Sitewide model group
Shilo Inn June 13, 2006

Sitewide conceptual models
Limitations – data gaps limits to making the model reliable and convincible

- Well drilling to maximize impact – working with GS and INL instrumenting to cover some of the data gaps USGS drilling deep wells to cover some data and quality issues
- Management support has been strong in the past

Mission Statement:

To develop a conceptual model that is reliable, testable, defensible and will position the team for potential future efforts in performance monitoring, long-term stewardship, and facility siting.

Produce a model that is robust, reliable, versatile, and defensible.

Science Issues:

- REV
    - Temporal and spatial variability
    - Scaling is an issues
    - K-field - field to regional scale
    - Where are the plumes really going 3-dimensionally, do they intersect or are they transient.
    - Are the monitoring wells in the appropriate place to capture the contaminant.
    - Novel approaches of building a 3-D model with 2-D data. 3-D data is sparse currently.
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- Biogeochemical processes – system wide processes
    - Biomarker – vertical communication
    - Biosignatures passing in the plume – help to characterize the vertical in the plume sample the horizon
    - Reduce metal in the system and fully oxidized aquifer – electron transfer
    - Long term impact of TCE plume at RTC
    - Demonstrate tracking history or chemical signatures
    - Coupled processes – in a fractured system, but how do we stimulate the processes in a dynamic system or process.
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- Vertical communication in the system

    - What happened when we change the vertical resoultion
    - Deeper wells are needed to monitor deep aquifer. USGS is planning on deepening wells over the next few years.
    - Temperature signature and temperature tracer, to characterize the vertical.
    - Different heads are not hydrostatic in the well-homogenize head measurements

- Assumption of representative samples
    - Head
    - Chemistry
    - Geology
    - Data is suspect because of man-made wells

- Recharge/BCs
    - Induce errors into the systems magnitude of the flux from the main drainage areas and water recharge systems.
    - Function of linear recharge from surrounding areas. Water levels are not consistent across the years.
    - Sensitivity function or sensitivity analysis to cover recharge issues. Is this an important issue.
    - Weakest link in the model is we don't know the discharge volume
    - Recharge/discharge issues need to be identified – boundary condition sensitivity is the main issue.
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- Modeling
    - Concentrate on a facility to characterize the model, but main focus needs to be site-wide
    - What testing criteria do we apply to our models
    - Use nested models to characterize the variability.
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    - Advanced modeling techniques
        - Adaptive grid refinement, etc

- Long-term legal reliability is key to future models – site wide issues may require a more complex model.

- Nested models

    - Geologic models of the area still need to be refined. Pending data input USGS core library data updates.
- Model needs to be flexible to test new data.
- Single-time stamp, adds addition information control on the model.

Raw comments/scrib notes.

General Statements:

1. Positioned to take over the legacy issues from the cleanup side of the lab. All WAGs will be rolled into the INL. Mainly WAG 10 and the CERCLA cleanup sites.

2. Using a nested feature gridding starting at ¼ mile and then going down from there.

3. Use a site-wide model with sub-grids or sub-models to model specific facilities and small scale issues to model plumes. Facility models extend into the saturated zone and are regulatory bound.

4. Variablity is necessary for current models to measure transients. Need to look at 3-D activity – nested models have excellent potential to measure these sources.

5. 90% plus wells are shallow and associated with facilities. 275 wells (out of over 1000) are being used in current models.

6. Facility models use source terms and coupling to link both the vadose and saturated zone. Model deep enough to cover both.

7. We know so little about the vertical stratigraphy of the site, and homogenous efforts are taking part in the problem.

8. Transient eposide events in the aquifer. Use Chloroflour CFCH carbon testing for dating the aquifer. Integrated to show 3-D flow. Model matching imperfect observations. Testing the veracity of the model.
9. Processes - how do the processes further our understanding of our models. Models need to be more accurate and consistent.

10. USGS tritium is calibration point for the new conceptual models.

11. Alternative conceptual models – at what point do you abandon a non-working model and begin with a different model. Where does the testing and observations in the field change the conceptual model.

12. Predicting down stream concentrations – how much mixing and dispersion of the contaminate is observed, and how can the model predict that.

13. Redox contaminants are a part of the future model.

14. What can we do to make the model better—

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- Reduce metal in the system and fully oxidized aquifer – electron transfer
- Biosignatures passing in the plume – help to characterize the vertical in the plume sample the horizon
- Verticle communication in the system
- Assumption of representative samples – head varies at the hold. Assumption of homogeneity in the representative sample.
- Temperature signature and temperature tracer, to characterize the vertical.
- Data is suspect because of man-made wells
- Different heads are not hydrostatic in the well
- Recharge – induce errors into the systems magnitude of the flux from the main drainage areas and water recharge systems.
- Function of linear recharge from surrounding areas. Water levels are not consistent across the years.
- Sensitivity function or sensitivity analysis to cover recharge issues. Is this an important issue.
- Concentrate on a facility to characterize the model, but main focus needs to be site-wide
- Coupled processes – in a fractured system, but how do we stimulate the processes in a dynamic system or process.
- Long-term legal reliability is key to future models – site wide issues may require a more complex model.
- Where are the plumes really going 3-dimensionally, do they intersect or are they transient. And if so are the monitoring wells in the appropriate place to capture the contaminant.
- Deeper wells are needed to monitor deep aquifer. USGS is planning on deepening wells over the next few years.
- What does the site-wide model need to have to stimulate the program office at DOE
- Geologic terrains (uniqueness) and model those terrains in the site-wide model. Nested models
- Geologic models of the area still need to be refined. Pending data input USGS core library data updates.
- Vertical variability is not possible in large geologic model. Use nested models to characterize the variability.

- Scaling is an issues
- Biomarker – vertical communication
- Demonstrate tracking history or chemical signatures
- What testing criteria do we apply to our models
- Piggy back on the research of others to model the current site.
- Time talent and energy now to provide the data of the future.
- Model needs to be flexible to test new data.
- Vertical control will enhance our modeling nearly instanteously.
- Single-time stamp, adds addition information control on the model.
- Weakest link in the model is we don't know the discharge volume
- Recharge/discharge issues need to be identified – boundary condition sensitivity is the main issue.
- Problem of building a 3-D model with 2-D data. 3-D data is sparce currently.
- Are there novel ways of dealing with this issue.
- Control of the plumes across the vertical and horizontal.
- Facilities have done a good job of modeling the plume, but dispersion is not measurable.
- Be able to account for mass.

Objectives

- How do you create a large scale model that incorporates the local regional models. (Orange County California)
- Methods for integrating small scale contaminant modeling into large scales regional models
- Worst-case scenario models
- Must calibrate model against current plumes
- Dual domain – dual processes – parameter choice becomes important.
- How are you going to parameterize your site wide models – dispersion at multiple scales. Science need.
- Define dispersion parameter at scale. Verticle dispersion coefficient. Velocity variability or velocity dispersion. Capture variability in the dispersion.
- Capture uncertainty – bound the problem
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