Very Large System Dynamics Models – Lessons Learned

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Abstract

This paper provides lessons learned from developing several large system dynamics (SD) models. System dynamics modeling practice emphasize the need to keep models small so that they are manageable and understandable. This practice is generally reasonable and prudent; however, there are times that large SD models are necessary. This paper outlines two large SD projects that were done at two Department of Energy National Laboratories, the Idaho National Laboratory and Sandia National Laboratories. This paper summarizes the models and then discusses some of the valuable lessons learned during these two modeling efforts.

Key Words: Large models, model validation

Introduction

The Idaho National Laboratory and Sandia National Laboratories have been developing capabilities in system dynamics. As national laboratories, the researchers are tasked with large complex problems that can have long and significant impacts to national policy. The nature of the problems that the labs address with system dynamics typically places the models in the category of large System dynamics models. Although large models are not the preferred modeling practice within the SD community there are times when it is necessary.[1] There are some valuable lessons to be extracted from the work we have done at the national laboratories developing large system dynamic models. The purpose of this paper is to discuss the lessons learned from developing very large SD models. This will be done through two recent case studies, one at the Idaho National Laboratory and the other at Sandia National Laboratories.

Case 1 – VISION

Model Description

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The United States Department of Energy's Advanced Fuel Cycle Initiative's (AFCI) System Analysis group is performing broad system analyses of future nuclear energy in the United States.[2] The Idaho National Laboratory (INL) has been collaborating with Argonne National Laboratory (ANL) and Sandia National Laboratories (SNL) in developing a system dynamics (SD) model of the U.S. commercial nuclear fuel cycle. The Verifiable Fuel Cycle Simulation (VISION) model is being used to analyze and compare various proposed technology deployment scenarios.[3] The model is designed to give a better understanding of the linkages between the various components of the nuclear fuel cycle that includes uranium resources, reactor number and mix, nuclear fuel type and waste management. The model has evolved into a very large dynamic simulation model. At the outset, the model was envisioned to be complex and complete but the relative size was not expected to be nearly as large as it has evolved to. Two of the reasons for the evolution from a mid-sized model to a large model are necessity and success. As the model evolved, it because evident that more detail was needed to be able to properly capture the dynamics of the system at the level of detail required by the customers. In addition, as the model developed other groups saw the value of this type of model are added their requirements to the mix of previously established requirements.

There are a number of distinct components in the nuclear fuel cycle. These components, as outlined in Figure 1, include mining and milling of raw uranium, fuel fabrication, reactors, spent fuel storage, spent fuel separations, and waste management. Each of these components although separate components are tightly connected to the nuclear fuel cycle but usually analyzed in isolation of the other parts. This model links these components into a single model for analysis and includes both mass flows and economics. VISION is intended to assist in evaluating "what if" scenarios and in comparing fuel, reactor, and spent fuel separation alternatives at a systems level for U.S. commercial nuclear power. The model is not intended as a tool for process flow and design modeling of specific facilities or for tracking discrete units of fuel or other material through the system. VISION is intended to examine the interactions among the components of the U.S. nuclear fuel system as a function of time varying system parameters and provide a comparative analysis of different scenarios; this model represents a dynamic rather than steady-state approximation of the nuclear fuel system.

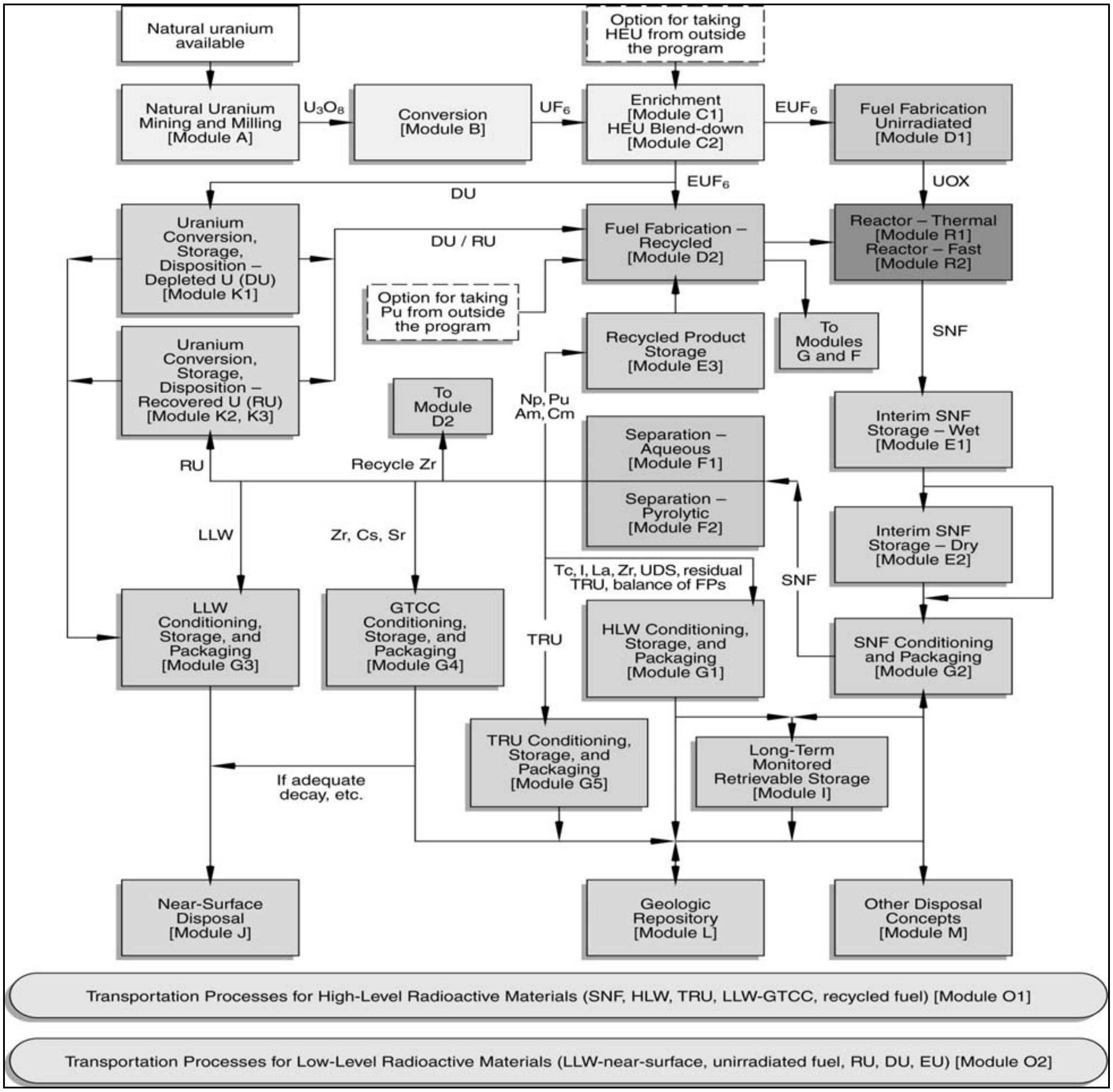

Figure 1: Schematic of VISION modules representing the nuclear fuel cycle processes and facilities and showing mass flow.

VISION is a large model by SD measures. The following list describes some of the model details:

- Composed of 42 modules (a module represents a separate component of the system)
- Approximately 3,300 variables
- 68 ranges (named arrays or matrix dimensions)
- 2,233,794 elements e.g. a variable with the dimension
- 4 sub-models.

In fact, the model is so large that the original version of the model which was developed in Stella[4] had to be rebuilt in Powersim Studio[5] because it became too large to add any more variables.

AFCI Systems Analysis group developed a set of four possible strategies that they were most interested in understanding and comparing. These four strategies basically covered the entire option space in terms of separations and waste management paths. In this context, a strategy is a general approach to fuel management that encompasses a range of options with similar characteristics. A strategy identifies nuclear reactor mix and recycle strategies. The four strategies are:

- The current U.S. strategy is **once-through -** all the components of spent fuel are kept together and eventually sent to a geologic repository. This strategy uses existing types of nuclear power plants, which are all thermal reactors.
- The second strategy is **limited recycle**, recycling transuranic elements once. Remaining transuranic elements and long-lived fission products would go to geologic disposal. Uranium in spent fuel, depleted uranium, and short-lived fission products would be disposed as low-level waste. This strategy uses existing types of nuclear power plants, which are all thermal reactors.
- The third strategy is **continuous recycle**, recycling transuranic elements from spent fuel repeatedly until destroyed. Continuous recycle is more technically challenging than limited recycle and therefore more research, development, and deployments would be required. Uranium in spent fuel can be recycled or disposed. Essentially no transuranic elements would go to geologic disposal. Long-lived fission products would either go to geologic disposal or some could be transmuted in power plants. Short-lived fission products would be disposed as low-level waste. This strategy would primarily use thermal reactors; however, a small fraction of fast reactors may be required.
- The fourth strategy is **sustained recycle**, which differs from transitional recycle primarily by enabling the recycle of depleted uranium to significantly extend fuel resources. This strategy would primarily use Generation IV fast reactors.

Figure 2 presents the four strategies in a diagram that outlines the path for each strategy. VISION was designed to simulate each of the above four strategies. Below are some results that demonstrate the outcomes and comparison capabilities that are available through VISION.

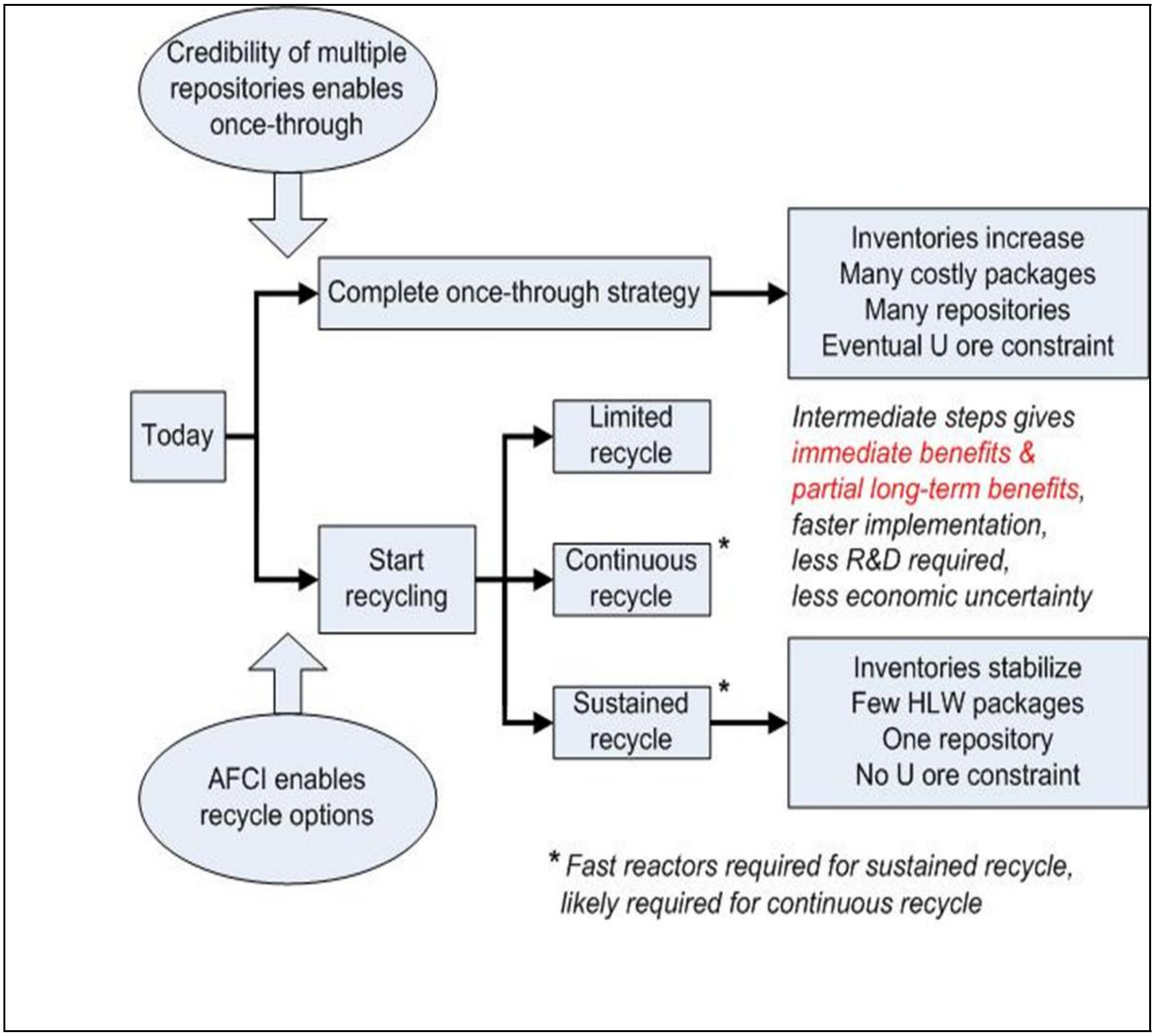

Figure 2: This diagram depicts the four basic strategies for nuclear growth in the US.

For each strategy, there are a myriad of options that need to be set, growth rate, fuel type, reactor parameters, process times. In order to make the comparisons useful, most of the parameters were held constant through out the scenario comparisons. Only those parameters necessary to match the basic strategy were modified.

We developed these five scenarios that covered the 4 key strategies listed above. The scenarios are:

- Once-through (current US strategy)
- Multiple recycles mixed oxide fuel
- Multiple recycles inert matrix fuel
- Thermal fuel supplying fuel to burner fast reactor with multiple recycles
- Thermal fuel supplying fuel to breeder fast reactor with multiple recycles

Each scenario starts in 2000 with spent fuel recycling starting in 2020 (where appropriate), and growth is 1.8% per year starting in 2010. Figure 3 shows a comparison of the 5 scenarios for total fresh uranium usage.

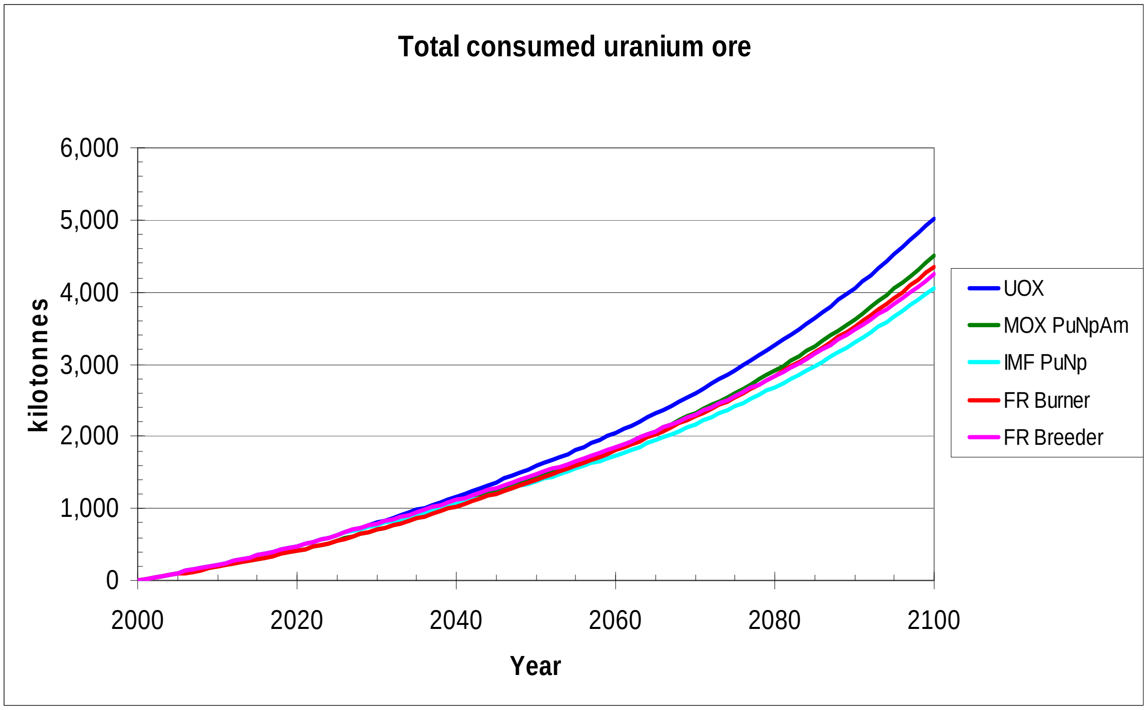

Figure 3: This chart shows a comparative graph of uranium consumption across the 5 different scenarios.

Figure 4 shows a chart for a single run that breaks the costs down across the five major cost elements, front end costs, back end costs, recycling costs, reactor operation costs and reactor capital costs. These types of charts are very useful in identifying the components that are most influential on the overall costs.

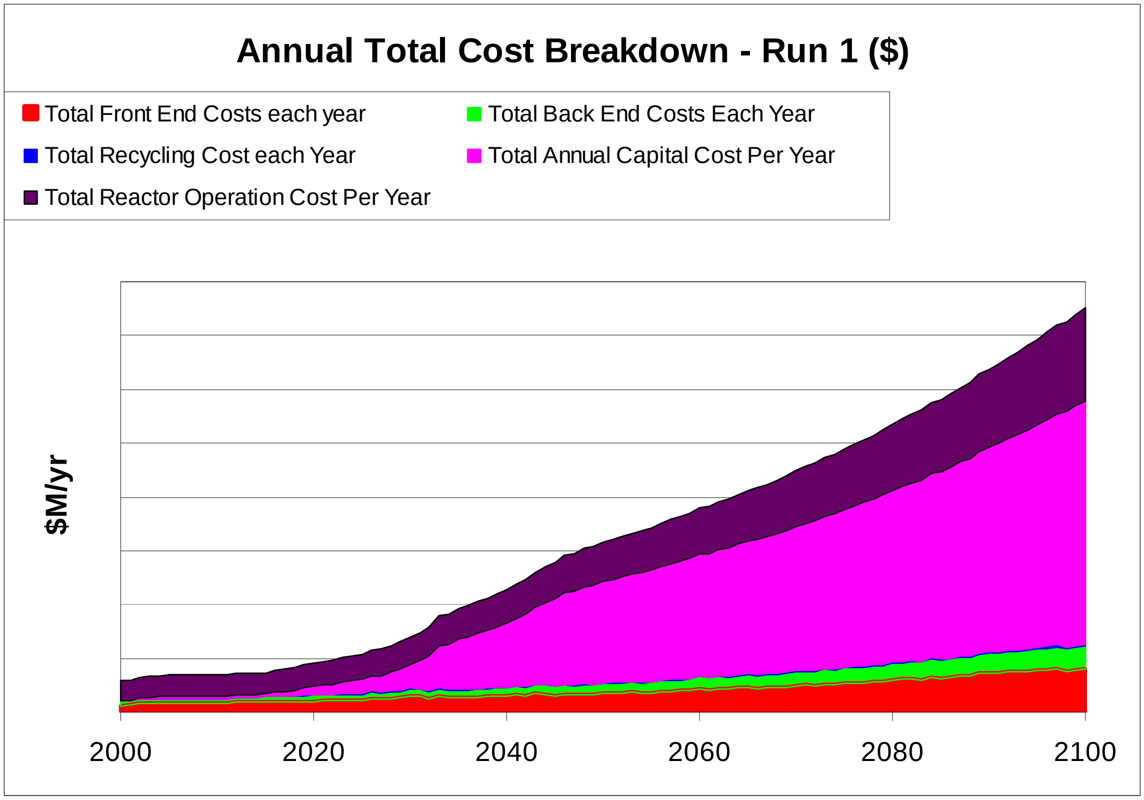

Figure 4: This charts shows the break down of the costs for a single run across the five major cost components.

VISION is able to produce a multitude of comparison charts such as the one shown above that allows for a quick comparison of different strategies on a variety of metrics.

Modeling Process

The INL has a set of requirements for every software development project which closely follows ANSI/IEEE 1058.1-1987 *Standard for Software Project Management Plans.*

Prior to any modeling activities it was necessary to develop a software management plan (SMP) and software requirements specifications (SRS) document.[6] The SMP outlines the development responsibilities, the development process, procedures for revision control and procedures for verification and validation. The SRS establishes the customer's minimum requirements that the model must meet at completion. In the SRS, it is important to outline not only what the model should do but also what the model is not intended to do. The document should capture the end-users expectations and make it clear what is expected. The SRS is a "living" document and can and should be updated as the modeling progresses. For very large models it is unlikely that all the specifications will be captured at the start of the process. Any changes to the SRS should be revision controlled so that the new requests are documented.

The SRS will also be helpful in determining the correct platform that the modeling should be done in. It is at this point that the programmer/modeler determines whether this is in fact a system dynamics model or if there is a more appropriate too for the application. It the end user desires discrete tracking or components throughout the lifecycle of the component then SD is probably not appropriate and forcing the model into that platform is going to lead to an inferior product.

VISION is about process flow of material, so the most natural way to divide up the model is by "plumbing". There were advantages to this process, such as, when working with subject matter experts in each area they were able to visually understand how we were modeling their sector by the views.

Modeling

VISION is the collective knowledge of subject matter experts from every area of the nuclear fuel cycle.

- Fuels
- Reactor Physics
- Waste Management
- Separations

There are many experts in each of the areas identified above but very few experts that understand every area of the nuclear fuel cycle and how those areas interact together in a unified system. VISION was able to capture the knowledge of subject area experts in each of the above areas and link the processes together into a functional system.

Benchmarking and Validation

Validation of large complex dynamic models is very difficult. It is important that good modeling practice be exercised from the start in order to facilitate the validation process. Naming convention, model structure, units should all follow a strict guideline that is established before any modeling is started.

During the modeling process it is very important to manage the customer and their requests. Any new request for enhancements needs to be evaluated for its value versus the complexity to add it to the model. Many requests add very little in terms of supplying understanding but a great deal in terms of complexity. The effects are in the "noise" but require a lot of modeling effort and validation. The modeler needs to be continuously asking the questions,

- "What is the value added with this enhancement"
- "How difficult is it to add to the model"
- "How difficult is it to validate the change"

From these questions, a return on investment can be estimated and the customer can determine if they are willing to pay the price for the enhancement. There are times when an enhancement will return little but the customer feels strongly enough about it that they want it added anyway. This can be very frustrating for a modeler when time and resources are being stretched to meet deadlines.

Models like most analysis activities have but one life. Anyone who uses the model and determines the model produces invalid results will lose confidence in the model results. It is very difficult if not impossible to re-establish their trust in the model. Therefore, it is essential that prior to any release of the model to verify and validate the model.

Due to the nature of the model and the intended end-use it was imperative that VISION be tested and validated at a very rigorous level. There were several levels of verification and validation performed on VISION. The first was done in-house. The model went through a number of tests including unit consistency, boundary adequacy, extreme conditions and integration error. In addition, the model was tested against other models.

The second step in the validation process was to have an outside source check the model. Modelers from Sandia National Laboratories that were not involved in the development of the model were requested to do an independent evaluation of the VISION model. Ideally they might have been involved in the modeling process as the model progressed.[7] The results were compiled in a report delivered to the INL upon completion. The basic finding of their report, using objective tests, verified that VISION was producing replicable and reasonable results.

The benchmarking activity was conducted to verify whether results obtained with the VISION model reasonably approximate system performance, as well as to provide a basis against which future model revisions can be subjected to regression. The five benchmark calculation methods included the DYMOND[8], CAFCA-II[9], and NFCSim[10] system analysis codes, analysis results from a recent NEA/OECD report, and Microsoft Excel spreadsheet calculations. Comparisons are made for alternative scenarios for four alternative model strategies of nuclear power plant fuel cycles, including the current once-through cycle, recycling of fuel through thermal reactors, a two-tiered combination approach for recycling using both thermal and fast reactors, and recycling through fast reactors alone.

Model Applications

It is important to note that VISION has been used for system level analyses since its first revision. The model was supplying an understanding of the complexity of the nuclear fuel cycle from the onset and so has been involved is supporting the AFCI and GNEP activities early on. It is important to note that an operational version of VISION has been necessary since the beginning. Because of this requirement the development of VISION has followed an incremental development process. Each installment of VISION has added new options and additional complexity to the analyses. Because VISION was demonstrating its benefits early on, the funding for the project was never interrupted or constrained even when other programs were experiencing cutbacks. Listed below are several of the activities that VISION has supported:

- VISION has been used to support the analyses that compile the annual AFCI Report to Congress. (2005, 2006, 2007)

- VISION is being used to support the analyses for the Global Nuclear Energy Partnership (GNEP) report to Congress. (Spring 2008)

- Three U.S. Universities are using VISION in their graduate level nuclear fuel cycle classes and six others have requested a copy. (Fall 2007, Spring 2008)

- Three masters of Science graduate students have developed sub-models as their master's projects.

- Five other students are working on sections of VISION for their master's and PhD projects.

VISION is proving to be a good analysis tool for AFCI and GNEP but is also proving to be a good educational tool for universities.

Case 2 – Rio Grande Model

Model Description

The MRG Model is structured as a dynamic water budget with each supply and demand component treated as a spatially aggregated, temporally dynamic variable. The spatial extent of the region is defined by the boundaries of Bernalillo, Sandoval, and Valencia counties in New Mexico. The various water supply, demand, and conservation terms are generally aggregated over the three-county region; however, in some instances features outside the planning region were simulated to accomplish required calculations (e.g., Rio Grande Compact balance is calculated for the entire Middle Rio Grande Basin).

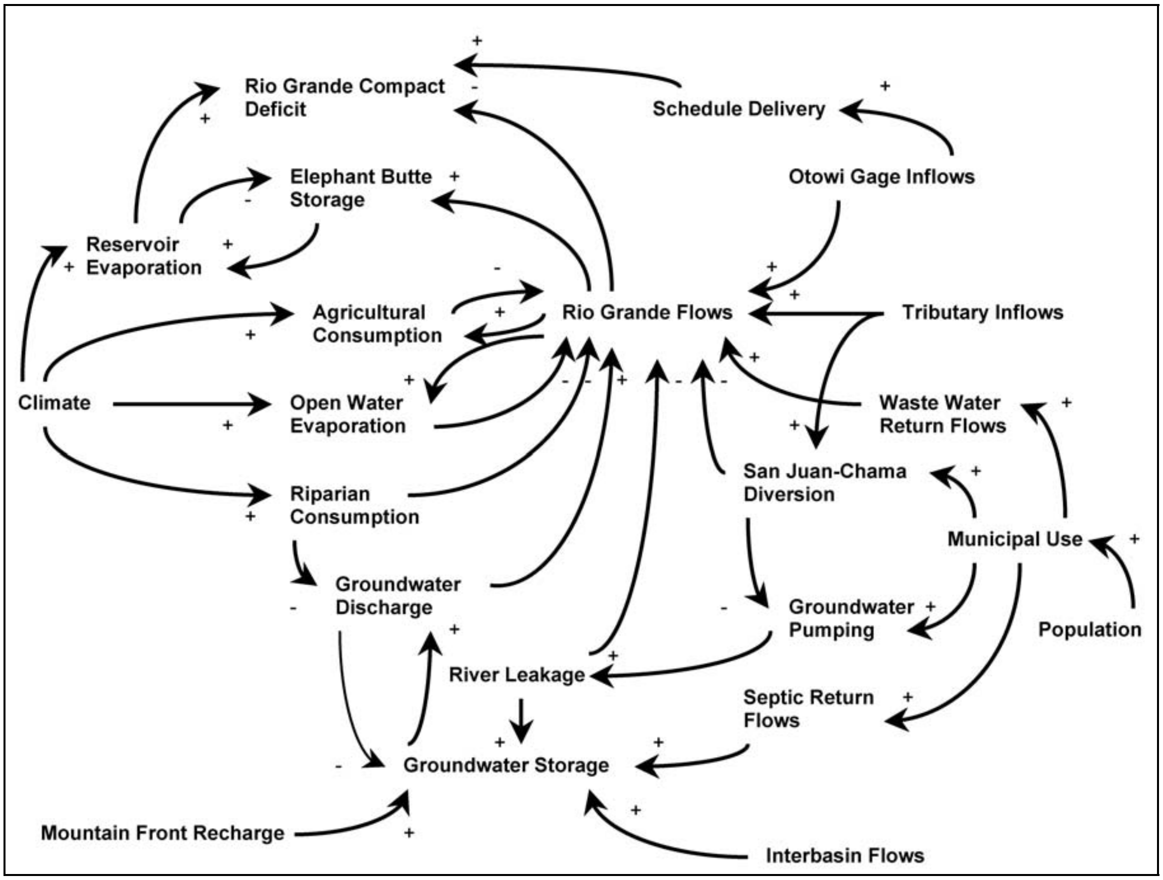

Figure 5**:** Causal loop diagram depicting the key elements influencing water supply and demand in the Middle Rio Grande Planning Region.

The MRG Model is also a large model by SD measures. The following list describes some of the model details:

- Composed of 13 modules (a module represents a separate component of the system
- Approximately 899 variables
- 3 ranges (named arrays or matrix dimensions)
- 5,437 elements e.g. a variable with the dimension

Modeling Process

As a result of the Middle Rio Grande cooperative water planning project growing in complexity it was determined that a model could assist in the planning process. A modeling project was initiated to:

1. provide a quantitative basis for comparing alternative water conservation strategies in terms of water savings and cost,
2. help the public understand the complexity inherent to the regional water system, and
3. engage the public in the decision process.

The team took a mediated modeling approach to the model building process. Although the actually model was built at Sandia National Laboratories, many people participated in bi-weekly modeling meetings. Table 1 lists the stakeholders and their roles in the modeling project. The Sandia National Laboratories team was a part of the CMT.

Table 1**:** List of stakeholders and their roles [11]

Stakeholder	Role
Interstate Stream Commission (ISC)	Manages treaty and interstate compact deliveries of water. Oversight of the statewide water planning process.
Mid Region Council of Governments	A board comprised of city and county officials. Purpose is to coordinate regional (MRCOG) planning.
Middle Rio Grande Conservancy District	Responsible for managing and delivering irrigation water to the farmers (MRGCD) of the Middle Rio Grande region.
City Utilities and Water Cooperatives	Responsible for managing and delivering water to urban and rural water users for domestic, commercial and industrial purposes. Also responsible for capturing and treating resulting wastewater.
Federal/State Agencies	Management of waters and ecosystems of the state. Provided data, models and system understanding in the water planning process.
Middle Rio Grande Water Assembly	Commissioned by the ISC with the responsibility of preparing the 50-year water (MRGWA) plan in cooperation with the MRCOG. Membership open to the public.
Cooperative Modeling Team (CMT)	Subset of MRGWA and MRCOG participants. Purpose was to develop an interactive model to assist in the water planning process.
General Public	Participation through volunteering on the MRGWA and/or participation at quarterly public forums.

Modeling

The model operates on an annual time step encompassing the period 1960–2050. This period includes a 41-year calibration period (1960–2000) and the prescribed 50-year planning horizon (2001–2050). An annual time unit was used because it matched the annual basis of calculation for key metrics in regional water planning (i.e., Rio Grande Compact obligations and groundwater depletions).

Sixty-six variables can be controlled in the model interface by slider bars or switches. The MRG Model like VISION is an application; an application is a model plus a detailed and complex interface or flight simulator. Users can easily simulate various combinations of hydrological, economic or demographic conditions, and then run the model and view output in seconds. This interactive modeling environment allows users in private or public settings to experiment with competing management strategies and evaluate the comparative strengths and weaknesses of each.

Benchmarking and Validation

The years 1960 to 2000 serve as the verification period for the MRG water-planning model. The verification process compares historical data with modeled data for four different variables, including groundwater depletions, Rio Grande Compact balance, Rio Grande flows at the San Acacia gage (located just south of the planning region), and storage in Elephant Butte Reservoir. The Rio Grande Compact legally delineates the water delivery requirements of water in New Mexico to downstream users (e.g. Texas and Mexico).

Model verification played an important role in the overall planning process. First, this effort provided a sense that the model was being tested for credibility and that the model was based on some level of reality. Second, verification of the model demonstrated that at an aggregated, surface/groundwater level, the modeled terms in the water budget achieve balance. Requiring the water budget to balance against historical data was important for several reasons; in particular, balancing the budget helped set reasonable bounds on parameters subject to uncertainty (e.g., mountain front recharge, agricultural consumption and bosque consumption). Balancing also increased confidence that the model could indeed produce output values consistent with other models, models that many of the stakeholders already had confidence in. Historical balancing also caused careful consideration of whether data gathered from disparate sources were all measured and/or calculated in a self-consistent manner. Finally, there were critics who argued, during the model development process, that a term in the water budget was incorrect. However, within the context of a historically balanced model any change made to one portion of the model required an equal and opposite change to another part of the model, and so indiscriminate changes to the model were precluded. Most importantly, the verification or balancing process made the team think more in the context of the whole system, dynamically, rather than the individual terms, detail.

Figure 6 shows the results of sensitivity analysis applied to surface and groundwater while varying rainfall and consumption via the Monte Carlo capabilities of the modeling tool.

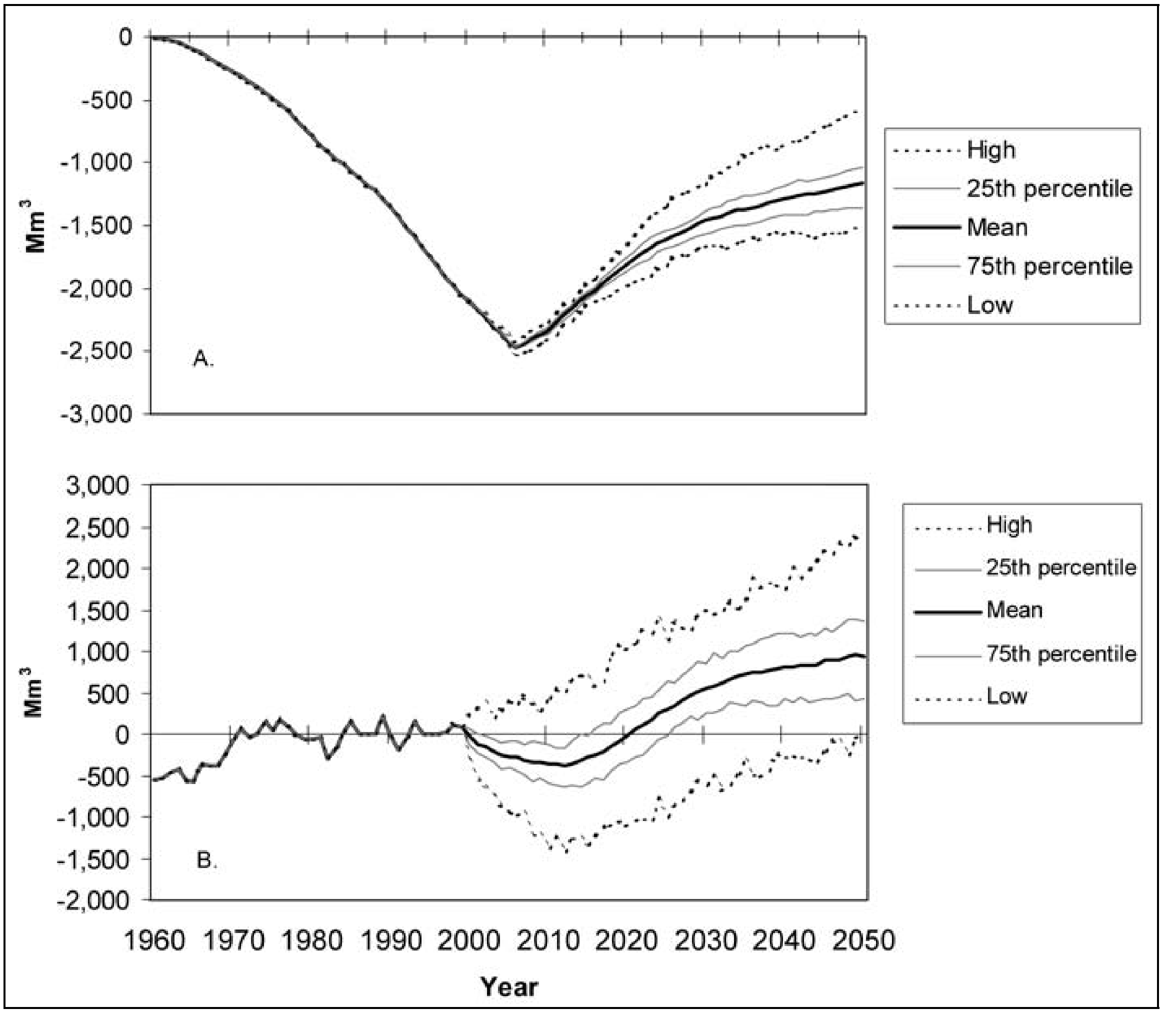

Figure 6**: (**A) Groundwater depletion and (B) Rio Grande Compact balance

Model Applications

Since the development of the MRG model several activities have taken place. The first was the realization that we now had model components, much larger than Molecules, that pertained directly to river basin management and that the model building process itself would lend itself to other resource allocation problems. The success of the MRG (partially due to its flight simulator nature) allowed the team to promote a modeling process that included stakeholder participation and rigorous hydrology and although mentioned, did not specifically promote system dynamics as the solution. Several other externally and internally funded projects have bee the result as shown below:

- River Basin modeling of the Willamette Basin to examine issues related to fish habitat and water temperature.

- Modeling of the Estancia Basin, in New Mexico, a basin with inflow but no surface water outflow.

- Modeling of the Gila and San Francisco River Basins in New Mexico to examine changes to come after legal settlement of water rights issues between New Mexico and Arizona.

- Water quality modeling for the Jordan and Zarqa Rivers in Jordan.

- Modeling of the entire surface water system in Iraq.

- Development of a Toolkit that contains components useful in watershed management including tools for surface and groundwater, population dynamics, non-use valuation, and regional economics.

- Collaboration with several universities and state and federal agencies.

Summary -- Big versus Small

It is important to justify why a system dynamics model develops into a large model and to separate it from the tendency for inexperienced modelers to develop large models. SD models that become very large are because they include a lot of detail complexity. But, as Peter Senge notes in his book, "The Fifth Discipline"[12], there are two types of complexity, detail complexity and dynamic complexity.

With VISION and the MRG Model it was necessary to capture both the detail complexity of the system as well as the dynamic complexity. The detail complexity was necessary because as is often times the case the "devil is in the detail". In the nuclear fuel cycle, it is necessary to track all flows, not at a mass level but at an isotopic level. In other words, it is necessary to track the flow of material at the level of isotopes; approximately 70 isotopes are currently tracked in VISION. Small changes in isotopic mixtures can cause significant changes in behavior. In addition, because of radioactive decay the inventory of isotopes is constantly changing as material sits in the various storage facilities.

With the MRG model, hydrologic rigor was required to alleviate concerns that the tools, which aggregated the hydrologic processes more that the standard hydrology modeling tools, could 'reproduce' the output of the latter. Although in many cases the system dynamics model performs as well as the standard tools, building confidence with the stakeholders typically requires more data and calibration than necessary.

Dynamic complexity is when an action has one set of consequences locally and a very different set of consequences in another part of the system at perhaps a much later time period. The nuclear fuel cycle also involves dynamic complexity. As an example, decisions on separations techniques could be very important for the type of separations facility needed but the impacts to future disposition of the waste which may not take place for years will be greatly impacted. The complex surface and groundwater interactions in the Middle Rio Grande Basin have been altered by modern human water use and management practices. The primary misunderstood interaction is the almost onesided transfer of groundwater to the surface water system and how residential and commercial water conservation practices can harm the surface water system. As Senge notes, “The real leverage in most management situations lies in understanding dynamic complexity, not detail complexity”. In the case of VISION and the MRG Models, it was necessary to capture both the dynamic complexity and the detailed complexity in order to capture the realistic behavior of the system.

When developing a model there are several ways to accomplish it. One is to start with a simple model that contains all the components of the finished product but with very little detail or complexity.

Ways of dividing up a model[7]

- By Loops
  -- Good for building a model
- By “plumbing” and decisions
  -- Good for dividing model between views – Visual understanding
- By Sectors
  -- Not so good, but common

Determining which way to divide up the model is very important. Remember, one of the strengths of system dynamics modeling is that the model diagrams should be visually stimulating and add to the understanding of the system. In fact some say that the actual model layout should be as informative as a causal loop diagram. Choosing the wrong method of dividing up the model may be detrimental to the model visualization.

The real danger of developing a large model, as Jim Hines noted in his *Modeling for Insights* class[13], is inadequate time and resources. So, it is important to understand the difficulties and time necessary when developing a large detail and dynamic complex model and to plan accordingly. It is also important to continuously manage the customer’s expectations. Only promise the customer what you can deliver on the time line agreed upon. In this sense, the modeling process resembles the software development process. Unfortunate as this may be, moving the customer away from static spreadsheet-like analysis is not a trivial task. Both the VISION and the MRG Model teams did extensive planning to understand the question and its scale.

Conclusions

Both projects were well funded and had an appropriate time lines to assure success. Most importantly, the models were able to show significant results early in the modeling process. Without the early success, continued funding and support from management would have been questionable.

The VISION model has been under development for over 2 years and is currently in its second version release. The model is supporting several important efforts which include a report to Congress on the Global Nuclear Energy Partnership (GNEP) and AFCI’s annual report to Congress. Because of the nature of the use of the model it is important that the model is reporting reasonable and prudent results. Take note that it was not stated as precise and accurate since those terms in any predictive model are over specifications of the models abilities.

The real value of the MRG Model has been advancing the premise that models can truly be of use, especially in contentious situations with various stakeholder groups. In addition the learning acquired in stakeholder management and model building has led to further work permitting much of the modeling team to stay together and continue work in this area and others.

The common and advocated approach to system dynamics model building does not encourage large model development. Both the VISION and MRG teams were well aware that much system insight could be gained from much simpler models. Nevertheless both teams succumbed or were forced to accept the detail complexity demanded by their customers. Actually, given the capabilities of today's system dynamics software, if dynamic complexity is handled well, detail complexity becomes more of a time and data management issue. Some lessons have been learned:

- When succumbing to detail complexity it is always important to ask the question: Is this added detail going to add to the quality of the model or will it simply make it more complicated?

- Validate the model early and then validate after every major update. Waiting till the end will make validation a daunting task.

- As model size increases, modeling becomes more difficult to manage. Applying the software engineering practices developed in the 1970s such as modularization, are essential.

- Use a standard naming convention for all variables and make sure you adhere to it all along the way.

- Add units to every variable that requires one. Unit consistency is the first and foremost objective check for model validity.

One of the ways of judging the success of a modeling project is by how many insights that a model generates. Insights can come from running a model or even when you are building the model. If at the end of a modeling exercise there are no "new" insights then the exercise probably has not been very fruitful. It simply verifies that you had a good understanding of the system prior to the modeling exercise. If however, there are many insights then the effort has at least generated some new understanding and knowledge. VISION and the MRG Model have, from the start, generated an uncountable number of new insights. As indicated above, this is directly a result of handling the dynamic complexity of the problem.

The most important lesson to take from these efforts is that before you embark on developing a large system dynamics model you be fully engaged with your customer and establish the requirements early in the process. The model specifications will help determine the time and funding requirements. At each step of the modeling process, keep the customer engaged and, as appropriate, modify the requirements specifications to meet any new requirements. The real success of the model is the acceptance of the model by the customer. Does the model end up developing a better understanding of the system and does the customer find it useful? That determines the success of the modeling effort.

U.S. DEPARTMENT OF ENERGY DISCLAIMER

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