Oil & Natural Gas Technology

DOE Award No.: DE-FE0001243

Clean and Secure Energy from Domestic Oil Shale and Oil Sands Resources

Quarterly Progress Report (October - December 2012)

Submitted by:
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Prepared for:
United States Department of Energy
National Energy Technology Laboratory

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Office of Fossil Energy

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155 S. 1452 E. Room 380
Salt Lake City, UT 84112

Principal Investigator: Philip J. Smith
Project Period: October 1, 2010 to September 30, 2013

Prepared for:
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EXECUTIVE SUMMARY

The Clean and Secure Energy from Domestic Oil Shale and Oil Sands Resources program, part of the research agenda of the Institute for Clean and Secure Energy (ICSE) at the University of Utah, is focused on engineering, scientific, and legal research surrounding the development of these resources in Utah.

Task 3, "Clean oil shale and oil sands utilization with CO_2 management," has been focused on the continued analysis of data from Uinta Basin oil and gas production and the development of a Matlab-based basin model. The Subtask 3.1 team evaluated well depth and well field for 6928 wells in the Uinta Basin and determined that well field had a significant effect on well depth. These results indicate that drilling costs should be tied to field in the Matlab model. For Subtasks 3.3 and 3.4, the project team continued work on a Matlab-based model that predicts drilling frequency and production levels from oil and gas wells in the Uinta Basin. Well counts were fit with a Poisson regression and the production data with an exponential decline curve.

Task 4 projects, "Liquid fuel production by in-situ thermal processing of oil shale/sands," range from the molecular to the basin scale. At the molecular scale, Subtask 4.9 researchers are synthesizing data and preparing a final publication on the details of kerogen and bitumen isolation and characterization from the three segments of the Skyline 16 core. At the core scale, Subtask 4.5 researchers completed their final task deliverable, a paper summarizing their work on oil shale structure before and after pyrolysis. Also at this scale, the Subtask 4.3 team completed tar analysis from demineralized kerogen samples from the Skyline 16 core. There was no noticeable difference in the types of compounds evolved from samples taken from different depths. Subtask 4.7 researchers carried out mechanical properties tests at 400°F and 800°F on larger White River oil shale samples. At the production scale, the Subtask 4.1 team performed a simulation Red Leaf's ECOSHALE capsule that included both a detailed property model and an operator splitting algorithm. Further work is required in order to balance the computational requirements of the short, fluid time scales and the long, thermal time scales. At the basin scale, Subtask 4.8 researchers described two cores of the Green River Formation. Detailed sedimentary and stratigraphic description was performed and photos were taken. X-ray flourescence data also collected at 3-foot stratigraphic intervals.

Task 5, "Environmental, legal, economic and policy framework," has one remaining project, Subtask 5.3. A summary report of research relevant to assessing the judicial and administrative framework for utilizing simulation science in the context of assessing environmental risks or harms is attached as an appendix to the report.

The Market Assessment (Subtask 6.3) was finalized in this quarter in preparation for sending it out to reviewers in October 2012. Subtask 6.1, which provided much of the engineering analysis for the assessment, will be completed once the process models and data have been uploaded to a webpage on the ICSE website.

Based on a project review of Task 7, Subtask 7.2 has been terminated and its remaining funds shifted to Subtasks 7.1 and 7.3. Expanded task statements based on revised budgets for Subtasks 7.1 and 7.3 are included in this quarterly report. Subtask 7.1 researchers proceeded with segmented linearization and development of constitutive modeling surfaces on American Shale Oil (AMSO) data. Subtask 7.3 researchers completed 15 simulations for their validation/ uncertainty quantification studies of the January heater experiment test conducted by AMSO.

PROGRESS, RESULTS, AND DISCUSSION

Task 1.0 - Project Management and Planning

During this quarter, there were no schedule/cost variances or other situations requiring updating/amending of the Project Management Plan (PMP). Internal budgeting reallocation occurred during this quarter as described under Task 7.0. Submission of a no cost time extension has been delayed until the first quarter of 2014.

Task 2.0 -Technology Transfer and Outreach

Task 2.0 focuses on outreach and education efforts and the implementation of External Advisory Board (EAB) recommendations. No further EAB scheduling decisions were made this quarter. Work has continued on identifying potential panelists for the 2013 ICSE Energy Forum event, which has been scheduled for April 2, 2013.

Task 3.0 - Clean Oil Shale and Oil Sands Utilization with CO_2 Management

<u>Subtask 3.1 (Phase I) – Macroscale CO_2 Analysis (PI: Kerry Kelly, David Pershing)</u>

There is one deliverable that has not been completed for Phase I of this project. The deliverable, a paper on potential greenhouse gas (GHG) emissions from Uinta Basin oil shale and oil sands development scenarios, is in draft form awaiting final inputs from Subtask 6.3.

The project team received updated assessment results in November and performed supplemental analyses to generate carbon footprints for each of the scenarios. Figure 1 shows the most recent well-to-pump GHG footprints for the Uinta Basin ex situ oil shale and oil sands and in situ oil shale scenarios without the use of oxyfiring for CO_2 capture using the November assessment results. These results are compared to literature values in the figure. Assessment results will be finalized in the next quarter, so the results in Figure 1 are preliminary.

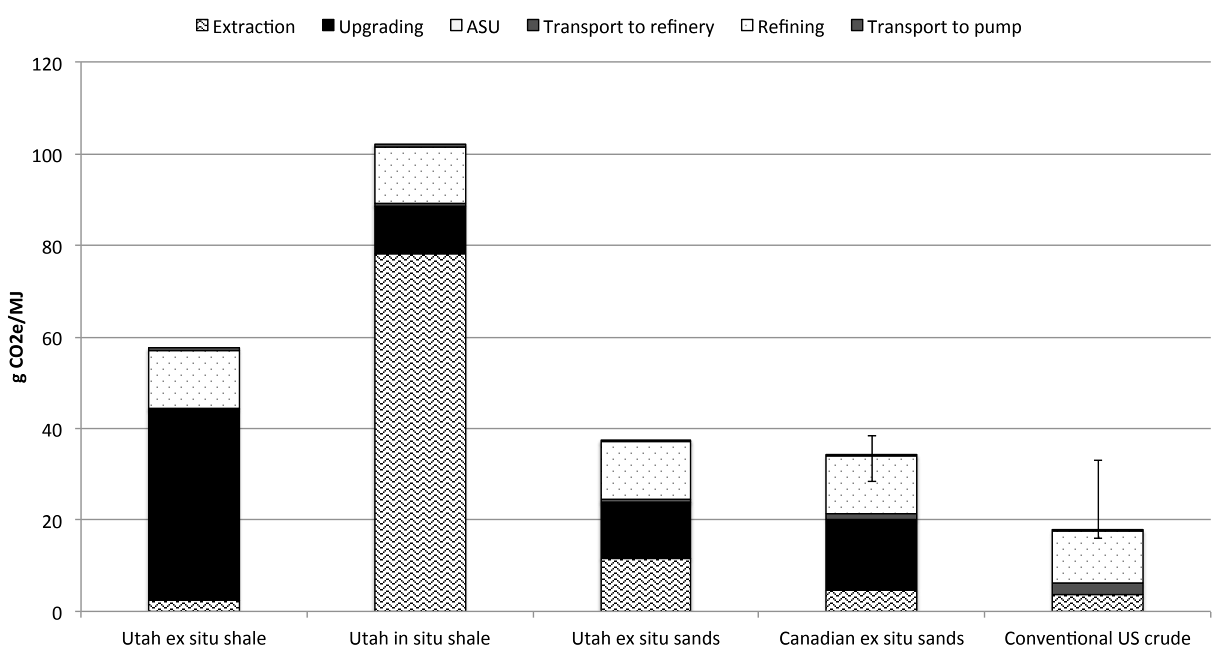

Figure 1. Preliminary comparison of well-to-pump GHG emissions for production of gasoline from in and ex situ Utah oil shale development, ex situ Utah and Canadian oil sands

development (ANL, 2012), and conventional crude oil (EPA, 2009). The error bars on the Canadian ex situ sands show the range of values reported in McKellar et al. (2009), and the error bars for conventional US crude show the range of values reported by DOE (2009).

In addition, refinements to the GHG analysis were made. The most significant was to estimate the energy requirements and GHG emissions associated with upgrading and refining based on the product properties (API gravity, composition including sulfur and nitrogen content) and relationships between these properties and processing/refining requirements (e.g., Rana et al., 2007; Brandt, 2012).

Subtask 3.1 (Phase II) – Lifecycle Greenhouse Gas Analysis of Conventional Oil and Gas Development in the Uinta Basin (PI: Kerry Kelly, David Pershing)

Using information collected from the Utah Division of Oil, Gas, and Mining database, team members evaluated well depth and well field for 6928 wells in the Uinta Basin to determine if the well field had a significant effect on well depth. Table 1 and Table 2 show the results for a two-sample t-test of unequal size and unequal variance at the 95% level of significance with the Bonferroni correction, which is used to correct for multiple comparisons and adjusts the p critical value from 0.05 to 2.16×10^{-4}. The t-tests were only performed for 22 fields with at least 15 wells drilled within the field. Of the 22 pairs of fields, which equals 132 possible comparisons (no duplicates), 57 (43%) comparisons indicate no difference in the mean depth, and 35 (26%) of the comparisons do not involve the same fields. Thus, it appears that the effect of field needs to be considered in the systems model for oil and gas development in the Uinta Basin.

Table 1. Student t-test results for the effect of field on well depth. The * indicates that the mean depth of the two fields does not differ at a 95% significance level. The p critical value was adjusted from 0.5 to 2.16×10^{-4} using the Bonferroni correction. Duplicates are not noted.

	Bluebell	8 mile flat	Monument butte	Bitter creek	South myton bench	8 mile flat north	Flat rock	Gusher	Gypsum hills	Hill creek	Kennedy wash
Bluebell	*										
8 mile flat		*									
Monument butte	*		*								
Bitter creek				*							
South myton bench					*						
8 mile flat north						*					
Flat rock		*		*		*	*				
Gusher	*		*					*			
Gypsum hills					*				*		
Hill creek					*			*	*	*	
Kennedy wash										*	*

Table 2. Student t-test results for the effect of field on well depth. The * indicates that the mean depth of the two fields does not differ at a 95% significance level. The p critical value was adjusted from 0.5 to 2.16×10^{-4} using the Bonferroni correction. Duplicates are not noted.

	Love	Natural buttes	Pariette bench	Red wash	Rock house	Uteland butte	White river	Wonsits valley	Windy Ridge	Big Valley

Love	*									
Natural buttes	*	*								
Pariette bench			*							
Red wash				*						
Rock house				*	*					
Uteland butte	*	*	*	*	*	*				
White river	*	*	*			*	*			
Wonsits valley	*	*				*	*	*		
Windy ridge				*	*	*			*	
Big valley	*	*	*			*	*	*		*

The project team also continues to monitor several potentially useful sources for validation data of GHG emissions.

Subtask 3.2 - Flameless Oxy-gas Process Heaters for Efficient CO_2 Capture (PI: Jennifer Spinti)

Work on the final deliverable for this task, a report detailing results of a validation/uncertainty quantification analysis, was on hold this quarter pending availability of the PI.

Subtask 3.3 - Development of Oil and Gas Production Modules for $CLEAR_{uff}$ (PI: Terry Ring)

The work on this subtask is being performed jointly with that of Subtask 3.4. Only one graduate student is left on the project, requiring the project team to combine resources to meet project milestones.
During this quarter, work began on developing a Matlab version of the system dynamics model $CLEAR_{uff}$ developed using the AnyLogic software. Using data and analysis from members of the research group, the simple Matlab model that has been created predicts (1) the number of wildcat oil wells that are drilled in response to the current price of oil and the number of wells drilled previously (well counts), and (2) the total amount of oil produced by all wells during each time step of the model. The next step is to build a version of the model that utilizes oil and gas price forecasts to determine the profitability of well. Profitability is then used as a basis for deciding whether or not the well is drilled. A revised overview of the Matlab model is shown in Figure 2.

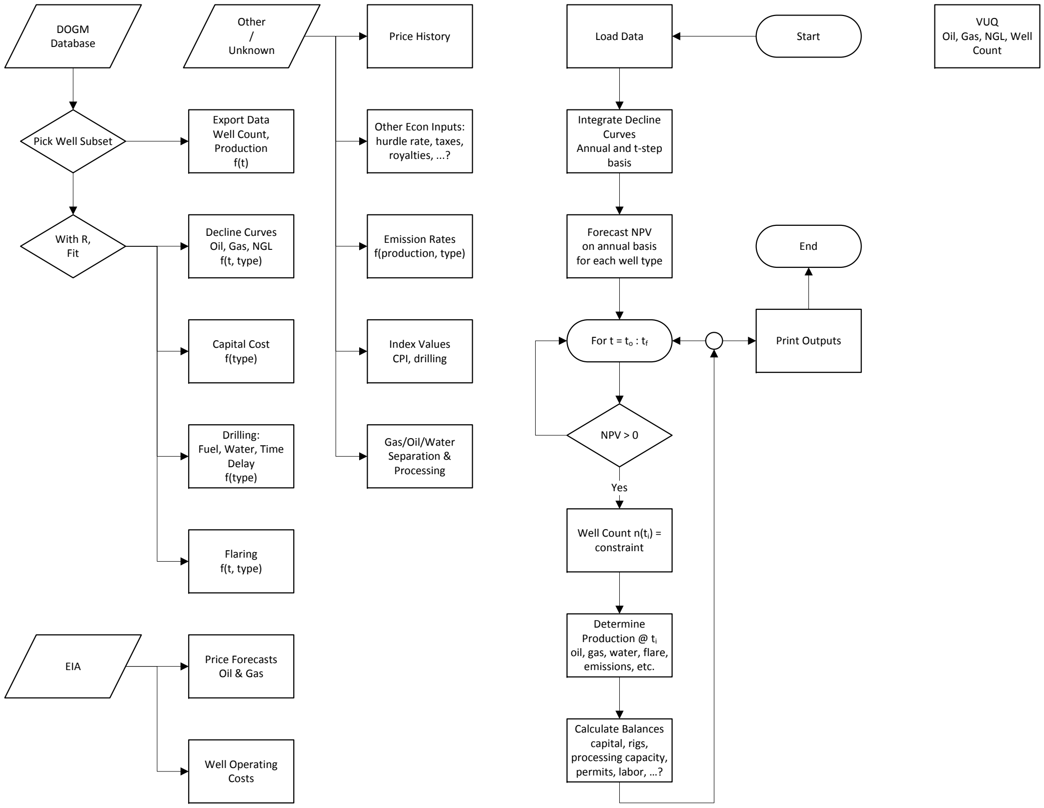

Figure 2. Overview of CLEAR model being developed in Matlab with application to oil and gas production in the Uinta Basin for model validation.

Well Counts

Data files have been generated that contain well counts as summed by month, quarter or year for the Brundage Canyon and Monument Butte oil fields; similar data can be given for other fields---these are mainly for testing. Each file has three columns: (1) "Index" - the date of the beginning of the time interval, (2) "count" - number of wells drilled during the interval, and (3) "price" - the inflation adjusted price of oil (unit is 2012 US$). A plot of the Brundage Canyon data is shown in Figure 3.

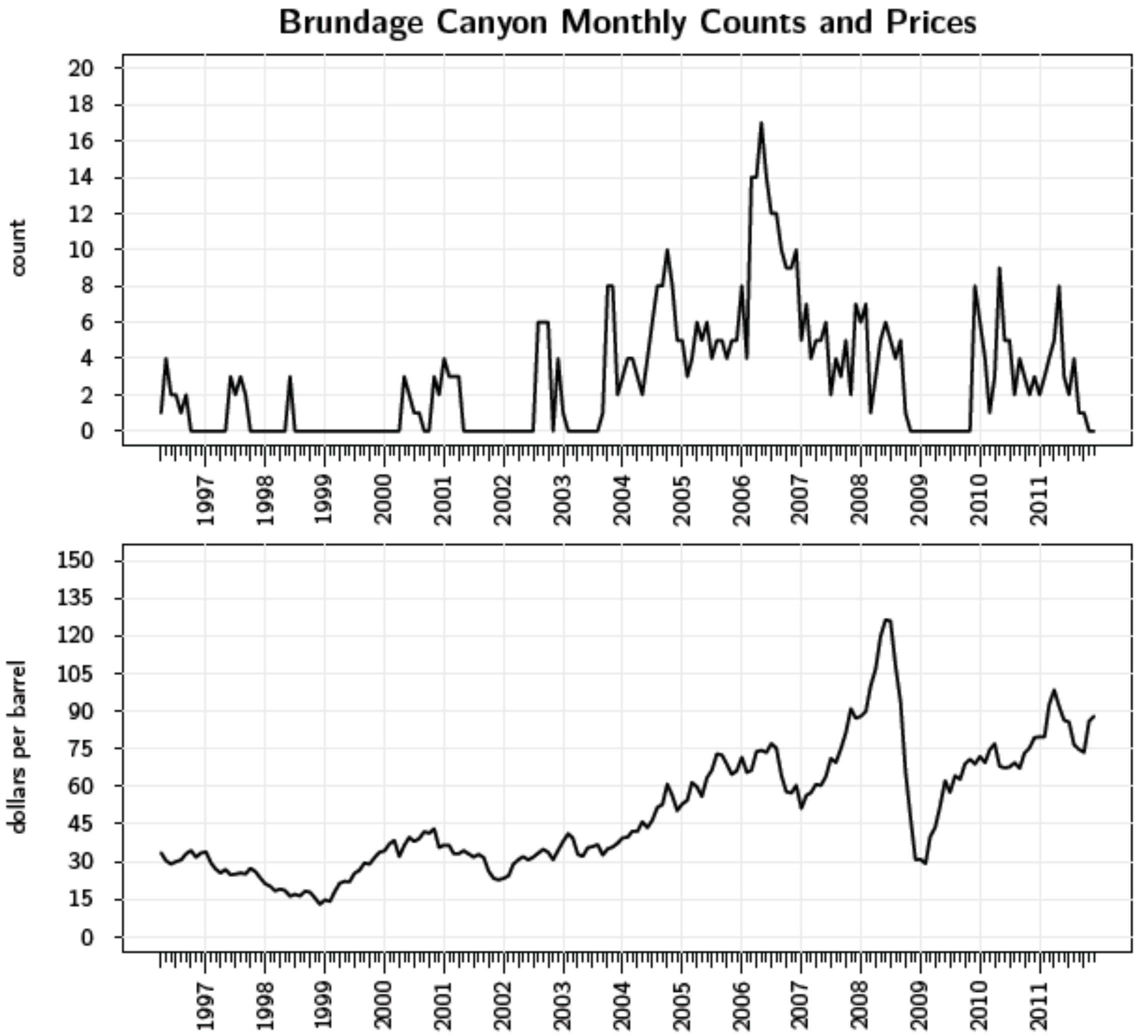

Figure 3. (top) Monthly well counts for Brundage Canyon oil fields. (bottom) Inflation-adjusted price of oil in 2012 US$.

The count data have been analyzed using Poisson regression. The model fit is mu_{t} = exp(x_{t} * beta), where x_{t} is a matrix whose first column is of ones, second column is of oil prices at time t, and third column is of prices in the month prior (t-1). The variable mu_{t} is the intensity parameter of a Poisson random variable. To make predictions from this model, one draws a vector hat(beta) from the posterior distribution of beta. Then the predicted count, hat(Y), is given by: hat(Y) = exp(x_{t} * hat(beta)}, where x_{t} is fixed at particular values (i.e. at given oil prices).

Decline Curves

Production curve estimates are included in this report as Appendix A. The observations Y_{it} are oil production from well i at time t. The simplest reasonable model of production is the exponential decline model: Y_{it} = alpha{i} + exp{delta{i} * t}. This is the model that is incorporated into the Matlab model described above.

Subtask 3.4 - V/UQ Analysis of Basin Scale $CLEAR_{uff}$ Assessment Tool (PI: Jennifer Spinti)

The work for this subtask has been performed jointly with that for Subtask 3.3 because of staffing issues. The focus this quarter has been on developing a model on which validation analysis can be performed.

Task 4.0 - Liquid Fuel Production by In-situ Thermal Processing of Oil Shale/Sands

Subtask 4.1 (Phase II) - Development of CFD-based Simulation Tools for In-situ Thermal Processing of Oil Shale/Sands (PI: Philip Smith)

In this quarter, the project team incorporated findings from past quarterly reports into one simulation. They implemented both a detailed property model and an operator splitting algorithm in simulations of thermal heating of oil shale inside Red Leaf's ECOSHALE capsule using a high performance computing (HPC)-based simulation tool.

Previously, they have described the implementation of directional, depth, and temperature-dependent properties into their HPC-based simulations in order to more accurately reflect a real modified in-situ oil shale process. They have also detailed the operator splitting algorithm that allows resolution of fluid flow inside the small cracks (small time scales) while simultaneously capturing the overall thermal effects (larger time scales). There needs to be a balance of computational cost such that the short, fluid time scales and the long, thermal time scales are both accurately captured in the simulation.

However, due to the complexity of the detailed-property implementation and the computational cost associated with the operator splitting algorithm (needed to resolve the short fluid time scales), the simulations did not progress as far as anticipated. Further tests were conducted with greater emphasis placed on the large, thermal scales. However, these simulations produced unrealistic results.

Because simulations this quarter were either too computationally intensive or produced unrealistic results, the plan in the next quarter is to achieve balance between the two and produce a simulation which more closely replicates the modified in-situ ECOSHALE process.

Subtask 4.2 - Reservoir Simulation of Reactive Transport Processes (PI: Milind Deo)

In preparation for writing the final report, thermal simulations using STARS have been performed by the Subtask 4.2 team. The Comsol modules, developed to incorporate heat and mass transfer with kinetics, have been tested with cores of different sizes and at various conditions. Using results from STARS and from the Comsol modules, the team will be able to compare experimental core pyrolysis results with models. Additionally, a new student, Hongtao Jia, started working on the Advanced Reactive Transport (ARTS) model.

Subtask 4.3 – Multiscale Thermal Processes (PI: Milind Deo, Eric Eddings)

During this quarter, the Subtask 4.3 team repaired the gas chromatograph/mass spectrometry (GC/MS) system and extracted data. They also completed tar analysis from demineralized kerogen samples GR-1.9, GR-2.9, and GR-3.9.

Tar/Char Analysis

Oil shale samples from the Green River Formation at different depths (corresponding to GR-1.9, GR-2.9 and GR-3.9 respectively) were pyrolyzed and separated into char, tar and light gas products. Tars taken at various temperatures in the pyrolysis process, corresponding to before, during and after the major decomposition of the kerogen, were then dissolved in methylene chloride and analyzed using a GC/MS system. The major components of the tar yield were identified using the MS data while the relative yield of each component were qualitatively determined using the GC data.

The power supply on the computer driving the GC/MS system for the pressurized thermogravimetric analyzer (TGA) failed this quarter. This is an old system donated by Chevron, making it difficult to obtain a replacement power supply. Fortunately, the new part was found and installed, a process that took two months. The repair permitted the project team to retrieve the GC/MS data from the computer.

The GC/MS analysis of tars from the three sets of demineralized kerogen (GR-1.9, GR-2.9, and GR-3.9) are displayed in Figures 4 through 6 showing the relative concentrations of the components of the tar samples at each temperature. Components are identified in Table 3 by the time of the observed peak. There was no noticeable difference in the types of compounds evolved from the samples taken from different depths. Pristane was observed early in the pyrolysis process in comparatively high amounts, while heavier compounds (docosane, tricosane, and tetracosane) were not observed until temperatures approached or exceeded 500°C. However, the major components of the tar at all temperatures were alkanes and alkenes between 10 and 20 carbons in length.

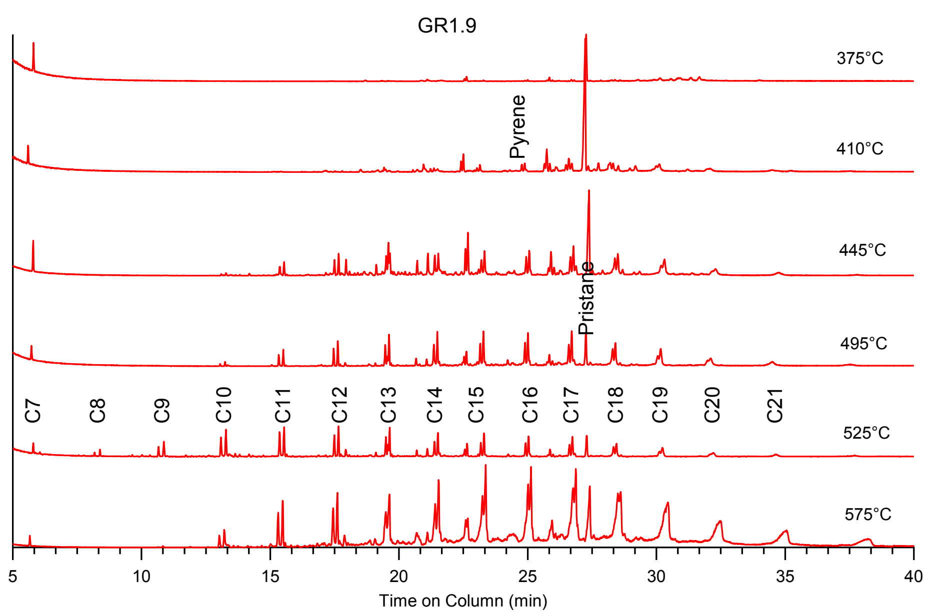

Figure 4. Gas chromatography spectra for tars collected in the kerogen retort at different temperatures from demineralized kerogen sample GR-1.9. Compounds are identified in Table 3.

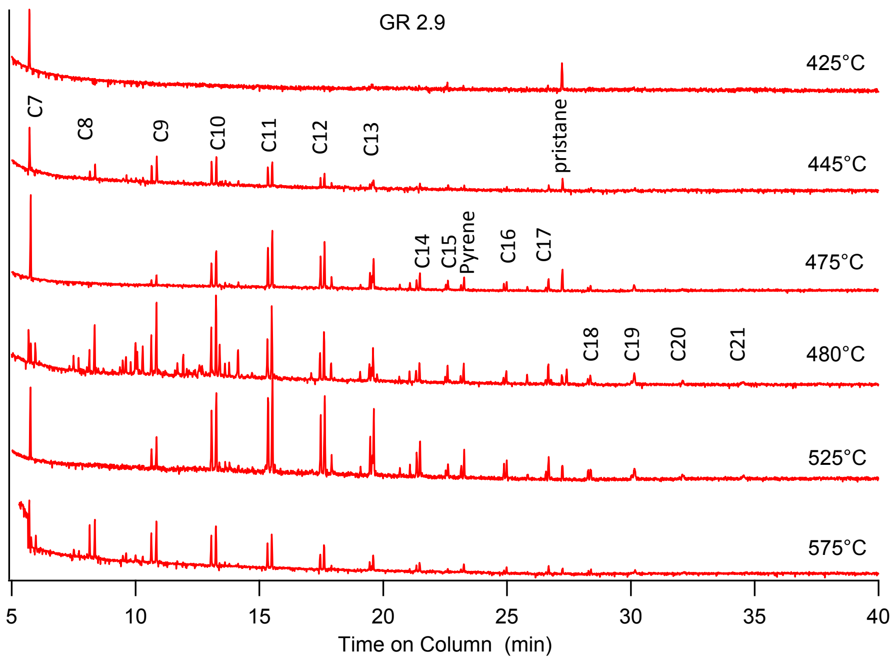

Figure 5. Gas chromatography spectra for tars collected in the kerogen retort at different temperatures from demineralized kerogen sample GR-2.9. Compounds are identified in Table 3.

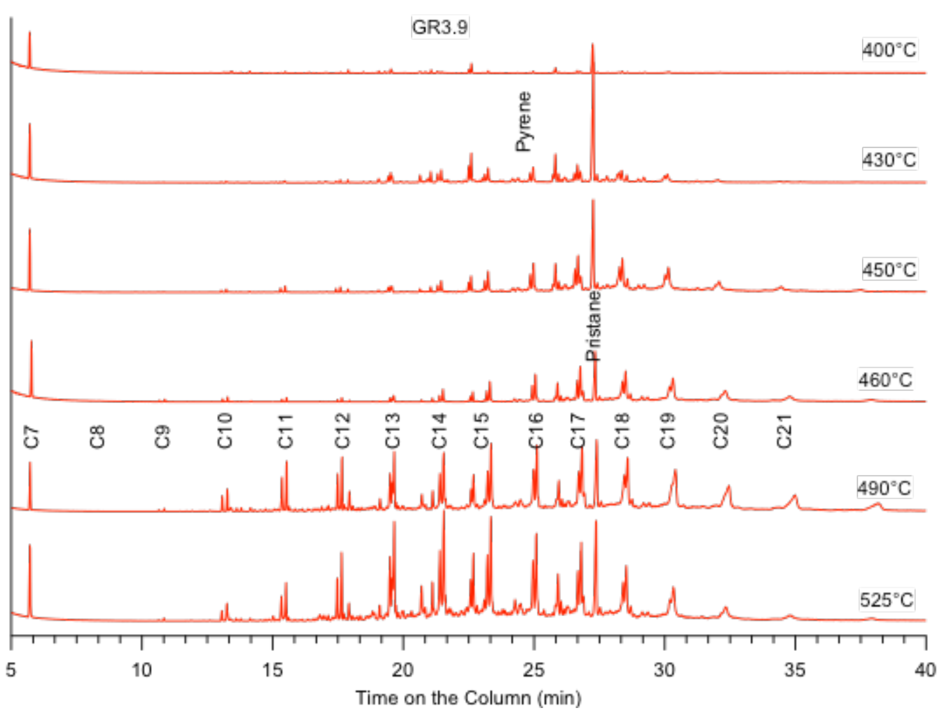

Figure 6. Gas chromatography spectra for tars collected in the kerogen retort at different temperatures from demineralized kerogen sample GR-3.9. Compounds are identified in Table 3.

Table 3. List of compounds detected in tars from kerogen pyrolysis using GC/MS, along with time of GC peak.

Time (min)	Compound	Time (min)	Compound
5.78	1-Heptene	21.7	Tetradecane
5.96	Heptane	22.84	2-Pentadecanone
8.21	1-Octene	23.4	1-Pentadecene
8.41	Octane	23.53	Pentadecane
10.7	1-Nonene	24.61	Pyrene
10.92	Nonane	25.19	1-Hexadecene
13.15	1-Decene	25.3	Hexadecane
13.35	Decane	26.12	2-Heptadecanone
15.47	1-Undecene	26.93	1-Heptadecene
15.63	Undecane	27.04	Heptadecane
17.6	1-Dodecene	27.58	Pristane
17.77	Dodecane	28.67	1-Octadecene
18.05	2-Tridecanol	28.79	Octadecane
19.22	Dodecanone	30.62	Nonadecane
19.65	1-Tridencene	32.64	Eicosane
19.72	2-Tridecanone	35.25	Heneicosane
19.79	Tridecane	38.39	Docosane
21.3	2-Tetradecanone	42.68	Tricosane
21.57	1-Tetradecene	48.4	Tetracosane

The project team has essentially completed the pyrolysis experiments along with the analysis of the gas and tar. They are assembling the data and analyses into the final report for this project. During the coming quarter, they will compare pyrolysis models developed by Professor Deo's group with CPD model predictions based on the measured chemical structure.

Subtask 4.4 - Effect of Oil Shale Processing on Water Compositions (PI: Milind Deo)

This project has been completed.

Subtask 4.5 - In Situ Pore Physics (PI: Jan Miller, Chen-Luh Lin)

The milestone to complete pore network structures and permeability calculations of Skyline 16 core (directional/anisotropic, mineral zones) for various pyrolysis temperatures and heating rates was completed during this quarter. The milestone originally included work at various loading conditions as well. However, samples are not available from Subtask 4.7, so the Subtask 4.5 team has chosen to modify the milestone and publish the work that has been completed. The final deliverable for the project, a topical report summarizing results of this work on the Skyline 16 core, has been replaced with a publication in *Fuel* entitled "Characterization of oil shale pore structure before and after pyrolysis by using X-ray micro CT." This publication will be submitted separately.

Subtask 4.6 - Atomistic Modeling of Oil Shale Kerogens and Oil Sand Asphaltenes (PI: Julio Facelli)

This project has been completed.

Subtask 4.7 - Geomechanical Reservoir State (PI: John McLennan)

In the last quarter, mechanical properties tests were carried out using White River oil shale samples. The experiments, unconfined compression at high temperature, were run in a structural loading frame in the Civil Engineering Department at University of Utah. One sample was tested at 400°F and another at 800°F. Equipment is being moved to another facility to carry out triaxial compression tests in the vessel that has been fabricated for that purpose. Thermal conductivity assessments were also carried out.

A new clamshell heater has been designed and fabricated for the purpose of measuring radial strain. The triaxial vessel is being fitted with feedthroughs for pressure, temperature and strain measurement. A condenser has also been designed and fabricated to collect the pyrolysis products. Apparatus debugging is now complete.

Triaxial testing will allow completion of the experimental matrix milestone by April 2013. Sunnyside and White River oil shale samples will be tested.

Subtask 4.8 - Developing a Predictive Geologic Model of the Green River Oil Shale, Uinta Basin (PI: Lauren Birgenheier)

There were two milestones due this quarter that were both met: (1) Detailed sedimentologic and stratigraphic analysis of three cores and, if time permits, a fourth core (Dec. 2012) and (2) detailed mineralogic & geochemical analysis of same cores.

With respect to the first milestone completion, Skyline 16 was described in summer 2011, Asphalt Wash 1 was described in January 2012, and SUB 12 and Red Wash 1 cores were described in this quarter, for a total of four cores. Asphalt Wash 1 was described by M. Rosenberg, an M.S. student currently supported by the project's cost share. Asphalt Wash 1 will constitute a portion of M. Rosenberg's thesis work. For the second milestone completion, X-ray fluorescence data that samples the full stratigraphic thickness of each core has been collected for all four cores. X-ray fluorescence data provides inorganic elemental abundances that is a proxy for mineralogy. As such, systematic stratigraphic changes in mineralogy can be identified quantitatively.

During this quarter, Lauren Birgenheier and Mike Vanden Berg described the SUB 12 (approximately 500 feet thick), and Red Wash 1 (approximately 800 feet thick) cores of the Green River Formation. Detailed sedimentary and stratigraphic description was performed and photos were taken. Additionally, X-ray Flourescence (XRF) data were collected at approximately 3-foot stratigraphic intervals through the thickness of the cores. Preliminary detailed measured sections have been drafted. XRF data have been calibrated and preliminary results have been graphed.

In the next quarter, drafted measured sections will be finalized and incorporated into the existing E-W cross section and the new N-S cross section. Geochemical data will also be synthesized.

Subtask 4.9 - Experimental Characterization of Oil Shales and Kerogens (PI: Julio Facelli)

A final deliverable, a paper on combined kerogen/bitumen structures and CPD reaction mode, remains to be completed for this project. During this quarter, researchers continued work on the paper. It will contain the details of the isolation of the kerogen and bitumen from the three segments of the Skyline 16 core and present the characterization work completed on the oil shale and kerogen, (solid state C-13 NMR, SAXS and PDF) and on the bitumen (solution H and C-13 NMR). The paper has been tentatively titled "Characterization of Shale, Kerogen and Bitumen from a Green River Oil Shale Core."

The research team will also be presenting a poster/paper at the 245th American Chemical Society National Meeting, New Orleans, April 7-11, 2013. A copy of the paper preprint is attached as Appendix B.

Task 5.0 - Environmental, Legal, Economic and Policy Framework

<u>Subtask 5.1 – Models for Addressing Cross-Jurisdictional Resource Management (PI: Robert Keiter, John Ruple)</u>

This project has been completed.

<u>Subtask 5.2 - Conjunctive Management of Surface and Groundwater Resources (PI: Robert Keiter, John Ruple)</u>

This project has been completed.

<u>Subtask 5.3 - Police and Economic Issues Associated with Using Simulation to Assess Environmental Impacts (PI: Robert Keiter, Kirsten Uchitel)</u>

Research efforts this quarter continued to focus on researching books, law review articles, and case law relevant to assessing the judicial and administrative framework for utilizing simulation science in the context of assessing environmental risks or harms. A brief summary report of that research is attached as Appendix C in satisfaction of the December 2012 milestone for this project, "White paper describing existing judicial and agency approaches for estimating error in simulation methodologies used in context of environmental risk assessment and impacts analysis".

6.0 – Economic and Policy Assessment of Domestic Unconventional Fuels Industry

<u>Subtask 6.1 Engineering Process Models for Economic Impact Analysis (PI: Terry Ring)</u>

Based on reviewer feedback, it was necessary to make some modifications to several of the process models. As a result, the milestone to upload all models used and data collected to the ICSE website was not completed.

The list of modifications that were performed includes:

- Adding the Paraho Direct retorting process to the ex situ oil shale scenario
- Extending the STARS simulation for in situ oil shale to run from 30 to 100 years and using the new production data to determine the overall energy balance of the process
- Creating new tables to show the operating/utility requirements for each scenario on a (unit) / bbl basis
- Updating cost indices (CEPCI, NFRCI, PPI, etc.) from end of 2011 to end of 2012 and generating new tables and figures for each scenario based on the updated numbers

- Replacing EIA 2011 price forecasts for oil, gas, and electricity with EIA 2012 forecasts

Subtask 6.2 - Policy analysis of the Canadian oil sands experience (PI: Kirsten Uchitel)

The final draft of the topical report for this subtask is being circulated amongst authors and researchers for final comments and edits. None of the four research assistants who worked on the project remain at ICSE, and as a result, securing their feedback has taken longer than expected. Despite the significant past delays associated with this report, it is now in the final stages of completion and will be ready for final submission to NETL shortly.

Subtask 6.3 – Market Assessment Report (PI: Jennifer Spinti)

Comments on the final draft report were received from reviewers in this quarter. Based on reviewer comments, additional work was required to prepare the report for final release. The changes described in Subtask 6.1 precipitated a cascade of changes to all the scenario sections and to the macroeconomic analysis. A subsection was also added to the end of each section that summarizes the economic analysis in the section and compares results with those from other published sources. The final report is being prepared for release on flash drives. It will also be available for download.

7.0 – Strategic Alliance Reserve

Based on feedback from a panel of scientists and representatives of American Shale Oil, LLC (AMSO), Genie Energy, and TOTAL that reviewed this project in September 2012, tasks and budgets have been realigned and reallocated to better meet the overall objectives of this industrial collaboration. Reflective of this redirection, Subtask 7.2 has been ended prior to the completion of its milestones and deliverables. The budget from this subtask has been reallocated to Subtasks 7.1 and 7.3. As a result of this budget shift, modified milestones and deliverables are presented in the respective subtask summaries below.

Subtask 7.1 – Geomechanical Model (PI: John McLennan)

New Focus

With the reallocation of funds from Subtask 7.2, the work program for this subtask has been accelerated. The program will be expanded to encompass basic reservoir simulations using commercial software to account for the thermal front propagation and the generation of permeability. The project team will also devote resources to further understanding the in-situ mechanics – generally and for AMSO's operations. Largely, this entails evaluation of the flow mechanics on a broader scale than was envisioned with the original task. These additional milestones have been added to the milestone table included with this report.

In the next quarter, the work program will be accelerated by involving another post-doctoral researcher to begin using commercial geomechanics software. Subsidence and compaction are being evaluated to meet the upcoming deliverable. This work is in response to the reallocation of funding. The effort will be to look at geomechanical and coupled production phenomena.

Report on Work from Last Quarter

Segmented linearization of the AMSO data was performed in this quarter, which partially fulfills the milestone to infer permeability-porosity-temperature relationships and to develop a model that can be used by other subtasks. The project team has digitized stress-strain data that AMSO collected from three vendors. They are characterizing discrete segments of these curves, represented by the loading regimes listed in Table 4, to infer how properties vary with temperature and confining pressure. Figure 7 shows synthetically generated curves of how the oil shale will deform under specific in-situ temperature and stress conditions.

Table 4. Regions for segmented linearization of AMSO data.

Segmented Linearization

Characteristic Loading Regimes:

1. Linear, nominally elastic may or may not be present
2. Yielding - Hyperbolic Linearization per Duncan and Chang
3. "Stabilized" region of strain hardening (usually)
4. Creep, Unload/Reload Segments
5. Unloading

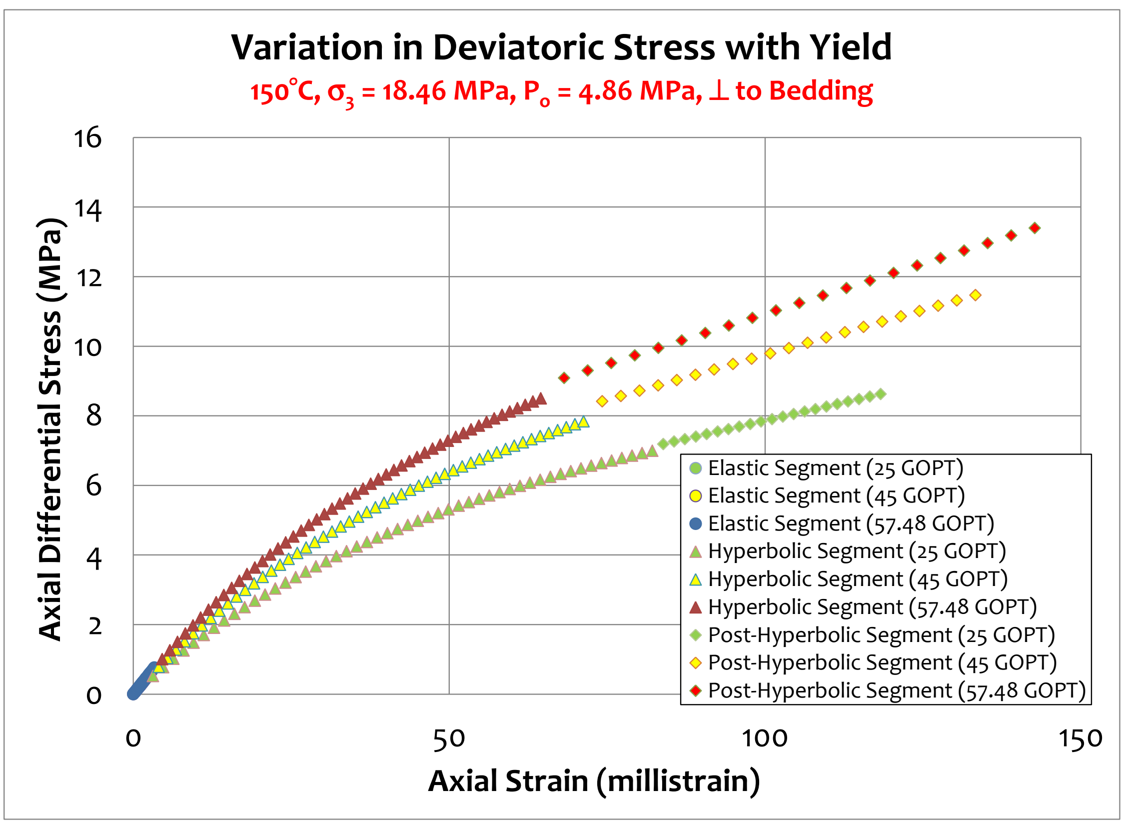

Figure 7. Variation in deviatoric stress with yield for various loading regimes.

Linearization and regression of four distinct regions from Table 4 (Region 5, “Unloading,” is considered unreliable) is guiding researchers to develop a regressed surface that tells how material deforms with temperature. As the deformation occurs, porosity develops, and this is quantified in the analyses to date. Once the temperature becomes high enough, pyrolysis occurs. The team will then assess porosity development due to phase conversion.

Testing in the large vessel is required to continue the development of these constitutive modeling surfaces. Hence, the milestone is only partially achieved up to now. As the research team develops the experimental database on the in-situ tests, they will be measuring deformation and porosity development due to stress conditions and pyrolysis. This step will allow them to develop the complete porosity curve; porosity develops because of converting solid kerogen and due to mechanical loading – they have data on the latter and are acquiring data on the former in the testing campaign from now through May 2013. Adding the permeability will also require the large scale testing that is currently in process. Initially there is no permeability. With deformation and phase conversion, the research team will determine if flowing nitrogen is able to remove the oil created, allowing the development of permeability. This segment of the analysis is contingent on the measurements through May with additional testing planned for June-July.

Subtask 7.2 – Kinetic Compositional Models and Thermal Reservoir Simulators (PI: Milind Deo)

Prior to the ending of this subtask, the team had studied the effect of geomechanics in thermal simulation using STARS. A complex kinetic model was incorporated and it was shown that geomechanics (subsidence and poroelastic changes) changes have significant impact on the results. Additionally, a thermal geomechanical model was incorporated into ARTS, a model developed at the University of Utah. This model was applied to a steam flooding example with a number of discrete fractures. The next task was to apply this tool to the AMSO problem. However, students working on these projects (Nan Zhao, Jake Bauman and Pankaj Tiwari) graduated and left the university. A post-doctoral fellow recruited to run these simulations also left for a job outside of the university, leading to the decision to terminate this project early and provide additional resources to Subtasks 7.1 and 7.3.

Subtask 7.3 – Rubblized Bed High Performance Computing Simulations (PI: Philip Smith)

New Focus

As stated in the Project Background for Task 7, this capstone project is intended to draw together the DOE funded oil shale research since 2006 to demonstrate computational simulation capability for the assessment and deployment of the shale oil production process commercialized by AMSO. In this integrated project, this simulation capability is coupled with experimental data from key small scale experiments conducted independently by AMSO in a formal validation process where the controlling uncertainties are accounted for and quantified. It is the project team’s thesis that the optimal risk assessment and decision-making regarding deployment of this new technology can most efficiently be accomplished by this formal simulation - validation and uncertainty quantification process. After having worked closely with AMSO personnel to accomplish this goal over the past year, team members have refocused the scope of the work to satisfy AMSO needs. This new focus is shown in the four task statements below, which have been incorporated into modified milestones for this task that have been incorporated into the milestone table included with this report. They have also learned that impacting the company and providing continuous timely research outcomes requires significantly more time commitment than originally anticipated. The reallocation of funds from Subtask 7.2 will be used to provide this manpower over the next year.

- Subtask 7.3.1 (completed milestone): Knowledge Collection - Collect AMSO background knowledge and data about the characteristics about the operation of the heated wells. This will include any known information about :
  - the geometry of the bed and its evolution over time as the formation is heated,
  - thermal properties of the shale,
  - operating conditions,
  - product yield models as a function of temperature,
  - physical and chemical characteristics of the shale.

- Subtask 7.3.2 (completed milestone): Generation 1 Simulation - Perform DEM, CFD and Thermal analysis of a characteristic section of the AMSO rubblized bed. This base case simulation will be built from the knowledge base acquired in Task 7.3.1 and the research accomplished under Task 7.1. It will then be extended to the heater test being conducted by AMSO on their site through the spring and summer of 2012. It will incorporate a simple thermal response model for the product yields (i.e. product yield as a function of shale temperature). The results of this task will be the first generation prediction of the production rates from the AMSO process. The resulting integration of these models that produces this base case simulation will become a product of this research and delivered to AMSO.

- Subtask 7.3.3 (deliverable): V/UQ of Generation 1 Simulator with AMSO Experimental Data - Experimental data collected from the AMSO heater test will be used in conjunction with the Generation 1 Simulator of Subtask 7.3.2 to produce a formal validation / uncertainty quantification (V/UQ) for the predictivity of the Generation 1 Simulator. This uncertainty quantification will include quantified uncertainties in the most important scenario parameters, model parameters, numerical parameters and experimental data. The intended use of the heater test and thus this V/UQ will be focused on the thermal analysis of the production zone. The V/UQ analysis will be delivered to AMSO and DOE and, after appropriate clearance for proprietary information, prepared for publication.

- Subtask 7.3.4 (milestone): Generation 2 Simulation - Incorporate the kinetic compositional models based on the publications of Allred (Marathon Oil), Campbell (Lawrence Livermore), Burnham (AMSO), Deo (UofU/ICSE), and Fletcher (BYU/ICSE). Also incorporate the geomechanics information from Subtask 7.1 as it becomes available. This becomes the Generation 2 Simulator. The geometry of the AMSO production zone will be input to this Generation 2 Simulation as opposed to being dynamically computed within the simulation. A demonstration simulation of this tool will be performed. The resulting simulation of the integrated models that produces this base case simulation will become the second generation product of this research and delivered to AMSO.

- Subtask 7.3.5 (deliverable): V/UQ of Generation 2 Simulator with AMSO Experimental Data - Ongoing experimental data collected from the AMSO tests will be used in conjunction with the Generation 2 Simulator of Subtask 7.3.4 to produce a formal V/UQ for the predictivity of the Generation 2 Simulator. This analysis will move beyond the V/UQ of Subtask 7.3.3 by building on the lessons learned from that task. The intended use of this simulation will be to provide product yield as well as thermal analysis for the operations of the ongoing RD&D tests at the AMSO facility. The resulting V/UQ analysis will be delivered to AMSO and DOE and, if cleared for release, made available to the public in the form of a scientific publication.

Report on Work from Last Quarter

In the past quarter, team members completed 15 simulations for their V/UQ studies of the January heater experiment test conducted by AMSO near Rifle, CO. They work closely with AMSO scientists, who guide the simulations to best answer questions that are relevant to them and their process. They continue to evolve their Generation I simulation tool and to include an increasing level of detail needed to accurately represent the AMSO in-situ oil shale process.

Before conducting the VUQ studies, the project team together with AMSO scientists identified the key quantity of interest for their January heater test - heating rate and its distribution inside the formation. This is the rate limiting step for an oil shale application. The V/UQ studies are therefore tailored to focus on this question. Team members selected thermal conductivity and the number of oil shale categories as two parameters which will vary over a specified range inside the Star-CCM+ simulations.

The computational domain for the simulations remained the same as described in the previous quarterly report. The simulations also incorporated all property variations based on depth, temperature and grade, also described in the last quarterly report.

Using this V/UQ matrix, the project team ran 15 Star-CCM+ simulations, producing 15 thermal response curves for each TM well for the January heater test. This ouput allowed team members to study the effect of the chosen parameters on the overall heat transfer distribution in the AMSO domain. A sample temperature distribution for one of the AMSO TM wells is shown in Figure 8.

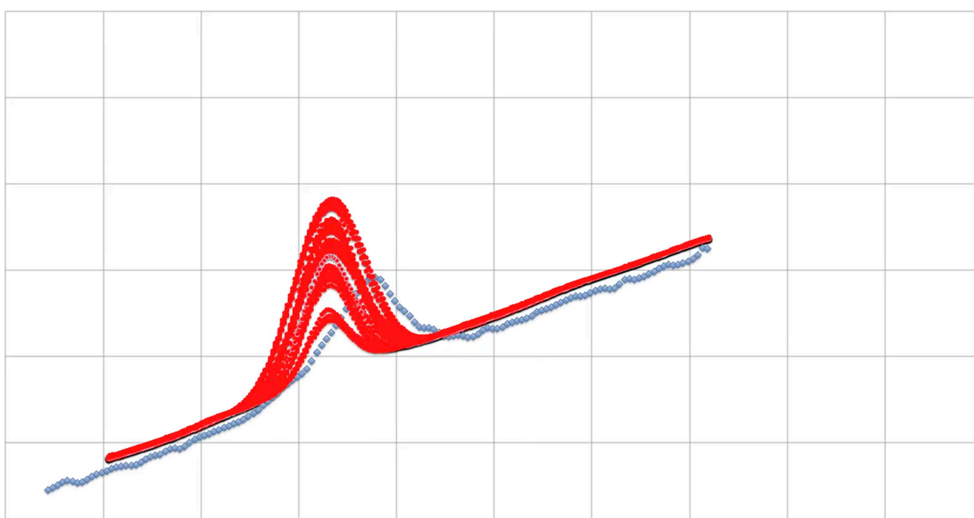

Figure 8. Comparison of temperature distribution for experimental results (blue markers) and 15 simulations (red markers) performed as a part of the V/UQ study in one of the tomography wells. Horizontal axis represents depth, while the vertical axis represents the temperature.

This methodology allows team members to study the effect of thermal conductivity and of groupings of oil shale (based on grade as a function of depth) on the overall heat distribution for the January heater test. Further, this methodology produces a range of possible temperature distributions for the AMSO heater test rather than a single temperature distribution. With this information, the most sensitive parameter for the overall heating rate can be determined.

However, based on feedback from AMSO scientists, the ranges for the sensitive parameters have been extended. Consequently, V/UQ studies for the Generation I simulator will not be completed until next quarter.

CONCLUSIONS

In this quarter, Subtask 4.5 was completed and summary papers/reports were drafted for Subtasks 4.9 and 6.3. The Market Assessment was released for final review and reviewer comments are being incorporated. Subtasks within Task 7 were adjusted due to the reallocation of funds from Subtask 7.2 to Subtasks 7.1 and 7.3. Additional milestones and deliverables associated with this reallocation are outlined in this report.

COST PLAN/STATUS

Baseline Reporting Quarter - PHASE I	Yr. 1								Yr. 2			
	Q1		Q2		Q3		Q4		Q5		Q6	
	7/1/09 - 12/31/09		1/1/10 - 3/31/10		4/1/10 - 6/30/10		7/1/10 - 9/30/10		10/1/10 - 12/31/10		1/1/11 - 3/31/11	
	Q1	**Total**	Q2	**Total**	Q3	**Total**	Q4	**Total**	Q5	**Total**	Q6	**Total**
Baseline Cost Plan												
Federal Share	484,728	**484,728**	484,728	**969,456**	484,728	**1,454,184**	484,726	**1,938,910**	323,403	**2,262,313**	798,328	**3,060,641**
Non-Federal Share	121,252	**121,252**	121,252	**242,504**	121,252	**363,756**	121,254	**485,010**	80,835	**565,845**	199,564	**765,409**
Total Planned	605,980	**605,980**	605,980	**1,211,960**	605,980	**1,817,940**	605,980	**2,423,920**	404,238	**2,828,158**	997,892	**3,826,050**
Actual Incurred Cost												
Federal Share	420,153	**420,153**	331,481	**751,634**	547,545	**1,299,179**	428,937	**1,728,116**	593,386	**2,321,502**	307,768	**2,629,270**
Non-Federal Share	29,456	**29,456**	131,875	**161,332**	151,972	**313,304**	100,629	**413,933**	191,601	**605,534**	45,101	**650,635**
Total Incurred Costs	449,609	**449,609**	463,356	**912,966**	699,517	**1,612,483**	529,566	**2,142,049**	784,987	**2,927,036**	352,869	**3,279,905**
Variance												
Federal Share	64,575	**64,575**	153,247	**217,822**	-62,817	**155,005**	55,789	**210,794**	-269,983	**-59,189**	490,560	**431,371**
Non-Federal Share	91,796	**91,796**	-10,623	**81,172**	-30,720	**50,452**	20,625	**71,077**	-110,766	**-39,689**	154,463	**114,774**
Total Variance	156,371	**156,371**	142,624	**298,994**	-93,537	**205,457**	76,414	**281,871**	-380,749	**-98,878**	645,023	**546,145**

Note: Q5 and Q6 reflect both CDP 2009 and CDP 2010 SF424a projections as the award periods overlap.

Baseline Reporting Quarter - PHASE II	Yr. 2				Yr. 3							
	Q7		Q8		Q9		Q10		Q11		Q12	
	04/01/11 - 06/30/11		07/01/11 - 09/30/11		10/01/11 - 12/31/11		01/1/12 - 03/31/12		04/01/12 - 06/30/12		07/01/12 - 09/30/12	
	Q7	**Total**	Q8	**Total**	Q9	**Total**	Q10	**Total**	Q11	**Total**	Q12	**Total**
Baseline Cost Plan												
Federal Share	712,385	**3,773,026**	627,423	**4,400,449**	147,451	**4,547,900**	147,451	**4,695,351**	147,451	**4,842,802**	245,447	**5,088,249**
Non-Federal Share	178,100	**943,509**	156,854	**1,100,363**	36,863	**1,137,226**	36,863	**1,174,089**	36,863	**1,210,952**	58,906	**1,269,858**
Total Planned	890,485	**4,716,535**	784,277	**5,500,812**	184,314	**5,685,126**	184,314	**5,869,440**	184,314	**6,053,754**	304,353	**6,358,107**
Actual Incurred Cost												
Federal Share	449,459	**3,078,729**	314,813	**3,393,542**	271,897	**3,665,439**	267,784	**3,933,223**	191,438	**4,124,661**	232,367	**4,357,028**
Non-Federal Share	48,902	**699,537**	48,835	**748,372**	105,695	**854,067**	40,652	**894,719**	33,092	**927,811**	44,294	**972,105**
Total Incurred Costs	498,361	**3,778,266**	363,648	**4,141,914**	377,592	**4,519,506**	308,436	**4,827,942**	224,530	**5,052,472**	276,661	**5,329,133**
Variance												
Federal Share	262,926	**694,297**	312,610	**1,006,907**	-124,446	**882,461**	-120,333	**762,128**	-43,987	**718,141**	13,080	**731,221**
Non-Federal Share	129,198	**243,972**	108,019	**351,991**	-68,832	**283,159**	-3,789	**279,370**	3,771	**283,141**	14,612	**297,753**
Total Variance	392,124	**938,269**	420,629	**1,358,898**	-193,278	**1,165,620**	-124,122	**1,041,498**	-40,216	**1,001,282**	27,692	**1,028,974**

Baseline Reporting Quarter - PHASE II	Yr. 4											
	Q13		Q14		Q15		Q16					
	10/01/12 - 12/31/12		01/01/13 - 03/31/13		04/01/13 - 06/30/13		07/01/13 - 09/30/13					
	Q13	**Total**	Q14	**Total**	Q15	**Total**	Q16	**Total**		**Total**		**Total**
Baseline Cost Plan												
Federal Share	146,824	**5,235,073**	146,824	**5,381,897**	146,824	**5,528,721**	133,794	**5,662,515**				
Non-Federal Share	36,705	**1,306,563**	36,705	**1,343,268**	36,705	**1,379,973**	35,906	**1,415,879**				
Total Planned	183,529	**6,541,636**	183,529	**6,725,165**	183,529	**6,908,694**	169,700	**7,078,394**				
Actual Incurred Cost												
Federal Share	128,349	**4,485,377**		**4,485,377**		**4,485,377**		**4,485,377**				
Non-Federal Share	79,871	**1,051,976**		**1,051,976**		**1,051,976**		**1,051,976**				
Total Incurred Costs	208,220	**5,537,353**		**5,537,353**		**5,537,353**		**5,537,353**				
Variance												
Federal Share	18,475	**749,696**		**896,520**		**1,043,344**		**1,177,138**				
Non-Federal Share	-43,166	**254,587**		**291,292**		**327,997**		**363,903**				
Total Variance	-24,691	**1,004,283**		**1,187,812**		**1,371,341**		**1,541,041**				

MILESTONE STATUS

ID	Title/Description	Planned Completion Date	Actual Completion Date	Milestone Status
1.0	Project Management			
2.0	Technology Transfer and Outreach			
	Advisory board meeting	Jun-13		
	Hold final project review meeting in format determined jointly by DOE/NETL and ICSE	Jun-13		
3.0	Clean Oil Shale & Oil Sands Utilization with CO2 Management			
3.1	Lifecycle greenhouse gas analysis of conventional oil & gas development in the Uinta Basin			
	Complete modules in $CLEAR_{uff}$ for life-cycle CO2 emissions from conventional oil & gas development in the Uinta Basin	Mar-13		
3.2	Flameless oxy-gas process heaters for efficient CO2 capture			
	Preliminary report detailing results of skeletal validation/uncertainty quantification analysis of oxy-gas combustion system	Sep-12	Oct-12	Report attached as appendix to Oct. 2012 quarterly report
3.3	Development of oil & gas production modules for $CLEAR_{uff}$			
	Develop preliminary modules in $CLEAR_{uff}$ for conventional oil & gas development & produced water management in Uinta Basin	Oct-11	Dec-11	Discussed in Jan. 2012 quarterly report
3.4	V/UQ analysis of basin scale $CLEAR_{uff}$ assessment tool			
	Develop a first generation methodology for doing V/UQ analysis	Oct-11	Nov-11	Discussed in Jan. 2012 quarterly report
	Demonstrate full functionality (integration of all modules) of V/UQ methodology for conventional oil & gas development in Uinta Basin	Mar-13		
4.0	Liquid Fuel Production by In-Situ Thermal Processing of Oil Shale/Sands			
4.1	Development of CFD-based simulation tool for in-situ thermal processing of oil shale/ sands			

ID	Title/Description	Planned Completion Date	Actual Completion Date	Milestone Status
	Expand modeling to include reaction chemistry & study product yield as a function of operating conditions	Feb-12	Mar-12	
4.2	Reservoir simulation of reactive transport processes			
	Incorporate kinetic & composition models into both commercial & new reactive transport models	Dec-11	Dec-11	Discussed in Oct. 2012 quarterly report
	Complete examination of pore-level change models & their impact on production processes in both commercial & new reactive transport models	Jun-12	Jun-12	Discussed in July 2012 quarterly report
4.3	Multiscale thermal processes			
	Complete thermogravimetric analyses experiments of oil shale utilizing fresh "standard" core	Sep-11	Sep-11	Discussed in Oct. 2011 quarterly report
	Complete core sample pyrolysis at various pressures & analyze product bulk properties & composition	Dec-11	Sep-12	Discussed in Oct. 2012 quarterly report
	Collection & chemical analysis of condensable pyrolysis products from demineralized kerogen	May-12	Sep-12	Discussed in Oct. 2012 quarterly report
	Complete model to account for heat & mass transfer effects in predicting product yields & compositions	Jun-12	Jun-12	Discussed in Oct. 2012 quarterly report
4.5	In situ pore physics			
	Complete pore network structures & permeability calculations of Skyline 16 core (directional/anisotropic, mineral zones) for various loading conditions, pyrolysis temperatures, & heating rates	Mar-12	Mar-12	Discussed in April 2012 quarterly report for 1 loading condition; samples never received from Subtask 4.7, so PI dropped loading condition as variable & considers task complete
4.6	Atomistic modeling of oil shale kerogens & oil sand asphaltenes			
	Complete web-based repository of 3D models of Uinta Basin kerogens, asphaltenes, & complete systems (organic & inorganic materials)	Dec-11	Dec-11	Discussed in Jan. 2012 quarterly report
4.7	Geomechanical reservoir state			
	Complete high-pressure, high-temperature vessel & ancillary flow system design & fabrication	Sep-11	Sep-11	Discussed in Oct. 2011 quarterly report
	Complete experimental matrix	Dec-12		PI stated that new completion date is April 2013

	Complete thermophysical & geomechanical property data analysis & validation	Mar-13		

ID	Title/Description	Planned Completion Date	Actual Completion Date	Milestone Status
4.8	Developing a predictive geologic model of the Green River oil shale, Uinta Basin			
	Detailed sedimentologic & stratigraphic analysis of three cores &, if time permits, a fourth core	Dec-12	Dec-12	Discussed in this quarterly report
	Detailed mineralogic & geochemical analysis of same cores	Dec-12	Dec-12	Discussed in this quarterly report
4.9	Experimental characterization of oil shales & kerogens			
	Characterization of bitumen and kerogen samples from standard core	Jan-12	Feb-12	Email sent to R. Vagnetti
	Development of a structural model of kerogen & bitumen	Jun-12	Jun-12	Discussed in July 2012 quarterly report
5.0	Environmental, legal, economic, & policy framework			
5.1	Models for addressing cross-jurisdictional resource management			
	Identify case studies for assessment of multi-jurisdictional resource management models & evaluation of utility of models in context of oil shale & sands development	Jun-11	Jul-11	Discussed in Oct. 2011 quarterly report
5.2	Conjunctive management of surface & groundwater resources			
	Complete research on conjunctive surface water & groundwater management in Utah, gaps in its regulation, & lessons that can be learned from existing conjunctive water management programs in other states	Aug-11	Aug-11	Discussed in Oct. 2011 quarterly report
5.3	Policy & economic issues associated with using simulation to assess environmental impacts			
	White paper describing existing judicial & agency approaches for estimating error in simulation methodologies used in context of environmental risk assessment and impacts analysis	Dec-12	Dec-12	Attached as appendix to this quarterly report
6.0	Economic & policy assessment of domestic unconventional fuels industry			
6.1	Engineering process models for economic impact analysis			
	Upload all models used & data collected to repository	Oct-12		Models had to be updated based on second round or reviews

ID	Title/Description	Planned Completion Date	Actual Completion Date	Milestone Status
7.0	Strategic Alliance Reserve			
	Conduct initial screening of proposed Strategic Alliance applications	Mar-11	Mar-11	
	Complete review and selection of Strategic Alliance applications	Jun-11	Jul-11	Discussed in Oct. 2011 quarterly report
	Implement new Strategic Alliance research tasks	Sep-11	Sep-11	Discussed in Oct. 2011 quarterly report
7.1	Geomechanical model			
	Infer permeability-porosity-temperature relationships, develop model that can be used by other subtasks	Dec-12		Partially completed as described in this report. Addn'l work will be completed in July 2013
	Make experimental recommendations	Aug-13		
	Basic reservoir simulations to account for thermal front propagation	Dec-13		
	Evaluation of flow mechanics	Dec-13		
7.2	Kinetic compositional models & thermal reservoir simulators			Project has been terminated
	Incorporate chemical kinetics into thermal reservoir simulators	Jun-12	Jun-12	Discussed in July 2012 quarterly report
	Demonstrate reservoir simulation of AMSO process	Sep-12		
	Incorporate poroelastic & geomechanical models into reservoir simulator	Jun-13		
7.3	Rubblized bed HPC simulations			
	Collect background knowledge from AMSO about characteristics & operation of heated wells	Jun-12	Jun-12	Discussed in July 2102 quarterly report
	Perform generation 1 simulation - DEM, CFD & thermal analysis of characteristic section of AMSO rubblized bed	Sep-12	Sep-12	Discussed in Oct. 2012 quarterly report
	Perform generation 2 simulation that incorporates kinetic compositional models from subtask 7.2 and/or AMSO	Jun-13		

NOTEWORTHY ACCOMPLISHMENTS

The Subtask 4.7 team completed measurements of stress and strain at 800°F.

PROBLEMS OR DELAYS

Responding to reviews received of the Market Assessment (Subtask 6.3) required additional modeling work in Subtask 6.1. That work included the analysis of a second oil shale retort for the ex situ oil shale scenario and performing a simulation out to 100 years for the in situ oil shale scenario. This unforeseen work will delay the completion of the Subtasks 3.1 (Phase I), Subtask 6.1, and Subtask 6.3 until June 2013. In Subtask 4.3, the computer that crashed in the previous quarter was repaired and the needed data was retrieved. Some of that data is presented in this report. Researchers in Subtask 4.5 have never received samples for testing from Subtask 4.7. Hence, rather than further delay the completion of their project, they opted to removed the variable of loading condition from their experimental matrix. A paper summarizing their work was recently published in *Fuel*. In Subtask 4.7, the experimental program at high temperatures has been challenging. The project team is currently debugging the radial strain measurement system. Fortunately, the axial strain measurement system is working well. The separator/condensation system is also being debugged. Completion of the milestone for Subtask 7.2 to infer permeability-porosity-temperature relationships and to develop a model that can be used by other subtasks has been delayed by the need to acquire data in a testing campaign that will be completed in May 2013 if all goes well.

RECENT AND UPCOMING PRESENTATIONS/PUBLICATIONS

Wilkey, J. (2011, December). Evaluation of the economic feasibility of heavy oil production processes for West Sak Field. MS Thesis, University of Utah, Salt Lake City, UT.

R. Keiter, J. Ruple, H. Tanana and R. Holt. (2012, January). Conjunctive surface and groundwater management in Utah: Implications for oil shale and oil sands development. Submitted to the Department of Energy under DOE Award No. DE-FE0001243.

Tiwari, P. & Deo, M. (2012, February). Detailed kinetic analysis of oil shale pyrolysis TGA data. *AICHE Journal*, *58(2*), 505-515.

Spinti, J. (2012, February 15). Presenter/panelist - *Oil sands: How Utah can improve on the Alberta model.* Utah Governor's Energy Development Summit, Salt Lake City, UT.

Deo, M. (2012, February 15). Presenter/panelist - *Oil sands: How Utah can improve on the Alberta model.* Utah Governor's Energy Development Summit, Salt Lake City, UT.

Tiwari, P. & Deo, M. (2012, April). Compositional and kinetic analysis of oil shale pyrolysis using TGA-MS. *Fuel*, *94*, 333-341.

Rosenberg, M., Birgenheier, L. & Vanden Berg, M. (2012, April) Outcrop examination and sequence stratigraphy of the lacustrine Green River Formation, Uinta Basin, Utah: Implications for conventional and unconventional oil and gas development. Poster presented at the annual meeting of the American Association of Petroleum Geologists Annual Convention, Long Beach, CA, April 22-25, 2012.

Eby, D., Chidsey, T., Vanden Berg, M. & Laine, M. (2012, April). Microbial carbonates from core and outcrop, Tertiary (Eocene) Green River Formation, Uinta Basin, Utah. Paper presented at the American Association of Petroleum Geologists Annual Convention, Long Beach, CA, April 22-25, 2012.

Badu, S., Pimienta, I. S. O., Orendt, A. M. Facelli, J. C. & Pugmire, R. J. (2012). Modeling of asphaltenes: Assessment of sensitivity of ^{13}C SSNMR to molecular structure. Submitted to *Energy & Fuels, 26(4),* 2161-2167.

Fletcher, T. H., Orendt, A. M., Facelli, J. C., Solum, M. S., Mayne, C. L. & Deo, M. (2012, May 15). Kinetics of Uinta Basin oil shale pyrolysis. Presentation at the 2012 University of Utah Unconventional Fuels Conference, Salt Lake City, UT.

Ruple, J. (2012, May 15). Wilderness quality lands and unconventional fuel development. Presentation at the 2012 University of Utah Unconventional Fuels Conference, Salt Lake City, UT.

Tiwari, P. (2012). Oil shale Pyrolysis: Benchscale experimental studies and modeling. Ph.D. dissertation, Department of Chemical Engineering, University of Utah.

Lin, C. L., Miller, Hsieh, C. H., Tiwari, P. & Deo, M. D. (2012, May). Characterization of core pore structure before and after pyrolysis using X-ray micro CT. Paper submitted to *Fuel*.

Tiwari, P., Deo, M., Lin C. L. & Miller, J.D. (2012, October). Characterization of the oil shale core pore structure before and after pyrolysis. Paper accepted for presentation at the 2012 AICHE Annual Meeting in Pittsburgh, PA, October 28-November 2, 2012.

Vanden Berg, M. D., Birgenheier, L. P. & Rosenberg M. J. (2012, September). Core-based sedimentologic, stratigraphic, and geochemical analysis of the lacustrine upper Green River Formation, Uinta Basin, Utah: Implications for conventional and unconventional petroleum development. Poster presented at the 2012 American Association of Petroleum Geologists - Rocky Mountain Section Meeting in Grand Junction, CO.

Rosenberg, M.J., Birgenheier, L.P, & Vanden Berg, M.D. (2012, October). Sedimentology and sequence stratigraphy of the Green River Formation, eastern Uinta Basin, Utah. Paper presented at the 32nd Oil Shale Symposium, Golden, CO.

Burnham, A., Day, R., Switzer, L., McConaghy, J., Hradisky, M., Coates, D., Smith, P., Foulkes, J., La Brecque, D., Allix, P., Wallman, H. (2012, October). Initial results of the AMSO RD&D pilot test program. Paper to be presented at the 32nd Oil Shale Symposium in Golden, CO.

Pimienta, I. S. O., Orendt, A. M., Pugmire, R. J., Facelli, J. C., Locke, D. R., Winans, R. E., Chapman, K. W. & Chupas, P. J. (2012, October). Three-dimensional structure of the Siskin Green River oil shale kerogen model: A comparison between calculated and observed properties. Submitted to *Energy and Fuels*.

Deo, M. (2012, October). *Oil shale liquefaction: Modeling and reservoir simulation*. Short course presentation to Statoil, Trondheim, Norway.

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APPENDIX A. Production curve estimates (see attached).

APPENDIX B. Paper entitled "Characterization of shale and kerogen from a Green River oil shale core."

APPENDIX C. Memorandum for Subtask 5.3.

Production Curve Estimates

Michael Hogue

August 16, 2012

1. Production Curves

In this document $q(t)$ be the *rate of production* at time t (e.g. barrels of oil per month in the $t = 10$th month of production).

Production curve analysis in the petroleum engineering literature has focused mostly on the following three types of production (or "decline") curves. Two of these, the exponential and harmonic curves, are limiting cases of the hyperbolic curve. The parameters of the curves are estimated from production data.

1.1. Exponential

$$q(t) = q_0 e^{-\delta t} \tag{1}$$

1.2. Hyperbolic

$$q(t) = q_0 \left(1 + \theta\delta t\right)^{-1/\theta} \tag{2}$$

1.3. Harmonic

$$q(t) = \frac{q_0}{1 + \delta t} \tag{3}$$

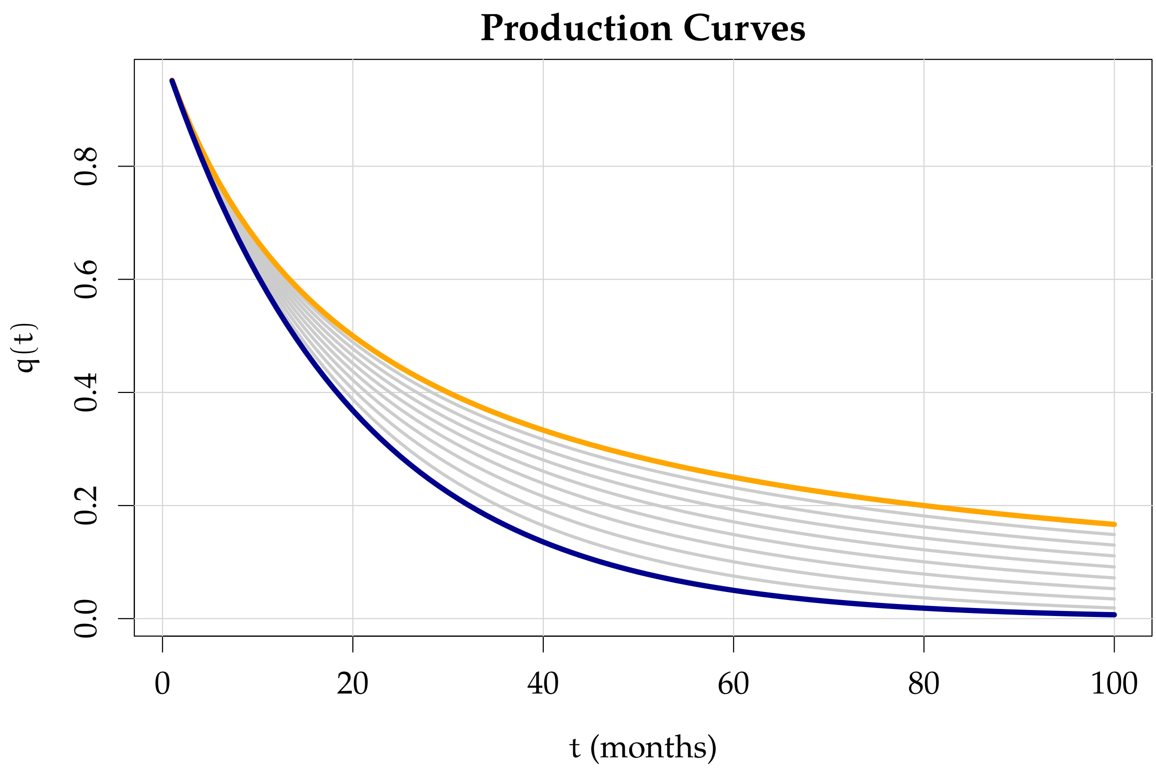

Figure 1: Gray curves represent various hyperbolic production curves, blue and orange curves the limiting cases of exponential and harmonic decline.

2. Fitting the Production Curves to Production Data

The following seven fields contain about 80 percent of the non-horizontal (i.e. vertical or slanted) oil wells drilled in the Uinta Basin since 1993.

Field Name	Field Name	OW Count
105	Monument Butte	1146
117	South Myton Bench	128
55	Altamont	92
590	8 Mile Flat North	250
60	Antelope Creek	97
718	Windy Ridge	94
72	Brundage Canyon	533

Table 1: Uinta Basin OW drilled between January 1993 and January 2012, by field.

$$\hat{q}(t) = \hat{q}_0 \left(1 + \hat{\theta}\hat{\delta}t\right)^{-1/\hat{\theta}]} \tag{4}$$

$$= 860 \times \left(1 + 1.8 \times 0.6 \times t\right)^{-1/1.8} \tag{5}$$

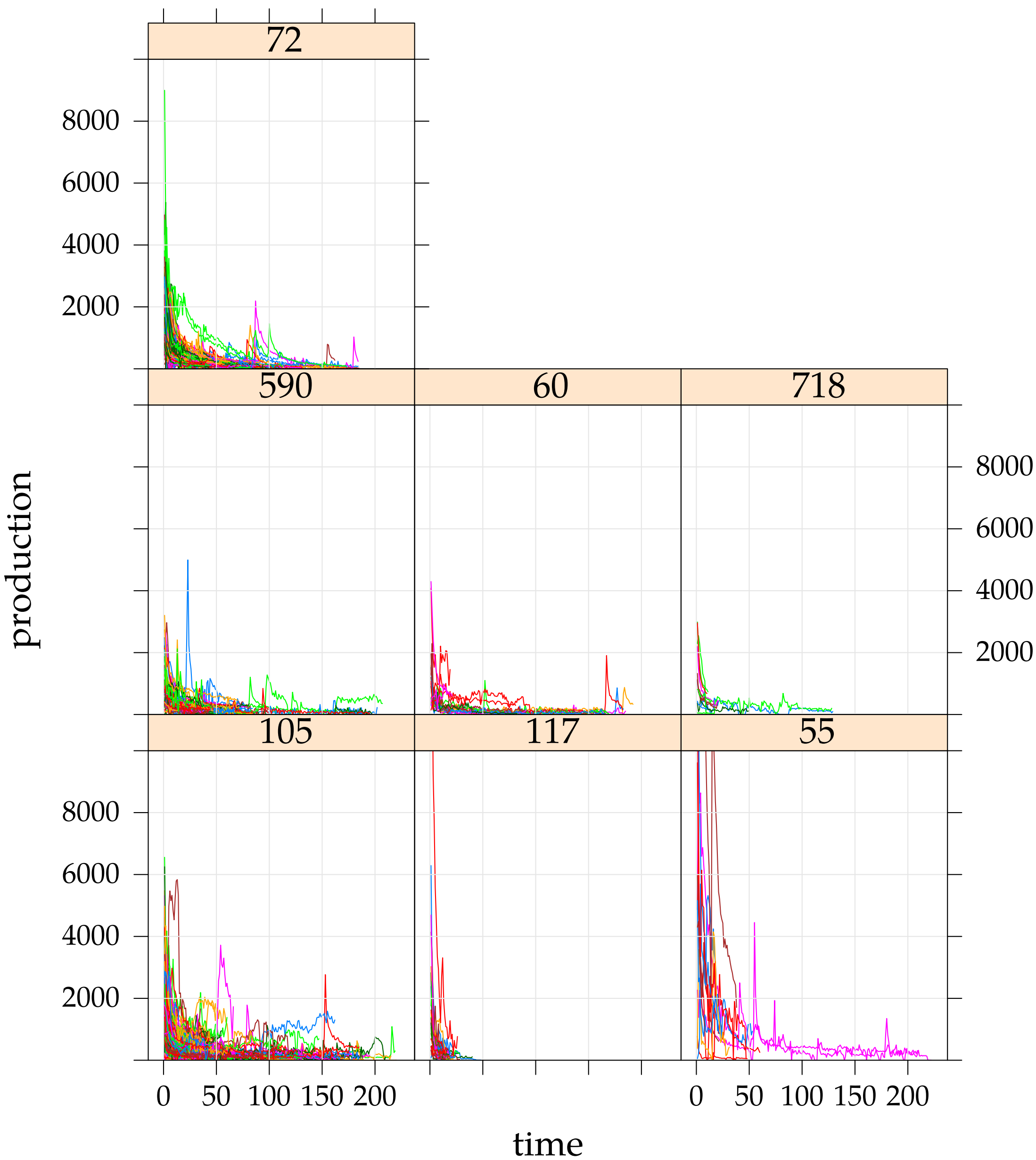

Figure 2: Production curves by field (see Table 2 for field names).

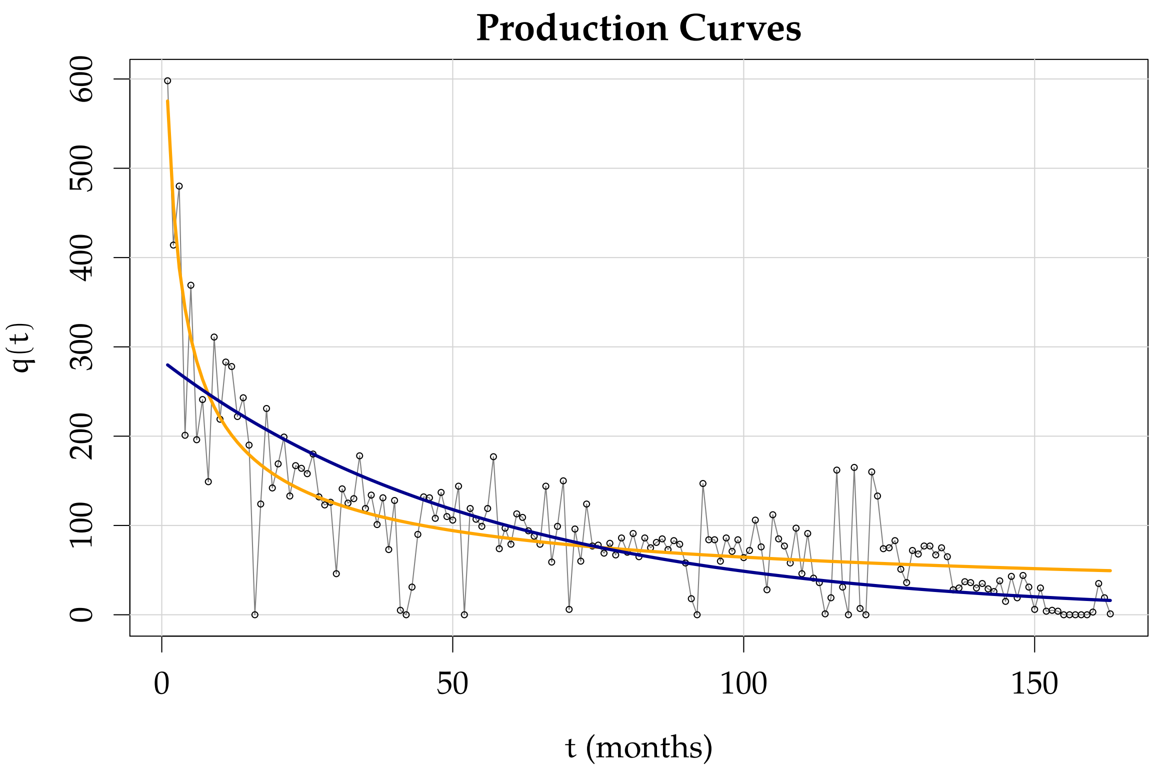

Figure 3: Exponential and hyperbolic curves fit to one well's production data. See equation 4 for the estimated hyperbolic.

Characterization of Shale and Kerogen from a Green River Oil Shale Core

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Introduction

A number of analyses, including solid state ^{13}C NMR, small angle X-ray scattering (SAXS), and atomic pairwise distribution function (PDF) measurements, have been completed on shale and kerogen samples from three sections of a well-defined, well-controlled, fresh oil shale core taken from the Green River Formation in the Uinta Basin in order to characterize the chemical nature of both the shale and the kerogen isolated from the shale. The geological nature of these three shale samples was also studied by other techniques such as scanning electron microscopy (SEM) and X-ray fluorescence (XRF). Each of the experimental techniques provides distinct information as to the composition and/or structure of the sample. The data obtained is analyzed to study the variation and similarities in both the shale and the organic matter between the segments.

Experimental

The Utah Geological Survey (UGS) and the University of Utah Institute for Clean and Secure Energy (ICSE) as part of its Oil Shale Program drilled a 1000 foot core (4 inch diameter) at the Uinta Skyline 16 location during Spring 2010. Three one-foot segments of this core were chosen to be studied; these segments are designated as GR1 (Mahogany zone rich), GR2 (Mahogany zone lean) and GR3 (Upper R6). Portions of these segments were powdered and sieved to 100 mesh for the analyses completed. The kerogen in these samples was isolated by a process adapted from that of reported by Vandergrift *et al*.[1]

The solid state NMR were obtained on a Varian Direct Drive oversampled spectrometer operating at a carbon frequency of 25.1562 MHz with a Chemagnetics 7.5 mm PENCIL rotor with a spinning speed of 4100 Hz. Experiments performed included a proton saturation recovery T1 experiment, variable contact time (VCT), dipolar dephasing (DD), a very good signal to noise CPMAS spectrum with a contact time of 3 ms for sub-integrals and a single pulse (SP) experiment for comparison with CP based experiments. The structural analysis developed in the Grant/Pugmire laboratory was completed.[2]

Measurements of the PDFs were completed on instrument 11-ID-B at the Advanced Photon Source (APS), Argonne National Laboratory. Samples were in kapton capillaries. High-energy X-rays (60 KeV, λ=0.2128Å) were used with a Perkin Elmer amorphous silicon based detector.[3] The 2D diffraction images were processed in Fit2D[4] software to perform x-ray polarization correction and radial integration for peak intensity. Extraction of the experimental pair distribution function from these data was made with PDFgetX2.[5]

The SAXS of these same samples in 1.0 mm OD glass capillaries were recorded on the 12-ID-B beamline at the Advanced Photon Source (APS), Argonne National Laboratory equipped with a Pilatus 2M detector. The data was analyzed using the IRENA software package.[6]

Acknowledgments: This work is supported by a grant from the U.S. Department of Energy, National Energy Technology Laboratory under DOE Award Number DE-FE0001243. Use of the Advanced Photon Source was supported by the U. S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract DE-AC02-06CH11357.

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Memorandum

To: Kirsten Uchitel
From: Heather Tanana
Re: Simulation Project

You asked me to perform preliminary research on the use of models and simulations from the judicial and administrative perspectives. A model is a tool "used to simulate some aspect of the real world."[1] Models and simulations have become increasingly common in environmental decision-making.

> Policymakers often must predict outcomes of complicated processes, and making those predictions would be all but impossible without models. Complex environmental systems often involve more variables, data, and interdependent feedback processes than people reasonably can organize in their minds, and interactions within these systems may create counterintuitive, nonlinear responses that are impossible to understand without models. Models can organize, manipulate, and process vast quantities of data and can simulate complex multivariable processes, and these capacities allow them to predict the future, compare alternative possible futures, test the ramifications of assumptions, and contribute to improved understanding of system interactions. These powers are invaluable in planning efforts.[2]

Many agency regulations depend on models to make science-based decisions, however, the agencies are encouraged to be forthcoming about their models' assumptions and limitations.[3] As a result, the EPA has set forth policy to guide model usage.[4] However, despite such guidelines, courts may be called upon to determine whether use of models and simulations were appropriate,

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[1] Robert L. Glicksman, *Bridging Data Gaps Through modeling and Evaluation of Surrogates: Use of the Best Available Science to Protect Biological Diversity Under the National Forest Management Act* 13 (2008) (quoting James D. Fine & Dave Owen, *Technocracy and Democracy: Conflicts Between Models and Participation in Environmental Law and Planning*, 56 Hastings L.J. 901, 903 (2005)).

[2] James D. Fine & Dave Owen, *Technocracy and Democracy: Conflicts Between Models and Participation in Environmental Law and Planning*, 56 Hastings L.J. 901, 912-13 (2005).

[3] Wendy Wagner, Elizabeth Fisher, & Pasky Pascual, Misunderstanding Models in Environmental and Public Health Regulation, 18 N.Y.U. Envtl. L.J. 293, 305-06 (2010).

[4] Susan R. Poulter, Environmental Risk Assessment – Science, Policy, and Legal Issues, 9 Risk: Health, Safety & Environment 7, 18 (Winter 1998); John W. Hayse, Using Monte Carlo Analysis in Ecological Risk Assessments 10 (Oct. 2000) (noting that EPA supports the use of probabilistic analysis techniques); Wendy Wagner, Elizabeth Fisher, & Pasky Pascual, Misunderstanding Models in Environmental and Public Health Regulation, 18 N.Y.U. Envtl. L.J. 293, 304 (2010) (discussing the EPA's Council for Regulatory Environmental Modeling, which provides oversight for models).

required, or properly done in particular cases.[5]

Model admissibility is subject to the following legal tests: *Frye*, *Daubert*, and Federal Rules of Evidence 702, or its state equivalent. The *Frye* test focuses on "general acceptance in the relevant scientific community."[6] "The *Daubert* factors expand upon the *Frye* test to include, among other things, whether the techniques have a known error rate, are subject to standards governing their application and enjoy widespread acceptance."[7] Additionally, under *Daubert v. Merrill Dow Pharms.*, the trial court must act as a gatekeeper to keep out speculative and unreliable opinions by performing "a preliminary assessment of whether the reasoning or methodology underlying the testimony is scientifically valid and of whether that reasoning or methodology properly can be applied to the facts in issue."[8] The Federal Rule of Evidence 702 states:

> If scientific, technical, or other specialized knowledge will assist the trier of fact to understand the evidence or to determine a fact in issue, a witness qualified as an expert by knowledge, skill, experience, training, or education, may testify thereto in the form of an opinion or otherwise, if (1) the testimony is based upon sufficient facts or data, (2) the testimony is the product of reliable principles and methods, and (3) the witness has applied the principles and methods reliably to the facts of the case.

Generally speaking, a strong presumption of validity exists in regards to agency regulations relating to technical subjects, including modeling.[9] Judges often "lack the competence to evaluate modeling evidence satisfactorily. The limited scientific expertise, training, and education of judges make it difficult to determine an appropriate level of review at the evidentiary screening state… [and] drawing a line between good and bad models is often not an easy task, even for those with the relevant scientific expertise operating outside the adversarial context of litigation."[10] Many courts also "perpetuate the pervasive misunderstanding and assume that since the model is mathematical, it is correct. As a result,

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[5] *See* Robert L. Glicksman, Bridging Data Gaps through Modeling and Evaluation of Surrogates: Use of the Best Available Science to Protect Biological Diversity under the National Forest Management Act 18 (2008) (discussing procedural requirements for model use, such as notice and comment).
[6] The National Judicial College, Hydrologic Modeling Benchbook: Dividing the Waters 52 (2010).
[7] *Id.* *See also* Matthew W. Swinehart, Remedying Daubert's Inadequacy in Evaluating the Admissibility of Scientific Models Used in Environmental-Tort Litigation, 86 Tex. L.Rev. 1281, 1301-11 (2008) (discussing the *Daubert* criteria).
[8] 509 U.S. 579, 593-94 (1993).
[9] *Lourdes Med. Ctr. of Burlington Country v. Bd. of Review,* 197 N.J. 339, 376 (2009).
[10] Matthew W. Swinehart, Remedying Daubert's Inadequacy in Evaluating the Admissibility of Scientific Models Used in Environmental-Tort Litigation, 86 Tex. L.Rev. 1281, 1299 (2008).

they pass the model through the system without much, if any, scrutiny…even in cases when there are reasons to suspect that the model may have significant problems."[11]

However, there is judicial precedent for rejecting models based on assumptions not supported by, or at odds with, ascertainable facts.[12] Courts have invalidated agency decisions that relied on modeling or simulation exercises where "they have found that a particular model was ill-suited to the activities to which it was applied or that the agency was unable to justify building the model on apparently arbitrary assumptions."[13] Challengers have also been successful when EPA declined to explain its decision or revise a supporting model after receiving comments attacking the model's methodology, as well as situations when the model was not applicable to a particular subset of industries, activities, or locations.[14] "Finally, if challengers disagree with embedded policy judgments, such as the risk adversity of assumptions built into a risk assessment, courts will sometimes invalidate a model and not defer to the agency."[15]

The enclosed literature review includes articles and case law that seeks to answer the following questions:[16]

- How do courts approach simulations of varying depth or quality?
- What are the relevant guidelines?
- Where are simulations and models acceptable and where are they not?

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[11] Wendy Wagner, Elizabeth Fisher, & Pasky Pascual, Misunderstanding Models in Environmental and Public Health Regulation, 18 N.Y.U. Envtl. L.J. 293, 320 (2010). *See Sierra Club v. U.S. Forest Serv.*, 878 F. Supp. 1295, 1310 (D.S.D. 1993) ("As long as an agency reveals the data and assumptions upon which a computer model is based, allows and considers public comment on the use or results of the model, and ensures that the ultimate decision rests with the agency, not the computer model, then the agency use of a computer model to assist in decision making is not arbitrary and capricious."

[12] *Leather Indus. Am., Inc. v. EPA*, 40 F.3d 392 (1994)).

[13] Robert L. Glicksman, Bridging Data Gaps through Modeling and Evaluation of Surrogates: Use of the Best Available Science to Protect Biological Diversity under the National Forest Management Act 20-21 (2008). *See Ctr. for Biological Diversity v. BLM*, 422 F. Supp. 2d 1115 (N.D. Cal. 2006) (reversing the FWS' reliance on modeling or simululation techniques on these grounds).

[14] National Research Council of the National Academies, Models in Environmental Regulatory Decision Making 77 (2007). *See State of Ohio v. EPA*, 784 F.2d 224 (6th Cir. 1986).

[15] National Research Council of the National Academies, Models in Environmental Regulatory Decision Making 77 (2007). *See State of Ohio v. EPA*, 784 F.2d 224 (6th Cir. 1986). *See Gulf South Insulation v. Consumer Product Safety Commission*, 701 F.2d 1137 (5th Cir. 1983).

[16] Relevant, but not yet reviewed, sources are noted at the very end.

Literature Review

Articles

1. Susan R. Poulter, Environmental Risk Assessment – Science, Policy, and Legal Issues, 9 Risk: Health, Safety & Environment 7 (Winter 1998)

    This article identifies policy questions regarding the use of Monte Carlo Analysis (MCA) in environmental risk assessment and possible administrative and judicial responses to them.

    "The EPA and the National Academy of Sciences, have recognized Monte Carlo methods as means of quantifying variability and uncertainty in risk assessments." 7-8. "To date, there has been little discussion of Monte Carlo simulations in court opinions – perhaps not surprising given the technical nature of this computational technique and courts' inclinations to defer to agency expertise."

    Background on MCA, including advantages and disadvantages. 8-14. Probability distributions created by MCA "display the location of any particular risk estimate within the range of risk." 11. "Monte Carlo techniques in and of themselves do not dictate any particular degree of protectiveness or conservatisms, they provide more information for implementation of such policy choices." 14. These techniques are more demanding of data and therefore more costly. 15. Additionally, "[u]nderstanding and interpreting the output requires more sophistication the public is usually credited with," potentially precluding meaningful public input and commentary on the risk assessment. 16.

    EPA policy specifies eight conditions that must be met when using MCA in a risk assessment, primarily full explanations of the underlying data, assumptions and methods. See EPA, guiding Principles for Monte Carlo Analysis (1997). Notably, MCA does not "obviate the hard policy choices, such as which groups deserve protection and at what levels." 18. These issues will affect the analysis design.

    "[M]odel uncertainty represents a lack of knowledge about the way that variables are related to each other and thus constitutes uncertainty about whether a model approximates a real-world process or relationship." 19. "Most practitioners appear not to have incorporated quantitative estimates of model uncertainty into their analysis," although they acknowledge it as an important issue. 21.

    "Judges will likely be disinclined to delve into [the intricacies of MCA,] likely characterized as technical and scientific and subject to a longstanding judicial deference." 22. However, MCA use may be challenged as a departure from prior agency practices, or claims that MCA should or should not have been used in a particular instance. 23.

    Discussion of *Sierra Club v. NRC*, 862 F.2d 222 (9th Cir. 1988) where licensing opponent relied on a probabilistic risk assessment.

MCA use may also be challenged on the basis that although warranted, it was improperly conducted. 25. "There is ample judicial precedent for rejection of modeling based on assumptions not supported by, or at odds with, ascertainable facts." 25 (citing *Leather Indus. Am., Inc. v. EPA*, 40 F.3d 392 (1994)). However, a court is likely to defer to the agency where "various factual interpretations are arguable." 25-26. "Policy issues are more clearly fair game for judicial intervention than are issues characterized as science, but even here, administrative agencies are entitled to deference in interpreting ambiguous statutory mandates." 26.

2. John W. Hayse, Using Monte Carlo Analysis in Ecological Risk Assessments (Oct. 2000).

This article provides background on the Monte Carlo Analysis (MCA), which is a statistical technique used to analyze the effect of uncertainty and variability on the estimate of risk. The MCA has been used with human health and ecological risk assessments to evaluate the likelihood of negative site-wide effects.

"Defining the statistical distributions (PDFs) that will be used for the model's input parameters is probably the most difficult aspect of a Monte Carlo analysis and is the step that leads to the most controversies over the use of Monte Carlo analysis." 6. Determining PDFs typically requires the collection of sample data.

"With appropriate explanations, the results of a Monte Carlo analysis may also be used to help interested parties, such as the public or regulators, understand the basis for risk management decisions." The decision to use a MCA depends on the individual case's financial, time, and personnel constraints.

EPA policy supports the use of probabilistic analysis techniques, such as the MCA. However, "[i]t is not the intent of this policy to recommend that probabilistic analysis be conducted for all risk assessments supporting risk management decisions." 10. Additionally, use of MCA in risk assessments is not *per se* cause for rejection of the risk assessment by the EPA.

The article further outlines conditions required for MCA acceptance:
- Clearly identify the purpose and scope of MCA
- Fully document the methods
- Provide a sensitivity analysis
- Consider correlation among input variables
- Present complete information for all input and output PDFs
- Include deterministic results

3. Wendy Wagner, Elizabeth Fisher, & Pasky Pascual, Misunderstanding Models in Environmental and Public Health Regulation, 18 N.Y.U. Envtl. L.J. 293 (2010).

This article "documents the pervasive misperception of models as truth machines" and sets forth proposals for making better use of models.

“[D]espite their extraordinary influence on environmental policy, models are often created, refined, and deployed in the backroom, behind the curtain, only to be hauled out for critical attention when things go very wrong.” 294. “[C]onfusion and even anxiety abounds within the regulatory sphere regarding the appropriate use and methods for assessing the reliability of models.” 295.

“Models are needed to synthesize raw data, often from multiple sources, into computational forms that provide a comprehensive picture about an ecosystem or environmental scenario under different conditions.” 297. [M]odels provide a means of assessing, measuring, and/or predicting exposure or harm. 298.

Models have been used under the CAA, CWACERCLA, SDWA and to bring toxic tort suits. 299-301. EPA developed the Council for Regulatory Environmental Modeling to provide oversight for models, added a models database to its website, and commissioned a National Research Council report to help it assess models in the future. 304.

A 2009 NRC report called for better models, better information about a model’s limitations and the need for formal analyses of model uncertainties. 305 (citing Comm. on Improving Risk Analysis Approaches Used by the EPA, Nat’l Research Council, Science and Decisions: Advancing Risk Assessment (2009)). The White House’s Office of Management and Budget also “issued a circular requiring all executive agencies to conduct their analyses with more transparency using formal model evaluation techniques. By issuing the circular, OMB recognized that most regulations depend on models and wanted to encourage agencies to be more forthcoming about their models’ assumptions and limitations. 305-06 (citing Office of Mgmt. & Budget, Circular A-4 on Regulatory Analysis (2003)).

Discusses various types of models. 306-08. Limitations of models include significant uncertainties and subjective judgments. “[T]he documentation that accompanies a regulatory model should contain enough information about the underlying data, assumptions , and analytical approaches to allow an interested and objective stakeholder to assess the domain of the model.” 309.

“[E]valuating a model’s soundness requires more than just comparing model outputs to other models or to historical data. It also requires information about the assumptions and analytical techniques through which a model was developed.” 312. However, “the modeling community has yet to establish a coherent, universally-shared set of guiding principles through which regulators and interested stakeholders can evaluate whether one model (or set of models) can be said to be more appropriate for a given situation than another.” 312.

“Models are embedded in and shaped by their institutional context, but from the perspective of the courts, many policymakers in Congress, and even the agencies, there is a widespread (though not uniform) misconception that models provide deterministic answers. 318. "In resolving challenges to models, most courts perpetuate the pervasive misunderstanding and assume that since the model is mathematical, it is correct. As a result, they pass the model through the system without much, if any, scrutiny…even in cases when there are reasons to suspect that the model may have significant problems." 320. See *Sierra Club v. U.S. Forest Serv.*, 878 F. Supp. 1295, 1310 (D.S.D. 1993) ("As long as an agency reveals the data and assumptions upon which a computer model is based, allows and considers public comment on the use or results of the model, and ensures that the ultimate decision rests with the agency, not the computer model, then the agency use of a computer model to assist in decision making is not arbitrary and capricious." 320. Some earlier courts did not even insist on a full explanation of the assumptions or basis for the model. 321. See Robert L. Glicksman, *Bridging Data Gaps through modeling and Evaluation of Surrogates: Use of the Best Available Science to Protect Biological Diversity Under the National Forest Management Act,* 83 Ind. L.J. 465, 492 (2008) ("The law is clear that a court may not second-guess methodological choices made by an agency in its area of expertise."). 321.

Although fewer in number, some courts have rejected a model "when there is evidence of unresolved issues or uncertain calculations." 321. See 701 F.2d 1137, 1146 (5th Cir. 1983) 107 ("To make precise estimates, precise data are required.). In Leather Industries of America, Inc v. EPA, the D.C. Circuit invalidated EPA's model partly because it was dissatisfied with an assumption built into the model, holding that more data-backed justification was required. 323. In Ohio v. EPA, the Sixth Circuit rejected an EPA air model for failure to "back up its regulations [and models] with checks against the real world data" generated for the particular site where the model is applied. 324. "The possibilities that this data might be quite expensive to collect, might be quite limited in terms of its local-specific value, and might take more than a year to gather were effectively dismissed as illegitimate reasons to depart from this rigorous validation requirement." 324. This decision limited an agency's ability to rely on models when data is too time-consuming or expensive to collect by requiring location-specific data to test the model.

"The misunderstanding of models as truth generators is reflected in the basic constitution of contemporary U.S. administrative law and expressed through a number of regulatory programs." 331-32. Although not truth generators, models do provide useful insights that aid deliberation and analysis. "Without an appreciation for the difference, the agency runs the risk of accepting badly incomplete answers and missing the true value of models." 332.

"The absence of a set of accepted best practice principles to guide high-quality computational modeling may be the most significant void in modeling science." 332. This may be partly due to the fact that models are developed by scientists in a range of disciplinary areas with few opportunities to communicate with one another. “The diversity of models and of disciplines using models make the communication of these fundamental uncertainties challenging because of the lack of a generally accepted approach to characterizing uncertainty.” 334.

Discussion of an industry challenge to EPA’s chloroform regulation in drinking water, assuming the relationship between a chemical dose and carcinogenic response is linear. “The rule was overturned when the Chlorine Chemistry Council argued successfully that EPA disregarded evidence that chloroform is a threshold carcinogen requiring an alternative, non-linear model.” 335.

“In a recent report, an NRC panel recommended that EPA replace a default assumption when the underlying evidence is ‘clearly superior’ to that for the default.” 335 (citing *NRC, Science and Decisions*, at 201). The panel equated the “clearly superior” evidentiary standard to a “beyond a reasonable doubt” legal standard. The panel highlighted the need to develop coherent rules for evaluating evidence embodied in a model and “hinted at the existence of some formal rules for model evaluation, pointing to the statistical P value as an analogy for how one might determine that evidence is ‘clearly superior.’” 336.

Discussion of agency benefits by relying on a model to generate “answers,” such as sidestepping accountability and insulating agency assumptions/modeling decisions from critical review. 337-39. However, demands for an unobtainable level of empirical certainty “may succeed not only in blocking the use of the model, but in blocking the policy as well.” 339. Climate change models are an example of models challenged for failing to meet the demand for “sound science.” 340-42. “Their objective is to destroy the credibility of ‘good’ or ‘plausible’ models by criticizing the model on every picky and generally insignificant detail.” 340-41.

“[B]ecause they are contingent and technically complex, and yet at the same time enter a policymaking world that is not well prepared to use them wisely, models are fodder for abuse and manipulation.” 344.

Discussion of contributions modes make to policy and environmental regulation (e.g., providing a better conceptual map about the real world than intuition and helping decision-makers evaluate sources of uncertainties). 345-46.

Proposes changes to the administrative process to correct the our current understanding of models, including 1) altering judicial review rules to ensure transparency of methods and assumptions and use of best practice guidelines; 2) allowing agencies to revise and evaluate models in a continuous process; 3) making agencies and legislatures part of the modeling process and communicating with modelers to ensure information and assumptions are shared between the two groups. 347-51. “[A] coherent treatment of evidence in models would: (1) describe the assumptions underlying an inference, (2) justify why the assumptions apply to the circumstances on hand, and (3) explain how the inferences derive from the interplay between the assumptions and the evidence." 352. "Ideally, a comprehensive explication of uncertainties, assumptions, and model framing would be based on best model practices that apply across the scientific fields. Since this seems unlikely to occur spontaneously, however, we recommend that EPA continue to take the laboring oar – working with scientists – to develop principles for qualifying and explaining the assumptions in models; for exposing alternative scenarios and model approaches; and for clarifying whether the inferences made were consistent with the assumptions. 353. EPA has taken steps in the right direction by providing a general set of practices for modeling. See Council for Regulatory Envtl. Modeling, EPA, Guidance on the Development, Evaluation, and Application of Environmental Models (2009). Balanced stakeholder participation (industry, scientists, agency) can also provide a check on exploiting model misunderstandings. 354-55.

4. Robert L. Glicksman, Bridging Data Gaps through Modeling and Evaluation of Surrogates: Use of the Best Available Science to Protect Biological Diversity under the National Forest Management Act (2008) (published in 83 Ind. L.J. 465 (2008)).

   This article discusses the lessons that may be drawn from the National Forest Service's shifting approach to the use of models and surrogates.

   Despite the pervasive uncertainty that surrounds environmental problems, "Congress has directed the agencies responsible for administering the environmental statutes to ground their policy decisions in science. . . . Agencies sometimes cope with the responsibility of making science-based decisions despite the presence of uncertainty by relying on scientific models, or otherwise using the limited information available to them, to make predictions about the impacts of agency decisions on the environment." 2. However, "competing models or differential applications of a single model may yield starkly divergent predictions about the effects of an agency's decision on the environment. As a result, litigation concerning the use of simulation models and surrogate parameters by environmental and resource management agencies has been plentiful." 3.

   Part I discusses the utility of modeling and how federal courts have reacted to challenges to reliance on these analytical techniques. 4-22. Modeling has become an important component of policy making in environmental law and is an integral part of implementing pollution control statutes. 10-11. Benefits and limitations of modeling discussed. 13-18.

   "In reviewing challenges to the use of agency models, the courts in environmental cases have recognized the importance of disclosing and providing an opportunity to comment upon the model's assumptions." 18. *See Lands Council v. Powell*, 395 F.2d 1019 (9th Cir. 2005) (finding that the agency's "heavy reliance" on the WATSED model to analyze cumulative effects of timber harvests on in-stream sedimentation violated NEPA because the agency did not disclose shortcomings of the model) and *Chem. Mfrs. Ass'n*, 28 F.3d 1259 (D.C. Cir. 1994) (finding that EPA afforded adequate notice of its intention to rely on a model in deciding whether to list a substance as a hazardous air pollutant under the CAA). "Substantive challenges to an agency's use of modeling in environmental decision making typically fact an uphill battle." 19. Courts tend to be very deferential to agency modeling decision and "have not been impressed by claims that an agency chose the wrong model from among competing alternative models, that deficiencies in the data the agency plugged into the model invalidated the results, that the model did not accurately predict or was not capable of actually predicting real world results, or that the agency should have deferred its decision until it could accumulate more information instead of relying on modeling results." 19-20. *See Miccosukee Tribe of Indians v. United States*, 420 F. Supp. 2c 1324 (S.D. Fla. 2006) (finding that the Corps of Engineer's reliance on limited modeling information was not arbitrary and capricious).

However, courts have invalidated agency decisions that relied on modeling or simulation exercises "in cases in which they have found that a particular model was ill-suited to the activities to which it was applied or that the agency was unable to justify building the model on apparently arbitrary assumptions." 20-21. *See Ctr. for Biological Diversity v. BLM*, 422 F. Supp. 2d 1115 (N.D. Cal. 2006) (reversing the FWS' reliance on modeling or simululation techniques on these grounds).

Part II discusses the use of models and surrogates in the specific context of the Forest Service's efforts to comply with NFMA requirements. 22-54.

Part III discusses criteria by which modeling and simulation techniques should be judged (e.g., realistic, collaborative, transparent, flexible). 54-61.

5. Matthew W. Swinehart, Remedying Daubert's Inadequacy in Evaluating the Admissibility of Scientific Models Used in Environmental-Tort Litigation, 86 Tex. L.Rev. 1281 (2008).

    This article analyzes Daubert's treatment of environmental models and suggests reformulating the inquiry to address modeling's unique challenges.

    "An 'environmental model' is a model – a mathematical representation of an object or process – that seeks to describe physical and natural systems, such as the fate and transport of contaminants in groundwater." 1282. The author argues that the Supreme Court's decision in Daubert v. Merrell Dow Pharmaceuticals, Inc. has proven inappropriate and inadequate in evaluating model reliability.

    "Models have long been a part of the scientific community's methodological arsenal. However, in recent decades, their influence in science and policy has dramatically increased, due largely to the confluence of two distinct phenomena: the advent of computers and the rise of intricate and demanding environmental regulatory regimes." 1284. Environmental models provide four main benefits in regulatory, legal, and research applications: 1) demonstrate complex relationships, 2) provide meaningful data frameworks, 3) incorporate information from multiple disciplines, and 4) used by scientists to explore new theories and to refine existing paradigms. 1286-88. However, models face two fundamental problems: uncertainty and an inherent lack of transparency. 1288-95.

The adversarial nature of environmental litigation also presents opportunity for the misuse of scientific evidence, including models. 1295-99. Models are impressive, "[b]ut they are not precise, and their remarkable value should not obscure the judicial inquiry into model reliability." 1296.

Judges often "lack the competence to evaluate modeling evidence satisfactorily. The limited scientific expertise, training, and education of judges make it difficult to determine an appropriate level of review at the evidentiary screening state… [and] drawing a line between good and bad models is often not an easy task, even for those with the relevant scientific expertise operating outside the adversarial context of litigation." 1299.

There are two basic ways to evaluate models: 1) see whether the model's results are relevant to the question and compare the model results to any available empirical data for consistence; and 2) look at the information that generated the model, including its theoretical underpinnings, the empirical data base, and independence of the evidence supporting the model. 1299-1300. "[W]hile it appears that courts may be well suited to assess the qualifications of a modeling expert, it does not necessarily follow that courts are inherently adept at wading through the enormously complex – and often opaque – models themselves." 1301.

The Daubert Court suggested the following four illustrative criteria for determining whether scientific evidence is reliable, and therefore, admissible: 1) the theory or technique is falsifiable, refutable, or testable; 2) the theory or technique has been peer-reviewed; 3) there is a known or potential rate of error; and 4) the underlying science has been generally accepted. Each of these criteria are discussed in turn, including their inability to sufficiently address the difficulties posed by models. 1301-11. In United States v. Dico, Inc., 266 F.3d 864 (8th Cir. 2001), the Eight Circuit Court of Appeals "treated general acceptance as virtually dispositive of the reliability of the modeling methodology at issue. . . . Although the court went on to discuss the accuracy of the underlying empirical data and model assumptions, it was clear that acceptance of the modeling methodology created a presumption in favor of reliability…." 1310. Courts as also tend "to equate general acceptance with peer review so that the fourth factor does not add anything to the analysis." 1310. *See e.g.,* Livingston v. Isuzu Motors, Ltd., 910 F. Supp. 1473 (D.Mont. 1995) (finding a model "generally accepted," using the same relative test as for the "peer review" analysis).

The Council for Regulatory Environmental Modeling drafted guidelines for regulatory environmental models in 2003, which include four primary components: 1) peer review, 2) quality-assurance and assessment procedures, 3) qualitative and quantitative corroboration of models, and 4) sensitivity and uncertainty analyses. 1311.

Suggestions for Daubert reform - a mandatory screening checklist: 1) is the modeler an expert in this particular methodology? 2) was the correct model chosen? 3) was the model applied correctly within its practical boundaries and theoretical limits? 4) is the real-world system too complex to model? 5) can conflicts of interest be mitigated? 6) was the model sufficiently tailored to the model's inputs and the natural system's unique conditions? 7) was all available empirical evidence considered? 8) to what extent is the model meaningfully communicable to the jury? and 9) how does the model contribute to the weight of the evidence?. 1312-25.

The authors suggest that courts require some showing that the modeler considered alternative models and an explanation of why the employed model is the "best available." 1316. Courts may also look to governmental agencies' evaluations of models, such as EPA's ranking of certain models based on their statistical performance. 1317-18. Notably, EPA recommends that all agency-endorsed models be peer-reviewed, but does not require it. 1318 (citing Pasky Pascual et al., Council for Regulatory Envtl. Modeling, U.S. Envtl. Prot. Agency, Draft Guidance on the Development, Evaluation, and Application of Regulatory Environmental Models (2003)).

6. Ira Giuffrida, Legal, Practical and Ethical Implications of the Use of Technology in European Courtrooms, 12 Wm. & Mary Bill of Rts. J. 745 (2004).

   This article explores how European courts are opening themselves to technology and to its various uses in courtrooms. Not really relevant because it does not discuss modeling, focuses instead on LiveTalk and electronic databases.

   "There is a fear associated with the use of technology in the courtroom that it may create a bias in the judicial process by affecting the judges or the jurors in their decision-making processes." 747. Discusses the need for technology in courtrooms.

7. Stephen P. Prisley & Michael J. Mortimer, A Synthesis of Literature on Evaluation of Models for Forest Carbon Accounting, Forest Ecology and Management 198 (2004) 89-103.

   This article reviews literature that may inform the development of guidelines for the application of models in areas with policy implications, such as forest carbon accounting.

   "It is commonly acknowledged that models are essential in many areas of ecological study and environmental management and regulation…. When such models are applied to inform public policy, some form of evaluation of a model's reliability is necessary." 90. No uniform evaluation exists. "A model must be evaluated in the context of its purpose, domain, and structure." 91. Discusses recommendations found in the literature for essential components to model evaluation, including scientific peer review of model composition; quantitative analysis of model results compared to field observations; and sensitivity analysis. 93-96.

"[T]he proposed use of scientific models must consider the potential for judicial scrutiny of the model, the model's particular application, as well as the policies followed in developing and adopting the model." 96. Federal courts have a lengthy history arbitrating the use of predictive models by federal agencies. 97 (citing Case, C.D. 1982. Problems in judicial review arising from the use of computer models and other quantitative methodologies in decisionmaking. Boston College Environ. Affairs Law Rev. 10(4), 251-363). A court's invalidation of a particular model may impair an agency's ability to use that model.

Discussion of the Data Quality Act, requiring nearly all federal agencies to prepare guidance to maximize the quality of information the agency publicizes or disseminates, including (presumably) models. 97-98.

Criteria that may or should be considered in assessing a particular model's application include: 1) stating the model's assumptions, disclosing the decision-making variables not dependent on the model, disclosing uncertainty, the degree of scientific acceptability, the use of peer review, and adequate empirical testing. 98.

In *Sierra Club v. U.S. Forest Service*, the court ratified the use of the agency's predictive model in part due the agency providing for and considering public comments. In *Chemical Manufacturers Ass'n v. EPA*, the court "noted that an overly rigid application of the model by the agency will subject the model and the agency's supporting evidence to heightened judicial scrutiny." 98. "While a court may be loath to second-guess the agency's choice of a model, or critique the model's inner workings, courts are much more receptive to ensuring that appropriate processes are followed prior to the employment of the model, particularly transparency in the model's assumptions and availability of the underlying data." 99.

See pg. 99 for summary of recommendations for models found in the literature: clearly define the scope, be clearly documented, be scientifically reviewed, be compared with field observations, conduct sensitivity analysis, be made available for evaluation, be periodically reviewed in light of new knowledge, and undergo public comment.

8. Camille V. Otero-Phillips, What's in the Forecast? A Look at the EPA's Use of Computer Models in Emissions Trading, 24 Rutgers Computer & Tech. L.J. 187 (1998).
   This paper traces the development of the CAA and the EPA's use of computer models to establish emission limitations. The author argues that computer

modeling should be used as a guide in developing a trading program to reduce the environmental impact of SO2 emissions on a national basis, rather than a state or regional.

Discussion of the EPA's use of computer-generated models to set emissions limitations at individual facilities. 204-08. Use of an atmospheric model depends on several factors, such as complexities of the area, level of detail and accuracy needed, and resources available. 205.

Under Title, EPA uses computer models to 1) project pollution levels, 2) evaluate and predict control program effectiveness, and 3) aid in the cost benefit analysis. 208-11.

Discussion of the court's reactions to the EPA's use of modeling. 212-15. "Courts have upheld the EPA's use ad choice of computer models in many areas of environmental decision-making." 213 (e.g., *Republic Steel Corp v. Costle*, 621 F.2d 797 (6th Cir. 1980), *Columbus & So. Ohio Elec. Co. v. Costle*, 638 F.2d 910 (6th Cir. 1980), and *P.P.G. Indus. V. Costle*, 630 F.2d 462 (6th Cir. 1980)). "The court's willingness to defer to the EPA's judgment on scientific matters, such as model selection, suggests a high likelihood that courts will continue to uphold the EPA's choice of models regardless of whether environmental impact is considered." 214.

To ensure accuracy, EPA recognizes the importance of validating models with data whenever possible. 215-217 (e.g., *Ohio v. EPA*, 784 F.2d 224 (6th Cir. 1986) and *Mision Indus., Inc. v. EPA*, 547 F.2d 123 (1st Cir. 1976)).

Discussion of emissions trading under Title IV. 218-221.

9. Eugene A. Lang, Jr., A Primer on Computer Simulation of Hydrocarbon Reservoirs, 12 Land and Water Law Review – University of Wyoming 1(1987).

This article discusses the use of computer simulations of hydrocarbon-bearing reservoirs in litigation.

"Given the important functions which computer simulations can perform, it is not surprising that expert testimony based upon simulations has been used in a wide variety of cases," including Southern Pacific Communications Co. v. Am Telephone & Telegraph Co.; Ideker, Inc. v. Missouri State Highway Commission; and Sorensen v. Lower Niobrara Natural Resources District. 1-2.

Describes reservoir simulation in detail. 2-9. Common misuses of reservoir simulation include 1) using a model that is too sophisticated and complex for the problem under consideration; 2) construction of a model without regard to cost; and 3) construction of models without adequate data. 8-9.

Legal problems arising from the use of reservoir simulators as the basis of expert testimony include: admissibility of such testimony and discovery. 9. Federal Rule of Evidence 703 requires the data underlying the expert's opinion to be of the type reasonably relied upon in his field of expertise. "Reasonable" has been interpreted by two leading commentators to be synonymous with "customarily." 10. Expert testimony based upon reservoir simulation is admissible under Rule 703, so long as the simulation is properly conducted. *See e.g.,* Soden v. Freightliner Corp., 714 F.2d 498, 502-07 (5th Cir. 1983); Zenith Radio Corp. v. Matushita Elec. Indus. Co., 505 F. Supp. 1313, 1329-30 (E.D. PA. 1981). Discovery relating to reservoir simulation is discussed (e.g., making the documentation relating to the model's programming available for the other party's inspection). 10-13.

10. Charles D. Case, Problems in Judicial Review Arising From the Use of Computer Models and Other Quantitative Methodologies in Environmental Decision Making, 10 B.C. Envtl. Aff. L. Rev. 251 (1982)

    This article discusses cases involving the judicial review of environmental decisions based on models to determine the proper role of judges and courts in such review. "The increasing use of quantitative models, particularly computer models, has placed a new burden upon the courts in their review of environmental decisions based on those models." 251.

    Environmental cases involving models should involve an evidentiary hearing to ensure sufficient analysis of the case. 252. A model is "an abstract, formal representation of a theory about, or empirical observation of, a defined set of facts of system. Models can range in complexity from a simple mathematical equation or expression to the most complex simulation models requiring computers to run them." 254. Models can be used to analyze existing data or to prediction future conditions.

    Discusses the use of models in the environmental decisionmaking process to: 1) project pollution levels, 2) evaluate environmental cleanup technologies and predict their effectiveness, and 3) aid in cost-benefit analysis. 256-59. Discusses the types of environmental models: mathematical and computer. 260-66. "Models are often used in environmental decisions to extrapolate from existing data because such decisions must e made on the basis of a sparse data base." 263.

    Discusses judicial review over agency action. 267-273. Reasons for increasingly widespread use of models in environmental decisions: 1) congressional mandates (e.g., CAA 1977 amendments), 2) congressional intent (e.g., statutes requiring use of best available evidence or latest available scientific data, which may be interpreted to require the use of models), and 3) increasingly complicated and intractable environmental problems. "A number of cases interpreting the Clean Air Act and NEPA establish the principle that the sophistication of the models used on computers must keep up with the current state of art." 271.

In general, environmental decisions are difficult for a court to review because: 1) vague statutory standards, 2) inadequate data base, 3) complexity of underlying science, 4) limitations of the environmental decisionmaker, requiring experts, and 5) inadequate and unclear presentation of data. 274-81. Institutional problems further contribute to the difficulties of judicial review in cases relying on environmental models, including "the self-perceived lack of scientific expertise on the part of judges, the lack of judicial access to technical resources to assist in the analysis of the technical issues involved in such decisions the limits on the court's ability to supplement or go outside the record, and the traditional deference which the courts give to administrative decisions." 293.

Use of environmental models raises two problems: 1) it may "increase the likelihood that a substantially incorrect decision will be reached due to the inability of environmental decisionmakers to deal with certain aspects of the use of models;" and 2) it may increase "the danger that wrong environmental decisions may not be detected and corrected by the reviewing court." 273-74.

"Cases involving challenges to environmental models take the form of allegations of insufficient underlying evidence. The cases normally raise questions of (1) whether the model from the evidence adequately supports the decision; or (2) whether the evidence used in the model justifies the model's use. . . . Allegations of insufficient underlying evidence in such environmental decisions do not often succeed because of the deference accorded to such decisions under the arbitrary and capricious standard applied to them, as contrasted with the more deferential substantial evidence and 'rule of reason' or reasonableness tests." 302. Cases involving challenges to models often separately discuss "the alleged errors in the methodology of the model and the data used in the model." "The fundamental questions on judicial review are simply the proper scope of review (how far the court should inquire into alleged errors in modeling methodology or data used in the model) and standards of review (to what extend the court should overlook apparent errors in the underlying data or modeling results)." 302.

There are four categories of cases involving environmental models: 1) emission standards and nonattainment designations under the CAA; 2) EIS under NEPA; 3) regulations promulgated on the basis of the models; and 4) permits and licenses under the various environmental statutes. 303. This article discusses the first two categories. See 303-335 for CAA and 336-358 for NEPA cases.

The cases reviewed "generally review that: (1) the role of the court in the decisions has been too restricted; and (2) the standards and scope of review applied by the courts has not been sufficiently searching to ensure the correctness of the factual underpinnings of agency decisions, since the methodology and data underlying the model or models used in the decision generally are not scrutinized." 358.

The author suggests that "[a] court properly may substitute its judgment for the agency's in several instances: (1) where the agency uses an incorrect model or a model that inexplicably falls short of the modeling art; (2) where the agency uses unexplained or unjustified assumptions or adjustments in the model; (3) where the agency uses data shown to be incorrect or inapplicable to the situation; where the agency uses an insufficient data base such as by using inexplicably out-of-date data, failing to validate and explain the procedures applied to ensure that the model was proper for the data base, failing to use monitoring data or other procedures to calibrate and validate the model, failing to cite to supporting technical and scientific literature or failing to distinguish apparently inconsistent technical literature, and failing to explain or correct apparently incorrect or imprecise methodologies or results; (4) where the agency fails to properly structure and summarize the supporting and nonsupporting data and methodology in an understandable index or appendix; and (5) where the agency fails to provide necessary data at a time at which meaningful comments and challenges to data and methodology could be raised, or fails to provide a realistic opportunity for the presentation of such objections." 359-60.

11. Bruce M. Kramer, Air Quality Modeling: Judicial, Legislative and Administrative Reactions, 5 Colum. J. Envtl. L. 236 (1978-1979)

    "This article reviews the history of the use of predictive models to ascertain the impact and relationship of a single emitter of air pollution on the ambient air." Air quality models are essential in determining existing ambient air quality for all major pollutants under the CAA, and "vital tools in designing SIP's." 238.

    Discusses the first case that dealt directly with the EPA's use of air quality modeling: *Texas v. EPA*. 243. "Because the Clean Air Act itself did not specify a standard of review, the court opted for a test that was first applied by the United States Supreme Court in *Citizens to Preserve Overton Park, Inc. v. Volpe*." 243. "The EPA, in its argument before the *Texas* court, did not contend that its model was a precise of accurate representation of reality. Rather, it argued that the use of the more complicated and untested Texas model should be rejected where that model led to marked differences with the more scientifically accepted, if simpler, rollback model." 246. The EPA model was also promulgated as part of an agency regulation, subject to the public review process. Ultimately, the court held that the EPA's decision to use the simplistic straight rollback model was not arbitrary or capricious. 247.

    EPA's air quality modeling techniques were criticized again in *South Terminal Corp. v. EPA*. 248. The EPA's database was based on a single day's reading from a possibly malfunctioning machine, and therefore insufficient to support the EPA's photochemical oxidant determination. As to the model itself, "[t]he *South Terminal* court concluded that the mere fact that there are conflicts as to the use of the model does not justify the court's substitution of its judgment for that of the EPA." 249.

In *Mision Industrial, Inc. v. EPA*, petitioners argued that EPA's predictive methodology permitted too great a likelihood of error. 250. However, the court "concluded that great deference was owed to the EPA in its area of expertise, and the court refused to substitute its judgment for that of the Administrator."

"In all three cases, *Texas, South Terminal,* and *Mision Industrial*, the courts recognized that the modeling used was crude, much dispute existed concerning background data, and the EPA was under tremendous time pressure because of the mandates of the 1970 [CAA] Amendments. . . . The judiciary's presumption in favor of agency expertise gave the EPA a distinct advantage over any challengers of agency air quality modeling decisionmakign both in modeling's initial, and later, more sophisticated, stages." 250-51.

In *Cleveland Electric Illuminating Co. v. EPA*, petitioners challenged the agency's use of a more complex model. 251. The court "refused to enter the speculative game of determining whether RAM was the best possible approach for developing a sulfur dioxide SIP. Rather, it compared RAM to the more simplistic rollback model, and found several significant points to support the EPA's selection of the former over the latter." 252. The court also held that predictive perfection was not required of the model, due to its recent development and conservative use.

Other court decisions reviewed "signaled the continuation of substantial judicial acceptance of the EPA's modeling decisions despite the lack of express congressional approval of modeling techniques at the time." 256.

Discussion of the 1977 CAA Amendments requiring EPA to designate appropriate air quality models. 259-262. "[T]he 1977 Amendments resulted in changing the EPA's position on air quality modeling from one allowing state flexibility to one mandating use of EPA-specified models." 262.

Books

1. National Research Council of the National Academies, Models in Environmental Regulatory Decision Making (2007).

   Recognizing that the use of computational models is an essential element of the environmental regulatory process, the National Academies sought to assess evolving scientific and technical issues related to the development, selection, and use of computational and statistical models in the regulatory process at EPA. This report provides advice concerning management, evaluation, and use of models at the agency. This following sections appeared most relevant:

   Trends in Environmental Regulatory Model Use – 20-26. Discusses the increase in model use for regulatory purposes at EPA in the past 25 years.

Regulatory Model Classifications – 43-51. The EPA's Council on Regulatory Environmental Models provides the most exhaustive inventory of individual models, including more than 100 models used by the agency. However, this section discusses models from a functional and regulatory perspective, and provides examples of EPA documents that incorporate modeling activities

Congressional and Executive Branch Influences – 62-69. "Federal environmental statutes, such as the CAA and CWA, usually contain statements of health and welfare goals, schedules and deadlines for meeting them, and, often, criteria for determining whether the goal has been met." 62. Producing the kind of regulations authorized by such health- or welfare-oriented legislation requires the use of models. 65. This section discusses how legislation affects EPA's use of models, as well as executive branch oversight of the regulatory process.

Oversight Processes Governing Regulatory Models at EPA – 69-79. This section discusses external review of EPA's models (e.g., peer, public, interagency). EPA's models are also subject to legal challenges. Interested parties may challenge agency action in court. "If the model supports a regulation and has been subject to notice and comment, the courts give EPA considerable deference. Thus, challenges to EPA models are successful only when the regulation (and/or underlying model) is in conflict with EPA's statutory mandate, has been determined to be inconsistent with the Administrative Procedure Act requirements, or is 'arbitrary and capricious' (5. U.S.C. § 706)." 76. *See Nat'l Oilseed Processors Ass'n v. Browner*, 924 F. Supp. 1193, 1209 ("This Court must not undertake an independent review of EPA's scientific judgments; our inquiry focuses only on whether the agency has met the statutory requirement for 'sufficient evidence.'"). If a model has not undergone notice and comment, the agency may receive less deference from the courts. 77.

EPA's models have been challenged, and in some cases, challengers have been successful. "For example, when EPA declines to explain its decision or revise a supporting model even after receiving comments refuting one of the model's critical assumptions, the courts have invalidated and remanded the model back to EPA. Challengers have also been successful when they establish that EPA's model is not applicable to a particular subset of industries, activities, or locations." 77. *See State of Ohio v. EPA*, 784 F.2d 224 (6th Cir. 1986). "Finally, if challengers disagree with embedded policy judgments, such as the risk adversity of assumptions built into a risk assessment, courts will sometimes invalidate a model and not defer to the agency." 77. *See Gulf South Insulation v. Consumer Product Safety Commission*, 701 F.2d 1137 (5th Cir. 1983).

Discussion of attempts to challenge agency action under the Information Quality Act. 78. While courts have refused to review these challenges, the agency must respond to complaints related to the reliability of models.

The Challenges of Modeling in a Regulatory Environment – 79-82. This section offers recommendations related to continuing improvements to the accessibility of regulatory modeling (e.g., technical reliability; transparency and accountability). Recognizes that time and resource limitations may lead to use of existing models outside their "application niche." 80.

Model Evaluation – 104-169. This section offers recommendations related to model evaluation; principles for model development, selection and application; and model management.

2. The National Judicial College, Hydrologic Modeling Benchbook: Dividing the Waters (2010).

   "The quality and reliability of hydrologic models is a regular feature of surface water and groundwater disputes that are challenged in court." 2. This benchbook summarizes the kinds of water cases in which hydrological models often appear, reviews the literature on model building and testing, describes proposed guidelines on model construction and testing, and presents techniques for case management.

   Judging the Adequacy of Models – 49-62.

   1) American Society of Testing and Materials (ASTM) Standard Guides
      The ASTM began issuing model guidelines in 1993. *See* Table V.1 Documentation Elements at 51.

   2) Daubert Criteria
      "The legal tests for model admissibility are *Frye, Daubert,* and FRE 702 or its state-court equivalent." The *Frye* test includes "general acceptance in the relevant scientific community." 52. "The *Daubert* factors expand upon the *Frye* test to include, among other things, whether the techniques have a known error rate, are subject to standards governing their application and enjoy widespread acceptance." 52. "[T]he Court emphasized that the admissibility inquiry must focus 'solely' on the expert's 'principles and methodology,' and 'not on the conclusions that they generate.' Not surprisingly, professional engineering and scientific associations and review panels have, in general, supported the decision and the implementation of *Daubert* criteria." 54. *See* Table V.3 at 54 (providing Western States criteria for evaluating scientific evidence). "In an adversarial setting, particularly a complex and high stakes case, it is very likely that each side will be able to assemble an expert group that can produce a model that meets the ASTM/*Daubert* standards." 55. Under FRE 702, if scientific, technical or other specialized knowledge will assist the jury, an expert may testify if "(1) the testimony is based upon sufficient facts or data, (2) the testimony is the product of reliable principles and methods, and (3) the witness ahs applied the principles and methods reliably to the facts of the case."

55. Rule 702 "has the benefit of barring junk science and improper causation evidence…[but] does so at the expense of excluding in some cases where data may be limited, speculative causation evidence from the courtroom, even though the evidence of causation has wide support among experts in a particular scientific field." 56.

"The majority of reference and guide material on scientific evidence and expert testimony revolves around *Daubert.*" 56.

3) Federal Judicial Center Reference Manual on Scientific Evidence This manual "analyzes several words – *evidence, theory, law, error*, and *mistake* – that have very different meanings in law and science." 56. Overall, "the court must serve as a vigilant gatekeeper to ensure science in the courtroom is reasonably right and [] it may do so by requiring well-defined and acceptable error levels of the science." 56.

"The presence of experts is nearly ubiquitous with use of computer models in water litigation. As such, courts need to ensure that expert testimony substantiates the models and that expert opinion about and founded on the models can be properly framed and evaluated by the finder of fact." 60. "Generally speaking, the qualifications of an expert on modeling will require the same judicial discretion as the certification of any other type of expert[:]…'by knowledge, skill, experience, training, or education.'" 60 (quoting FRE 702). Discussion of permissible testimony. 60-62.

Case Examples of the use of Models in Complex Adversarial Proceedings – 71-80.

1) Arkansas River Compact: *Kansas v. Colorado* where Kansas filed suit against Colorado, claiming that Colorado allowed well development in violation of the Arkansas River Compact. H-IM is a model that simulates the physical and operational features of the Arkansas River. Both Kansas and Colorado adopted the model, but independently adjusted and modified it over the years of the trial.

2) Republican River Compact: *Kansas v. Nebraska and Colorado* where Kansas filed suit against Nebraska for violating the 1943 Republican River Compact by allowing unimpeded development of wells. The Final Settlement Stipulation contained provisions for the cooperative development of a groundwater model to serve as the basis for future compact administration.

3) *Park County Sportsmen's Ranch* where PCSR proposed a project to store water. The court found that the model in this case was not sufficiently reliable because it was not calibrated in accordance with accepted standards, no sensitivity analysis was conducted, experts

were unable to explain anomalous results, and an independent peer review was not completed.

4) San Luis Valley of Colorado where the Colorado State Engineer adopted new rules governing the major aquifers. The Court found that the "'groundwater model was developed following proper protocols and procedures, that it is calibrated to a degree sufficient for its intended uses under the Rules, and that the inputs to said model are reasonably accurate and may be relied upon for the purposes of the Rules.'s . . . The Court clearly found that the model was carefully and adequately developed." 80. However, the Court recognized that over time, the model may be open to re-examination utilizing the scientific model.

See also Appendix E: Admissibility of Expert Opinion Based on Computer Modeling – What Does Daubert Require? (Environmental Law Advisory, June 2003) at 101.

Cases – Pulled from keyword search

1. Commercial Union Insurance Co. v. Boston Edison Company, 591 N.E.2d 165 (Mass. 1992) – customers sued utility seeking compensation for overcharges resulting from faulty steam meter.

   The Court held that the computer-generated model for estimating energy usage was admissible, although customers were not required to accept the utility's estimate of energy usage.

   Admissibility of computer-generated models or simulations, like other scientific tests, is conditioned upon sufficient showing that: "(1) the computer is functioning properly; (2) the input and underlying equations are sufficiently complete and accurate (and disclosed to opposing party, so they may be challenged); and (3) the program is generally accepted by appropriate community of scientists." 549.

   "Generally courts have permitted computer models in cases not easily susceptible of other forms of proof. See, e.g., *Seattle Master Builders Ass'n v. Pacific Northwest Elec. Power & Conservation Planning Council,* 786 F.2d 1359, 1370 (9th Cir.1986), *cert. denied,* 479 U.S. 1059, 107 S.Ct. 939, 93 L.Ed.2d 989 (1987) (allowing use of computer simulations of value of energy conservation methods based on principles derived from American Society of Heating, Refrigerating and Air Conditioning Engineers "Handbook of Fundamentals" to determine energy conservation value); *Perma Research & Dev. v. Singer Co.,* 542 F.2d 111, 115 (2d Cir.), *cert. denied,* 429 U.S. 987, 97 S.Ct. 507, 50 L.Ed.2d 598 (1976) (results of computer simulation used to form basis of expert testimony regarding feasibility of perfection of automobile anti-skid device); *United States v. Dioguardi,* 428 F.2d 1033, 1037 (2d Cir.), *cert. denied,* 400 U.S. 825, 91 S.Ct. 50, 51, 27 L.Ed.2d 54 (1970) (computer analysis employed to determine when defendant would have exhausted his inventory, had he not concealed assets); *Pearl Brewing Co. v. Joseph Schlitz Brewing Co.,* 415 F.Supp. 1122, 1134 (S.D.Tex.1976) (computer simulation used to test varying market conditions in price-fixing case); *United States v. United Technologies Corp.,* 1977-2 Trade Cas. (CCH) par. 61,647, 1977 WL 1470 (1977) (econometric model used in antitrust case); *In re Sugar Indus. Antitrust Litig.,* 73 F.R.D. 322, 353 (E.D.Pa.1976) (expert could rely on statistical model to formulate his opinion as to class damages in complex antitrust case); *Messex v. Louisiana Dep't of Highways,* 302 So.2d 40, 44 (La.App.1974) (computer simulation of automobile accident used to assist court in determining whether defendant had reasonable opportunity to avoid accident)." 549-50.

The court held that computer-generated model of actual steam usage in building was admissible due to its general acceptance in relevant community of scientists and use by engineers and other professionals to model energy consumption. The trial court judge's obligation extended only to determining "(1) the completeness and accuracy of the data and underlying equations, and (2) whether program was generally accepted by appropriate community of scientists," not whether all the complex, underlying coding was complete and accurate. 552.

2. Oceana, Inc. v. Evans, 384 F.Supp.2d 203 (D.C. Cir. 2005) – environmental organization challenged the Secretary of Commerce's approval of an amendment to Atlantic Sea Scallop Fishery management Plan.

Plaintiffs contend that "the agency's use of the SEFSC 2001 model constituted an 'irrational[] rel[iance] on the model to do something it is simply not built to do,' while defendants counter that the model represented a reasoned methodology give the paucity of available data." 214.

The court held that the Secretary's use of NMFS' model to analyze whether scallop fishery would jeopardize loggerhead sea turtles was not rendered irrational by the fact that the model was prepared to assess the impact of shrimp-trawl regulations on loggerhead populations or that the model relied on mortality data collected in the mid 1970s and late 1980s. The model was the best available science, in-water survey data did not exist, and no expert offered any alternative for analyzing jeopardy. 217.

Plaintiffs argue that the model is so uncertain as to be arbitrary. Although the "best available science" does not always pass must under a rationality test, in this case, the agency's choice of methodology was not irrational since the necessary quantitative data simply does not exist. 220.

In *Columbia Falls*, the D.C. Circuit established that "[a]n agency's use of a model is arbitrary if that model 'bears no rational relationship to the reality it purports to represent.' 139 F.3d 914, 923 (D.C. Cir. 1998)." 220. The *Columbia Falls* court found the use of a model to be arbitrary and capricious because evidence showed that the byproduct would actually be exposed to disposal conditions different from those simulated by the model. However, in this case, "even if flawed or limited in its application, the model bears a rational relationship to the reality it purports to represent." 221.

3. State of Conn. v. EPA, 696 F.2d 147 (2d Cir. 1982) – State of Connecticut sought review of EPA's final rule permitting an electric company in NY to continue burning 2.8% sulfur content fuel until Sept. 24, 1984.

   The Court rejected challenges to the statistical modeling used by the EPA in assessing the impact of the plant's emissions upon Connecticut's air. Petitioners alleged that the Agency contravened its own Guideline on Air Quality models when it decided to rely on the CRSTER model. 158. However, the guidelines ultimately state that "each complex situation be treated on a case by case basis with the assistance of expert advice." 159. The EPA adopted this case-by-case approach, adjusting the model to account for terrain complexities in Connecticut and providing a detailed technical rationale for the inadequacy for other proposed models. 159.

   See also Alabama Power Co. v. Costle, 636 F.2d 323 (D.C. Cir. 1979), upholding EPA modeling regulations under the CAA. "Of great importance is a reasoned agency response to substantial questions of fact, policy or science raised in comments on recommended models or in proposals to employ new techniques." 387. Modeling "is on 'the frontiers of scientific knowledge,' but the lack of scientific certitude about modeling techniques increases rather than reduces the need for the agency to critically examine all substantial questions of fact and science emerging from the commenting process." 387-88.

4. West Virginia v. EPA, 362 F.3d 861 (D.C. Cir. 2004) – two states and several businesses and energy policy entities petitioned for review of EPA's rules requiring various states to revise SIPs.

   "'While courts routinely defer to agency modeling of complex phenomena, model assumptions must have a rational relationship to the real world.' Appalachian I, 249 F.3d at 1053." 866-67.

   Under the arbitrary and capricious standard of review set forth by the CAA and APA, "'[a]gency determinations based upon highly complex and technical matters are entitled to great deference' . . . particularly when we review the use of computer models, because 'their scientific nature does not easily lend itself to judicial review.' *Appalachian Power Co. v. EPA*, 135 F.3d 791, 802 (D.C. Cir. 1998). The EPA has 'undoubted power to use predictive models' as long as it 'explain[s] the assumptions and methodology used," and the court will "defer to the agency's decision on how to balance the cost and complexity of a more elaborate model against the oversimplification of a simper model[;]" although court will vacate if agency's conclusions drawn from this model are unreasonable. 867-68.

5. Novartis Corp. v. Ben Venue Laboratories, Inc., 271 F.3d 1043 (2001) – patentee brought action against alleged infringer relating to patent on forms of crystalline pamidronate

disodium. The court held that the patentee failed to create a genuine issue of material fact as to whether the claimed product formed during alleged infringer's manufacturing process.

> "There is nothing inherently unreliable or suspect about computer simulations as evidence, but every simulation of a physical process embodies at least some simplifying assumptions, and requires both a solid theoretical foundation and realistic input parameters to yield meaningful results. Without knowing these foundations, a court cannot evaluate whether the simulation is probative, and it would be unfair to render an expert's opinion immune to challenge because its methodology is hidden in an uncommented computer model." 1054.

6. Natural Resources Defense Council v. Herrington, 768 F.2d 1355 (D.C. Cir. 1985) – Petitioners challenged DOE's final rules determining that mandatory energy-efficiency standards were not justified for eight types of household appliances.

   DOE's use of econometric computer model to project future energy consumption of household appliances was not arbitrary or irrational since the agency provided a reasoned basis for use of its model. However, the use of statistics for annual hours of operation of central air conditioners, in an econometric model designed to project energy savings from standards, was not supported by substantial evidence.

   "'An agency may utilize a predictive model so long as it explains the assumptions and methodology it used in preparing the model. If the model is challenged, the agency must provide a full analytical defense.' *Eagle-Picher Indus., Inc. v. EPA*, 759 F.2d 905, 921 (D.C. Cir. 1985). However, we will defer to an agency's judgment to use a particular model if the agency examines the relevant data and articulates a reasoned basis for its decision. *See id.* at 921-22; *Small Refiner Lead Phase-Down Task Force v. EPA*, 705 F.2d 506, 535 (D.C. Cir. 1983); *Sierra Club v. Costle*, 657 F.2d 298, 332-33 (D.C. Cir. 1981)." 1385.

   The ORNL model utilized by the DOE was not developed specifically for this rulemaking. The model's algorithm "quantified DOE's assumption that as fuel prices go up, market distortion…will go down." 1385-86. The algorithm reflects three specific propositions about the consequences of higher fuel prices on the market: consumers will purchase more efficient appliances, consumers will accept longer payback periods, diminishing market distortion, and the expected change in market distortion can be quantified in a specific mathematical formula. 1387. Although petitioners challenged these propositions, the DOE acknowledged the problems raised and offered a reasoned defense to its conclusions (e.g., defects were extremely difficult to fix and of relatively minor moment to the rulemaking).

   Although the DOE's efforts to verify the algorithm empirically proved disappointing, commenters did not provide another method of predicting future market distortion. 1390.

"The safety valves in the use of such sophisticated methodology are the requirement of public exposure of the assumptions and data incorporated into the analysis and the acceptance and consideration of public comment, the admission of uncertainties where they exist, and the insistence that ultimate responsibility for the policy decision remains with the agency rather than the computer. With these precautions the tools of econometric computer analysis can intelligently broaden rather than constrain the policymaker's options and avoid the 'artificial narrowing of options that [can be] arbitrary and capricious.' *Sierra Club v. Costle,* 657 F.2d 298, 334-35 (D.C. Cir. 1981)."1391.

7. Natural Resources Defense Council v. U.S. Army Corp. of Engineers, 2001 WL 1491580 (S.D.Fla. June 28, 2001) – challenge to the implementation of a hydrological model in accordance with the ESA

   The Corps' Hydraulic Engineer, Dr. Richard Punnett, used the South Florida Water Management Model (SFWMM) rather than the Service's recommended MODBRANCH computer because the SFWMM Model was widely accepted as the best available model for the task at hand.

   "On judicial review, the role of the Court is not to attempt to become a tie-breaking technical expert." *9.

8. City of Wichita v. Trustees of APCO Oil Corp., 306 F.Supp.2d 1040 (D.Kan. 2003) – City brought CERCLA action against potentially responsible parties, seeking contribution for prior response costs and declaration of responsibility for future response costs.

   Expert testimony on computer modeling of groundwater flows was insufficiently reliable to be admissible because the expert failed to correlate model results with field data, assumed relevant ground conditions without obtaining confirmation, and deviated from usual modeling methodology. 1107.

   "If properly used, computer models appear to be an invaluable tool in approximating the complexities of underground fluid flow. Without these modes, the scientists and engineers would be limited to guessing at sources and fluid flow characteristics based on the limited number of wells that penetrate the aquifer… Unfortunately, there are no true crystal balls – the models are only as good as the data placed into them. In this case, the data inputs and methods for configuring the models provided fertile ground for disagreement. Nonetheless, the court concludes that computer modeling of plume size is an appropriate basis for allocating costs. The real question is simply whose model to use." 1106-07.

   "Computer modeling is an accepted and, in appropriate circumstances, reliable method for use in determining groundwater flow and contaminant transport in an aquifer, and to evaluate the effectiveness of remedial alternatives. . . . Nevertheless, even in the best of circumstances, a model is only an estimate and the accuracy of the estimate depends to a considerable extent on the data selected for use in the computer model, the quality and reliability of that data and, of course, the skill of the modeler." 1108.

9. Principi v. Survivair, Inc., 2005 WL 5960352 (M.D.Fla. Oct. 18, 2005) – Plaintiff brought action for negligence and strict liability as to the design and manufacture of a breathing apparatus.

   Plaintiff argues that Defendant's expert witness' opinions are unreliable because they are based on a simulation that deviated from the actual occurrence in several material ways. As a result, the court analyzed the reliability of the simulation conducted.

   "[T]he Court disagrees that the simulation must replicate exactly all of Plaintiff's activities during the CTT for it to be reliable. . . . Any differences may be addressed on cross-examination and in argument." *4.

10. Oceana, Inc. v. Locke, 674 F.Supp..2d 39 (D.C. Cir. 2009) – fishing company alleged final rule promulgated by NMFS regarding amendment to standardized bycatch reporting methodology violated various Acts.

    "Where a scientist challenges the manner in which an agency has relied upon her own research, her unique familiarity with the meaning of that research can constitute 'particularly relevant' background information about the basis for the agency's decision. Carlton v. Babbitt, 26 F.Supp.2d 102, 108, 111 (D.D.C. 1998) (ruling that agency should have considered scientist's declaration…because agency ultimately relied solely upon that scientist's research article for certain conclusions….). 47.

11. BCCA Appeal Group v. EPA, 355 F.3d 817 (5th Cir. 2003) – industries, local government, and environmental groups petitioned for review of EPA's rule approving Texas' state implementation plan for ozone attainment (notably the CAA requires that an attainment demonstration be "based on photochemical grid modeling." 42 U.S.C. § 7511a(c)(2)(A).

    EPA's reliance on the state's photochemical grid modeling to determine whether the proposed SIP would satisfy the CAA requirements was not arbitrary, capricious, or contrary to law. 832-33. Although such models "are imperfect tools for predicting future air quality, a modeled attainment demonstration 'provide[s] a reasonable expectation that the measures and procedures outlined will result in attainment of the NAAQS by [the statutory deadline.' . . . "'[A] reviewing court must remember that the [agency] is making predictions, within its area of special expertise, at the frontiers of science. When examining this kind of scientific determination, as opposed to simple findings of fact, a reviewing court must generally be at its most deferential.' *Baltimore Gas 7 Elec. Co. v. NRDC*, 462 U.S. 87, 103 (1983). The court's role is to evaluate whether the EPA's projections represent arbitrary or capricious exercises of its authority, not whether they are accurate." 833.

    EPA determined that the Texas model provides reasonable predictions as confirmed by comparisons with monitoring data and therefore can provide an acceptable estimate of the amount of emissions needed for attainment. The model was validated by various diagnostic and sensitivity analyses and graphical and statistical performance measures (e..g, normalized bias, gross error). "This explanation is reasonable and is supported by the record, and, therefore, EPA's determination is entitled to deference." 832. Overall, the EPA recognized the model's shortcomings and provided plausible explanations that were supported by the record. 834.

12. League of Wilderness Defenders Blue Mountains Biodiversity Project v. FS, 615 F.3d 1122 (9th Cir. 2010) – conservation groups brought action against FS alleging that project authorizing logging violated NFMA and NEPA.

    "In creating the EIS, the Forest Service conducted computerized simulations to determine the effects of wildfires on the Project area under three different treatment scenarios…." 1127.

    Deference to an agency's decision "is highest when reviewing an agency's technical analyses and judgments involving the evaluation of complex scientific data within the agency's technical expertise." 1130.

    Dissent: criticizes the FS' reliance on a computer simulation that is not grounded in any actual information about fire frequency in the area of concern. 1148.

13. San Luis & Delta-Mendota Water Authority v. Salazar, 760 F.Supp.2d 855 (E.D. Cal. 2010) – water districts, state water contractors, and water users brought action under ESA challenging FWS' biological opinion addressing the impact of state water projects.

    The FWS' failure to employ a quantitative life-cycle model did not violate the ESA's best-available-science requirement. 881. Instead, the BiOp used a relatively simple, non-quantitative, conceptual life-cycle model. 882. Uncertainty in survey data, due to random sampling error and bias, complicated model fitting. As a result, at the time the BiOp was issued, an appropriate life-cycle model did not exist. "[I]n the absence of such a model, and because one could not be developed during the time allowed for this consultation, the techniques used by USFWS do reflect generally-accepted scientific standards and practices." 884.

    Under the APA, "[c]ourts are not required to defer to an agency conclusion that runs counter to that of other agencies or individuals with specialized expertise in a particular technical area." 872.

    "As a general rule, choices regarding modeling methods are exactly the sort of choices that, under the APA, are left to the expert agency in the exercise of discretion. *NWF v. EPA*, 286 F.3d at 565. A court 'may reject an agency's choice of a scientific model only when the model bears no rational relationship to the characteristics of the data to which it is applied.' *Id.* at 565 (internal quotations and citations omitted). *Lands Council* instructs that a court is 'not free to impose on the agency [its] own notion of which procedures are best. . . . Nor may [it] impose procedural requirements not explicitly enumerated in the pertinent statutes.' 547 F.3d at 993." 908-909.

"Comparison of Calsim II to Dayflow model runs created potentially material bias in the BiOp's evaluation of the impact of Project operations…. FWS' failure to address or explain this material bias represents a failure to consider and evaluate a relevant factor and violates the ESA and APA." 968. In NWF v. EPA, the EPA applied a particular model to predict whether businesses were likely to go bankrupt as a result of additional regulation. NWF criticized the model on several grounds, including its error rate of 15%. However, the D.C. Circuit rejected each critique, reasoning that none called into question the model's reliability. However, in this case, undisputed expert testimony calls into question the manner by which FWS utilized two models to evaluate the impact of project operations. "Unlike *NWF v. EPA*, where the agency applied a model that was deemed reliable, here, FWS has not addressed or explained the material bias created by its methodological choices." 909.

"FWS' use of a linear stock-recruit model, although scientifically criticized, was not arbitrary, capricious, or clear error." 969. Plaintiff's expert testified that linear models are not effective for modeling fish populations and standard practice is to use a multiplicative stock-recruit model. 920. "Multiplicative models are the textbook standard for modeling fish and other populations." 921. The FWS also received several comments recommending the use of a logarithmic model. "A court 'may reject an agency's choice of scientific model only when the model bears no rational relationship to the characteristics of the data to which it is applied.' NWF v. EPA, 286 F.3d at 565; see Nat'l Ass'n of Metal Finishers v. EPA, 719 F.2d 624, 657 (3rd Cir. 1983) ('the choice of scientific data and statistical methodology to be used is best left to the discretion of the [agency])…." 922. Scientific dispute exists among experts and some evidence exists that use of the linear model is not totally inappropriate. "It is a close call. Absent agency bad faith, Plaintiffs have not established that this modeling dispute proves FWS violated the best available science standard." 922.

14. Cleveland Elec. Illuminating Co. v. EPA, 572 F.2d 1150 (6th Cir. 1978) – Companies and the state of Ohio petitioned the court to review imposition of EPA's sulfur dioxide pollution control plan.

The court held that the use of the real-time-air-quality-simulation model by the EPA was a rational choice and not arbitrary or capricious. "It is, of course, no part of the responsibility of this court to determine whether the RM model represents the best possible approach to determining standards for the control of sulfur dioxide emissions. Our standard of review of the actions of United States EPA is whether or not the action of the agency is 'arbitrary, capricious, an abuse of discretion, or otherwise not in accordance with law.'" 1161. Overall, the EPA's use of the Ram model is supported by sufficient evidence: 1162-63

1) EPA's use of a "rollback" model was strenuously object to at public hearings.
2) EPA responded by devising and adopting the Ram model

3) The RAM model can be applied to many individual sources of pollution and employs a wider, more complete and accurate data base than any prior model.

Cases – Westlaw Most Cited[17]

C [Cited 4 times for this legal issue]

Eclipse Electronics v. Chubb Corp., 176 F.Supp.2d 406

157 EVIDENCE

157XII Opinion Evidence

157XII(D) Examination of Experts

157 k557 k. Experiments and results thereof.E.D.Pa.,2001

Engineer's expert opinion was reliable as to effect of environmental conditions on electronic connectors stored in warehouse in action to recover for damages to inventory of connectors, even though expert did not actually test all connectors in warehouse, **where opinion was based on widely-accepted industry study used in creation of standards for simulating environmental conditions that mirrored real world environmental conditions, model carried with it low actual and potential error rate, expert had extensive experience as engineer, and lack of extensive testing went to weight, not admissibility, of testimony**. Fed.Rules Evid.Rule 702, 28 U.S.C.A.

H [Cited 3 times for this legal issue]

Ruff v. Ensign-Bickford Industries, Inc., 171 F.Supp.2d 1226

D.Utah.C.Div.,2001

Degradation pathway for royal demolition explosive (RDX) predicted by McCormick was generally accepted in scientific community, and thus was sufficiently reliable to permit dose estimation expert to base his prediction upon model in action alleging that explosives manufacturer's release of RDX and its breakdown properties caused non-hodgkins lymphoma cancers**, despite one other study predicting another degradation pathway; manufacturer's expert stated that McCormick's theory represented most widely cited model and cited McCormick pathway in his recent pre-litigation scientific publications, McCormick pathway was peer-reviewed and had been cited 41 times in peer reviewed literature, and at least three scientists had published studies confirming existence of RDX and its breakdown products as predicted in McCormick study.**Fed.Rules Evid.Rule 702, 28 U.S.C.A.

H [Cited 0 times for this legal issue]

Abarca v. Franklin County Water Dist., 2011 WL 140371

E.D.Cal.,2011

Scientific factual disputes concerning reliability of hydrologist's groundwater model, including reliability and accuracy of sampling data from allegedly contaminated well and monitoring wells, reliability of model in light of its exclusion of such sampling data and hydrologist's failure to calibrate entire model,

[17] Highlighted cases appear to be most relevant.

and existence of substantial impermeable clay layer beneath allegedly contaminated well, warranted admission of model at trial on issue of groundwater contamination caused by former wood-treatment facility in action for, inter alia, negligence, trespass, nuisance, and wrongful death brought by current and former area residents against, among others, former owners of facility's operators, **subject to court's reserved authority to strike model if trial proceedings ultimately showed that it was not supported by proper scientific foundation.** Fed.Rules Evid.Rule 702, 28 U.S.C.A.

[Cited 7 times for this legal issue]
Liquid Dynamics Corp. v. Vaughan Co., Inc., 449 F.3d 1209
C.A.Fed.Ill.,2006
Competitor's **challenge to computer simulations** used by patentee's expert to establish infringement of helical-and rotational-flow claim limitations of patent directed to method and apparatus for handling waste water slurries in storage tanks **went to the weight of the evidence rather than the admissibility of expert's testimony and analysis**; competitor did not challenge reliability of computational fluid dynamics (CFD) analysis used by expert, but instead argued that the expert applied inaccurate parameters. Fed.Rules Evid.Rule 702, 28 U.S.C.A.

[Cited 1 times for this legal issue]
In re Flood Litigation Coal River Watershed, 668 S.E.2d 203
W.Va.,2008
Report by state agency and testimony of two engineers were sufficiently reliable for admission as expert testimony as proffered by property owners in first phase of action against timbering companies arising from flooding allegedly caused by upstream timbering activities, in which jury determined if company had materially increased peak flow of surface water from its property, if increase materially caused or contributed to causing streams in watershed to overflow their banks, and if company's use of its land was reasonable; authors and engineers had extensive training and professional experience, and **computer models they used were an accepted methodology within engineering profession**. Rules of Evid., Rule 702.

[Cited 0 times for this legal issue]
Abarca v. Franklin County Water Dist., 2011 WL 140371
E.D.Cal.,2011
A half-calibrated model is, by definition, inadequately calibrated and excluded under *Daubert*test for determining admissibility of expert testimony. Fed.Rules Evid.Rule 702, 28 U.S.C.A.

[Cited 0 times for this legal issue]
Cantrell v. Ashland Oil, Inc., 2010 WL 1006391
Ky.,2010
Alleged acceptance by scientific community of linear-no-threshold (LNT) **model** for analyzing health risks of ionizing radiation did not render reliable testimony of property owner's expert witness as to possible future harm to owners' property as result of radiation contamination caused by oil company's allegedly negligent oil production, in

owners' trespass suit against company; LNT **model measured only future risks of radiation exposure, but owners were required to prove that contamination unreasonably interfered with their current use and enjoyment of their property** in order to prove an actual harm or injury and be entitled to actual damages.

H [Cited 0 times for this legal issue]
In re Static Random Access memory (SRAM) Antitrust Litigation, 264 F.R.D. 603
N.D.Cal.,2009
Expert opinions of indirect purchaser plaintiffs' experts were admissible at the class certification stage of antitrust proceedings; economic principles and **regression models relied upon by the experts were solidly grounded in the academic literature**, and they cited extensive facts and data from the case that they reviewed and relied upon in rendering their opinions. Fed.Rules Evid.Rule 702, 28 U.S.C.A.

H [Cited 0 times for this legal issue]
In re Matter of Complaint of Atlantic Marine Property Holding Co., Inc., 570 F.Supp.2d 1363
S.D.Ala.S.Div.,2008
Meteorologist's proffered expert testimony as to wind speeds at shipyard where barge broke loose from its moorings during hurricane was not rendered unreliable, and thus inadmissible in barge owner and charterer's action seeking exoneration from or limitation of liability for property damage allegedly resulting from barge's breakaway, by his **use of computer model used to project path of a hurricane, although the model was used principally by another individual and it was unknown what peer review it had received, where meteorologist's use of the model was not basis for his conclusion regarding wind speeds, and his testimony regarding path of hurricane predicted by the model would not be offered to show its accuracy**. Fed.Rules Evid.Rule 702, 28 U.S.C.A.

H [Cited 0 times for this legal issue]
Green Mountain Chrysler Plymouth Dodge Jeep v. Crombie, 508 F.Supp.2d 295
D.Vt.,2007
Expert's testimony on impact of future climate change in the region was reliable and relevant in suit challenging regulations establishing greenhouse gas (GHG) emissions standards for new automobiles; **testimony was based in part on climate models prepared by other scientists which had been selected by the United States government for use in the U.S. Global Climate Change Research Project's assessment of regional global warming impacts.** Fed.Rules Evid.Rules 702,703, 28 U.S.C.A.

H [Cited 0 times for this legal issue]
Acker v. Burlington Northern and Santa Fe Ry. Co., 347 F.Supp.2d 1025
D.Kan.,2004
Proposed expert testimony regarding height of flood waters on property was sufficiently reliable to warrant its admission in property owners' action alleging that train's presence on tracks near property caused flooding on property, **despite railroad's**

contention that expert's model was inaccurate with respect to actual surveyed flood depths, that expert calibrated his hydrologic model on irrelevant past flood, and that expert's use of effects of embankment and bridge on flood were time-barred, where fact issues remained as to surveyed flood depths, flood elevations for past flood were known, expert used slightly modified version of model approved by Army Corps of Engineers, and it would be impossible to model effect of train without also considering bridge and embankment. Fed.Rules Evid.Rule 702, 28 U.S.C.A.

H [Cited 0 times for this legal issue]
Lyons v. J.A. Auger, Inc., 821 So.2d 536
La.App.2.Cir.,2002
It was proper for the trial court to allow accident reconstruction expert to testify as to results of computer simulation of accident, without performing a *Daubert* analysis of the simulation, if it believed that expert's reliance on the simulation was a reasonable one for experts in his field. LSA-C.E. art. 705.

See also 105 American Law Reports, Federal 299 (1991)
29A Am. Jur. 2d Evidence § § 708-753 (Reliability of scientific technique and its acceptance within scientific community as affecting admissibility, at federal trial, of expert testimony as to result of test or study based on such technique--modern cases).

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3. Thomas O. McGarity & Wendy E. Wagner, Legal Aspects of the Regulatory Use of Environmental Modeling, 10 Envtl. L. Rep. 10,751 (2003).
4. Daniel A. Farber, Modeling Climate Change and its Impacts: Law, Policy, and Science, 86 Tex. L. Rev. 1655 (2008).

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