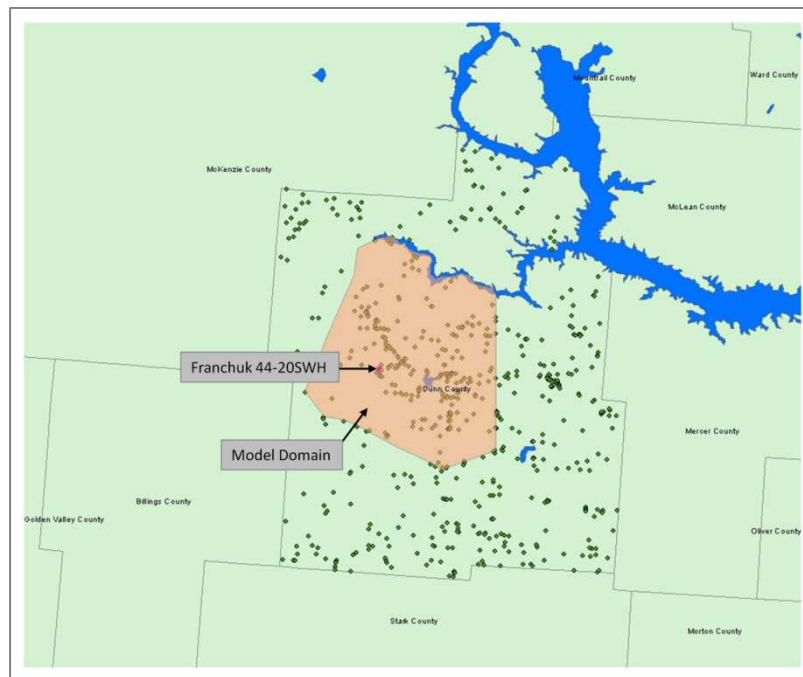


Figure 3, the extent of modeling area which is bounded on the north by the Little Missouri River, on the east by an artificial boundary, on the south by the Knife River, and on the west by the Killdeer Mountains Range.

The stratigraphic model will be developed through a combination of data sources including products and data from USGS Earth Resources Observation and Science Center, North Dakota oil and gas layers information from North Dakota Industrial Commission, Department of Mineral Resources, Oil and Gas Division, Data reported from the project: Williston and Powder River Basins Groundwater Availability Study by USGS, and hydrogeological information explored from the case study. The model will refine the understanding of the stratigraphy of the study area through the analysis, integration and interpretation of: (1) borehole data acquired from the information source (existing oil/gas wells and water wells); (2) geospatial data set for geologic structural frameworks created by USGS. The stratigraphic data from all of the various data sources will be used to assess three-dimensional interpolation and modeling techniques for investigating subsurface stratigraphy and alluvial architecture. With the support by GIS (geographic information systems), a static three-dimensional model will be produced using these data sets that will cover the entire study region.

Task Duration: From the beginning of the project to 7/31/2013

Task 2: Delineate spatial distribution of the shallow aquifer system including the Killdeer Aquifer and the Sentinel Butte Aquifer in the study area.

Based on the framework from task 1, this task aims to investigate the shallow and deeper section to delineate the groundwater aquifers. According to the report of ground-water resources of Dunn County, North Dakota (Klausing, 1979), two main aquifers, including the Killdeer Aquifer and the underlying Sentinel Butte water yielding formation, are potentially hydraulically linked to the HF fluids releasing site. The subsurface would be dissected and generalized to provide the geologic section and aquifer characteristics of geologic units in the study area. Two main water-yield formations would be delineate with digital map. The basic hydrogeological features, including the boundaries of aquifer system, the top and bottom elevation of the formations, rock properties and hydraulic conductivities will be digitally available. This model may serve as the basis for creating more detailed flow and transport model.

Task Duration: From 8/1/2013 to 8/15/2013.

Task 3: Create groundwater flow.

This task creates a three-dimensional groundwater flow model using the data explored from Task 1, Task 2 and the case study. The model domain encompasses an area depicted in Figure 3, vertically including all aquifers from the ground surface to the bottom of the Sentinel Butte formation. The model boundaries are chosen to coincide with specific hydrological features that provide physical boundary conditions. On the north and south, the Little Missouri River and the Knife River may provide a suitable model boundary where the constant water heads are given to represent the river stage. On the west, the Killdeer mountain range acts as the groundwater flow divides where no-flow conditions are assumed. On the east edge of mode domain, there is no physical boundary available in an adequate distance. However, a large number of water

wells exist along the boundary, which may provide a known water head condition based on observed multi-year water levels in the wells. The model domain is set in a relatively large area, spanning about 25 miles (40 kilometers) from the west to the east and 31 miles (50 kilometers) from the south to the north.

Model Inputs

The simulation of groundwater flow requires a thorough understanding of the hydrogeologic characteristics of the study area. The basic information used for creation of groundwater flow model will include the following:

- Extent and thickness of aquifers, confining units, and structural controls.
- Hydrologic boundaries that control the rate and direction of movement of groundwater.
- Hydraulic properties of the aquifers and confining units.
- Initial distribution of hydraulic head throughout the modeled area.
- Distribution of groundwater recharge, pumping, leakage to or from surface water bodies.

Creation of Flow Model

GMS 8.3, (Groundwater Modeling System) will be used to create the flow model. The model packages will include:

- Basic package, including 3D finite difference grid and layer type setting
- Layer Property Flow
- Wells
- Recharge
- River
- lake
- Observation

Task Duration: From 8/16/2013 to 8/31/2013

Task 4: Investigate flow pattern of groundwater in the aquifer system.

This task focuses on the flow processes in the aquifer system, investigating flow characteristics of groundwater under the specific model conditions such as precipitation, evapotranspiration, water extraction from wells, and interaction of groundwater and surface water, as well as water loading from the location where the hydraulic fracturing incident occurred. The simulations are intended to:

- Understand system dynamics to identify and quantify controlling and significant - processes. -
- Predict a future change or impact in response to the intense recharge of HF fluids.
- Evaluate sensitivity of the system to model uncertainty and/or magnitude of stresses.
- Identify capture zones or source protection areas.

- Characterize preferential flow of groundwater that is potentially connected with HF - fluids releasing site. -

Task Duration: From 8/17/2013 to 9/30/2013

Task 5: Create the fate and transport model.

This task creates a three-dimensional groundwater transport model using the data gained from the flow model. The model focuses on the basic characteristics of the transport around the incident site. The model domain is selected to cover the area of the flow model. The location of the contamination source (Franchuk 44-20SWH well) is approximately located at the center of the area. The zero concentration boundary condition for the transport model could be reasonably accepted for such space scale. To capture the characteristics of rapidly varying fluid fronts in a full field model, the model grid will be refined around the well Franchuk 44-20SWH.

Model Inputs

The simulation of the contaminants transport requires successful modeling of the groundwater flow in the study area. Model inputs will include:

- Spatial distribution of groundwater heads and velocity determined by a calibrated - groundwater flow model. -
- Boundary conditions for the concentration of contaminants.
- Initial distribution of the contaminants.
- Location, history and mass loading rate of the contaminants.
- Effective porosity.
- Soil bulk density.
- Adsorption and degradation parameters.

Creation of Transport Model

GMS 8.3, (Groundwater Modeling System) will be used to create the transport model. The model packages will include:

- Advection
- Dispersion
- Adsorption
- Reaction
- Source and Sink
- Observation

A specific work in this task is to develop the user-defined reaction package that can be integrated into RT3D. The decay chain of two species (tBuOOH and TBA) will be involved in the model. The reaction equation system is described as:

$$\frac{dC_{tBuOOH}}{dt} = -\frac{k_{tBuOOH}}{R_{tBuOOH}} C_{tBuOOH}$$

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$$\frac{dC_{TBA}}{dt} = \frac{k_{tBuOOH}}{R_{TBA}} \frac{w_{TBA}}{w_{tBuOOH}} C_{tBuOOH} - \frac{k_{TBA}}{R_{TBA}} C_{TBA}$$

Where, C is the concentration of species [mg/L]; k is the first order decay constant [1/day]; R is the retardation factor associated with the adsorption of species; w is the molecular weight; the subscript $tBuOOH$ and TBA respectively indicates tert-Butyl hydroperoxide and tert-Butyl alcohol, the indicator compounds. The reaction model will be coded in FORTRAN and tested under Intel Visual Fortran development environment with a small scale test model, and then integrated into RT3D as the user-defined reaction package.

Task Duration: From 10/1/2013 to 10/15/2013

Task 6: Simulate the fate and transport of the contaminants under the mass loading conditions associated with the incident of the hydraulic fracturing activities.

Based on the results of flow modeling, this task will implement the fate and transport models to simulate the movement and chemical change of contaminants as they move with groundwater through the subsurface. The contaminants will include the following indicator compounds that are used to detect the possible presence of HF fluids in the aquifer:

- tert-Butyl hydroperoxide (tBuOOH), as the parent species
- tert-Butyl alcohol (TBA), as the daughter products of the decaying contaminants

Fate and transport models require the development of a calibrated groundwater flow model that is based on field data. The model simulates the following:

- Movement of contaminants by advection and diffusion
- Removal or release of contaminants by sorption or desorption
- Decay of the contaminants, tBuOOH → TBA

Task Duration: From 10/16/2013 to 11/15/2013

Quality Objectives and Criteria for Model Inputs/Outputs

In this project the quality objectives are:

- To obtain data to support modeling studies that are of known quality
- To document the correct application of data interpretation and analysis methods
- To document steps in model development
- To ensure the consistency of model input and outputs
- To assess uncertainty in the model results
- To retain records that document the activities of the project

Acceptance criteria: the site hydrogeological and environmental data will be acquired from the case study, from The National Geologic Map Database of USGS, from published peer-reviewed

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journal papers, federal agency reports, and state agency-accepted data. The quality of data acquired from the case study will have been evaluated as part of the project (Hydraulic Fracturing Retrospective Case Study, Bakken Shale, Killdeer and Dunn County, ND, TASK No. 26278, QA ID No. G-16094). Data acquired from the case study is expected to include: water heads at existing wells, measured concentration of target contaminants at monitoring wells, and locations of HF wells.

Performance criteria: The concept of target population is applied to measurements, estimates, or predictions of quantities of environmental concern (USEPA 2006, Section 4.1). In this case, the predicted quantities will be the predicted spatial distributions of (a) water heads, (b) groundwater velocities, (c) flow path of tracking particles, (d) characteristics of captured zones, and (e) concentration of compounds of HF fluids. The performance criterion for these predictions will be their consistency with the input data. The uncertainty of predicted values will be assessed by sensitivity studies in which input data will be varied through ranges consistent with the uncertainty of the input data.

Selection of modeling tools: GMS (Groundwater Modeling System) will be employed to build the numerical models. GMS is a complete program for building and simulating groundwater models. It features 2D and 3D geostatistics, stratigraphic modeling and a unique conceptual model approach. GMS fully supports MODFLOW2005 (Harbaugh, 2005) and RT3D (Clement, 1997). MODFLOW2005 will be used as the simulator to model flow in the aquifer system. MODFLOW2005 is popular model in ground water community, which is commonly used for simulating flow in subsurface environment. MODFLOW2005 can model three-dimensional ground flow process and involve most hydrogeological features and conditions that naturally occur. The model consists of modules which correspond to specific hydrogeological features and can be easily assembled. The model is of deterministic characteristics; giving the parameters, such as hydraulic conductivity, geometric domain and other definition conditions, the model outputs hydraulic head and flux in model cells. The model provides several available solvers (algorithm for solving matrix equations), including pre-conditioned conjugate gradient method (PCG) (Hills, 1990), strong implicit procedure (SIP) (Weinstein, Stone, and Kwan, 1969), and direct solver (DE4) (Harbaugh, 1995). Depending on the computer resources available, space grid can be refined to capture geological heterogeneity. RT3D will be used to model the transport of compounds of HF fluids in groundwater. RT3D is a three-dimensional transport simulator that accounts for many build-in and user-defined reaction packages. RT3D models the migration of contaminants in the flow field simulated by MODFLOW2005. RT3D solves the convection-dispersion equations, the time step automatically determined in accordance with the stability condition. RT3D is also a modular model. The main input parameters include: porosity, dispersivity, and reaction-related parameters.

A specific reason for selecting RT3D is that the user-defined reaction package is available and supported by RT3D. The reaction package can be developed by users based on the specific reaction process occur in Killdeer site. In the study area, the contaminants include two species

which form a decay chain ($t\text{BuOOH} \rightarrow \text{TBA}$). The fate and transport of the decay chain can be fully simulated by RT3D.

Availability of model tools: MODFLOW2005 and RT3D both are public domain sources. There are no specific requirements for application of the selected models. MODFLOW2005 and RT3D are both written in FORTRAN and can be compiled and executed under Windows environment. MODFLOW2005 and RT3D are both fully supported by GMS (Ground water Modeling System), in which pre- and post-treatment tools are adequately provided. In addition, GMS is developed and sponsored by DoD (Department of Defense) and freely available for EPA.

Analysis of uncertainty: Any numerical model is of uncertainties, including uncertainties of input and uncertainties of model results. The uncertainties will be assessed by sensitivity analyses in which the important input parameters will be varied and their effects investigated. All significant input data that can reasonably be expected to affect the results will be varied through a range of expected or typical values. The OAAT (one-at-a-time) method will be used for the analysis, i.e. one variable will be varied and others held constant when evaluating the model.

Conceptual model: The conceptual model is described in Figure 4. Flow and transport in three-dimensional space will be simulated. The key processes to be simulated in the models are fluid flow in aquifer system, advection, dispersion, mass loading and dissolution of contaminants (compounds of HF fluids) in groundwater.

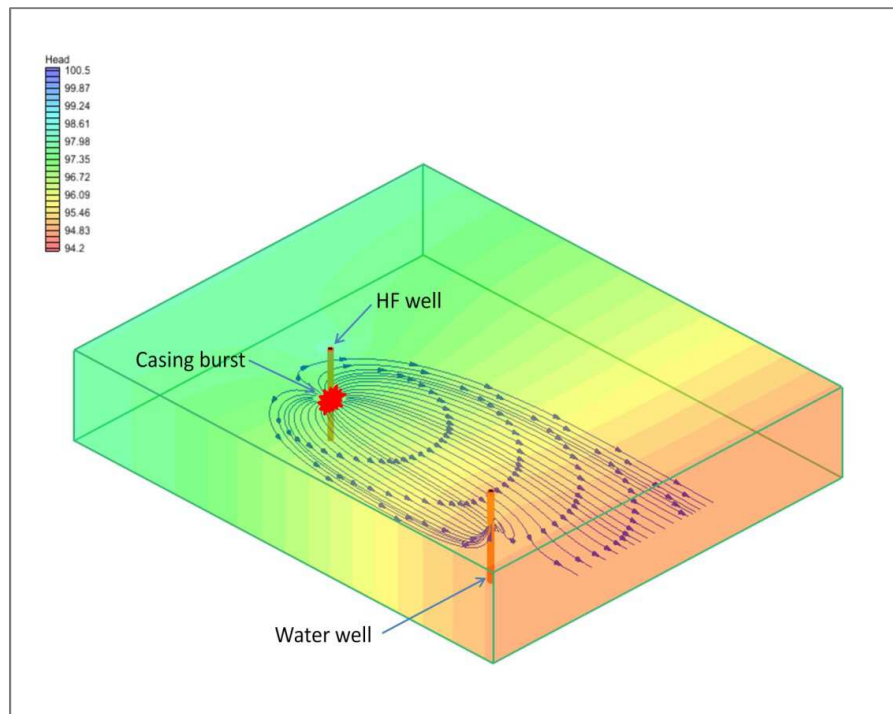


Figure 4, Conceptual model of study area -

Characteristics of subsurface are the stratigraphy, properties of various rock layers (e.g. porosity, density, hydraulic conductivity, dispersivity, and adsorption and degradation parameters). The subsurface environment (flow status and contaminants concentration) change as a result of water extraction and releasing of composites of HF fluids, and these changes must be incorporated in the models.

The final project report will explicitly state and justify all assumptions used to the models. The assumptions that are specific to this work are: 1) groundwater flow and transport in saturated zones, 2) flow model has the constant water head boundary conditions along the northern, eastern and southern boundaries, and no-flux boundary condition along the western boundary, 3) contaminants are treated as a solute, 4) reaction includes adsorption and natural attenuation; adsorption complies with the equilibrium linear isotherm and natural attenuation is described by first-order decay process.

Input data required for these simulations will be obtained from the case study (Hydraulic Fracturing Retrospective Case Study, Bakken Shale, Killdeer and Dunn County, ND) and the technical literatures. Table 1 lists the parameters and their availability.

Table 1, Data and parameters for flow and transport modeling

Data/Parameters	Availability
Geographic coordinates of study area	National map viewer, downloadable from http://nmviewogc.cr.usgs.gov/viewer.htm
Area of model domain	25 miles by 31 miles centered at the Killdeer site
Information of oil/gas wells	Database of API, Database of North Dakota Industrial Commission, Department of Mineral Resources, Oil and Gas Division
Information of water wells	National Water Information System (NWIS) groundwater database of USGS , the Map and Data Resources of the State Water Commission, North Dakota
Water heads in water wells	Case study, Map and Data Resources from North Dakota State Water Commission
Contaminants concentration in monitoring wells	Case study
Hydraulic conductivity	Literatures, Klausning (1979), Fischer (2013)
Specific storage	Literatures, Klausning (1979), Fischer (2013)
Dispersivity	Estimation, in accordance with properties of aquifer materials
Porosity of formations	Estimation, in accordance with properties of aquifer materials
Recharge (precipitation/evapotranspiration)	Estimation, The National Water Information System of USGS
Adsorption parameter	estimation based on empirical data

Degradation parameter	estimation based on empirical data
Soil/rock density	estimation based on empirical data

It is not expected that all these data have been, or can be, measured in the field. For data not available from direct measurements, values will be taken from the scientific literature or assumed and justified based upon values in the literature. Uncertainty of input data will be justified based upon values in the literature.

Special Training Requirements / Certification

The required qualifications of the members of the project team are:

- 1) Advanced degree in the field: geophysics, geochemistry, environmental sciences and engineering, or hydrogeology.
- 2) Experience in numerical computation of hydrogeological problems.
- 3) Record of peer- reviewed publications.

No special training is necessary other than to the QA requirements of this project.

Documents and Records

To ensure that all personnel identified in project have the current version of the QAPP, email will be used to distribute electronic copies of the QAPP and record acknowledgment of receipt.

The product of this work will be development and application of the models for flow and transport of groundwater in the Killdeer site, North Dakota.

This work will be documented in

- 1) - EPA report describing the method and approach, and presenting representative simulations. This report will provide information on model structure, model data file, and modeling analysis results.

The following documents will be stored electronically on GWERD computers assigned to the researchers:

- 1) Model files created in the course of development of the models, including site geographic and geological map files.
- 2) Final GMS project files and input and output files used to generate results.
- 3) Records documenting planning and communication between project team member.
- 4) Records documenting in-house review of final report.

All documentation shall provide enough detail to allow for reconstruction of the project activities. All records will be deliverable in electronic format at the end of the project for archiving. The record package will include a directory to facilitate location of particular records.

The final project report will contain the following elements:

- 1) Background and description of the problem -
- 2) Development of stratigraphic model -

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- 3) Development of numerical models to simulate groundwater flow
- 4) Development of numerical models to simulate the contaminants transport
- 5) Model assumptions, referenced data and estimated data
- 6) Calibration for groundwater flow model
- 7) Simulation of flow and transport for specified model scenarios
- 8) Discussion of simulation results
- 9) Conclusions and recommendations

Proper document control and distribution procedures

- 1) Details on document storage
- 2) Backup plan for records stored electronically

Work will be done on personal computers and backed up automatically on remote servers. Copies will be maintained of all work documents, including script codes, input files, and output files necessary for a qualified individual to reproduce the work.

Description of the change control process: Any change to this QAPP will be approved by the Principal Investigator, case study Technical Lead and EPA QA Manager. The revised QAPP will be distributed to all participants of this project.

Length of retention periods for each record: All records will be deliverable in electronic format at the end of the project for archiving. The record package will include a directory to facilitate location of particular records. Because this is a level 1 QA Category project, all project records require permanent retention per the Agency Records Schedule 501, *Applied and Directed Scientific Research*. Records will be stored in Dr. Huang's office in the GWERD until they are transferred to GWERD's Records Storage Room. At some point in the future, records will be transferred to a National Archive facility. In addition, records shall be moved to the HF project O: drive when work is completed.

Data assessment reports, interim project progress reports: Interim project progress reports will be submitted to the case study Technical Lead as requested by the EPA project manager.

Model science formulation report, peer review reports: The model science formulation will be documented in the final project report which will be peer-reviewed.

Measurement and Data Acquisition

Sampling Process Design: -

This project includes no sampling. This section is not applicable. -

Sampling Methods: -

This project includes no sampling. This section is not applicable. -

Sample Handling and Custody: -

This project includes no sampling. This section is not applicable. -

Analytical Methods: -

This project includes no analysis of samples. This section is not applicable. -

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Quality Control: -

This project includes no direct measurement or data acquisition. This section is not applicable. -

Instrument/Equipment Testing, Inspection, and Maintenance: -

This project will use no measurement or test equipment. This section is not applicable. -

Model Calibration: -

Calibration is the process of modifying the input parameters to a groundwater model until the output from the model matches an observed set of data. The tool of automated parameter estimation (Doherty J. and Hunt R. J., 2010) provided in GMS 8.3 (MODFLOW PES) will be used to assist in the process of calibrating the flow model. The trial and error method (Neuman, 1973, 1982; Yeh, 1988; Brooks et al., 1994; Rama Rao et al., 1995; Sun et al., 1995) will be used to calibrate the fate and transport model. -

As an optional approach used to calibrate the flow model, a parallel genetic algorithm will be developed based on the microGA [Carroll, 1996]. The approach will integrate parallel GA and MODFLOW2005 into an optimizer running under parallel computation environment supported by Environmental Modeling and Visualization Laboratory of EPA. The model domain will be divided into 13 zones for hydraulic conductivity and 14 zones for recharge rate in accordance with the local geological sediment environment. In total, 27 model parameters will be estimated by fitting the water head observations. Several subroutines are required to set model parameters and extract water head. The subroutines will be coded in FORTRAN and integrated into MODFLOW2005. The modified MODFLOW2005 will then be called by parallel GA to minimize the objective function. -

Calibration Criterion for flow model: -

The flow model will be calibrated to the steady-state conditions. The criterion proposed in the calibration of flow model is to minimize the water head error residual term. When computed water heads are imported, the residual errors can be calculated as (objective function): -

$$F_{obj} = \sqrt{\frac{1}{N} \sum_{i=1}^N (H_i - h_i)^2}$$

where, H_i and h_i are respectively the observed and computed water heads at monitoring well i , N is the total number of observation points. The objective function depends on the model parameters. In the calibration, the model parameters include hydraulic conductivities defined in number of model parameter zones. The model parameter zones will be divided based on the surficial geology (Killdeer aquifer) and shallow geology (Sentinel Butte Formation). The optimized hydraulic conductivities will be used to simulate the flow and transport in the aquifer system.

Calibration Criterion for fate and transport:

The criterion proposed in the calibration of fate and transport model is to minimize the contaminants concentration error residual term. When computed concentrations are imported, the residual errors can be calculated as (objective function):

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$$T_{obj} = \sqrt{\frac{1}{NM} \sum_{j=1}^M \sum_{i=1}^N (C_i(t_j) - c_i(t_j))^2}$$

where, C_i and c_i are respectively the observed and computed concentration at observation point i , t_j is the observed time point, N is the total number of observation points, M the total number of time series records at the observation point. The objective function depends on the hydrodynamic dispersivities and adsorption and decay constants defined in the parameters zones. The fate and transport model will be calibrated by manually adjusting the model parameters to fit the observation data.

Inspection/Acceptance of Supplies and Consumables: -

This project will use no supplies or consumables. This section is not applicable. -

Non-Direct Measurements (Data Acquisition Requirements): -

The case study has completed acquiring data, in another project (Hydraulic Fracturing - Retrospective Case Study, Bakken Shale, Killdeer and Dunn County, ND). Input data for the models will be acquired from the case study and from scientific literature. This project will not use any measuring or test equipment. -

Data Management and Hardware/Software Configuration

The following data (including script codes and input and output files) will be managed by this project:

1) DATA

Environmental and process data will be acquired from the case study or from the scientific literature as described earlier. The quality of data from the case study has been evaluated as part of another project (Hydraulic Fracturing Retrospective Case Study, Bakken Shale, Killdeer and Dunn County, ND). Data quality from both these sources will be accepted for use on this project as described in section on Data Validation. Accurate transcription of these data into input files will be verified by line-by-line hand checking (direct comparison of input files with the source data).

2) SOFTWARE

Simulators, MODFLOW2005 and RT3D both are highly credible sources. Code verification is unnecessary. Both simulators are supported by GMS (Groundwater Modeling System). The project files of GMS will be archived and documented in the project reports. GIS (Geographic Information System) will be used to manage ground surface elevation, water wells location and hydrological features of the study area. The data set is exported to the format compatible with GMS. The scripts of MATLAB will be used to reformat data downloaded from the data sources, the scripts also will be used to verify the correctness of the data set.

Assessment and Oversight

1) Assessments and Response Actions -

Plans for science and product peer review: The final project report will be peer reviewed. -

Audit: A Technical Systems Audit will be conducted by a QA support contractor with oversight - by the EPA QA Manager, early enough in the project to allow for identification and correction of - any issues that may affect data quality. Detailed checklists, based on the procedures and - requirements specified in this QAPP will be prepared and used during the audit. -

Assessors do not have stop work authority; however, they can advise the PI if a stop work order - is needed in situations where data quality may be significantly impacted, or for safety reasons. - The PI makes the final determination as to whether or not to issue a stop work order. -

For assessments that identify deficiencies requiring corrective action, the audited party must - provide a written response to each Finding and Observation to the QA Manager, which shall - include a plan for corrective action and a schedule. The PI is responsible for ensuring that audit - findings are resolved. The QA Manager will review the written response to determine their - appropriateness. If the audited party is other than the PI, then the PI shall also review and - concur with the corrective actions. The QA Manager will track implementation and completion - of corrective actions. After all corrective actions have been implemented and confirmed to be - completed, the QA Manager shall send documentation to the PI and his supervisor that the - audit is closed. Audit reports and responses shall be maintained by the PI in the project file and - the QA Manager in the QA files, including QLOG. -

At the conclusion of a TSA, a debriefing shall be held between the auditor and the PI or audited - party to discuss the assessment results. Assessment results will be documented in reports to - the PI, the PI's first-line manager, and the Technical Research Lead. If any serious problems are - identified that require immediate action, the QAM will verbally convey these problems at the - time of the audit to the PI. -

The PI is responsible for responding to the reports as well as ensuring that corrective actions - are implemented in a timely manner to ensure that quality impacts to project results are - minimal. -

2) Reports to Management -

Quarterly progress reports and a final report will be submitted to the GWERD Research Lead, - Ms. Smith and the principal Investigator Dr. Douglas Beak. -

All final audit reports shall be sent to the first-line manager of the PI, the Technical Research - Lead, and copied to the PI. Audit reports will be prepared by the QA Manager with input from - the QA support contractor where audit performance was delegated. Specific actions will be - identified in the reports. -

Data Validation and Usability

1) Data Validation

Environmental and hydrogeological data will be acquired from the case study or from the scientific literature. Attributes to be considered for acceptance will include whether the data were collected: (1) using standard methods, (2) according to approved procedures, and (3) under a QA program.

2) Validation methods

Model compounds such as three-dimensional stratigraphic model, model package options and model boundaries assignment will be validated by technical review. To a great extent, the theory and mathematical and numerical procedures used in these simulators have already been validated by technical review, peer review, and acceptance by the scientific community. Outputs of simulations are not guarantees but are reasonable expectations, based upon the quality of input data, and uncertainty estimated from sensitivity of outputs to uncertainty of inputs. Limitations on the use of outputs of simulations will be discussed in the reports.

The scripts of MATLAB will be used to check the reasonability of data sets: borehole screen elevations will be checked to confirm that the vertical coordinates are higher than that of the borehole bottom and bed rock surface elevations are not larger than the ground surface elevation. Data identified with this check will prompt further review and if confirmed, this data will not be used. GIS mapping will be used to check the location of water wells. The spatial coordinates of wells should be bounded by the study area. Well locations identified to be outside the study area will not be used.

3) Reconciliation with User Requirements

The project final reports will describe and justify any deviations from this plan, and will include discussion of assumptions and results, and will discuss limitations of the use of output data for users of the report.

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Table 2. QAPP revision history.

Revision Number	Date Approved	Revision
0	5/16/2013	New document
1	9/19/2013	<p>QAPP revised to address Observations from Technical Systems Audit:</p> <ul style="list-style-type: none"> • Task 5: added description of user-defined reaction package • Quality Objectives and Criteria for Model Inputs/Outputs: added justification for using RT3D • Documents and Records; Assessment and Oversight: removed peer reviewed journal article as a product • Measurement and Data Acquisition: added model calibration using a parallel genetic algorithm • Data Management and Hardware/Software Configuration: added information on using GIS to manage certain information and the use of scripts to reformat downloaded data and to verify correctness • Data Validation and Usability: added use of scripts in MATLAB to check reasonableness of data • References: added a reference • Added Revision History Table