Simulation Modeling: A Reviewer's Perspective

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- Simulation modeling is increasingly being used in problem solving and decision making.
- Simulation models are reviewed by the model developers, regulators, and other stakeholders.
- The objective of the review process is to develop confidence in the model results and decisions based on those results.

Presentation Outline

- Reviewing Simulation Models
  - Reviewability
  - Complexity
  - Support
  - Other considerations
- Identifying Risk Significant Components of Simulation Models
  - Risk informing
  - Determining risk significant components

Simulation Modeling: Reviewability

- Simulation models must be able to be independently reviewed and understood.
  - Consider objective of the model
  - Consider audience
  - Models don't make decisions, humans make decisions

- Documentation of the modeling is as important as the modeling itself.

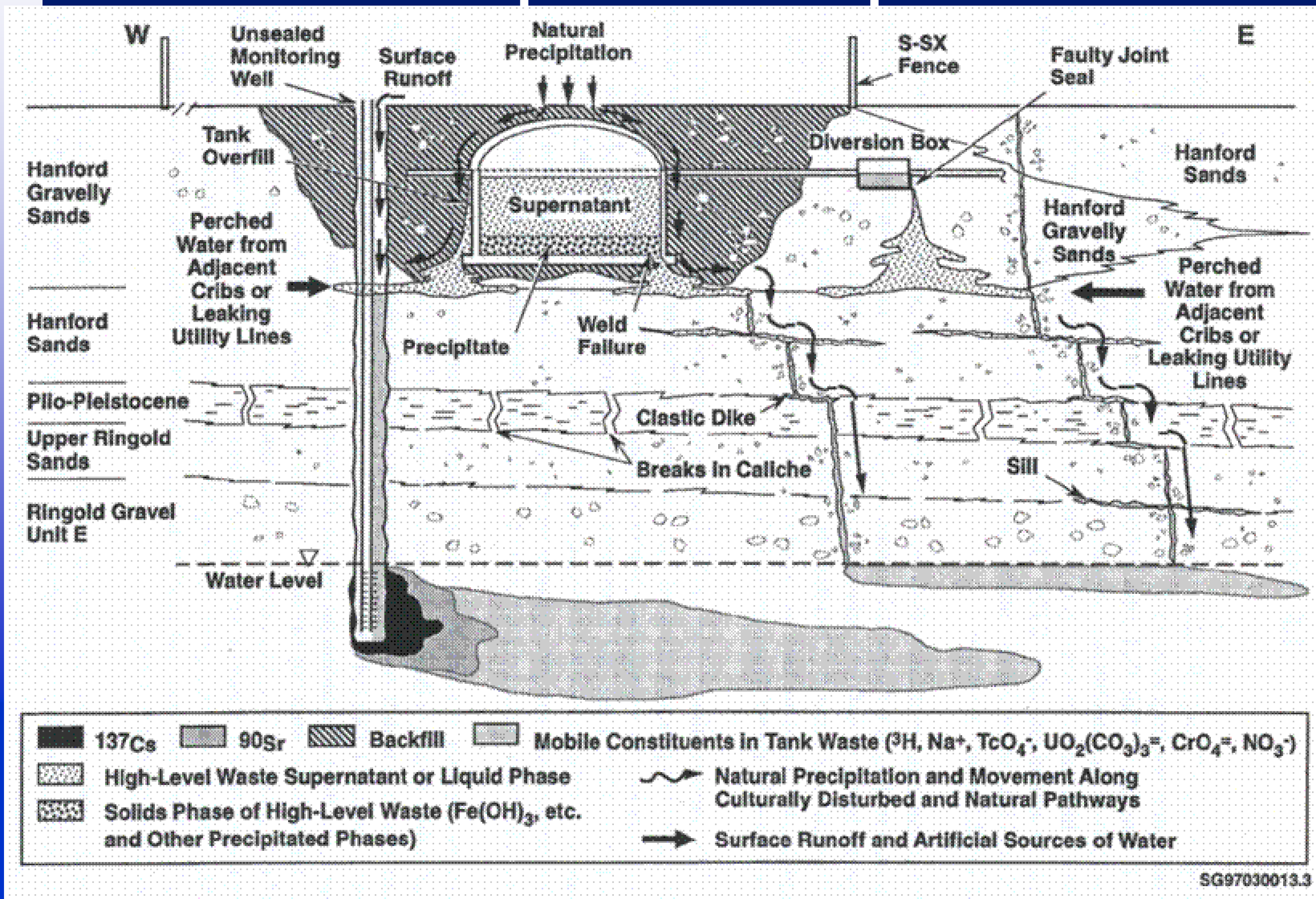
- The analysis and documentation must be transparent and traceable.

- Data should be traceable to the source to facilitate the review of data validity.

Simulation Modeling: Reviewability

- The modeling and documentation should be consistent.
- Documentation and explanation (and therefore cost) increases with model complexity.
- A model that is not understood is unlikely to be accepted.
- Consider review effort:
  - 100,000 lines of FORTRAN code compared to a 100 element visual simulation model? GoldSim models are inherently easier to review.

Example of a complex site



Simulation Modeling: Complexity

- Review effort increases exponentially with increasing model complexity.
- Model complexity should be commensurate with available supporting information.
- However, the analysis approach should test whether additional complexity may have a significant impact on the model results.
- Model building is a dynamic process in itself. If complexity is added to a model and found not to have a significant influence on the results (either favorable or unfavorable), it should be removed.

Simulation Modeling: Complexity

- Complex does not necessarily mean better.
- However, sometimes complexity is unavoidable and necessary.
- Example:
  - INTRAVAL, Synthetic Migration Experiment, Phase 1 Case 6 [copies of the report are available from the Swedish Nuclear Power Inspectorate (SKi)]
  - A modeler who used hand calculations to estimate fracture properties did as well, and in some cases considerably better, at predicting the experimental results than much more sophisticated calculations (e.g., geospatial techniques).

Simulation Modeling: Support

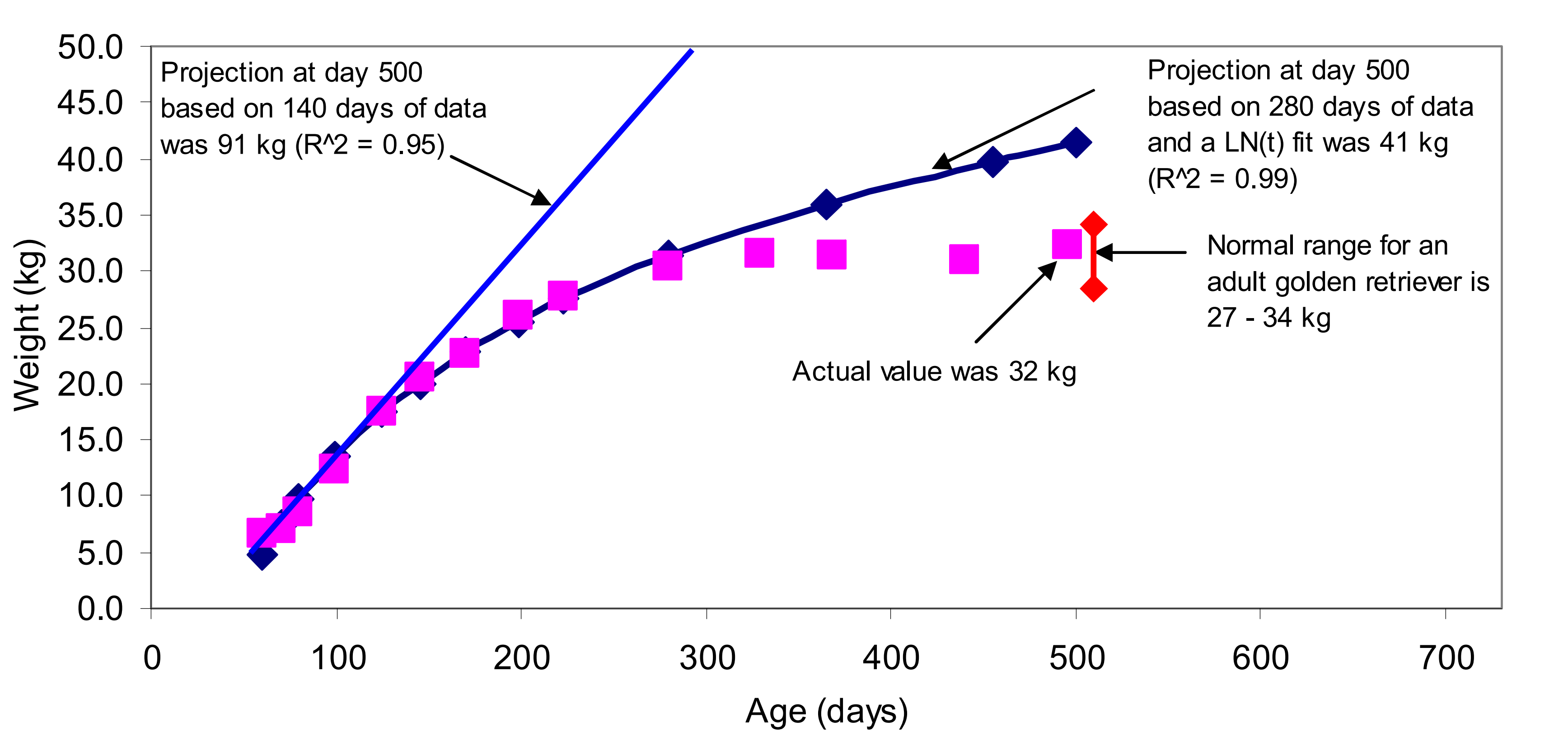
- Model support is arguably the most essential element to successful simulation modeling.
- Simulation modeling should have support, at a minimum, in the form of verification and validation:
  - Verification – Solving the equations right
  - Validation – Solving the right equations
- A variety of elements can be part of the model support process, including the following: internal review (QA), independent external review, documentation of verification efforts, and a multi-faceted validation effort.

Simulation Modeling: Support

- Simulation modeling that allows for the independent review and understanding of intermediate outputs is strongly encouraged.
- Documentation and openness about shortcomings of the modeling generally increases confidence for the reviewer.
- Natural and dynamic systems can be inherently difficult to predict.
- Simulation modelers, by their nature, are biased to being overconfident in their ability to predict a system.
- Example: Causal inference

Simulation Modeling: Support

- Consider transient nature of the system and ability of short-term data to validate model that makes long-term predictions.



Simulation Modeling: Other Considerations

- Consideration of uncertainty and variability is typically essential for successful simulation modeling.
- Understanding the impact of uncertainty can be difficult using sensitivity analysis of a deterministic model when the system being modeled is complex.
- When model support is limited, a simple, highly-uncertain simulation model is generally preferable to a complex, deterministic model.

Developing and Presenting Risk Information

- To the extent practical, the simulation model development and subsequent analysis process should have an objective of identifying risk information.
- Risk is defined here to be those things most likely to impact the decision.
- For example, in problems that NRC reviews, there may be 500 parameters in the analysis:
  - The reviewer wants to focus on those 10 to 20 most likely to impact the decision.
  - The analyst should want to identify the same parameters, so they can increase the support for those parameters.

Developing and Presenting Risk Information

- There are many methods for determining important parameters and uncertainties (e.g., regression analysis, genetic algorithms, parameter trees).
- Our experience is that one method is not the best, and usually multiple methods should be used.
- The analyst should develop an understanding of the model, which can be as important as quantitative analysis techniques.
- The understanding of the analyst can be very important to adequately performing the analysis.

Developing and Presenting Risk Information

- The reviewer may not have the time to review all of the information available.
- <u>Produce the most convincing argument (with the least amount of information)!</u>

Developing Risk Insights: Example

- An independent PA model was used to develop risk insights for the review of the Saltstone Disposal Facility (SDF) at the Savannah River Site (SRS)
- NRC staff typically uses independent performance assessment (PA) models to develop risk insights
- In this context, a performance assessment is a model to project the long-term (e.g., thousands of years) performance of natural and engineered systems for the disposal of radioactive waste.

Developing Risk Insights: Example

- 49 operational high-level waste tanks at SRS
- The Department of Energy (DOE) plans to:
  - Remove salt waste from the tanks
  - Mix treated liquid salt waste with dry ingredients to create a cementitious wasteform called "saltstone"
  - Dispose of approximately 5 million cubic meters of saltstone in concrete vaults on site

Developing Risk Insights: Example

- NRC staff had to review a PA model initially developed in 1992, updated in 1998, and a supporting analysis performed in 2002.
- The DOE analysis was deterministic, performed with a variety of software products in which the outputs were manually transferred between programs.
- The analysis was documented in a 1992 document of over 700 pages, a few main supporting documents of many hundred pages each (and many hundred references).
- There was no clear linkage of the analysis, the data used, and the documentation.

Developing Risk Insights: Example

- NRC staff, in this case and commonly, does not have an unlimited amount of time to perform the review.
- What do you review? How do you review it?
- What are the essential questions to ask?
- What is driving the results of the analysis?
- What is the impact of uncertainty?

Developing Risk Insights: Example

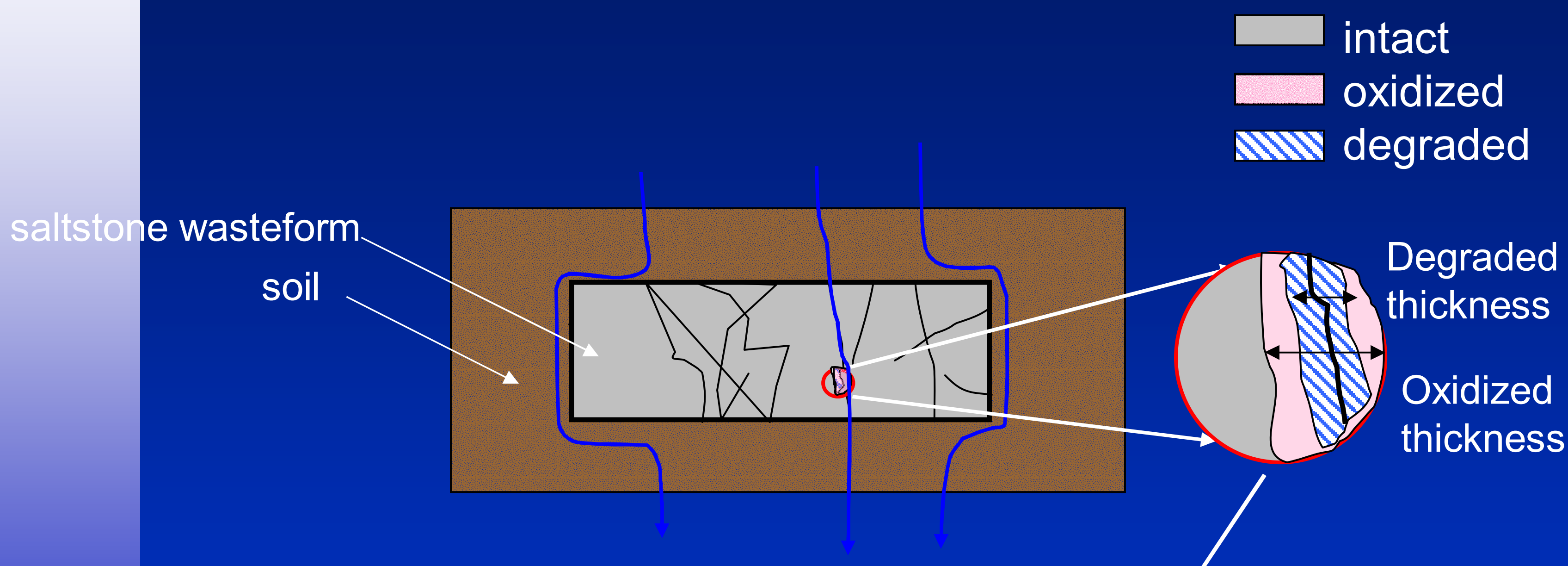
- Model developed using GoldSim Software:
  - Probabilistic assessment
  - Specialized elements facilitate radionuclide transport modeling
  - 1150 elements, more than 300 stochastic elements

- Submodels included:
  - Degradation of engineered cap
  - Oxidation of saltstone
  - Physical degradation of saltstone
  - Release of radioactive material
  - Transport in unsaturated and saturated subsurface zones as well as surface water
  - Exposure pathways
  - Dose assessment

Developing Risk Insights: Example

- Preliminary results were sensitive to wasteform degradation assumptions
- Preliminary results indicated need to model degradation and oxidation as a function of time
- Model refined to include submodels of:
  - Grout oxidation
  - Physical degradation of wasteform
- Simulation modeling using risk insights is typically iterative.

Developing Risk Insights: Example



Number of half cells modeled depends on user-defined fracture spacing

Risk Insights Example – Analysis Approach

- Run probabilistic base-case model
- Develop confidence in model
  - Individual realizations physically reasonable
  - Results insensitive to time-stepping and number of realizations
- Run genetic analysis of base-case probabilistic results using Neuralworks Predict®
- Limit number of stochastic variables
- Re-run genetic analysis
- Evaluate alternate cases

Uncertainty Analysis with Genetic Algorithms for the Base Case, Using a Shortened Variable List

Variable Name	Description	Importance Factor
GW_flow	Average Darcy velocity of fluid in the saturated zone transport pipe. Influences dilution and transport times.	0.98
Fracture_spacing	Average spacing of fractures in the wasteform. Influences the amount of oxidation and degradation during the simulation period and the diffusive path length of contaminants to the fractures.	0.97
Water_intake	Consumption rate of drinking water. Directly influences the drinking water dose.	0.96
Bound_waste_deg_rate	Rate at which contaminants are available for release and transport. Conceptually represents dissolution of the wasteform.	0.93
Mg_conc	Concentration of Mg in the fluids contacting the wasteform. Influences the amount of degradation predicted to occur during the simulation period.	0.86
Infiltration_rate	Rate of infiltration of water into the subsurface. Influences the release and transport of contaminants from the wasteform.	0.71

Risk Insights Example – Conclusions

- Risk insights (in this case developed by the reviewer) were used to focus the review on key elements of the simulation model.
- Requests for additional information were reduced (compared to if risk insights were not used).
- A simple, highly uncertain model was refined and the complexity increased based on initial analyses.
- By identifying and emphasizing risk-significant elements of the modeling, the confidence in the decision should be enhanced for all stakeholders (e.g., that public health and safety will be protected).

Conclusions

- The reviewability of the model should be considered when a simulation model is developed.
- Transparent and traceable analysis and documentation can be as important as the details of the modeling.
- Model complexity should be increased as needed, and removed if it is not materially affecting the decision.
- Model support is essential to validating a model and increasing confidence in model results.
- Developing and presenting risk information can accelerate the process of achieving credibility of the modeling and developing confidence in the resultant decisions.