Final Report: Integrated Assessment of Energy Technologies

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ABSTRACT
This project involved two related areas of examination. The first, “Assessing the Value
of New Energy Technologies” focuses on two main tasks. (1) Developing ways to
represent the performance and costs of new energy technologies at representative years in
the future probabilistically with and without GCEP support, and (2) Developing a
demonstration portfolio valuation model designed to give a probabilistic representation of
the contribution of resources invested in each GCEP program area to the overall value of
the GCEP portfolio. The second, “Modeling the Transition to a Hydrogen and/or Solar
Economy”, focuses on two main tasks: (1) Modeling several quantitative scenarios of the
introduction and growth of hydrogen use in light duty vehicles, examining the
consequences for economic and environmental impacts as well as impact on other U.S.
natural resource use, and (2) An investigation of how policy actions may accelerate
reductions in the cost of PV-generated electricity so that it may compete economically
with fossil-fuel generated electricity.

This research was accomplished through the use of a number of empirical, theoretical and
mathematical modeling approaches. The models employed varied in scope and
complexity, but all were grounded in the relevant economic, engineering and systems
analysis theories and tied into trends and relationships that are consistent with empirical
data. The R&D portfolio work generally utilized more comprehensive, but less detailed,
analyses, while the hydrogen and solar transition work highlighted some critical elements
of those potential transitions in more detail..

Several frameworks for assessing the value of new energy technologies were developed
and refined during the course of the project. This work highlighted the vast uncertainties
in both new technology development and in the market into which the new technologies
would need to compete. Not surprisingly, one of the most basic results from all this work
was the desirability of a portfolio of energy R&D investments to hedge against both
technological and market uncertainties. Although each technology area is expected to
have benefits that are at least several times their costs (even with discounting of the
future benefits), it was not difficult to construct alternative plausible future market and
technology development scenarios that multiplied the benefits of R&D in each area by a
factor five to ten or more. These “option” values were even larger than originally
expected owing to non-linearities in the payoffs when other parts of the portfolio turn out
to be less successful than expected and the market for low carbon technologies turns out
to be more substantial than expected. The two most important sensitivities outside the
portfolio turned out to be the pace of improvement in end-use energy efficiency in the
world’s economies and the future role of nuclear power in the world’s economies. Although these sensitivities have significant impacts on the efficacy of the GCEP portfolio they are not expected to decrease it to anywhere near the breakeven point. In fact, more rapid improvements in end-use efficiencies than anticipated could substantially reduce the heavy burden new low carbon supply alternatives that it is currently envisioned they would need to play in stabilizing atmospheric concentrations of greenhouse gases. Finally, the choice of policy instrument employed to limit greenhouse gas emissions can alter the relationship between the impacts of alternative technologies with price oriented policies generally leading to greater complementarity and caps leading to more substitutability.

Several observations can be made regarding likely payoffs from research in the various GCEP technology areas. First, improvements in electric power and automotive conversion technologies are likely to have the most immediate large scale impacts on greenhouse gas emissions. This result is obtained because most of the world’s current energy supply consists of fossil fuel based technologies, so improving these conversion efficiencies by a few percent have a large and immediate impact on carbon emissions. This is especially true in China and India where the most rapid growth in emissions is projected to occur. If we want to reduce carbon emissions substantially over the next two to three decades improving the combustion efficiency of fossil fuels is the way to go. This is true over a very wide range of variations in future energy market and alternative technology development scenarios.

Carbon capture and sequestration can also have large benefits, but since it is now only used in a small number of projects where the carbon sequestered has value in accompanying enhanced oil recovery projects, experience is limited and costs are relatively high. Additional research can drive down the price for sequestration and especially for separation and both elements are part of the GCEP portfolio. A key uncertainty governing the market penetration of CCS is whether or not an explicit price will be put on carbon. Without an explicit carbon price, penetration will be limited to a relatively small number of applications where the carbon has value for other purposes. Another issue with CCS is public acceptance because of concerns about public safety from carbon leaking out of storage sites, and the possibility of large scale leakage of carbon from such sites that can create a sudden new source of carbon emissions. Project research on the likelihood of leaks and the costs of monitoring carbon reservoirs for leaks and repairing them if found suggest that these concerns can be overcome, but they may delay the wide spread use of CCS beyond what the economics suggest. In sum, CCS has very high value in most scenarios.

Direct solar photovoltaic conversion and advanced biofuels look like they can contribute to carbon emission reductions at the giga-ton level by about mid century over a fairly wide range of scenarios. Large cost reductions (up to a factor of ten) in both seem possible, especially if learning about advanced technologies as experience is gained leads to cost reduction rates in the way they have for current first generation technologies. This project included several systematic investigations of learning curves and their implementation, including facilitating policies, in energy market modeling.
Hydrogen is a virtually non-polluting fuel form at the point of use, but elemental hydrogen does is not abundant in nature. In order for hydrogen to be used in a greenhouse gas mitigation strategy, non-carbon producing and affordable methods of producing it, efficient ways of distributing it, low cost and light weight methods for storing it (especially onboard motor vehicles), and economical devices to use it (e.g., PEM fuel cells or hydrogen fueled internal combustion engines) all need to be developed in parallel. Since advances in all these areas are challenging this may be an area where a well designed research program can have a large impact, but co-ordination of progress in all four areas within and outside of GCEP is important and will not be easy. In this study, alternative hydrogen vehicle transition pathways were examined in great detail. These studies show that it will take a long time to phase in a substantial number of hydrogen vehicles even if all the technical challenges can be met and that a hydrogen internal combustion engine may serve as a valuable short term substitute to a hydrogen fuel cell vehicle because much less technology development would be required to make it economic. Despite the challenges hydrogen remains an attractive energy fuel option for large scale use in the second half of the century. Substantial reductions in the cost of photovoltaic generated electricity generation seem likely in the next couple of decades and the GCEP portfolio in that area is both deep and broad which promises to accelerate the pace of cutting-edge technology development in this area. At the same time innovative market mechanisms designed to bring this technology into more widespread use and drive down the costs of each generation of PV technology that is introduced more rapidly are being experimented with in several regions (e.g., Japan, Germany and California). These programs enhance the payoff from the development of new generations of the PV technology because they can be refined and proliferated to enhance their rate of market penetration as well.
Introduction and Overview

Background

This research involves two related areas of examination. The first, “Assessing the Value of New Energy Technologies” focuses on two main tasks.

- Developing ways to represent the performance and costs of new energy technologies at representative years in the future probabilistically with and without GCEP support.

- Develop a demonstration portfolio valuation model designed to give a probabilistic representation of the contribution of resources invested in each GCEP program area to the overall value of the GCEP portfolio.

The second, “Modeling the Transition to a Hydrogen and/or Solar Economy”, focuses on two main tasks:

- Modeling several quantitative scenarios of the introduction and growth of hydrogen use in light duty vehicles, examining the consequences for economic and environmental impacts as well as impact on other U.S. natural resource use.

- An investigation of how policy actions may accelerate reductions in the cost of PV-generated electricity so that it may compete economically with fossil-fuel generated electricity.

These two related areas will be examined separately in the next two sections of this report, entitled “Results: Assessing the Value of New Energy Technologies” and “Results: Modeling the Transition to a Hydrogen and/or Solar Economy”. A number of additional sub-projects are described in subsequent sections. Those sections fill out some of the details for items presented in this overview and lay out some future research directions.

Results: Assessing the Value of New Energy Technologies

Assessments of the impacts of new technologies depend on assessments of both their likely cost and performance characteristics (including carbon emissions and other environmental impacts), and their likely market penetration under a wide range of possible energy futures. The approaches used to accomplish these two tasks are now presented.

Advanced Technology Representation

This task involved alternative ways of representing the performance and cost of fundamentally new energy technologies with and without GCEP funding. This involved assessments of the probability of demonstrating the technical feasibility of the technology and separate assessments of the probability distributions over the cost and likely environmental impacts of employing these technologies to reduce carbon emissions at
future dates of interest. We experimented with assessing these impacts using a large number of different probability distributions, and different levels of structural modeling of future energy devices and processes.

Also important in projecting the costs of new energy technologies are projected shifts in the assessed distributions over time and decreases in costs with level of implementation resulting from limits on rates of introduction, as well as siting, intermitancy of availability, and resource supply considerations. Land use, water use, and noble metal availability are examples of resources whose prices may increase if demand for them increases significantly to support the wide-scale introduction of new energy technologies.

Obviously these assessments require a great deal of input from technical experts in the areas being assessed. Here we used our strong traditional expertise in probabilistic risk assessment and system economics, but now with much more input from GCEP’s central systems group and technology assessment staff to bring in their expertise in technology assessment. In fact, we are participating in a DOE sponsored project headed by a former PhD student now at the University of Massachusetts on assessing probabilities of the cost and performance of new energy technologies. We involved experts in specific technologies and relevant areas of scientific research here at Stanford (including GCEP PIs) and the research community at large in this endeavor. Particularly valuable here continue to be input from technical experts at the sponsoring companies. One example of the approach to new technology assessment that we are pursuing is discussed in the sections below on carbon capture and sequestration technologies.

**Portfolio Valuation**

Given information regarding the characteristics of the new energy technologies resulting from R&D (expressed via ranges or probability distributions over costs and performance at specific future dates of interest), assessments of the value of those specific new technologies depend on what other new technologies have been developed, the rate of improvement in existing technologies, and conditions in energy markets. Conditions in energy markets are reflected in energy prices and depend on many factors including population levels, economic output, the structures of the world’s economies, resource availabilities, energy producer (and especially oil exporter) behavior, the set of available technologies for producing, transforming and consuming energy, and government energy, economic, and environmental policies.

The key factors that determine the future value of new energy technologies are highly uncertain and the relationships between them can be quite complex. One approach to energy policy assessment is to run sensitivity analysis on external factors through models of the energy system. Results from these types of exercises are extremely illuminating but generally consider only one reference scenario for one basic set of input and parameter values for each model. There are extremely large uncertainties about both sets of inputs over the course of a century and these uncertainties can have a significant impact on how we value the products of long-term R&D on new energy technologies. During this project, the elements of this system have been specified in enough detail to
allow the development of a full demonstration version of the technology assessment system.

**Design Criteria for Evaluation Framework**

At the beginning of this project, preliminary design criteria for the evaluation framework were developed. It was recognized that large-scale energy system models are often designed for purposes other than long-run energy technology assessment (e.g., short-run mitigation analyses, assessing international trade impacts of climate policies, emissions target setting and emissions trading analyses) and, therefore, include a level of complexity that makes extensive sensitivity analysis, let alone formal uncertainty analysis, infeasible. The approach employed here is to use reduced-form energy models (calibrated to the more large-scale models) as the central element of an uncertainty-oriented technology evaluation approach. We continue to use literature reviews, structural models, and expert assessments to develop probability distributions about key inputs to the models. This is crucial because these inputs are generally more important determinants of the values of the new technologies than the parameters included in the models.

We have identified the important drivers of the valuation equations and calibrated them to available modeling results. In addition, we know what information to seek via expert assessments, e.g., ranges of possible economic growth rate assumptions, fossil fuel resource base estimates, evolution of conventional energy technologies, oil exporter behaviors, etc. Based on these assessments, we are working with a set of integrated probabilistic scenarios. These scenarios represent a wide range of future states of the world and are mutually exclusive and collectively exhaustive so that probabilities can be assigned to them. This enables us to compute impact values for the new technologies across a wide range of possible technological and socio-economic futures. Figure 1 shows the key elements of the technology evaluation system.
We designed these scenarios to be as informative as possible about the efficacy of the GCEP R&D portfolio. For example, they range from a (relatively low probability) case where there is no future concern about climate change to one in which (say twenty years from now) climate change is perceived to be a (relatively low probability, but plausible) much more serious problem than currently expected. In the former case, only a small number of low-/non-carbon emitting technologies (e.g., perhaps advanced-technology combustion engines) will be adopted, whereas in the latter many low-/non-carbon emitting technologies that are more expensive than conventional carbon emitting technologies will be adopted. This comparison illustrates the “option value” associated with the development of new technologies. If new technologies are developed they can be introduced and diffused if they are needed, but kept “on the shelf” (and perhaps put into further development to make them more economical) if they are not needed.

Uncertainty about the cost and performance of the technology being evaluated and those of other new technologies is represented by sampling from the probability distributions for those characteristics. Over time more sophisticated ways of incorporating the actual probability distributions into the analysis were adopted, and the representation of R&D effort has been broken down into stages, reflecting the technical challenges that need to be met to bring the technology to fruition as well as open up the option of improving its performance over time. This information allows us to look at the optimal R&D portfolio more fully as a sequential decision making problem over time where stages of the R&D on a particular technology may be pursued with subsequent
stages either canceled or accelerated depending on how the energy system and the climate problem evolve.

Finally, the technologies are being evaluated in groups in hopes of finding the most valuable portfolio(s) of technology options given the uncertainties about technology costs and performances, scenario variables, and valuation model parameters. Here we use the whole portfolio as a hedge against future uncertainties as well as using individual elements of the portfolio as hedges against lack of technical or economic success in the other elements of the portfolio.

Overview of Demonstration Valuation Framework

To describe the demonstration evaluation system we start with a description of the prototype developed early in the project and then add detail regarding the demonstration version. The starting point for both systems was the gathering of information regarding the characteristics of the new energy technologies resulting from R&D (expressed via probability distributions over costs and performance at specific future dates of interest as described above). Assessments of the value of each new technology depend on what other new technologies have been developed, how fast existing technologies are improved, and conditions in energy markets. Thus, these evaluations require a type of “integrated assessment” of all technologies under all possible market conditions. The basic approach pursued in the design of the prototype evaluation system was initially to divide the world up into two parts: (1) what the GCEP Portfolio can provide in terms of supplies of carbon energy substitutes at various price levels, and (2) what the world might demand of this portfolio under a wide range of future energy market futures. Obviously, both the technology assessments and market assessments are very complex and highly uncertain.

The prototype assessment system started with a highly simplistic and aggregate representation of key elements of the system, but was designed in a way in which more detailed information from any source could easily be added as necessary (in modeling parlance this framework has been designed to be highly scalable). The value of each individual GCEP research program was evaluated in terms of its contribution to the value of the whole GCEP portfolio, which was, in turn, evaluated in terms of its contribution to key energy sectors in key world regions at specific times in the future.

The simplest aggregated version of the framework looked at the GCEP enabled supply and rest-of-world demand for non-carbon energy at various future dates of interest. The supply side of that framework consisted of the collection of stochastic GCEP R&D program supply curves described above. These consisted of a single subjective probability of technical success of the program and a probability distribution over the cost of employing the new technology commercially.

The demand for non-carbon energy takes into account possible future conditions in the global energy system including the implications of alternative fuel price scenarios, improvements in non-GCEP technologies (through learning over time, with respect to non-GCEP R&D funding, and with respect to cumulative experience), critical materials
or infrastructure constraints on the rates of new technology adoption, economic growth rates, structural changes in the global economy, and government policies including those directly related to climate change. Forecasting how all these factors will work towards creating a market for advanced non-carbon technologies is extremely complicated and highly uncertain. But it is just this wide range of possible outcomes that can create a very large value for advanced technology development.

Conceptually, one could construct these demand curves for non-carbon energy by taking any of the leading global energy models for one set of model parameters, one set of model drivers and one set of policies and add a fictitious source of non-carbon energy at a very low price and observe the demand for it, subsequently increasing the price again and again until more non-carbon energy is demanded. In this way a demand curve for non-carbon energy for one model implemented state of the world could be developed. Since the focus of GCEP is on long-run pre-competitive R&D to help prepare for a very wide range of future states of the energy system it would be cumbersome and probably infeasible to run a large-scale model thousands of times to develop the demand side of the framework. In addition, large-scale models may impose too much structure on the world energy system to be appropriate for this task. Thus, we started with very aggregated energy system models which could be calibrated to the existing set of large-scale energy models, but also took inputs from a number of other sources including relevant empirical work and expert opinion.

In the demonstration model we used a simplified version of an existing global energy systems model as the primary source of baseline energy system and energy technology projections. In other words, baseline carbon emissions are calibrated to the baseline emissions produced by the model and most of the baseline technology assumptions come from that baseline or extrapolations from it. The model used for this purpose is the Energy Information Administration’s (EIA’s) new System for the Analysis of Global Energy (SAGE-EIA, 2003a & 2003b). This model was used for the first time to produce the projections included in the EIA’s 2004 International Energy Outlook (IEO-EIA, 2004) which was released in April 2004 (IEO 2005 is now scheduled to be released on July 15, 2005). This is a technology rich global model which has grown out of set individual country/regional MARKAL models in the past few years. An early application of a MARKAL type model to national energy R&D planning can be found in Weyant (1984).

The ETSAP (Energy Technology Systems Analysis Programme) network which includes representatives from most of the MARKAL (ETSAP, 2005a) teams has developed a general global energy technology systems modeling framework called the TIMES model (ETSA, 2005b). This “model” is a set of data files (spreadsheets, databases, simple ASCII files), which fully describes the underlying energy system (technologies, commodities, resources and demands for energy services) in a format compatible with the associated model generator (MARKAL or TIMES). In addition to the SAGE model, instances of global models based on the TIMES architecture include the Energy Technology Perspectives (ETP) project MARKAL model of the IEA, the Global MARKAL-Macro of the Paul Scherrer Institute, and the European Fusion
Development Agreement TIMES model; the national models of the ETSAP partner institutions; and various regional and municipal models developed by other institutions. Each set of files defines one model (perhaps consisting of a number of regional models) and is "owned" by the developer(s).

SAGE was selected here because it is the most public of the existing TIMES variants and as the documentation is brought up to EIA’s normal high standards should be the most transparent version. In addition, the baseline and sensitivity cases produced as part of the IEO (including the energy market and technology inputs) are compared with other projections, assessed and debated publicly on a regular basis (EIA, 2004).

Calibrating to – but simplifying from - an existing model like the SAGE model has several other advantages. First, it allows us to focus in on key strategic regions/sectors on relevant time scales and used reduced form representations of the sectors/regions/dynamics not focused on to create a comprehensive picture of how the energy system would affect - and be affected by - new GCEP stimulated technologies.

The second benefit of the scalability provided by the partial co-integration with an existing model is the ability to look at the dynamics of technology development and crucial implications of assumptions about the degree of foresight assumed to be used by the businesses and consumers whose behavior is represented in the models. These dimensions of the technology assessment process are typically not well reflected in existing large-scale general purpose integrated assessment models.

A third benefit of the model integration strategy we are employing is that it allows us to expand rapidly into new areas as the GCEP portfolio expands or as new areas are proposed. For example, the current system focuses on energy conversion/use in key regions for electricity generation, transportation and large thermal uses in the industrial, residential and commercial end-use sectors. Should a more comprehensive and explicit treatment of end-use energy become desirable, the detail in this area included in SAGE could easily be assimilated (and assessed and modified) in a way that would require only minimal modifications to the rest of the system.

In order to be useful for long-run technology portfolio assessment under uncertainty, a number of modifications and simplifications were made to the basic structure of the SAGE model. First, the time horizon of the model was extended to 2100 from the 2050 to which the model has been run for the EIA’s International Energy Outlook and the 2025 time frame through which results were reported in that document. Second, in part by lengthening the time periods considered from five years to 25 years each, many of the short-run dynamics in the SAGE model were eliminated or greatly simplified. Finally, much of the detail on the operation of the electricity transmission and distribution system and daily/seasonal patterns of electricity demands were simplified or eliminated because again it is anticipated that these dynamic constraints will not impact the assessments of the introduction of fundamentally new energy technologies over many decades very much. In effect, the assumption made here is that the T&D and scheme for temporal pricing of electricity can be designed around the new technologies given sufficient lead
times. These simplifications greatly reduced the time required for a single run of the full SAGE model. Although this has not been fully tested, it is estimated that this reduced-form global energy model would run in about .01% to .1% of the time it takes to run the full SAGE model in a comparable computing environment.

This calibration to the SAGE baselines and technology data does not (as will become obvious) preclude adopting model structure, parameters and inputs from other modeling and analysis efforts where appropriate. For example, cost and diffusion parameters for hydrogen fueled vehicles are drawn from National Research Council (2004), and carbon capture and sequestration from Heddle, Herzog, and Klett. (2003), and Dooley and Friedman (2004). This is another advantage of the flexible assessment architecture adopted here. In other words, if the overall architecture of the assessment system were optimization or computable general equilibrium oriented this would immediately limit the types of formulations that could be integrated into it. Moreover, as others modeling systems continue to become more technology rich, any set of technology assumptions and scenarios can be employed in our assessment system.

The integrated assessment framework consists of eight regions, five conversion/use sectors, and five time periods. The eight regions are China, India, Other Developing, Former Soviet Union and Eastern Europe, Western Europe, Japan, United States, and Other Developed. This regionalization allows the focus to be on the largest current and likely future GHG emitting countries/regions in a way that is consistent with existing data collection/modeling efforts. Following SAGE we also divide the US into 4 regions and China into two; greater regionalization of China and India could be added in the near future as the requisite data is developed. These sub-country regionalizations are especially important in assessments of the potential of distributed and renewable resources.

The current breakdown of conversion/end-uses includes electricity generation, transportation, industrial steam/process heat, residential and commercial heating, and other non-electric uses. This breakdown is a bit unconventional, but again focuses well on where large reductions in GHG emissions may be possible with very advanced new technologies and where current GCEP R&D programs lie.

As in SAGE, demands for the outputs of the first four of the five end-use/conversions sectors are based on computing supply-demand equilibria at projected fuel prices and cost and performance parameters for individual supply technologies. For each level of demand, supplies are produced by the cost-minimizing mix of technologies, given fuel prices. In the other non-electric demands sector fuel demands are computed as reduced-form functions of fuel prices, although individual technology data from SAGE could ultimately be used for these uses as well.

The five time periods considered are 2005-2015, 2016-2025, 2026-2050, 2051-2075, and 2076-2100. The 2000-2025 period of last year was split into two ten year periods this year to allow tracking of the dynamics of introduction of known new technologies over that time period. These time periods are long enough to allow most of the energy
producing, transforming, and using equipment to be turned over (excepting some large power plants and other similar scale facilities), which seems appropriate for assessing the impacts of “step out” energy technologies. Despite the length of these time periods, many shorter run capacity and transition limitations can be considered when necessary through the use of growth rate assumptions and various kinds of constraints on the absolute or market share contributions of individual technologies.

While it is not possible to include a comprehensive list of all the technologies and their assumed performance characteristics included in the demonstration assessment framework here, we can give a flavor for the level of detail employed by briefly describing some of the main SAGE technologies (EIA, 2003a). Technologies for electricity generation, automotive transport, residential space heating, and steam/process heat for ferrous and non-ferrous metals, chemicals, and paper and pulp making.

The electric generation technology descriptors consist of the number of the grids within the region where the facility is to be installed (often there is only one), the year of availability, the fuel required, and the basic technology employed. For each technology, the SAGE data base includes its efficiency, annual utilization or capacity factor, lifetime, investment cost, and fixed and variable maintenance costs. For renewable electricity generation from wind, solar and biomass (in both central station and distributed modes) the availability of appropriate resources by quality category (e.g., average wind speed, solar insolation level, and productivity of biomass sources) are also key inputs. Fossil fuel prices come from scenario assumptions modified by aggregate demand changes caused by new technology introductions. Distributed generation technologies receive a transmission and distribution credit (negative O&M charge) reflecting their closer proximity to load centers. Similar descriptors are used to describe the transportation, residential building and industrial technologies.

With 8 regions, five energy uses and five time periods included, 200 sets of constrained technology comparison/optimizations (each with dozens of technology options) must be computed, although only about 10% of these strongly influence the results obtained. Thus, additional simplifications like scaling results from one region to another or from one time period to another are sometimes employed without biasing the results.

In the assessments, fuel demand interactions and feedbacks are captured by integrating the fuel demands from the optimal mix of energy technologies in each sector region and time period with simple fuel supply functions. For example, if there is a large increase in the demand for natural gas because it is the most economic way to make hydrogen for fuel cell vehicles this will lead to an increase in natural gas prices and a decrease in gasoline prices. These adjustments in fuel prices will make gasoline fueled cars somewhat less expensive and hydrogen fuel cell vehicles somewhat more expensive to operate with respect to the case where fuel price feedbacks are ignored. At present, land, water and noble metal usages are calculated, but feedbacks from those markets are not yet accounted for.
Unexpected changes in the fuel price outlook occurred during this project due to the persistence of higher oil and gas prices than anticipated. We were already considering a wide range of future price expectations last year, but the level of oil and gas prices over the last two years has lead some observers to conclude that current price levels may be sustained for the next several decades. While we do not believe that is the most likely scenario, it is more likely than last year, leading to an increase in the high end of our price range and a higher probability attached to that range.

There are uncertainty representations (i.e., probability distributions) for energy demand levels, fuel prices, and climate policies that are similar to the new technology supply uncertainty specifications described above. Given probability distributions for the demand for energy and constraints on carbon emissions in the future and for the supply of each technology included in the GCEP portfolio, stochastic simulation techniques are used to generate thousands of possible supply/demand equilibria each including a level of contribution by each technology in the portfolio for each simulated state of the energy system.

At this point another modeling challenge comes into play – how much foresight and rationality to attribute to the firms and consumers whose behavior is represented in the analysis. Typical modeling practice has been to assume either no foresight, meaning the actors whose behavior is being represented make their investment decisions assuming that current prices and technologies will prevail into the indefinite future (this is sometimes referred to as a “recursive dynamic” formulation, reflecting the carry-forward of capital equipment), or that they have perfect foresight based on perfect forecasts of future fuel prices and technologies. In the first case we can add the uncertainties in after the decisions are made to get distributions over actual market outcomes, while in the second we apply the probabilities to the perfect decisions that are ultimately made to find out what our uncertainties as analysts imply about the distributions over key outputs (like carbon emissions or net surplus). As these two sets of assumptions are typical modeling practice we explored the implications of both in our integrated assessment framework.

On the other hand, neither of these two sets of polar opposite assumptions seems completely realistic – firms and consumers probably do have some foresight in making energy investment decisions, but it is far from perfect over the several decades much energy capital equipment lasts. Thus, decisions are made under uncertainty and investors will hedge against bad outcomes by investing in technologies that are robust over outcomes on market conditions and technology performance weighted by their probabilities. Model formulations that reflect this approach to investment decision making are rare and have generally been limited to considering only two or three uncertainties.

In addition, here we separate the investment uncertainty from the R&D uncertainty by conditioning the investment uncertainty on whether the technical uncertainties have first been resolved (no success at that stage means no new technology to invest in) and the resulting cost projected for the technology. The R&D investment reduces, but does not eliminate, uncertainty about the cost of the new technology. Using advanced flexible
optimization techniques like approximate dynamic programming, neural networks and genetic algorithms (see, e.g., Bertsekis and Tsitsiklis, 1996; Bertsekis, 2000; Davis, 1991, Goldberg, 1989, and Whinston, 2000) we were able to analyze the implications of this set of assumptions regarding foresight and decision making strategies to compare the results obtained and implications for advanced technology research investing with the other two setups.

Impact Measures
There are a wide range of benefit measures that could be used to quantify the benefits of the GCEP portfolio for each supply and demand realization. Given GCEP’s objectives, one important metric is the reduction in carbon emissions attributable to the new technologies that are developed. In making such assessments, though, it is important to include not only a range of possible energy sector futures, but also a range of outcomes regarding the costs, performances and contributions to carbon emission reductions of other new energy technologies. These carbon emission reductions come from efficiency improvements, sequestration of carbon emissions and fuel substitutions.

Another frequently used benefit metric is the increase in net surplus to the economy resulting from the new technologies. For simple supply and demand curves such as those shown in Figure 2, the net social surplus gain can be computed as the area under the demand curve less the area under the supply curve for energy in each region/sector considered. The area under the demand curve represents the total value of energy to consumers and intermediate goods producers while the area under the supply curve represents the total draw on societal resources required to produce the alternative energy. Net social surplus is maximized at the point where supply equals demand (also known as the market equilibrium) because to the left of the point the marginal area under the demand curve exceeds the marginal area under the supply curve and that relationship reverses to the right of the market equilibrium point.

In the demonstration model the market equilibrium is found by solving a linearized optimization problem represented by the area under the demand curve for energy in the region/sector less the least-cost mix of energy supply options given the availability of new (and old) technologies and any constraints on the energy supply system.

In Figure 2 we can see how net surplus is reduced as carbon emissions are constrained because many of the least expensive energy supply options produce carbon emissions. The inclusion of new technologies resulting from GCEP research leads to increases in net benefits in two ways: (1) providing lower cost ways to reduce carbon emissions (for example, via coal-fired electricity generation with carbon capture and sequestration); and (2) possibly providing lower-cost sources of non-carbon energy than some of the original carbon emission producing sources (the goal of the project is breakthrough technologies after all).

Using the net benefits triangle, it is thus easy to calculate the net benefits of the GCEP portfolio for one particular set of technology outcomes and one particular future state of the world energy system. Given the complexities and uncertainties involved
though, this set of calculations might need to be repeated thousands to millions of times to capture the effect of the full range of outcomes.

This capability is implemented through Monte Carlo Simulation in which each probability distribution is sampled through the use of appropriate random number generators to sample from the GCEP technology and market environment probability distributions. For example, if an R&D project on a new technology has a .2 chance of demonstrating the technical feasibility of a new carbon free energy technology, a random number between 0 and 1 is generated and the technical demonstration is assumed to be successful if that number is .2 or less and unsuccessful otherwise. Then the cost of the new technology is determined by another random draw used to pick an outcome corresponding to that probability number in the cost distribution for that technology. For example, if .5 is drawn, the mean of the probability distribution over future costs is selected. The process is repeated over all the uncertainties many times over to generate probability distributions over various output measures, including the net benefits of what ever portfolio is being analyzed.

![Diagram](image)

**Figure 2.** GCEP Technology Assessment: Conceptual Overview

**Example Results**

In this section we illustrate a few of the different uses of the demonstration evaluation system. Figure 3 shows a range of calibrations to the 2005 IEO cases. The Reference, High and Low Baselines are based on the IEO reference, high and low economic growth rate assumptions. Here we use the GCEP fuel price uncertainties, but (as in the IEO) do
not assume any additional climate policies. The reference baseline reaches 25 GT of carbon emissions in 2100, while the high and low scenarios reach 37 GT and 16 GT in that year, respectively. These results are very similar to those included in the IEO for the first half century. Also shown are the emissions projections that result from the baseline reference assumptions with technologies frozen at their 2005 efficiency and cost levels, and the WRE carbon emissions trajectory which is projected to lead to a CO₂ concentration in the atmosphere of 550 ppmv. The former case leads to slightly over 50 GT of carbon emissions in 2100, while the latter shows emissions by that date at 5.8 GT and heading down.

The R&D evaluation framework is not designed primarily to make small sets of carbon emissions projections like those shown in Figure 3, but to assess the impacts of new technologies over a plausible range of energy market futures determined by economic growth rates, fuel prices, and climate policies. A sample probabilistic range covering 84 percent of the possible outcomes is shown in Figure 4. Here we use the IEO economic growth rate cases probabilistically (with 50% weight on the reference level and 25% on each of the high and low assumptions) as well as fuel price and climate policy uncertainties. This lowers the mean of the distribution down to slightly over 20 GT of global carbon emissions in 2100, with the 9th percentile at about 14 GT and the 93rd percentile at about 30 GT by that date. This means there is a 9% chance actual emissions will be below 14 GT in 2100 and a 7% chance they will be over 30 GT by the end of the century.
From these carbon emission scenarios we can project the carbon emission reductions that would be expected to result from the GCEP R&D portfolio. Recall the high low and reference refer to the economic growth levels, with each projection resulting from a range of fuel price and climate policy assumptions. Here we use the decision making under uncertainty formulation to model investments in energy using plant and equipment. By 2100 reference case carbon emissions are lowered from a little over 20 GT to about 10GT, in the high case the reduction in carbon emissions is from 30 GT to 13 GT, and in the low case from 14 GT to 8.5 GT. Over the century these expected reductions are all fairly substantial.

These simple global emission and technology introduction projections are still not the main objectives of the technology assessment system, they only set the stage for integrated technology assessments. As a simple example of the overall evaluation methodology, consider the case where world energy demand is aggregated and there are only four technology areas in the GCEP portfolio – renewable energy, advanced combustion, hydrogen and carbon sequestration. Figure 5 shows results for this portfolio. This collection of technology programs is referred to as a “mini” portfolio here because although it only includes 4 of the 11 GCEP areas – they are the ones in which there are currently the most active R&D projects. Also shown is the distribution of emission reductions for the mini-portfolio without the renewables element, the difference between
the two being the incremental value of adding the renewables program to the other program elements.

The expected level of carbon emission reductions for the min-portfolio is a little over 400 GT. There is also much less chance of a no payoff from the program which results from diversification: that is, the probability of all projects in all four technology areas proving to be technically infeasible (about a 2% chance) is much less than any individual technology program proving to be infeasible. Finally the probability of very large benefits is larger (about 1.0% for cumulative carbon emissions of 1000 giga-tons) as it is better to have two or more areas with chances at a technically feasible and relatively low cost carbon free technology than only one area when the demand for carbon free energy is simultaneously high due to high economic growth, tight fossil fuel market conditions and public policies designed to reduce carbon emissions significantly.

![Cumulative Carbon Emission Reductions Through 2100 (GT)](image)

**Figure 5. Incremental Contribution of Renewables Program**

Rather than repeat this picture of the incremental shift in the probability distribution over carbon emission reduction levels for all 32 cases, we summarize the results for all those cases in Table 1. Table 1 shows the expected carbon emissions reductions for each of the areas conditional on already having none, one, two or three of the other areas in the portfolio. The subscripts in Table represent 25th percentile values for projected carbon emission reductions. For example, if the sequestration program is added to a portfolio that already includes renewables the expected additional carbon emission reductions during the century is 103 GT, there is a 75% chance that it will be greater than 7 GT, and a 10% chance it will be greater than 267 GT.
### Table 1
Incremental Contributions of GCEP R&D Areas to Cumulative Carbon Emission Reductions (GT Carbon)

<table>
<thead>
<tr>
<th>Areas Already in R&amp;D Portfolio</th>
<th>R&amp;D Area Added to Portfolio</th>
<th>Adv. Comb.</th>
<th>Sequestration</th>
<th>Renewables</th>
<th>Hydrogen</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nothing</td>
<td></td>
<td>62157&lt;sup&gt;305&lt;/sup&gt;</td>
<td>12143&lt;sup&gt;317&lt;/sup&gt;</td>
<td>45141&lt;sup&gt;378&lt;/sup&gt;</td>
<td>1590&lt;sup&gt;267&lt;/sup&gt;</td>
</tr>
<tr>
<td>Adv. Comb.</td>
<td></td>
<td>-</td>
<td>10134&lt;sup&gt;301&lt;/sup&gt;</td>
<td>23123&lt;sup&gt;314&lt;/sup&gt;</td>
<td>1380&lt;sup&gt;179&lt;/sup&gt;</td>
</tr>
<tr>
<td>Sequestration</td>
<td></td>
<td>43142&lt;sup&gt;277&lt;/sup&gt;</td>
<td>-</td>
<td>992&lt;sup&gt;67&lt;/sup&gt;</td>
<td>15118&lt;sup&gt;249&lt;/sup&gt;</td>
</tr>
<tr>
<td>Renewables</td>
<td></td>
<td>40140&lt;sup&gt;282&lt;/sup&gt;</td>
<td>7103&lt;sup&gt;267&lt;/sup&gt;</td>
<td>-</td>
<td>1584&lt;sup&gt;189&lt;/sup&gt;</td>
</tr>
<tr>
<td>Hydrogen</td>
<td></td>
<td>52133&lt;sup&gt;291&lt;/sup&gt;</td>
<td>8141&lt;sup&gt;345&lt;/sup&gt;</td>
<td>32157&lt;sup&gt;356&lt;/sup&gt;</td>
<td>-</td>
</tr>
<tr>
<td>Adv Comb, Sequestration</td>
<td></td>
<td>-</td>
<td>-</td>
<td>773&lt;sup&gt;233&lt;/sup&gt;</td>
<td>14105&lt;sup&gt;176&lt;/sup&gt;</td>
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<td>-</td>
<td>1383&lt;sup&gt;179&lt;/sup&gt;</td>
</tr>
<tr>
<td>Adv Comb, Hydrogen</td>
<td></td>
<td>-</td>
<td>7121&lt;sup&gt;273&lt;/sup&gt;</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Sequestration, Renewables</td>
<td></td>
<td>31130&lt;sup&gt;263&lt;/sup&gt;</td>
<td>-</td>
<td>-</td>
<td>1295&lt;sup&gt;165&lt;/sup&gt;</td>
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<tr>
<td>Sequestration, Hydrogen</td>
<td></td>
<td>34112&lt;sup&gt;259&lt;/sup&gt;</td>
<td>-</td>
<td>572&lt;sup&gt;242&lt;/sup&gt;</td>
<td>-</td>
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<tr>
<td>Renewables, Hydrogen</td>
<td></td>
<td>28121&lt;sup&gt;261&lt;/sup&gt;</td>
<td>487&lt;sup&gt;242&lt;/sup&gt;</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Adv Comb, Sequestration,Renewables</td>
<td></td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>1279&lt;sup&gt;151&lt;/sup&gt;</td>
</tr>
<tr>
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<td>575&lt;sup&gt;227&lt;/sup&gt;</td>
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<td>Adv Comb, Renewables, Hydrogen</td>
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<td>-</td>
<td>381&lt;sup&gt;231&lt;/sup&gt;</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Sequestration, Renewables, Hydrogen</td>
<td></td>
<td>2399&lt;sup&gt;262&lt;/sup&gt;</td>
<td>-</td>
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</tr>
</tbody>
</table>

Technology Strategy for Climate Change: Optimal R&D Investment and its Interaction with Abatement Policy

The sectoral, regional, time and technology disaggregation of the demonstration evaluation framework seems adequate for placing approximate values on R&D in the technology areas, and for developing useful insights regarding the design of the R&D portfolio. Nonetheless, improvements in the representation of the dynamics of new technology introduction and diffusion would help improve the realism of the system and lead to refinements in the portfolio valuations as well as additional insights. An approach to improved dynamics for the electricity sectors of the US and China is described in the
This study describes several considerations for basic research investment strategy in environmentally motivated technologies. In particular, these considerations are important in the context of global climate change, in which the need for long-term, fundamental technological change is acute. Market-based abatement policies are effective mechanisms for bringing about the diffusion of existing technologies and can even spur incremental improvements through learning and induced applied R&D. Thus abatement policy is a mechanism for getting technologies “off the shelf”. However, because of long timeframes and limited appropriability in basic research, a second mechanism is required to put new abatement technologies “on the shelf”. An optimal response to the climate change problem must include both mechanisms.

From a planner's perspective, uncertainty plays a large role in the design of climate policy. One major uncertainty is the severity of damages from accumulating greenhouse gas concentrations. While information about this uncertainty may be obtained through scientific research, the underlying distribution is exogenous to the decision-maker: We can learn about the relationship between emissions and environmental impacts, but we cannot change it. The future state of technology is another major uncertainty important to policy-makers. As opposed to uncertainty about damages, the distribution over the technology state space can be partially controlled; moreover, the basic R&D strategy is the control variable. This characterization defines the interplay between the two mechanisms, and demonstrates that they must be considered jointly.

The first part of the problem is to define the form of an optimal R&D strategy. Increasing investment in an R&D program translates into increasing probability of success, with decreasing returns to scale. The value of success is measured by improvements to both baseline and policy-modulated welfare. Separating probability from value reveals two possibly unrelated sides to a prospective technology: its technical potential for advance, and the market potential of an advance. The optimal level of investment balances these two sides by equalizing the product of marginal probability and value with the opportunity cost of investment. Individually optimal investment levels, based only on the intrinsic characteristics of the program in isolation, may be altered in a portfolio of research programs due to interactions on both the probability and value sides. On the probability side, interactions are referred to as spillovers, and their presence tends to increase the effectiveness of investment and thereby reduce optimal levels. Market interactions determine the incremental value of a development when other technologies have also arrived; in general, substitution effects lead to lower overall investment and a less diversified portfolio, while complement effects lead to the reverse. A budget constraint on overall investment can reduce the number of funded programs by raising the required value threshold. However, the diversification properties of a R&D investment portfolio are fundamentally different from those in a financial portfolio.
The characterization of an optimal investment portfolio in any context has become closely linked with the objective of diversification since the ascendance of modern portfolio theory sparked by Markowitz. Diversification is motivated in a portfolio of financial securities by the risk aversion of the investor. By dividing funds among several uncorrelated assets rather than investing in a single asset, the same expected return can be achieved with lower variance. However, the technology strategist in this model is risk neutral, meaning that variance is of no concern; thus any justification for a diversified research portfolio must come from elsewhere. Within the current analytical framework, three factors may be identified that drive the diversification of the optimal R&D portfolio posed in this problem. These are decreasing returns to scale, uncertainty, and heterogeneous applications.

First consider the case of decreasing returns. Applying the optimality condition of equal marginal productivity across investment options, a single research program will not dominate, since as its marginal returns fall with increased funding, it will be optimal to move funds to programs with higher marginal return to the first dollars spent. In this way investment is spread across several programs to exploit the most productive range in each. However, this property does not always lead to diversification—a research program may receive no funding if it has a lower marginal return at zero investment than the marginal returns from funded programs at optimality. In general, there will be a ranking of research programs, with the highest ranked programs receiving the highest funding priority. The presence of a binding budget constraint further limits diversification by increasing the value threshold required at optimality, thereby making it more difficult for a program to enter the portfolio. The consequence of decreasing returns to scale is that diversification occurs sequentially in investment—as more funding is made available, a wider array of programs is pursued.

The effect of uncertainty on diversification in a public R&D portfolio is distinct from the effect of risk in a financial portfolio. In the latter case, an investment with a wide range of possible returns (i.e. high risk) requires a hedging strategy because the investor prefers less variance to more, and in fact is willing to sacrifice some expected return in order to reduce variance. In the case of investment in basic research, a wide range of possible outcomes (i.e. high uncertainty) requires a hedging strategy because the (risk neutral) R&D planner simply prefers more expected return to less, with no preference as to variance. In particular, uncertainty about the extent of climate damages affords opportunities for several research programs to provide value. For example, a rapid transition to a low-carbon set of technologies may be justified if the damages are severe, whereas a slow transition from fossil fuels might be justified if the welfare consequences of continued emissions are mild. A diversified portfolio can increase expected return by addressing both of these possibilities.

Uncertainty about which research programs will achieve technical success plays a different role in shaping the optimal portfolio than uncertainty about market conditions. Often diversification is invoked as a response to the low-probability, high-payoff nature of basic research. According to this argument, because success in any given individual program is an unlikely event, several programs should be funded so that the probability
of at least one success is reasonably high. This line of reasoning may be clarified using the current framework. First, suppose the programs in question are independent from a market perspective, so that the expected value of a success in one is not diminished or increased by success in another. Then funding should be allocated according to marginal productivity only, without regard to the underlying distribution (assuming risk neutrality). The level of diversification among low-probability programs should be identical to that among high-probability programs with the same marginal relationship between probability and investment. Now suppose there are market interactions among the research programs. If the programs are substitutes, diversification is actually discouraged. However, when success probabilities are quite low, market interactions become less important, because success in an individual program is most likely to occur on its own. Thus a portfolio of low-probability substitutes should be more diversified than a portfolio of high-probability substitutes because the negative co-externalities of market competition are mitigated in the low-probability case. Finally, if the programs are complements, diversification is naturally encouraged, but market interactions will again have a muted role.

The third driver for diversification in the R&D portfolio modeled here is heterogeneous applications. Because the environmental goal of reducing greenhouse gas (GHG) emissions may be met in a variety of ways, there are many different possible technological applications for abatement. Even within a single sector, several technologies may be deployed simultaneously because of regional variation in costs, access to infrastructure, or other idiosyncratic factors. Although observed heterogeneity in today's systems does not necessarily impose a similar condition on systems in the future, it is generally agreed upon that no single technology can facilitate a transformation to a carbon-free world. This conclusion can be interpreted as an argument for diversification in the sense that heterogeneous applications lead to market independence, and away from substitution, among research programs.

Optimal investment levels are also dependent on assumptions about the behavior of the future policy-maker. The diffusion of abatement technologies, and therefore their value, depends on the policy incentives in place when they are developed. Therefore, the value of a successful development is maximized when the policy incentive is determined optimally in response to the outcome of the research program. If constraints, such as fixed targets, are placed on the policy-maker such that an \textit{ex post} suboptimal incentive is enacted when a program succeeds, its value is diminished and less investment is justified. On the other hand, if constraints cause a suboptimal incentive only when a program fails, the value of success is actually increased in relative terms. These effects describe one part of the interaction between R&D strategy and abatement policy, but they do not address the considerations of a simultaneous interaction. This interaction must be based on the way the abatement policy-maker's decision depends on beliefs about the future state of technology.

To address the question of simultaneous interaction, the study combines the R&D strategy model with a dynamic abatement policy model. The standard view of this interaction is that the two instruments are substitutes. An important result is that this rule
need not be true. When damages increase gradually with emissions, rather than as a step function imposed by a stabilization target (or a cost-effectiveness criterion), the primary factors motivating the substitute rule are removed, and the interaction is based on marginal effects which could point in either direction. Increased abatement effort at the same time as R&D investment could enhance the value of both activities. Moreover, an observation throughout is that planning based on stabilization target scenarios, while removing the troublesome necessity of specifying a damage function, changes the problem significantly from a sequential decision-making cost-benefit analysis. In addition to distorting the valuation of technology outcomes, as described above in the context of fixed policy targets, a cost-effectiveness analysis can fundamentally alter the relationship between R&D investment and concurrent abatement to the point of changing the sign.

These insights can be applied to decisions facing R&D managers in a variety of institutions, including governmental agencies, national labs, non-governmental organizations (NGOs), universities, and industry consortia aiming for long-term, collaborative strategic goals. The portfolio in this study represents the amalgamation of basic research efforts from all of these sources and is managed as if by a single optimizer, but in reality the problem involves multiple decision-makers. The applicability of the current approach therefore depends importantly on open communication among research actors, and a shared commitment to widespread technological diffusion. To achieve the effect of a centrally optimized portfolio, institutions must interact as in a cooperative game in which individual portfolio managers take into account the work being done at other organizations when determining which programs to pursue, and each seeks to serve a unique niche, avoiding duplication of effort. In general, this type of interaction contrasts with observed institutional behavior, in which actors are concerned with a smaller subset of costs and benefits and accordingly pursue a targeted research portfolio independent of the global optimum. For example, a national government may focus only on technologies that are relevant to its economy, or perhaps to a particular industry, but this approach risks ignoring more attractive investment opportunities in research areas that apply elsewhere. This behavior is especially problematic for climate change, where damages are incurred globally and emissions reductions anywhere are equally effective.

Understood in the preceding context, the results of this work highlight for R&D managers the key strategic elements of the investment decision. The value of success in a proposed program is comprised of its ability to diffuse in a possibly carbon-constrained market, and the effects of that diffusion on economic welfare in the baseline and as modulated by the future abatement policy regime. Concepts of uncertainty, program interaction, timing, and information value have all been incorporated into this definition. The value calculation does not translate directly into investment, but must be weighed against a probabilistic representation of the program's effectiveness. Also important to decision-making are the motivation behind diversification and, in particular for public managers, the implications for concurrent abatement policy. Finally, the framework is useful as a blueprint for implementation with a numerical model, thus applying the leverage of existing integrated assessment capabilities to specific R&D planning questions. This study implements the framework with an illustrative integrated
assessments. The numerical results offer several technology-specific insights: for example, they suggest that improvements to fossil efficiency may be an important area for R&D investment, and that the role played by market interaction effects is strongest for renewable technologies, but in aggregate may be small. Financially, the expected benefits of investment appear to far outweigh the costs. However, in general, the implementation exercises demonstrate the value of the framework rather than providing robust recommendations. The approach described here has provided new high-level decision-making insights about the joint goals of technology development and emissions abatement.

Another New Direction in the Development of the Assessment Framework

Another area of research in this project was improvements in the assessment of the results of the GCEP R&D technology areas. Including more technological process detail drawn from thermodynamics, petroleum geology, electro-chemistry, biology, bio-engineering and other relevant disciplines in the assessment process were a fruitful area for research. In appendices B and C we include papers on “Carbon Capture and Storage – Estimating the Costs” and “Quantifying the Leakage Rate Associated with Carbon Storage,” which described an approach to a combined structural/expert assessment of the leakage rates from carbon sequestration sites. Building on that work we built a preliminary assessment framework for trading off the costs of monitoring carbon storage sites against the benefits such a program would provide in terms of early detection of leaks and possible repair before the carbon dioxide reaches the surface. This work is summarized in appendix D entitled. “Optimal Frequency of Time-Lapse Seismic Monitoring in Geological CO₂ Storage.”

In addition, Appendix F entitled “Knowledge Stock and Cost Curves: A Firm Based Approach,” attempts to bridge the theoretical and econometric analysis of cost curves. Cost curves are used to predict the cost trajectory of a technology in the future. This paper suggests a dynamic programming model to build cost curves. All parameters of the model, however, may be estimated econometrically. Combining theoretical as well as an econometric approach provides a powerful tool to capture various factors which are ignored in any one analysis. Although the methodology is general it has been tailored to predict the cost of renewable energy technologies, in particular the cost of photovoltaic cells. Firm-based cost curves (instead of industry based cost curves which are used commonly) are developed as a function of the firm's knowledge stock (which maybe defined as the knowledge gained through experience, R&D expenditure and spillovers). Each firm optimally invests in R&D expenditure and decides how much to produce, which in turn, increases its knowledge stock in the next period. The model captures the strategic interaction between firms (i.e., competitive versus collusive behavior), optimal R&D investment, the relationship between optimal R&D, profits and extra and in-industry spillovers, uncertainty in R&D productivity and finally the decrease in the cost of production with increasing knowledge. We consider initially a two-period model which we extend to T-periods. Parameters such as cost curves, R&D productivity and the demand curve needed for the above analysis maybe estimated econometrically. This work complements the work on Solar Photovoltaic cost curves described in Results II below.
Results II: Modeling the Transition to a Hydrogen and/or Solar Economy

This part of the work was done on the micro level and included several more detailed explorations of possible transitions to a hydrogen and/or solar economy.

Results: Modeling the Transition to a Hydrogen Economy

This year’s work in micro level analysis of technologies focused entirely on models designed to examine implications of a possible transition to a hydrogen economy, or more precisely, of a transition to using hydrogen in place of gasoline as fuel for light duty vehicles. This modeling and analysis was developed jointly for GCEP and for the National Research Council (NRC) “Committee on Alternatives and Strategies for Future Hydrogen Production and Use”. This work was incorporated in the National Academies’ recently published study: The Hydrogen Economy: Opportunities, Costs, Barriers, and R&D Needs.

A final version of the National Academies’ study is available online at www.nap.edu. The methodology for the study is summarized here and some of the key results of it are included here as Appendix A. It should be noted that this modeling and analysis included intellectual contributions by all members of the NRC committee and by its consultants, in addition to the contributions by James Sweeney.

The Modeling and Analysis: Summary of Methods

The goal of the modeling and analysis was to develop insights into the implications of moving to hydrogen as fuel for light duty vehicles. But there are still many technical, institutional, regulatory, and economic barriers to the use of hydrogen as an automotive fuel. This modeling and analysis is based on explicit assumptions that an aggressive research and development effort is successful in reducing the costs of proton exchange membrane (PEM) fuel cells, is successful in solving the challenge of on-board storage of sufficient quantities of hydrogen, is successful in developing safety and other regulatory standards. The analysis is based on the assumption that, as a result of the R&D and of the regulatory progress, the total production and maintenance costs of fuel cell vehicles becomes equivalent to that of hybrid vehicles fueled by gasoline, or that any additional costs of such vehicles is matched by increased functionality that vehicle purchasers would find attractive enough to compensate for the additional production and maintenance costs. The work conducted for GCEP does not make a judgment about whether the R&D will be so successful, but rather provides analysis of the implications of such successful R&D.

The modeling and analysis started with mathematical models which build up estimates of the unit costs (costs per kilogram of hydrogen) that could be expected for the various hydrogen-supply technologies. These models are designed to estimate unit costs of the production, transportation, and dispensing of hydrogen for use in automobiles. These models incorporate estimates of the major components of cost, including the capital depreciation and amortization, feedstock costs, costs of electricity or other energy inputs, costs of separating carbon dioxide from the gas stream, costs of sequestering
carbon dioxide, and operations and maintenance costs. Consistent assumptions about economic conditions, interest rates, electricity costs, and carbon prices (if any) are used across the various technology estimates. These models were first developed by SFA Pacific to be used by the NRC committee. They were subsequently modified as a result of deliberations by the NRC committee members.

The unit cost models are available in two versions. The first includes estimates of costs that would be incurred if current technologies were utilized. The second version includes estimates of unit costs, conditional upon technological advances. The latter version depends on the technological judgments of the members of the NRC “Committee on Alternatives and Strategies for Future Hydrogen Production and Use”.

Linked to this the first group of unit cost models are models designed to examine the quantitative impacts of various technologies if successful. Currently the primary such model is a relatively simple vintage capital representation of automobile use of fuels. The model uses as inputs the assumed fractions of new vehicles in any future year which would be fueled by hydrogen and the assumed fractions of new gasoline-powered vehicles that are hybrid vehicles or conventional vehicles. This model then keeps track of the projected number of vehicles produced in any year, the capital stock of automobiles from the various vintages, the average fuel efficiency of each vintage, the fraction of vehicles from each vintage that would be fueled by hydrogen as opposed to gasoline, the assumed differential fuel efficiency of new hydrogen vehicles, the growth of vehicle miles traveled, and the resulting consumption of hydrogen and gasoline.

In addition, these consumption estimates have been combined with estimates of carbon dioxide emissions from gasoline-based consumption and the carbon dioxide emissions from the various hydrogen-producing technologies in order to estimate how implementation of various hydrogen production technologies might decrease or increase the emissions of carbon dioxide into the atmosphere and the quantities out of carbon dioxide sequestered.

Similarly, based on estimates of the unit cost of producing hydrogen from various technologies, the model are used to provide quantitative estimates of changes in the total cost of fuel for vehicles, conditional on implementation of the various hydrogen-production technologies. For the NRC study, these unit costs are based on the unit cost models described above.

Finally, these models are used to estimate quantities of other resources that would be used to produce the hydrogen. Estimates currently have been developed for use of natural gas, coal, and land, conditional on various technological pathways for hydrogen production. In addition, for scenarios in which carbon dioxide is separated and sequestered, the annual quantities and cumulative quantities of sequestered carbon are estimated. For an in depth discussion of the “chicken and egg” nature of the establishment of a hydrogen vehicle market see Appendix E.
In addition to systematic assessments of scenarios for the introduction of hydrogen fuel cell vehicles in the U.S., this project included: (1) work on identifying barriers and opportunities for the introduction of hydrogen internal combustion engines, and (2) work on modeling the cost and benefits of solar photovoltaics. An overview of research in these two areas follows.

**Hydrogen Internal Combustion Engine Vehicles: Identifying Opportunities and Barriers**

In recent years, there has been increasing interest in the promising concept of a hydrogen economy, where our transportation sector would be powered by hydrogen rather than oil. The heart of this promise lies in the possibility of producing hydrogen from low-emission, domestic energy sources, and using that hydrogen in high-efficiency vehicles. But, there are many obstacles that must be overcome before this opportunity can be realized. For example, considerable technological development remains to be done before cost-effective hydrogen fueled vehicles are ready to hit the road at a large scale. Moreover, it is not entirely clear which technological avenue to pursue.

Hydrogen vehicles powered by fuel cells have received the greatest attention, but other technology options are also being developed, the most prominent of which is the hydrogen internal combustion engine (ICE) vehicle. The Ford Motor Company has developed a prototype hydrogen ICE vehicle, the “Model U,” which it believes is a viable alternative to hydrogen fuel cell vehicles. But, open questions remain about the potential of hydrogen ICE technology relative to hydrogen fuel cell technology.

This research project aims to address some of these open questions through an in-depth examination of the hydrogen ICE technology, with an eye to the relative merits of hydrogen ICE when compared to the existing gasoline hybrid technology and the future hydrogen fuel cell technology. This examination involves both the characteristics of the technology and the economics of an application of these technologies at the large scale. As such, this research agenda fits squarely in the first of the two of the three primary objectives of the Stanford Global Climate and Energy Project (GCEP): (1) “identify promising opportunities on technologies for low emissions, high-efficiency energy supply,” (2) “identify barriers to the application of these new technologies at large scale,” and (3) “conduct research into technologies that will help to overcome barriers and accelerate global applications.”

More specifically, this research aims to address the following questions: (1) what are the key technological characteristics that define hydrogen ICE vehicles; (2) how do these characteristics compare with those of other technology options; (3) what are some plausible scenarios of hydrogen ICE adoption; (4) what are the barriers that would need to be overcome for these scenarios to occur; and finally (5) what are the economic and environmental consequences of hydrogen ICE adoption? In concert, these questions aim to provide basis for assessing the desirability of promoting hydrogen ICE technology relative to other promising vehicle technologies.

*What are the key technological characteristics of hydrogen ICE vehicles?*
There is a long history of using hydrogen in internal combustion engines, beginning in 1807, when Issac de Rivas built the first hydrogen internal combustion engine. Indeed, hydrogen in internal combustion engines even predates gasoline in internal combustion engines (Taylor 1985).

However, there are difficulties to running ICE vehicles on hydrogen that only recent technological developments have begun to overcome. Many of these difficulties stem from critical tradeoffs between different desirable attributes. Understanding these tradeoffs is essential to understanding of the economics and market potential for hydrogen ICE vehicles.

The first important relevant tradeoff is whether to run the hydrogen ICE $\text{lean}$ (with a low density of hydrogen to air), or at a higher hydrogen-air ratio. This amounts to a tradeoff between higher engine efficiency and lower criteria air pollutant emissions (e.g., nitrous oxides) with a lean fuel mixture, and greater power with a higher density fuel mixture. The higher emissions associated with a fuel mix that provides more power can be reduced by the use of technologies such as three-way catalysts, but at the cost of higher manufacturing costs. With higher engine efficiency, a smaller fuel tank is also possible, which ties in directly with the tradeoff between fuel tank size and vehicle range. Depending on the fuel economy of hydrogen ICE vehicles, a very large tank size may be required to achieve a marketable vehicle range (Kliesch and Langer 2003).

As the hydrogen ICE technology is further developed, engineers will have to reconcile these competing demands. How this is accomplished will have a considerable influence on the application of the new technology on a large scale. This research includes a detailed examination of the technical details of hydrogen in ICEs, insofar as they are relevant to the effects of a large-scale application of hydrogen ICE vehicles.

How do these characteristics compare with those of other technology options?

An important element in this research is to provide a sense of the relative merits of hydrogen ICE vehicle technology in comparison to other prominent competing technologies. Specifically, the characteristics of hydrogen ICE vehicles are compared to those of conventional gasoline vehicles, hybrid gasoline vehicles, and future hydrogen fuel cell vehicles. While many of the details of how the technology will progress in each of these areas is highly uncertain and endogenous to the policy process, rough estimates of the characteristics of each of these vehicles types can be found or derived.

As such, Table 2 provides a comparison of the salient characteristics of each vehicle type. Note that several of the quantitative estimates are highly uncertain. In particular, the fuel economy estimates are rough approximations of what the average on-the-road vehicle fleet fuel economy might be in the relatively near future if the technologies are developed as hoped for or expected.

Several points brought out in Table 2 are worth highlighting. First, due to the nature of using hydrogen in the vehicle, both hydrogen ICE vehicles and hydrogen fuel cell vehicles are most likely to also be using a hybrid transmission with an electric motor, much as today’s hybrid gasoline vehicles do. Second, hydrogen ICE vehicles are likely
to have an engine efficiency advantage over today’s gasoline hybrid vehicles, although not as great of an advantage as hydrogen fuel cell vehicles would enjoy.

Third, under high loads (e.g., towing a boat up a hill), both gasoline vehicles and hydrogen ICE vehicles are likely to be able to provide sufficient power. Issues of efficiency losses and increased criteria pollutant emissions would need to be worked out for hydrogen ICE vehicles, but the potential would still be there to provide the power. In contrast, hydrogen fuel cell vehicles would be constrained by the number of fuel cells—once all fuel cells are working at capacity, very little additional power can be squeezed out. Unfortunately, the only solution to this issue for fuel cell vehicles is to add more fuel cells, which happen to be one of the most expensive components of the engine.

Finally, the concept of hydrogen in internal combustion engines is reasonably well understood. While much additional research would need to be done before commercialization of a hydrogen ICE vehicle, the technology is much closer to commercialization than hydrogen fuel cells, which remain prohibitively costly and with a short life-span.

Analyzing the differences between the technological characteristics of the leading competing options with hydrogen ICE vehicles provides insight into the value of promoting each technology, and the relative consequences of a wide-spread introduction of each.

*What are plausible scenarios of hydrogen ICE introduction and how might they occur?*

This research builds upon knowledge of the technical characteristics of the different vehicle types to develop plausible scenarios of wide-spread introduction hydrogen ICE vehicles. In the development of these scenarios, the most important barriers to the introduction of hydrogen ICE vehicles become apparent, many of which appear to be more closely related to the lack of a hydrogen infrastructure than to the vehicle technology itself. These barriers also hold for hydrogen fuel cell vehicles, so it may be that if infrastructure issues are solved, a critical barrier to hydrogen ICE vehicles is competition from hydrogen fuel cell vehicles.

*What are the economic and environmental consequences of hydrogen ICE vehicle introduction?*

Given these scenarios of hydrogen ICE vehicle introduction, this research goes on to examine the economic and environmental consequences of these scenarios. Of particular interest is how these consequences compare to a baseline of all conventional vehicles, a scenario of wide-spread introduction of hybrid vehicles, and a scenario of wide-spread introduction of hydrogen fuel cell vehicles. These other three scenarios are taken from the National Research Council (2004) Report on the Hydrogen Economy. Relevant metrics used to compare the different scenarios include fuel economy, total gasoline use, and carbon dioxide emissions.

This component of the research agenda provides insight into the relative value of promoting each of the competing technologies, as well as a deeper understanding of the economics of hydrogen ICE vehicles.
Research Methodology and Conclusions

This research has relied heavily on interviews with experts in the field, as well as technical papers that address some of the critical questions about the details of hydrogen ICE technologies. The economic scenario analysis components of the research have followed the methodology of the NRC (2004) Report, providing a similar economic and environmental analysis.

It appears that hydrogen ICE vehicles may have a place in a future hydrogen economy, although it is likely to be limited, depending on the technology advance of fuel cell vehicles. The same difficulties in implementing the hydrogen economy will equally apply to hydrogen ICE vehicles and hydrogen fuel cell vehicles, but the potential fuel economy improvement benefits are greater for fuel cell vehicles. However, the expense of adding additional fuel cells on vehicles that face high load demands (e.g., trucks, buses) may imply that it would be more cost-effective to utilize hydrogen ICE technology in those cases.

<table>
<thead>
<tr>
<th>Table 2. Comparison of Different Vehicle Types</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Gasoline ICE</strong></td>
</tr>
<tr>
<td>Engine Type</td>
</tr>
<tr>
<td>Average engine efficiency</td>
</tr>
<tr>
<td>Max engine Efficiency</td>
</tr>
<tr>
<td>Transmission Type</td>
</tr>
<tr>
<td>Transmission Efficiency</td>
</tr>
<tr>
<td>Fuel Economy (mpg equiv.)</td>
</tr>
<tr>
<td>Power</td>
</tr>
<tr>
<td>Fuel Tank Size (constant range)</td>
</tr>
<tr>
<td>Cost of Fuel</td>
</tr>
<tr>
<td>Criteria Pollutant Emissions</td>
</tr>
<tr>
<td>State of technology</td>
</tr>
</tbody>
</table>
Modeling the Cost and Benefits of Solar Photovoltaics

This study utilizes learning curves to model and predict cost reductions in photovoltaic modules relevant for electric power generation. By extending the existing learning curve theory to a two-factor model, this analysis accounts for the impacts of both R&D and production activities on technology cost. Results suggest that increasing production activity or increasing R&D activity, but not both, may be inexpensive policy methods to reduce PV unit costs to fossil-fuel levels. Also, a cost-benefit analysis suggests that the economic justification of continued production activity and R&D efforts depends on one’s assessment of the value of carbon. With a balanced look at both the costs and benefits of certain policy actions, the study recognizes that increasing production activity may be the best way to reach cost-competitive PV generated electricity. Programs like subsidies and tax incentives for solar installations may have substantive impacts on the cost of photovoltaic systems.

In order to model cost reductions, a two-factor learning curve was used with the form,

\[ C_t = C_0 Q^{-\alpha} R^{-\beta} \]

where \( C_t \) is the cost at time \( t \) in $/W_{\text{peak}}\), \( C_0 \) is cost of the first unit in $/W_{\text{peak}}\), \( Q \) is the cumulative production in MW_{\text{peak}}\), \( \alpha > 0 \) is the learning-by-doing ("LBD") parameter, \( R \) is the cumulative R&D expenditures in Million 2000 $, and \( \beta > 0 \) is the learning-by-searching ("LBS") parameter. This formula, first introduced by Kouvaritakis et al. in 2000, measures the contributions to cost reductions from both production and R&D activities.

Pathways

To address how to best accelerate PV cost reductions in the future, expressions for \( Q_t \) and \( R_t \) over time are needed. A closed form, analytical expression for an optimal path of \( Q_t \) and \( R_t \) could not be derived, so instead, this analysis utilizes low, base, and high growth rates for each, estimated from historical data. Each pair of \( Q_t \) and \( R_t \) growth rates was called a policy pathway and illustrated how cumulative production and cumulative R&D expenditures would increase each year. Five pathways were analyzed:

<table>
<thead>
<tr>
<th>Pathway</th>
<th>Low Q growth</th>
<th>Base Q growth</th>
<th>High Q growth</th>
</tr>
</thead>
<tbody>
<tr>
<td>High R growth</td>
<td>Low R&amp;D</td>
<td>Optimistic</td>
<td></td>
</tr>
<tr>
<td>Base R growth</td>
<td>Status Quo</td>
<td>High Production</td>
<td></td>
</tr>
<tr>
<td>Low R growth</td>
<td>Pessimistic</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

These pathways represent, in an approximate form, differing policy actions. A pathway like High R&D may reflect an increased focus on PV technology in R&D
funding, for example, while High Production may reflect increased demand for PV systems as a result of subsidies or public interest. These pathways, then, are how this study analyzes policy actions.

Pathways are also needed to translate the relevant factors in the learning curve into time-relevant scenarios. That is, the most illustrative measure of technical progress in photovoltaics may be the time until cost-competitive PV is achieved, not the units or dollar amounts – the learning curve (as specified) does not account for any temporal issues. The option to form a learning curve where time is the driving factor was not made for two reasons. First, it has been shown that in single-factor models, cumulative production is a more accurate factor than time (Argote and Epple, 1990). Second, using time as a factor precludes any analysis of policy actions and alternatives – the only option is to wait for costs to decrease!

Cost Structure

The cost of each constructed pathway was computed to provide a quantitative means of comparison. This cost includes research and development expenditures, as well as the production cost of the technology. Research and development’s contribution to the total cost of a pathway in a particular time period is defined as

\[ C_r(t, R_{t-1}) = R_t - R_{t-1} \]  

(2)

where \( R_t \) is the cumulative research and development expenditure at the end of time period \( t \).

As previously stated, the production cost is assumed to follow a two-factor learning curve, so the marginal cost of each unit produced is less than that of the previous unit. Thus, the total cost of production of a pathway in a particular time period is defined as

\[ C_q(t, Q_{t-1}, R) = \int_{Q_{t-1}}^{Q_t} C_0 \cdot q^{-\alpha} \cdot R^{-\beta} dq \]  

(3)

where \( Q_t \) is the cumulative production level at the end of time period \( t \), \( C_0 \) is the initial production cost, \( \alpha \) is the learning-by-doing parameter, and \( \beta \) is the learning-by-searching parameter. The level of \( R \) to use in calculating the production cost depends on the time lag between investing in research and the research contributing to cost reductions. The cost of production is bounded below by the case where \( R=R_t \), i.e., R&D expenditures during time \( t \) have full effect on production cost in time \( t \). An upper bound can be placed on cost by assuming a time lag between investment in research and the research contributing to cost reductions. In this analysis, the upper bound assumes that the time lag of research is one year, i.e., investing in research today has full impact a year from today; this assumption is represented by the case where \( R=R_{t-1} \). These two bounds imply that

\[ C_q(t, Q_{t-1}, R_t) \leq C_q(t, Q_{t-1}, R_{t-1}) \leq C_q(t, Q_{t-1}, R_{t-1}) \]  

(4)

where \( C_q(t, Q_{t-1}) \) is the actual production cost in time period \( t \).

The total cost of each pathway computed is reduced to reflect the expenditure that would be necessary regardless of technology choice. The assumption is that the service provided by the technology in question would need to be met by some source. In this analysis, it is assumed that new electricity capacity is needed and that capacity can either
be from conventional technologies or solar photovoltaics. The cost of building conventional technologies is defined as

$$C_c^t (Q_t, Q_{t-1}) = C^* (Q_t - Q_{t-1})$$ (5)

where $C^*$ is the per unit cost of the conventional technology (and the target cost of photovoltaic technologies). This formulation assumes that the conventional technology’s cost is constant and thus the technology experiences no learning effects.

Combining each of the above equations and summing over time determines the total cost of a pathway. In each time period, the total cost is defined as

$$C^t (Q_t, Q_{t-1}, R_t, R_{t-1}) = C^t_c (Q_t, Q_{t-1}) + C^t_q (Q_t, Q_{t-1}) - C^t_c (Q_t, Q_{t-1})$$ (6)

Summing this equation over time (with discounting) yields the total cost of an individual pathway, i.e.,

$$C (Q, R) = \sum_{t=1}^{T} C^t (Q_t, Q_{t-1}, R_t, R_{t-1}) \cdot e^{-rt}$$ (7)

where $Q$ is the vector of $Q_t$’s, $R$ is the vector of $R_t$’s, and $r$ is the discount rate.

Data

To parameterize the learning curve, three separate data series were necessary: cumulative production of photovoltaics, cumulative research and development expenditures, and the unit cost of a photovoltaic module. Photovoltaic shipments in the United States were used to estimate cumulative production.\(^1\) The shipment data is from the Energy Information Administrations’ (EIA) Annual Energy Review 2004, Table 10.5. This data series is measured as photovoltaic modules received by US companies; the data series needed is photovoltaic modules produced by US companies. Thus, the proxy used for production is total shipments plus exports minus imports. The EIA data is only provided for 1982 to 2003. Production in 1979 and 1980 were estimated from the graph provided in Richard Swanson’s paper. The cumulative R&D expenditure data series was constructed from information provided by the Energy Information Administration on the Department of Energy’s annual research funding for photovoltaic technologies, in “Department of Energy Historical R&D Budget, Fiscal Years 1978-1999.” EIA only provides data for 1978 to 1999. The annual photovoltaic R&D expenditure in the US for the years 2000 to 2002 is from the International Energy Agency. Photovoltaic module prices for 1989 to 2003 are from the Annual Energy Review 2004, Table 10.5. Prices in 1979, 1980, 1985, and 1986 are from Swanson’s paper and reflect years where Swanson specifically stated module cost, rather than simply graphing the value. All data was converted to constant 2000 dollars using the GDP deflator provided by EIA in the Annual Energy Review 2004, Table D1. The cumulative production, cumulative R&D, and cost data are provided in Table 4.

\(^{1}\) Photovoltaic Installed Capacity was also considered as a proxy for production. However, this data series has theoretical flaws and provided a low $R^2$ in the estimation.
Table 4: Learning Curve Data

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>1979</td>
<td>3</td>
<td>$335</td>
<td>$30.74</td>
</tr>
<tr>
<td>1980</td>
<td>6</td>
<td>$600</td>
<td>$20.97</td>
</tr>
<tr>
<td>1985</td>
<td>53</td>
<td>$1,212</td>
<td>$10.76</td>
</tr>
<tr>
<td>1986</td>
<td>62</td>
<td>$1,269</td>
<td>$10.07</td>
</tr>
<tr>
<td>1989</td>
<td>105</td>
<td>$1,414</td>
<td>$6.54</td>
</tr>
<tr>
<td>1990</td>
<td>125</td>
<td>$1,457</td>
<td>$6.97</td>
</tr>
<tr>
<td>1991</td>
<td>146</td>
<td>$1,513</td>
<td>$7.25</td>
</tr>
<tr>
<td>1992</td>
<td>170</td>
<td>$1,583</td>
<td>$7.07</td>
</tr>
<tr>
<td>1993</td>
<td>204</td>
<td>$1,656</td>
<td>$5.93</td>
</tr>
<tr>
<td>1994</td>
<td>246</td>
<td>$1,739</td>
<td>$4.94</td>
</tr>
<tr>
<td>1995</td>
<td>296</td>
<td>$1,830</td>
<td>$4.95</td>
</tr>
<tr>
<td>1996</td>
<td>352</td>
<td>$1,895</td>
<td>$4.36</td>
</tr>
<tr>
<td>1997</td>
<td>430</td>
<td>$1,958</td>
<td>$4.36</td>
</tr>
<tr>
<td>1998</td>
<td>514</td>
<td>$2,037</td>
<td>$4.08</td>
</tr>
<tr>
<td>1999</td>
<td>642</td>
<td>$2,118</td>
<td>$3.70</td>
</tr>
<tr>
<td>2000</td>
<td>789</td>
<td>$2,182</td>
<td>$3.46</td>
</tr>
<tr>
<td>2001</td>
<td>938</td>
<td>$2,256</td>
<td>$3.34</td>
</tr>
<tr>
<td>2002</td>
<td>1,110</td>
<td>$2,324</td>
<td>$3.59</td>
</tr>
</tbody>
</table>

To compute the target cost of photovoltaics, the cost and performance of competing electric generating technologies are needed, as well as fossil fuel prices. The cost and heat rate of new electric generating technologies are from EIA’s Assumptions to the Annual Energy Outlook 2005, Table 38. The capacity factors for coal and natural gas electric generation are from EIA’s Electric Power Annual 2000, Figure 4. The capacity factor for solar photovoltaic electric generation is from EIA’s Assumptions to the Annual Energy Outlook 2005, Table 75. The fuel price data is the data estimated for the year 2005 in EIA’s November 2005 Short-Term Energy Outlook, Table 4. All costs are in constant 2000 dollars. Cost and performance data used in the analysis are presented in Table 5.

Table 5: Electric Generating Technology Cost and Performance Data

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Coal</td>
<td>8,844</td>
<td>$1,286</td>
<td>$25.82</td>
<td>$0.004</td>
<td>71%</td>
<td>$1.42</td>
</tr>
<tr>
<td>Natural Gas</td>
<td>7,196</td>
<td>$601</td>
<td>$11.70</td>
<td>$0.002</td>
<td>29%</td>
<td>$7.37</td>
</tr>
<tr>
<td>Photovoltaic</td>
<td>10,280</td>
<td>$4,735$ (^2)</td>
<td>$10.96</td>
<td>$0.000</td>
<td>24%</td>
<td>$0.00</td>
</tr>
</tbody>
</table>

Parameter Estimation: Learning Curve

Ordinary Least Squares (OLS) was first used to parameterize the two-factor learning curve. This method simultaneously determines the learning-by-doing parameter, \( \alpha \), the learning-by-searching parameter, \( \beta \), and the initial cost, \( C_0 \). However, two-factor learning curves (2FLC) have been plagued historically with multicollinearity, leading to

\(^2\) This value, solar photovoltaic capital cost, is the one used in the AEO 2005. Its value will be varied later to find \( C^* \), the cost that makes solar photovoltaic technologies competitive with coal and natural gas.
instability (Kouvaritakis et al., 2000; Miketa and Schrattenholzer, 2005). A test of the condition number for the data used in this analysis suggests that the 2FLC for PV also exhibits multicollinearity. To correct for this problem, an OLS regression of cost on cumulative production and cumulative R&D with β fixed was performed, as suggested by Kouvaritakis et al. and used by Miketa and Schrattenholzer. This regression yielded an estimate of α and C₀ for each β specified. The value of β was then varied to find the best goodness-of-fit, i.e., the highest R². Table 6 shows the estimates of α, β, and C₀ for the simultaneous estimation case, the single-factor learning curve, as well as various values of β in the fixed β case. In addition, the table includes the R² and a 95% confidence interval on the parameter estimates. Figures 6 and 7 show the estimated and actual values of module cost versus cumulative production and cumulative R&D expenditures, respectively.

Table 6: Learning Curve Parameter Estimation

<table>
<thead>
<tr>
<th></th>
<th>C₀</th>
<th>-α</th>
<th>95% CI on -α</th>
<th>LBD Rate</th>
<th>-β</th>
<th>95% CI on -β</th>
<th>R²</th>
</tr>
</thead>
<tbody>
<tr>
<td>Simultaneous</td>
<td>101</td>
<td>-0.342</td>
<td>(-0.401, -0.283)</td>
<td>21%</td>
<td>-0.139</td>
<td>(-0.931, 0.653)</td>
<td>0.984</td>
</tr>
<tr>
<td>Single Factor</td>
<td>45</td>
<td>-0.384</td>
<td>(-1.582, -0.229)</td>
<td>23%</td>
<td>0.000</td>
<td>N/A</td>
<td>0.983</td>
</tr>
<tr>
<td>β Fixed 1</td>
<td>176</td>
<td>-0.313</td>
<td>(-1.501, -0.160)</td>
<td>20%</td>
<td>-0.234</td>
<td>N/A</td>
<td>0.983</td>
</tr>
<tr>
<td>β Fixed 2</td>
<td>292</td>
<td>-0.287</td>
<td>(-1.501, -0.130)</td>
<td>18%</td>
<td>-0.322</td>
<td>N/A</td>
<td>0.983</td>
</tr>
<tr>
<td>β Fixed 3</td>
<td>9,793</td>
<td>-0.104</td>
<td>(-1.834, 0.120)</td>
<td>7%</td>
<td>-0.931</td>
<td>N/A</td>
<td>0.965</td>
</tr>
</tbody>
</table>

A confidence interval on β can only be computed for the simultaneous determination cases. In all other cases, β is fixed.

Figure 6: Module Cost versus Cumulative Production
Three different learning scenarios were constructed by varying the parameters of the learning curve. The Base case learning scenario uses the learning parameters that maximize the goodness-of-fit ($R^2$). The Low learning scenario fixes the learning-by-searching rate at 0% and then estimates the learning-by-doing rate and initial cost; this scenario is identical to a single-factor learning curve. The High learning scenario fixes the learning-by-searching rate at the upper bound on the 95% confidence interval for the joint estimation and then calculates the learning-by-doing rate and initial cost. Table 7 shows the learning curve parameter values used in the analysis.

**Table 7: Learning Scenarios**

<table>
<thead>
<tr>
<th></th>
<th>$C_0$</th>
<th>$\alpha$</th>
<th>LBD Rate</th>
<th>$\beta$</th>
<th>LBS Rate</th>
</tr>
</thead>
<tbody>
<tr>
<td>Low</td>
<td>45</td>
<td>0.384</td>
<td>23%</td>
<td>0.000</td>
<td>0%</td>
</tr>
<tr>
<td>Base</td>
<td>101</td>
<td>0.342</td>
<td>21%</td>
<td>0.139</td>
<td>9%</td>
</tr>
<tr>
<td>High</td>
<td>9,793</td>
<td>0.104</td>
<td>7%</td>
<td>0.931</td>
<td>48%</td>
</tr>
</tbody>
</table>

**Parameter Estimation: Target Cost**

To find $C^*$, the target cost for photovoltaic technologies, the levelized cost of generating electricity from new coal and new natural gas plants was first calculated. Next, the capital cost of a solar photovoltaic plant was selected to equate the cost of electricity from solar with the cost of electricity from coal and natural gas. Table 8
shows the calculation of the electricity cost for coal, natural gas, and three values of PV capital cost.\textsuperscript{4}

Table 8: Cost of Electricity Generation

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Coal</td>
<td>6,220</td>
<td>55.01</td>
<td>$78.26</td>
<td>$205</td>
</tr>
<tr>
<td>Natural Gas</td>
<td>2,540</td>
<td>18.28</td>
<td>$134.78</td>
<td>$96</td>
</tr>
<tr>
<td>Photovoltaic 1</td>
<td>2,102</td>
<td>21.61</td>
<td>$0.00</td>
<td>$756</td>
</tr>
<tr>
<td>Photovoltaic 2</td>
<td>2,102</td>
<td>21.61</td>
<td>$0.00</td>
<td>$103</td>
</tr>
<tr>
<td>Photovoltaic 3</td>
<td>2,102</td>
<td>21.61</td>
<td>$0.00</td>
<td>$194</td>
</tr>
</tbody>
</table>

Three scenarios for target cost of solar photovoltaic technologies were created based on the electricity cost estimates previously described. In the base case, the target cost is chosen such that solar is cost competitive with natural gas. In the low case, the target cost is chosen such that solar is cost competitive with coal, the low cost producer. This cost was not used as the base case because coal provides base load generation, whereas solar provides peaking power. Thus, solar is not likely to replace coal generation and will not need to match the cost of coal. The high case is simply the analysts’ judgment of an upper bound on the target cost. Table 9 shows the values of $C^*$ used in the analysis.

Table 9: Target Cost Scenarios

<table>
<thead>
<tr>
<th>C$^*$ (2000$/W)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Low</td>
</tr>
<tr>
<td>Base</td>
</tr>
<tr>
<td>High</td>
</tr>
</tbody>
</table>

Figures 8-10 illustrate level sets of each learning curve scenario at the three target cost scenarios. In each, points on the same line indicate different pairs of changes in R and changes in Q that achieve a particular technology cost.

\textsuperscript{4} The first PV capital cost is the assumption used in the Annual Energy Outlook. The second is the level needed to equate solar electricity cost with coal. The third equates solar with natural gas.
Figure 8: Base learning curve level sets

Figure 9: Low learning curve level sets
Parameter Estimation: Growth of Q and R

Low, base, and high growth rates of Q and R were estimated from historical data. By examining the historical behavior of Q and R, it becomes apparent that cumulative R&D expenditures are best modeled with a per-year absolute growth, while the cumulative production is best modeled with a per-year percentage growth. Also, there are two major regimes – one from 1978 to 1981 and the other from 1982 to the present. From these observations, growth rates are estimated using these authors’ judgment.

Table 10: Growth rates of Q

<table>
<thead>
<tr>
<th>High Q growth</th>
<th>Growth rate</th>
<th>Comment</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>28% pa</td>
<td>CAGR of cumulative prod. 1979-2003</td>
</tr>
<tr>
<td>Base Q growth</td>
<td>19%</td>
<td>CAGR of cumulative prod. 1984-2003</td>
</tr>
<tr>
<td>Low Q growth</td>
<td>5%</td>
<td>Authors’ judgment</td>
</tr>
</tbody>
</table>

Table 11: Growth rates of R

<table>
<thead>
<tr>
<th>High R growth</th>
<th>Growth rate</th>
<th>Comment</th>
</tr>
</thead>
<tbody>
<tr>
<td>Base R growth</td>
<td>70 M 2000 $</td>
<td>Average of 1982-2002</td>
</tr>
<tr>
<td>Low R growth</td>
<td>20 M 2000 $</td>
<td>Authors’ judgment</td>
</tr>
</tbody>
</table>

These growth rates are illustrated in Figures 11 and 12.
Therefore, the five pathways examined are:

1. **Status Quo**: Q grows at 19% pa, R grows at $70M pa
2. **High R&D**: Q grows at 19% pa, R grows at $213M pa
3. **High Production**: Q grows at 28% pa, R grows at $70M pa
4. **Optimistic**: Q grows at 28% pa, R grows at $213M pa
5. **Pessimistic**: Q grows at 5% pa, R grows at $20M pa

**Results**

For each learning curve (Low, Base, and High), the five pathways were applied to determine how cost reductions occur in each. Recall that each pathway represented how \( Q_t \) and \( R_t \) changed in time; adding the learning curve framework allows us to examine how \( C_t \) behaves in time for each pathway. Together, these are fifteen different \( C_t \) curves.

In Figures 13 to 15, each graph illustrates a single learning curve case. In each, the Pessimistic pathway represents, in a sense, an upper bound on costs in the model. A comparison of the other four pathways shows that Status Quo and Optimistic, as expected, bookend High R&D and High Production. What perhaps is more interesting is the location of these latter two pathways.

![Figure 13: Technology cost over time, Base learning curve](image)

In the Base LC case (Figure 14), higher R&D expenditures, as expressed in High R&D, have little effect on costs as compared to Status Quo. The difference here is never more than $0.10/W_{peak} throughout the 20 year period, despite the non-zero LBS parameter. On the other hand, higher production rates, as expressed in High Production, have a more substantial effect on costs, often driving them down $0.30/W_{peak} or more from the Status Quo pathway. For the Base LC, this is as expected, as the LBD rate of 21.1% (taken to be \( 1-2^{-\alpha} \)) is over twice the LBS rate of 9.2% (taken to be \( 1-2^{-\beta} \)). Using the base target cost of $1.21/W_{peak}, cost-competitive PV is reached by all pathways between 2013 and 2018 (8-13 years), with the exception of the Pessimistic pathway, which never attains that cost.
In the Low LC case (Figure 14), recall that the LBS rate is zero and thus this scenario acts as a single-factor learning curve. R&D expenditures (or increases in expenditures) have no effect and the only recourse to accelerate cost reductions is to increase production rates. This is the classic theory of learning curves, and illustrates the limits of its usefulness in the recommending policy actions.

Figure 14: Technology cost over time, Low learning curve

Figure 15: Technology cost over time, High learning curve
In the High LC case (Figure 15), the effect of increased R&D expenditures and increased production rates are reversed as compared to the Base LC case. As you would expect with a higher LBS rate, increased R&D expenditures lead to decreased costs.

**Figure 16:** Technology cost over time, Status Quo

**Figure 17:** Technology cost over time, High R&D
Examining the pathways individually (Figures 16 - 20), both the Low LC case and Base LC case have similar dynamics. The High LC case results in costs that are nearly uniformly higher.

![Graph: High Production Technology Cost Over Time](image)

**Figure 18:** Technology cost over time, High Production

![Graph: Optimistic Technology Cost Over Time](image)

**Figure 19:** Technology cost over time, Optimistic
The cost of each previously defined pathway was computed and compared for the three sets of learning parameters. In this section, the results of the base case are presented. The base case assumes a target cost of $1.21/W and a discount factor of 5%. Both the target cost and discount factor are varied later in the sensitivity analysis. Figures 21, 22, and 23 show the annual cost of each pathway over time for the Base, Low, and High learning scenarios, respectively, in the base case.

The cost of each pathway increases initially due to increased production of the technology, and then eventually declines as production and R&D impact the unit cost of the technology. Under Base learning parameters, the Optimistic pathway has the highest cost in the initial period due to the large investment in R&D and high production. This pathway, however, reaches the target cost first. The Pessimistic pathway has the lowest initial cost, but does not meet the target cost by the year 2050.

The Low learning parameters are similar enough to the Base learning parameters that the annual cost of each pathway takes on the same shape and ordering of initial costs. Under the Low learning parameters, however, the High Production pathway reaches the target cost slightly before the Optimistic pathway, and the Status Quo pathway reaches the target cost slightly before the High R&D pathway; the opposite is true under the Base learning parameters.
Figure 21: Annual cost of pathways, Base learning parameters

Figure 22: Annual cost of pathways, Low learning parameters
Figure 23: Annual cost of pathways, High learning parameters

Under the High learning parameters, the High Production pathway cost increases much more quickly than the other four pathways. This pathway assumes production increases substantially; however, the High learning parameters put little weight on production in the reduction of unit cost.

The previous three graphs show the annual cost of each pathway over time. However, the cost ordering of pathways changes as time progresses. Thus, in order to rank the pathways in terms of cost, another metric is necessary. Figure 24 shows the net present value of the cost of each pathway under each of the three learning scenarios.5

As seen in Figure 24, each pathway has approximately the same NPV under the Base learning parameters. The High Production pathway has marginally lower cost ($4.6 billion) and the High R&D pathway has marginally higher cost ($5.2 billion), but each pathway costs approximately $5 billion. Under the Low learning parameters, the pathway costs are also relatively similar. The High Production pathway is the least expensive, costing only $3.7 billion, and the High R&D pathway is the most costly, at $5.2 billion. Under the High learning parameters, however, the difference in cost between the most and least expensive pathways is substantial. The High Production costs $39.6 billion, almost eight times as much as the High R&D pathway. This large cost is due to the rapid growth of production and moderate R&D assumed in the High Production pathway. The High learning scenario assumes that a cumulative doubling of production only reduces unit cost by 7%; thus, rapid expansion of PV production has little effect on the cost of photovoltaics.

5 The Pessimistic pathway is not included in this graph because it does not reach the target cost by the year 2050.
One interesting observation from the NPV graph is that the High R&D pathway is relatively robust with respect to learning parameters. In each of the three learning scenarios, the High R&D pathway costs approximately $5 billion and reaches the target cost in 2017. Thus, if there is uncertainty in the learning parameters, the High R&D pathway is the least risky in terms of cost.

The previously presented analysis aimed to find the cost and time necessary to render PV technologies economically competitive with fossil fuel technologies, under several different learning scenarios and pathways. The results suggest the least costly pathway depends on the learning curve parameters specified. For example, in the Low and Base learning scenarios, the High Production pathway is the least costly, while the High R&D is the least expensive in the High learning scenario. The High R&D scenario is robust in terms of learning curves, having roughly the same cost and time to target under each learning scenario. The analysis also suggests that the preferred pathway depends on the target cost. For example, the High R&D scenario is the least expensive means of reaching a target cost of $0.61/W. The High Production pathway is preferred for target costs of $1.21/W and $2/W.

The benefit of solar PV technology in terms of carbon emissions reductions was also analyzed. The analysis finds that a carbon value of $48/ton C for coal or $106/ton C for natural gas will set the discounted value of reduced carbon emissions equal to the discounted costs in the Status Quo pathway under Base learning parameters. Therefore, from a reduced carbon emissions perspective, the economic justification depends on one’s assessment of the value of carbon.

A cost-effectiveness study suggests that alternative pathways may be preferred to the Status Quo pathway. In particular, the High Production pathway is less costly and
achieves more benefits than the Status Quo under Low and Base learning parameters. This finding is consistent with historical cost reductions in the solar PV industry. Conversations with Bill Yerkes, the Chief Technology Officer of Solaicx, indicate that historic PV cost reductions have been driven by production. The High Production pathway relies on increased production to reduce costs of solar to an economically competitive level. Under High learning parameters, the High R&D and Optimistic pathways are deemed cost-effective. A sensitivity analysis on the carbon value suggests that increasing the value of carbon to $54/ton C makes the High Production pathway cost-effective under the High learning parameters.

Publications


Publications


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Appendix A: Highlights of The Hydrogen Economy: Opportunities, Costs, Barriers, and R&D Needs.

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In what follows are graphical summaries of results of the modeling and analysis, as included in the National Academies’ recently published study: *The Hydrogen Economy: Opportunities, Costs, Barriers, and R&D Needs*. The interested reader can read more detailed discussions of these results in that study, currently available online at www.nap.edu.

Figure 1 shows the estimated unit costs of the various technologies, based on currently available state of technology. The heights of the bars represent the unit costs, expressed as dollars per Kg of hydrogen. The four bars on the left are all central station technologies (CS), large enough to produce 1.2 million Kg of hydrogen per day, roughly enough to fuel 2 million light duty vehicles from each such plant. Two use coal as a feedstock (Coal) and two use natural gas (NG). For one coal and one natural gas technology carbon dioxide is separated and sequestered (Seq); for the other two technologies carbon dioxide generated during the production process is vented into the atmosphere (no label). The two bars in the center are all mid-size (MS) technologies, large enough to produce 24,000 Kg of hydrogen per day, roughly enough to fuel 40 thousand light duty vehicles from each such plant. They use biomass (Bio) as a feedstock, which is gasified for producing hydrogen.

The next four bars are distributed (Dist) technologies, large enough to produce 480 Kg of hydrogen per day, roughly enough to fuel one thousand light duty vehicles from each such station. The first of these distributed technologies is a small reformer, using natural gas as a feedstock. The other three use electrolyzers, in which electricity is used to dissociate water, producing hydrogen and oxygen. One of these three is based on electricity taken from the grid; such electricity is represented as being generated by mix of primary energy sources typical of the U.S. grid. The second is based on two sources of electricity: electricity is generated from wind turbines (WT) during the time sufficient electricity is available from these turbines; electricity is taken from the grid at all other times. The third is also based on two sources of electricity: electricity is generated from photovoltaic (PV) cells during the time sufficient electricity is available from these PVs; electricity is taken from the grid at all other times.\(^6\)

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\(^6\) We also examined electricity derived entirely from wind turbines or from photovoltaic cells, not using grid electricity as a backup. However, these would require substantially larger electrolyzers, since the electrolyzer would be operating only a small fraction of the time. The increased capital cost of the larger electrolyzer leads to significantly greater unit costs than those pictured in this graph.
The final bar represents gasoline, expressed in a per-mile hydrogen-equivalent basis. This bar represents the cost to produce enough gasoline to drive one hybrid vehicle the same number of miles as a fuel cell vehicle can be driven using one Kg of hydrogen. In this discussion, that will be referred to as the “per-mile hydrogen equivalent” gasoline cost. This gasoline cost is based on nation-wide U.S. estimates, for crude oil prices of $30 per barrel. This estimate is very sensitive to the assumptions about the future price of crude oil.

In Figure 1, five different components of costs are presented for the central station and the mid-size technologies: production, distribution by pipeline or truck, dispensing, CO₂ disposal (sequestration), and “carbon imputed cost”. The “carbon imputed cost” is an estimate of environmental cost of carbon dioxide release, based on an assumed environmental cost of $50 per tonne of carbon. However, for the distributed station, the production and dispensing cost are modeled as being part of one integrated operation; there is no distribution cost because the hydrogen is produced on site. Thus only the total distributed cost and the “carbon imputed cost” are included for these technologies.

Figure indicates that even with current technologies, if the U.S. were to have large enough hydrogen production plants, it would be possible to produce hydrogen using either coal or natural gas as a feedstock, at delivered unit costs that would be very similar to unit costs (on a per-mile hydrogen equivalent basis) of using gasoline in hybrid vehicles. This implies that if the challenges of producing fuel cell vehicles were solved,
so that these vehicles had production and maintenance costs equivalent to these costs for hybrid vehicles, then at a large scale of hydrogen production the fuel costs for fuel cell vehicles would also be very similar to fuel costs for hybrid vehicles. Thus such vehicles could be competitive with hybrid vehicles.

Figure 1 also indicates that unless current technologies are improved, hydrogen produced from renewable energy or by electrolyzing water would be substantially more expensive than hydrogen produced from fossil fuels.

More detailed cost estimates are shown in Figure 2 for the same current technologies. In this figure, the production costs are further broken down into several cost components:

**Figure 2.** Details of Unit Cost Estimates for Currently Available Technologies

capital charges, feedstock costs, electricity cost, non-fuel operations and maintenance (O&M) and fixed costs. These categories are also shown for the distributed hydrogen production technologies.

Figure 2 shows that for hydrogen generated using electrolysis, the cost of electricity is the most important cost element, followed by capital costs, primarily capital costs of electrolyzers and of storage facilities. Capital costs are large components of the cost of biomass. In addition, distribution costs of these mid-size facilities are large, since
distribution by pipeline increases sharply on a per-unit basis for these smaller facilities. Distribution by truck seems to be the lowest cost option.

We have developed similar cost estimates for potential future technologies. These estimates were based on the technical judgments by the members of the NRC “Committee on Alternatives and Strategies for Future Hydrogen Production and Use”. They are meant to represent moderately optimistic judgments about the improvements in these technologies, if an aggressive R&D program is directed toward the technologies and is successful. Figure 3 presents these cost estimates, using the same scale as used in Figure . Only one new technology is introduced: nuclear energy (Nu) in a reactor run at high enough temperatures to cause direct dissociation of hydrogen from oxygen in water.

Figure 3 shows that with technological advances, hydrogen could be generated from fossil fuels, distributed, and dispensed to the consumers at costs lower than the costs of gasoline (with $30 per barrel crude oil prices.) Cost of hydrogen from wind-turbines, from distributed natural gas reforming, and from nuclear power would be more expensive than gasoline costs, but not very much more expensive.

The potential future generation of hydrogen by electrolysis, using wind turbines for the electricity is based on the wind turbines being used to provide all of the electricity. If
the cost of fuel cell stacks drop sharply, then costs of electrolyzers are likely to drop sharply as well. Such a change would make low quality, intermittent electricity economically attractive for electrolysis: it would be more economical to invest in large electrolyzers and to use them only when the wind turbines are generating electricity.

Gasification of biomass and electrolysis from grid-derived electricity or from photovoltaics is expected to be substantially more expensive, even with the technology advances we have postulated.

More detail on these cost estimates is provided in Figure 4. This figure shows that the high cost of electricity is expected to be the dominant factor in the unit costs of electrolysis-based hydrogen production. It shows that the high costs of distribution of hydrogen from mid-sized plants is a key factor, but not the only factor, in the high unit costs of biomass gasification. This suggests that methods of reducing this cost, say through a network of pipelines that could connect mid-sized plants could significantly reduce these cost estimates.

Additional discussion of these cost estimates is provided in the National Academies’ study: *The Hydrogen Economy: Opportunities, Costs, Barriers, and R&D Needs.*

![Possible Future Technologies: Cost Estimates](image)

**Figure 4.** Details of Unit Cost Estimates for Possible Future Technologies

Unit estimates of carbon releases into the atmosphere from light duty vehicles are provided in Figure 5 for currently available technologies and in Figure 6 for possible future technologies.
These graphs suggest none of the technologies would increase the unit emissions of carbon dioxide into the atmosphere above the amounts that would be associated with use of gasoline in hybrid vehicles. Technologies involving capture and sequestration of the carbon dioxide could sharply reduce the unit releases of carbon dioxide. Generation of hydrogen through electrolysis could reduce unit emissions, but for current technologies the reduction would not be very large. However, with potential future technologies, use of wind turbines could reduce emissions to zero, since in this case no grid-based electricity would be used. Use of natural gas could reduce emissions, but again, not by large amounts, absent carbon dioxide sequestration.

![Current Technology Estimates: Carbon Released to Atmosphere](image)

**Figure 5. Unit Estimates of Carbon Releases for Currently Available Technologies**

Biomass technology is particularly interesting from a carbon management perspective, if the carbon dioxide is separated and sequestered when the biomass is gasified. In that case, only a very little carbon dioxide would be released into the atmosphere at the point of gasification. None would be released at the point of use. However, growing of the biomass would take carbon dioxide out of the atmosphere. Most of this carbon dioxide would be sequestered. Thus, on net, use of biomass could reduce the amount of carbon dioxide: on net it could lead to negative emissions of carbon dioxide, if the carbon dioxide were separated and sequestered.
The unit estimates discussed above were incorporated into a vintage capital model of the light-duty vehicle evolution over time in order to create several quantitative scenarios of the introduction and growth of hydrogen use in light duty vehicles. We turn now to that discussion.

As discussed above, the analysis assumes that the maintenance and production costs of fuel cell vehicles can be made equivalent to the costs of hybrid vehicles. In order to meet this end, fuel cells would need very large improvement from their current state. In particular, it would be necessary to meet cost targets for the fuel cell stack of about $50 per KW. The stacks would need much longer lives than is now the case, on the order of 4,000 to 5,000 hours of operation over the normal lifetime of a passenger car. On board storage of hydrogen must be improved in order to provide an adequate range between refuelings, on the order of 300 miles. In what follows, in some scenarios we assume all these goals have been met.

![Figure 6. Unit Estimates of Carbon Releases for Possible Future Technologies](image)

We have developed three scenarios in order to estimate quantitatively the impacts of fuel-cell vehicles. The first scenario, perhaps the most unlikely, is one in which the goals are not met, so that hydrogen vehicles are never introduced in large scales. In addition, in this scenario hybrid vehicles never command a large market share, so that almost all of the vehicles remain conventional gasoline-fueled light duty vehicles.
The second scenario is also one in which the goals are not met, so that hydrogen vehicles are never introduced in large scales. But in this scenario hybrid vehicles grow steadily in market share, ultimately replacing all conventional vehicles.

The third scenario is one in which the fuel-cell vehicle goals are met and hydrogen progressively becomes the dominant fuel for light duty vehicles. In this scenario, hybrid vehicles first replace conventional vehicles over time; then H2 vehicles replace hybrid vehicles. The number of conventional vehicles follows same time trajectory whether or not hydrogen vehicles are successfully introduced.

The second and third scenarios allow the comparison between a successful introduction of hydrogen fuel cell vehicles and no successful such introduction. The first scenario provides a baseline for projections of the current system.

![Fuel Economy Over Time Assumed for Three Vehicle Technologies](image)

**Figure 7.** Fuel Economy Over Time Assumed for Three Vehicle Technologies

The analysis depends on assumptions about the changes over time in the fuel efficiency of the three types of vehicles. We assume that in each scenario the fuel efficiency of conventional vehicles again begins grow. We assume that hybrid vehicles have a 45% gain in fuel efficiency over conventional vehicles and that fuel cell vehicles have a 66% gain over hybids. Figure 7 shows projected fuel efficiencies over time, measured in miles per Kg of hydrogen or miles per gallon of gasoline, of the fleet of new light duty vehicles. Note that these estimates include not just small vehicles, but a mix of differing weights and sizes of light duty vehicles.
Figure 8 shows the assumed penetration rates of the new vehicles in the second and third scenario. (In the first scenario there is no penetration of either hybrid or fuel cell vehicles.) In the second scenario, hybrid vehicles increase to 100% market share of new vehicles and conventional vehicles decrease to zero market share by 2035. In the third scenario, the growth of hybrids is interrupted by the rapid growth of hydrogen fuel cell vehicles, which increase to 100% market share before 2040.

![Assumed Fractions of New Vehicles](image)

Figure 8. Assumed Fractions of New Vehicle Types: Three Scenarios

The entire inventory of vehicles on the road adjusts only with a lag to the adjustments in new vehicle sales, since in any year, the inventory is dominated by previous vintages of vehicles. Figure 9 provides estimates of the on-the-road inventory of vehicles, using a very simple vintage capital model of the vehicle fleet.

Figure 8 and Figure 9 represent an optimistic assessment of the rate at which new fuel cell vehicles can penetrate into the market and the rate at which the fleet of vehicles would evolve. They show that if hydrogen technologies are successful, the evolution of the system would occur only over many decades, converging to 100% market share of hydrogen vehicles no earlier than about 2050.

In order to determine the consumption of gasoline and of hydrogen in the various scenarios, it is also necessary to estimate how much vehicles would be driven, the vehicles miles of travel. We assumed that the total vehicle miles would increase by 2.3% per year over the time horizon. The assumed trajectory of vehicle miles traveled is shown in Figure 10.
Figure 9. Estimated On-the-Road Fractions of Vehicle Technologies

Figure 10. Assumed vehicle miles of travel (Growing 2.3% per year)
The assumptions described above lead to projections of gasoline use over time in the three scenarios. These estimates are shown in Figure 11. This figure shows that absent either hybrid vehicles or hydrogen fuel cell vehicles gasoline consumption would steadily increase over time. The second scenario shows that a market shift toward hybrid vehicles could stop the growth of gasoline consumption, at least temporarily. However, if hydrogen fuel cell vehicles were to follow the diffusion pattern of scenario three, then by 2050 consumption of gasoline would be completely phased out.

![Gasoline Use by Light Duty Vehicles](image)

**Figure 11.** Gasoline Use by Light Duty Vehicles: Three Scenarios

As gasoline consumption is decreased in the third scenario, hydrogen consumption would be increased over time. Figure 12 shows the projected increase in hydrogen consumption over time, if hydrogen fuel cell vehicles penetrate the market consistently with the third scenario.

Figure 12 shows that it would be not until about 2027 that hydrogen use for light duty vehicles would be as large as the current U.S. production of hydrogen. However, by 2050, the use of hydrogen for vehicles could increase to over 100 billion Kg per year, or over 100 billion tons of Kg per year.

In what follows, it will be assumed that the hydrogen production and use for light duty vehicles follows the growth path of Figure 12.
However, various pathways are possible for producing the hydrogen, including each of the technologies shown in Figure 11 and Figure 2. In order to examine the implications of the various technologies, impacts of moving to a hydrogen economy are examined under the assumption that all of the hydrogen is produced using a single technology. The graphs in the subsequent portion of this report are based on 100% of the hydrogen being generated from a single technology.

In fact, moving toward a hydrogen economy would not lead to all hydrogen production being based on a single technology. It is more likely that a mix of technologies would be utilized. In that case, the various impacts would be based on a weighted average of the impacts estimated for the various single technology scenarios.

We turn now to an examination of the impacts of hydrogen technologies on carbon dioxide released into the atmosphere.

Under these assumptions, the transition to hydrogen could greatly influence the emissions of carbon dioxide into the atmosphere. If no hydrogen were introduced into the system, but hybrid vehicles grew in market share consistently with scenario two, the emissions of carbon dioxide into the atmosphere would increase until the year 2010 and would then remain roughly constant through the year 2040. This is shown by the orange curves in Figure 13 below.
Figure 13. Carbon Releases into the Atmosphere from Light Duty Vehicles: Hydrogen Produced from Fossil Fuels
Figure 13 shows carbon dioxide releases for the current technologies and the possible future technologies, (upper panel and lower panel, respectively), for fossil-fuel based production of hydrogen plus hydrogen generated from direct thermal dissociation of hydrides.

For both the current technologies and the possible future technologies, generation of hydrogen using natural gas can significantly reduce the carbon dioxide emissions. Emissions could be sharply reduced by capturing and sequestering the carbon dioxide. Generation of hydrogen from nuclear facilities would even further reduce the emissions.

Figure 14 shows emissions of carbon dioxide for hydrogen made with renewable energy – biomass, photovoltaics, wind turbines – and hydrogen electrolyzed using grid-based electricity. Carbon dioxide releases would be reduced if hydrogen were generated using photovoltaics, wind turbines, nuclear power, or biomass. However, using grid-based electricity to when the wind turbine or photovoltaics was not producing electricity would reduce the degree to which these technologies reduce the carbon dioxide releases.

This graphs show the dramatically negative releases of carbon dioxide from use of biomass when, after the biomass is gasified, the carbon dioxide is separated and sequestered.

We have also examined the impacts of the various hydrogen pathways on the use of other natural resources.

Figure 15 shows the amounts of natural gas that would be used by the various technologies that use natural gas as a feedstock. This graph also plots the projections, to the year 2025, from the Energy Information Administration, of natural gas production, consumption, and exports, not counting use for hydrogen production. The large amount of natural gas that would be needed for hydrogen production could not be supplied from domestic resources. These quantities would likely lead to increased imports of natural gas.

This impact can be quantified by comparing the reductions in oil use – and hence oil imports – with the increase in natural gas consumptions – and hence imports. These comparisons are shown in Figure 16, for potential new technologies. A graph based on potential future technologies would look very similar. This graph shows that, on an energy equivalent value, the increases in natural gas imports would be very similar in magnitude to the reductions in oil imports. Such a shift cannot be expected to contribute to energy security.
Figure 14. Carbon Releases into the Atmosphere from Light Duty Vehicles: Hydrogen Produced Using Current Non-Fossil Fuel Technologies
Figure 15. Natural Gas Used to Generate Hydrogen: Current and Future Natural-Gas-Based Technologies

Figure 16. Impacts on Gasoline Use vs Natural Gas Use: Possible Future Technologies
For hydrogen generation using coal, however, the results are quite different. Figure 17 shows the amount of coal that would be used if all of the hydrogen were produced from coal. The EIA projections of U.S. coal production and use are also plotted on the same graph. Although coal used for hydrogen production could be a significant fraction of the projected use of domestic coal, this increase in production could be satisfied from domestic coal production.

![Graph showing coal used to generate hydrogen](image_url)

**Figure 17. Impacts on Coal Use: Current and Future Technologies**

If biomass were used as the feedstock, then it would be necessary to grow the biomass. Figure 18 provides estimates of the amount of land that would be required if all of the hydrogen were produced using biomass. This suggests that 300,000 to 600,000 square miles of land would be needed to produce all the hydrogen from biomass. In order to put this in perspective, it can be noted that the U.S. currently uses 700,000 square miles of land as crop land and 900,000 square miles of pasture land. This suggests that, although one could use biomass to produce some hydrogen, it would not be viable to use it as the primary source of hydrogen.
The final natural resource examined is sites for sequestration of carbon dioxide. Figure 19 shows the annual amount of carbon dioxide that would be sequestered for those technology pathways that involve sequestration. Figure 19 shows the cumulative amount of carbon dioxide that would be sequestered. These suggest that between 0.8 and 1.6 billion metric tonnes would be sequestered annually, leading to a cumulative amount sequestered by 2050 of between 10 and 20 billion metric tons. Cumulative carbon sequestration totals are shown in Figure 20. Much research is still needed to ascertain the amount of carbon dioxide that could be safely sequestered. However, for perspective, it can be noted that the estimated capacity of depleted U.S. oil and gas reservoirs is between 25 and 50 billion metric tonnes. In unminable U.S. coal seams there is an estimated capacity to sequester carbon dioxide of 15 billion metric tonnes.
Carbon Dioxide Sequestered from Automobile H2: Future Technology

Figure 19. Annual Amount of Carbon Dioxide Sequestered: Future Technologies

Cumulative Carbon Dioxide Sequestered from Automobile H2: Future Technology

Figure 20. Cumulative Amount of Carbon Dioxide Sequestered: Future Technologies
Finally is the issue of cost for the supply of fuel for the nation’s fleet of light duty vehicles. Using the unit cost estimate in combination with estimates of the rate of introduction of hydrogen vehicles allows estimation of the total costs to the fuel system. These estimates appear in Figure 21 through Figure 24. Figure 21 and Figure 22 provide estimates for hydrogen produced from fossil fuels, while Figure 23 and Figure 24 provide estimates for hydrogen produced with renewables.

With current technologies, distributed generation of hydrogen from natural gas would remain less costly than use of gasoline in conventional vehicles until the late 2030s. By 2030, without new technologies, the size of the hydrogen market would have increased enough that the cost of distributed generation of hydrogen using natural gas would exceed even the cost of gasoline in conventional vehicles. However, with the potential new technologies, all of the fossil fuel sources of hydrogen would result in a total fuel system cost less than would be the cost of gasoline used in conventional vehicles. Total costs would be similar to costs of the system if hybrid vehicles came to dominate the market.

![Figure 21. Fuel Costs for Light Duty Vehicles: Current Fossil-Fuel-Based Technologies](image)

On the other hand, hydrogen from electrolysis based on renewables or grid-based electricity, or hydrogen from biomass, would lead to sharp increases in the entire fuel system cost with current technologies. (See Figure 23) Even with the potential new technologies (Figure 24) most hydrogen production using renewables would be more expensive than the use of gasoline in conventional vehicles and substantially more costly than the use of gasoline in hybrid vehicles.
Figure 22. Fuel Costs for Light Duty Vehicles: Possible Future Fossil-Fuel-Based Technologies

Figure 23. Fuel Costs for Light Duty Vehicles: Current Non-Fossil-Fuel-Based Technologies
Figure 24. Fuel Costs for Light Duty Vehicles: Potential Future Non-Fossil-Fuel-Based Technologies

References

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Appendix B: Carbon Capture and Storage – Estimating the Costs

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Introduction
This section examines the cost structure of Carbon Capture and Storage (CCS). The analysis highlights the highly heterogeneous nature of Carbon Capture and Storage. Capturing this heterogeneity in a cost distribution is important as results using average values of the cost of carbon capture and storage in economic models may under or overestimate the role of CCS as a mitigation option in both the short and the long run.

This procedure overcomes the difficulty in arriving at overall cost estimates in the absence of detailed data. From underlying component distributions of cost, an aggregate marginal cost curve is built for carbon capture and storage that can be used in larger economic or dynamic system models.

Background
Carbon Capture and Storage is an add on strategy to mitigate climate change, i.e. it adds on top of the existing fossil-fuel technology set rather then replaces elements in that set. It allows the continued use of the existing fossil fuel base at lower emissions.

The overall cost of CCS technologies can be disaggregated into (1) the energy cost of CO2 capture (2) capital costs for the CO2 capture/separations unit, and (3) the cost of CO2 transport and storage.

![CCS Cost Chain](image)

Figure 1. CCS Cost Chain.

The Total Cost of Carbon Capture and Storage can be expressed simply as the Cost of Capture + Cost of Transport + Cost of Storage. As shown in Figure 1, the individual costs depend on the specific source, capture technology, distance to storage.
reservoir, and type of reservoir. There are therefore many combinations possible in this cost chain leading to several sequestration pathways.

Calculating Costs
The following functional relationships give the costs for each element in the chain:
- Cost of Capture = Capital Costs + Energy Penalty = \( f(\text{plant type, technology}) \)
- Cost of Transport = \( f(\text{distance to sink, location, volume}) \)
- Cost of Storage = Cost of Injection + Monitoring & Verification = \( f(\text{reservoir type, reservoir characteristics, volume, location}) \).

The next sections will examine each element in greater detail.

Capture Costs
One of the key barriers to the introduction of CO\(_2\) capture and storage technology has been identified as the high cost of capture. The high cost is principally associated with the extensive equipment required to scrub the CO\(_2\) from exhaust gas streams from power plants whose exhaust streams contain CO\(_2\) in low concentrations (8-14\% by volume). However, many industrial processes generate exhaust gas streams that can contain high purity (>90\%) CO\(_2\), which means that the capture costs will be significantly lower.

Electric Power Sector - The electric power sector accounts for a substantial portion of greenhouse gas emissions in the developed world and a growing fraction in developing countries. In the U.S., electricity generation accounts for about one-third of all greenhouse gas emissions. Table 1 shows reference capture costs for three main plant types. The three main plant types considered are: 1) natural-gas-fired combined cycle (NGCC), (2) integrated gasification combined cycle (IGCC), and (3) pulverized coal (PC). The cost of carbon capture can be calculated by attributing the additional cost of power generation from plant fitted with separation technology to the carbon dioxide captured.

Capture Cost = \( (P_c - P_{nc})/(E_{ct} - E_c) \) where
- \( P_c \) = generation cost from plant with carbon dioxide capture ($/kWh)
- \( P_{nc} \) = generation cost without capture ($/kWh)
- \( E_{nc} \) = emissions from plant without capture (kg/kWh)
- \( E_c \) = emissions from plant with capture (kg/kWh)
- \( E_{ct} \) = quantity of carbon dioxide produced in plant with capture (kg/kWh)

Carbon Dioxide Produced \( E_{ct} = E_{nc} \times G_{nc}/G_c \) where
- \( G_c \) = generation efficiency with capture technology fitted
- \( G_{nc} \) = generation efficiency without capture technology fitted

Table 1. Cost of CO\(_2\) Capture for different plant types.

<table>
<thead>
<tr>
<th>Plant Type</th>
<th>Cost of CO(_2) removal ($/tCO(_2))</th>
<th>Emissions without CO(_2) Capture (kg/MWh)</th>
<th>Emissions w CO(_2) Capture (kg/MWh)</th>
</tr>
</thead>
<tbody>
<tr>
<td>PC plant</td>
<td>$35</td>
<td>800</td>
<td>80</td>
</tr>
<tr>
<td>IGCC plant</td>
<td>$25</td>
<td>670</td>
<td>67</td>
</tr>
<tr>
<td>NGCC plant</td>
<td>$28</td>
<td>370</td>
<td>37</td>
</tr>
</tbody>
</table>

Source: Bechtel Corp 2002.
The total costs of sequestration for old coal-fired plants will be much higher as PC fired coal plants would have almost twice as much CO₂ to sequester than an equivalent gas fired plant because of the greater carbon content of the fuel. Therefore under an actual carbon tax regime, it may be more cost-effective in the long term to fuel-switch, load balance or build new gas-fired power plants instead of retro-fitting old coal fired power plants. 

*Non electric sources* - Recent estimates state that globally there are more than 14,600 large CO₂ point sources. More than 45% of these point sources are from various industrial plants and not such as cement kilns, steel mills, chemical refineries, gas processing facilities, etc., that could also be addressed via the deployment of CCS technologies. (Dooley 2002). These non-electric power CO₂ point sources potentially represent early opportunities for capturing CO₂ at low cost.

*Transportation Costs*

The total annual transportation cost per tonne of CO₂ is found by annualizing the construction cost using a capital charge rate of 15 percent per year and adding this to the annual O&M cost. Pipeline costs are estimated to be of the order of $1/tonne CO₂/100 km. For the Weyburn project, the CO₂ is being supplied via a 205 mile (325 km) long pipeline (costing 100 million US$) from the lignite-fired Dakota Gasification Company synfuels plant site in North Dakota to the Weyburn oilfield in Canada. The total project would add 20 Mt of CO₂ over its lifetime (IEA).

*Storage Costs*

As shown in Table 2, storage costs show great variability even within a reservoir class. The lowest possible costs can be achieved by using CO₂ in value added markets viz. Enhanced Oil Recovery (EOR) and Enhanced Coal Bed Methane (ECBM) where CO₂ can be used to displace previously unrecoverable oil and gas. The use of CO₂ for EOR will provide early sequestration opportunities at negative cost as EOR operations currently purchase CO₂ for around 50 $/tC (Heddle et al. 2003). While there is much less industry experience with ECBM than with CO₂-EOR, it appears that ECBM provides substantial potential for CO₂ sequestration at low cost. The cost for EOR and ECBM depends on many factors including injection well depth, formation thickness and permeability, reservoir geometry, CO₂ effectiveness, recycle rate, no. of injection wells etc. With large numbers of abandoned wells in depleted oil and gas reservoirs, workover, monitoring and verification costs can increase substantially. Higher oil and natural gas prices expand the scope for EOR and ECBM.

<table>
<thead>
<tr>
<th>Table 2. Storage Costs. Source (Herzog 2004)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Storage Type</td>
</tr>
<tr>
<td>EOR</td>
</tr>
<tr>
<td>ECBM</td>
</tr>
</tbody>
</table>

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IEA GHG has inventoried all large CO₂ point sources worldwide. The total emission of the inventoried sources (14 652 in total) sums up to 13.5 Gtonnes of CO₂ per year. This amounts up to about 60% of the estimated total anthropogenic emission worldwide (22.6 Gtonnes).
Depleted Oil/Gas Reservoir | Range: $2 to $20, Base: $5
---|---
Saline Aquifer | Range: $1 to $12, Base: $3
Ocean | Range: $10 to $25, Base: $15
Mineral Carbonates | $70?

The cost steadily increases moving to storage in saline aquifers and oceans although the variability decreases. Finally one could also consider permanent storage in mineral carbonates although with current technology, the cost is quite prohibitive.

**Total Cost**

Putting the cost chain together, Figure 2 shows the total cost for different CCS system configurations. For example an NGCC plant disposing of CO$_2$ in the deep ocean 400 miles away in the North Sea for example would incur a total cost of $50/tCO$_2$ whereas a PC plant injecting CO$_2$ for ECBM would incur a total cost of $15/tCO$_2$.

![CCS Cost Chains](image)

**Figure 2. Total Cost of different CCS configurations**

Therefore in building a marginal cost curve for CCS deployment a bottom up source-sink modeling approach may be more appropriate. In this model as shown in Figure 3, the most appropriate or least-cost source sink pairs are matched up for a region. Once the sink capacity is consumed, we would have to move to the next most expensive grade of reservoir. (Fig. 4). The marginal cost then at a certain level of CO$_2$ sequestered $Q$ will be equal to the cost of the least cost source-sink available pair at that point. i.e. $MC(Q) = C(u_i,v_j)/Q$. 

![Marginal Cost](image)
Figure 3. Source Sink Matching.

Figure 4. Storage Costs. Red line mirrors a rising marginal cost of storage as each reservoir option is exhausted.

Modeling Heterogeneity and Uncertainty
It is important to distinguish between heterogeneity and uncertainty. Heterogeneity in the case of CCS refers to the variety and spatial distribution of storage options available as well as the number of source types and capture technologies. Uncertainty on the storage side exists around the characterization of storage reservoirs and consequently the fate of CO₂ migration and leakage. On the capture side there is uncertainty in the evolution of capture technology.

Most macro broad based or ‘top down’ economic studies analyzing the potential of carbon capture and sequestration technologies (CCT) have used either a single cost based on a reference case or average costs (Dooley 2002). However, as is evident from the preceding analysis that – 1) the availability and cost of geological storage is highly variable and site-specific and 2) CCT technology will change with time and adoption = f(R&D) + f Quantity Sequestered = f(cumulative Installed Capacity)).

Bottom-up engineering models have greater spatial and temporal detail. In the case of CCS, a full-scale Geographic Information System (GIS) model would be needed to determine the most appropriate source-sink connections. Dooley, Dahowski et al. have developed a tool to facilitate the analysis of sources and geologic reservoirs for the long-term storage of CO₂ in the United States. Figure 5 shows a very rough cost curve for the 185 existing coal- and natural gas-fired power generation units in the United States located in Illinois, Indiana, Ohio and West Virginia assuming that they can not transport their CO₂ more than 100 miles from the power generating unit (Dooley 2002). At a
carbon tax of $50/ton, approximately 250 million tons of CO₂ can be sequestered out of approximately 600-700 million tones emitted, roughly 40% of total emissions.

Even with a GIS model there is the practical difficulty of estimating the actual cost of storage associated with a certain reservoir or storage site. This is akin to the inverse problem of petroleum resource extraction where it is difficult to estimate cost before an actual survey is conducted. Reservoir data does exist for depleted oil and gas reservoirs but for coal beds and saline aquifers little data is available.

To bridge this practical difficulty, a cost distribution for each of the source and sink types can be estimated using the studies, data, information, models and expert assessments currently available. These individual cost distributions can be combined in a statistical mixture model to generate an aggregate marginal cost curve for each region. As more information from experiments, CO₂ sequestration demonstration projects, simulations and assessments become available, the cost distributions can be updated. Broadly speaking this modeling approach belongs to the Bayesian school of thought. Its advantage lies in its ability to generate aggregate instead of site-specific information that can be used in economic models. Figure 7 illustrates this conceptual framework.
Figure 7. Conceptual Model of the CCS Analysis Framework

Using a Mixture Model to Capture Heterogeneity

Mixture modeling refers to modeling a statistical distribution by a mixture (or weighted sum) of other distributions.

Basic definition of a mixture model

A mixture model is given by the observation of $n$ independent random variables $x_1, x_2, \ldots, x_n$ from a $k$-component mixture density:

$$f(x_i) = \sum_{j=1}^{k} p_j f_j(x_i), i = 1, \ldots, n,$$

$$p_j > 0, \quad j = 1, \ldots, k; \quad p_1 + \ldots + p_k = 1$$

$$f_j(x) \geq 0, \quad j = 1, \ldots, k.$$

The parameters $p_1, p_2, \ldots, p_k$ are called the mixing weights and $f_1(x), \ldots, f_k(x)$ are the component densities of the mixture.

In our mixture model, the mixing weights are the proportions of the available reservoir storage types and CO$_2$ source-capture technology combinations. The cost distributions for the storage and capture components are the component densities of the mixture. These cost distributions are modeled by prior Bayesian probability distributions.

Methodology

The prior cost distributions are built for each geological storage type and for each of the capture technologies, both current and future, in the technology cost chain. It is assumed that any type of source or sink can be matched up, i.e. source-sink groups are independent of storage type and source type. In practice, important criteria for a source-sink match-up is proximity, storage capacity, seal integrity and cost. These factors are implicit in the cost estimates being used (Herzog et al. 2004). The distribution of total
cost is then obtained by sampling from the individual technology distributions and the reservoir costs in the cost chain and summing over those costs. Cost distributions for this study have been built using a Bayesian approach. The Bayesian approach combines sample information with other available and pertinent prior information. The actual cost estimates have been based on the cost analysis conducted by Herzog et al. (2004). In their study Herzog et al used ‘rules of thumb’ to define the engineering parameters needed to estimate costs. These ‘rules of thumb’ were derived based on information from experts in the field and the literature (Table 2). Using the high, low and base cases triangular distributions were generated for each of the storage types.

![Figure 8. Triangular distribution](image)

The triangular distribution is a well known distribution in quantitative risk analysis/ estimation and is commonly used in the absence of hard data. Its advantages are that it is simple to use and intuitively plausible. The weight for each storage component is equal to its percentage of the total available storage. Available storage refers to storage site within an acceptable distance from a source. Similarly on the capture side one would need to know what percentage of CO₂ emitters are coal plants, natural gas plants etc. This is where aggregate statistics from a GIS model would be very useful. A GIS model could answer questions like: What percentage of storage is located close enough to sources and far away enough from populated areas such that they are not a major risk – both for environmental and safety reasons? What percentages of reservoirs are large enough, i.e. greater than the threshold storage capacity?

**Monte Carlo Sampling** - A Monte Carlo sampling procedure is used to draw from each of the underlying probability density functions in the ratio of their respective weights. In the analysis for the United States weights of 20% EOR, 20% ECBM, 60% Aquifer and Depleted Oil and Gas Reservoirs are chosen.

The results of the mixture model analysis are shown in Figures 9 and 10. Figure 9 describes the cumulative distribution of storage costs for each of the storage classes – EOR, ECBM, Aquifer, Depleted Oil and Gas, as well as for the overall mixture, i.e. Total Storage. The results show that up to approx. 26% of available CO₂ storage capacity can be filled at negative cost. The curves for each of the storage classes basically indicate the cumulative distributions of cost if 100% of storage capacity were contained in that class.
The storage class with the widest range is EOR and the narrowest, Saline Aquifer. It is expected that after ‘value added’ early opportunities like EOR and ECBM, the Saline Aquifer class will dominate CO₂ storage, the primary reason being the abundance and uniform distribution of saline aquifers across most regions.

Figure 9 shows the marginal cost curves for storage and for total cost (= storage + capture) respectively. The marginal cost curve is obtained by inverting the cumulative distribution of cost. This is based on the premise that the lowest cost options will be deployed first. The storage cost curve in effect is the lower limit of the total cost curve since it is not expected that the geological storage costs of CO₂ will decrease with time substantially, at least not in the near future. The CO₂ capture costs on the other hand are expected to be a decreasing function of time through R&D and learning. Figure 11 shows the 10-50-90 distribution. In the case selected, 80% of the cost of storage falls within the range of -$18 to $20.
Figure 22. 10/50/90 curve by storage class.

Extensions and Future Work

Modeling Technological Change

Modeling technological change is a complex task. Technological change responds to policy, is highly uncertain and technological diffusion differs in time and between countries and regions (Clarke and Weyant 2002). The most important question we would like to answer is how costly will CCT be in the future. Rubin et al (2002) have used the concept of ‘learning’ in modeling technological change. They used experience over the past 30 years in the U.S. and other countries with reducing emissions of sulfur dioxide (SO$_2$) using flue gas desulphurization (FGD) systems (also commonly known as SO$_2$ “scrubbers”) to serve as a guide to technological progress in managing CO$_2$ emissions. This was plausible since SO$_2$ “scrubbers” and currently commercial CO$_2$ capture systems have similar principles of operation. For CCT a combination of learning and subjective probability assessment may be more appropriate, especially since these technologies have not yet been deployed at any significant scale. Since initial conditions have not exactly been set, it is worth considering a portfolio of several distinct technological possibilities incorporating spillover effects from advances in other areas like materials, nanotechnology etc. In the case of CO$_2$ separation, operating cost is closely linked with the energy penalty of the particular separation method. An exergy assessment (thermodynamic potential) can give us a good estimate of the minimum cost or technical limit associated with any future separation technology
**Incorporating the results of scientific research**

If geologic storage of CO$_2$ is to take place at large scale the issue of leakage risk seems very important - 1) when accruing for storage, monitoring and verification costs 2) regarding the location and appropriateness of sites and 3) calculating environmental and political cost. For example in the case of EOR, not all oil and gas reservoirs are good candidates for CO$_2$ flooding. Fluid properties are important. Heavy oil is more amenable to steam flooding than CO$_2$ flooding. It is also well known from the oil and gas industry that stress changes associated with injection or depletion can affect the integrity of the geologic seals that contain the fluid. Highly fractured carbonate reservoirs such as those in California may not be good CO$_2$ seals. Much less is known about coal beds and saline aquifers. It is evident from these issues that domain specific scientific knowledge is important in examining the role of CCS as a viable climate change mitigation option.

How can scientific research be integrated into our modeling efforts?

**Simulation** - One option is to run coupled reservoir-geomechanical simulations to determine leakage rates and CO$_2$ movement for a set of reservoir characterizations spanning the range of reservoir parameters and injection scenarios – Figure 13. This will allow us to determine leakage rate distributions for a set of reservoir classes. The results of the simulations can also show us the temporal profile of CO$_2$ migration and leakage which will be important in determining monitoring and verification costs. This is especially useful since monitoring and verification costs have not yet been treated with any significant rigor in the costing literature.
References


Kinder Morgan CO₂ Company. 2002. Presentation at IOGCC Geological Sequestration and EOR.


Appendix C: Quantifying the Leakage Rate Associated with Carbon Storage

Investigators
James Sweeney, Professor of Management Science and Engineering; John Weyant, Professor of Management Science and Engineering; Oscar Mascarenhas, Graduate Researcher.

Introduction
Establishing the permanence of geological storage of CO₂ is critical to the deployment of Carbon Capture and Storage. Leakage rates must be acceptable from the perspectives of climate change, the environment and human health and safety. On a global level, slow leaks could eventually build up to current fossil emissions levels. A 1% leakage rate from one trillion tons of sequestered fossil carbon sequestered carbon would create ten billion tons of annual emissions, comparable to the current annual total of seven billion tons. On a local level, leaking CO₂ can contaminate of drinking-water aquifers. The quantification of leakage risk and leakage rate is however yet to be rigorously analyzed and quantified on the macro scale. Studies evaluating the feasibility and potential of Carbon Capture and Storage have suggested a maximum leakage rate of approximately 0.001 – 0.01 % taking into account possible scenarios for future CO₂ emissions through fossil fuel usage (Benson, 2002) A leakage rate of 0.01 % would ensure that 90 % of the carbon dioxide would remain underground over a 1000 year time period. Leakage rates of 1 % imply that most of any stored carbon dioxide would return to the atmosphere after only 400 years (Benson, 2002). This emphasizes the need for the quantification of leakage risks.

Background

Leakage pathways
Several pathways exist for possible leakage both 'natural' and 'anthropogenic'. These include:
1) Diffuse leakage across caprock formations,
2) Concentrated leakage through natural faults and fractures, and
3) Leakage through human-made features such as wells:
   Depleted oil and gas reservoirs have large numbers of abandoned wells greatly increasing the potential for leakage. In areas where little oil and gas exploration has occurred, there are relatively few existing wells, and potential for leakage through existing wells is not a major concern.

Trapping CO₂
There are several trapping mechanisms to store CO₂ in the subsurface:
1) Structural Trapping
2) Geochemical Trapping
   a. Solubility trapping
   b. Ionic trapping
   c. Mineral trapping
3) Residual Gas trapping

**Structural trapping**

Structural trapping refers to permeability and capillary barriers created by the formation caprock. Trap effectiveness depends on the specific geometry and structure of the reservoir as well as the caprock type which can broadly be classified under shale, clay or carbonates. Permeability barrier effectiveness varies with rock properties increasing from gravel and coarse sands to clay and shales. Capillary barrier effectiveness increases moving from shales to carbonates.

Structural traps are classified under: 1) Closed Traps and, 2) Open traps. *Closed traps* physically retain the CO₂. These include structures such as anticlines, unconformities, sealed faults and facies changes. *Open traps* permit lateral migration of the CO₂ but prevent rapid upward migration of CO₂. Open trap structures include synclines and transmissive faults.

**Geochemical trapping**

Geochemical trapping broadly refers to chemical reaction of the CO₂ with brines and rock to form stable carbonates. The effectiveness of this trapping mechanism is determined by the volume and the rate of chemical reactions which are dependent on formation chemistry.

**Residual Gas trapping**

Residual gas trapping refers to the trapping of gas as it flows through the porous medium. Once the gas in injected, there is a hysteresis loss and some of it cannot flow out. Residual gas trapping depends on both pore-network characteristics and gas saturation.

**Overall Reservoir trapping potential**

Potential leakage rate is therefore a function of the overall trapping potential of the reservoir or more precisely - a function of the structural, geochemical and residual gas trapping potentials. The trapping mechanisms are however not necessarily independent of one another. A strong structural seal allows more time for geochemical reactions to take place further reinforcing the geochemical trap. In practice however, strong structural and geochemical traps may not coexist. Carbonate reservoirs have high geochemical trapping potential but are highly fractured in nature allowing concentrated high permeability pathways for CO₂ leakage.

**Uncertainty**

The uncertainties involved in the storage of CO₂ are of two main types (Figure 1) – the first type represents the inherent variability associated with geologic storage which includes the spatial heterogeneity of intrinsic permeability and porosity, the multiplicity of rock types and structural geometries and the randomness of external events like earthquakes. The other type of uncertainty also termed as epistemic uncertainty stems from an incomplete knowledge of the fundamental phenomena involved such as geochemical degradation of the reservoir or induced seismicity. In order to capture
epistemic uncertainty, risk scenarios must be constructed on a set of all known hypotheses regarding the nature of fundamental mechanisms (Paté-Cornell, 1996). These mechanisms must be structured as a set of mutually exclusive and collectively exhaustive elements in accordance with the fundamental laws of probability.

Figure 1. Uncertainty taxonomy for the geological storage of CO₂

*Simulation* - One option is to run coupled reservoir – geomechanical simulations to determine leakage rates and CO₂ movement for a set of reservoir characterizations spanning the range of reservoir parameters and injection scenarios. All of these data and parameter uncertainties create a problem that has a complex multi-dimensional parameter space with potentially wide ranges of possible values along the parameter axes. Because of the scale disparity and the large degree of uncertainty, and the resultant large number of simulations that will be needed to perform a risk analysis, computational efficiency of models becomes a concern, and different modeling options need to be considered. A systems approach is described in the following section.

**A Systems Approach to Modeling**

The complexity of geological storage of CO₂ makes it a good candidate for a ‘Systems’ approach to modeling. A systems model divides a system into a collection of components or elements linked together by form, process or function. The system can be expressed in terms of an input-output model and characterized by state variables at any point in time.

**Model Structure**

At a high level, a typical CO₂ reservoir system can be divided into blocks or zones as shown in Figure 2. CO₂ will be initially trapped beneath a relatively impermeable layer. Driven by diffusion, buoyancy, and regional hydraulic gradients, the CO₂ will move. Some will dissolve or become trapped beneath the caprock. The CO₂ that escapes will do so if the caprock fractures or when the moving front encounters a conduit such as a fault or an abandoned well with a failed concrete seal. It will then migrate upward, spreading horizontally as it moves, until it encounters another relatively impermeable layer, and the
whole process will begin again, similar to a jump-diffusion process. A fraction will never escape and the rest will escape with a distribution of time lags. The amount of CO$_2$ retained and the distribution of time lags will vary from reservoir to reservoir.

In reality, a real reservoir would contain many confining layers and copartment. The reservoir system can be decomposed still further into contiguous blocks both conceptual and physical. The flow or transfer or migration or ‘leakage’ of CO$_2$ between these system blocks can be expressed by a probability $P_{ij}(t)$ that can be interpreted as the expected fraction of flow between the $i^{th}$ and $j^{th}$ blocks. The transition probabilities $P_{ij}$ form the elements of a stochastic matrix $P$. The matrix $P$ essentially represents system structure.

$$
\begin{bmatrix}
P_{11} & P_{12} & \ldots & P_{1n} \\
P_{21} & P_{22} & \ldots & P_{2n} \\
\vdots & \vdots & \ddots & \vdots \\
P_{n1} & P_{n2} & \ldots & P_{nn}
\end{bmatrix}
$$

$$
\sum_{j=1}^{n} P_{ij} = 1 \quad \text{for all } i = 1, 2, \ldots, n
$$
The sum of all elements in each row of $P$ sums up to 1. Each row of matrix $P$ is a called a probability vector because of this property. This representation is essentially a Markov chain or a special class of a dynamic system that evolves probabilistically. The possible locations for the migrating at each step in time $CO_2$ can be thought of as states of the system. The future evolution of the process is described by a vector of probabilities at each step in the process. Successive probability vectors are generated by the recursion:

$$x(k+1)^T = x(k)^T P(k)$$, where $k$ is the time step of evolution.

Note that the transition probabilities depend on the number of steps ($k$) that have occurred in the evolution or in other words are a function of time. This follows from the physics of $CO_2$ migration and the timescales involved with the analysis. This formulation allows a rich set of analyses drawing on the theory of Markov processes. One example is the computation of the probability that a specified state location will ultimately be reached. Another is the average length of time to reach a specified state or group of states. This opens up interesting application possibilities, one of which is in the design of an optimal risk monitoring and control regime.

A systems analysis approach to assessing risk has been successfully applied to the field of radioactive waste disposal (Stenhouse et al., 1993). A central part of this approach is a rigorous and exhaustive documentation of the ‘FEP’s’ to describe the disposal concept which is to be evaluated. FEP’s are features, events, and processes relevant to the assessment of the behavior of a carbon dioxide disposal system. Features of the sequestration system could include rock and fluid properties, reservoir geometry, cement quality, such as unsealed or inadequately sealed boreholes, the quality (composition) of $CO_2$, undetected geological structures, etc. Events include seismic events, faulting, human error, etc. Processes include the mechanisms that govern the evolution of the disposal system, such as flow and diffusion of $CO_2$, chemical reactions with reservoir and cap rock etc. The transition probabilities are in essence functions of the ‘features, events and processes’ of the system components and their interfaces.

Motivation for a probabilistic approach
The $CO_2$ disposal system can be classified as an organized complex system or a system with structure – one involving large numbers of non-linear differential equations with many interactions among a large number of components and variables that define the system. Problem solutions related to such models of organized complexity tend to converge to statistically meaningful averages (Klir and Wierman, 1998). This sets the basis for a probabilistic approach to modeling this complex system.

Assessing Probabilities

Influence Diagrams
In order to assess probabilities, the dependencies between the key variables that represent the system FEP’s should be established. For example, the solubility of CO$_2$ in water may influence the degradation of borehole seals. An influence diagram can graphically represent this relationship between system variables, both uncertain and deterministic. It is an intuitive way of capturing complexity in a concise graphical form. Influence diagrams also serve to reduce the uncertainty space associated with the problem. The development of an influence diagram involves identifying the system state variables, deciding on appropriate states, determining the dependencies among events, and assigning likelihoods to the states. Uncertainties are represented by ovals. The uncertainty to be estimated - leakage through the well is represented by a hexagon. An event with no predecessors, that is, no arrows pointing to it, is an independent variable. An arrow pointing to an uncertainty represents probabilistic dependence.

**Figure 4. Influence diagram for wellbore leakage**

Consider the influence diagram shown in Figure 4 that represents a simple probabilistic model of leakage through an abandoned well. It is plausible that a migrating CO$_2$ plume can contact an abandoned well especially in areas like Texas which have close to a million wells drilled. Leakage through a wellbore will depend on the reactivity of CO$_2$ which are influenced by the cement quality, the materials used, well completion standards etc. all of which are believed to show a high degree of variability. (Norbotten et al., 2005)

**Expert Assessment**

The high uncertainty, variability and system complexity limits analytic modeling and makes simulation modeling a time intensive process. Since policy decisions need to be made in a timely manner, we have decided to conduct an expert assessment to assess probabilities.

Using much of the structure and modeling tools outlined in the previous sections, the CO$_2$ storage system will be broken down into well-defined components, lower level probabilities assessed, and then combined mathematically to arrive at a distribution of leakage rates. A Bayesian approach to assessing probability allows the incorporation of all available evidence including statistical data, physical models and expert opinion. Specific techniques will be used to account for motivational and cognitive biases and resolve differences of opinion.

The assessment meeting will comprise three stages. Participants will:
1) Assess the current state of knowledge and available evidence; Identify and address the key questions and issues related to CO₂ migration and leakage.
2) Agree on a structural model of leakage in the form of an influence diagram.
3) Identify leakage scenarios and quantify key uncertainties in the form of probability distributions. The uncertainty is propagated through a probabilistic model to obtain an overall distribution over leakage.

We will limit the assessment to sites that are suitable candidates for CO₂ disposal in North America. The reservoir classes considered will be 1) Depleted Oil and Gas Reservoirs, 2) Saline Aquifers, 3) Coal Beds.

It is reasonable to assume that sites will be selected to minimize the risk of leakage and unsuitable sites will not be considered. The major requirement is suitable geology.

An injection reservoir must generally have:
1. Sufficient depth (generally greater than about 2,500 ft) to maintain the injected fluid as a supercritical liquid,
2. Enough thickness and lateral extent to provide capacity for large injection volumes,
3. Sufficient porosity and permeability to accept injection fluids,
4. Impermeable caprock layers above the injection layer to provide containment,
5. A structurally sound setting free of faults and fractures, and
6. Suitable chemistry to prevent adverse interaction between the rock and injection fluid.

Since we are estimating likely leakage rates given suitable geology, we will therefore need an expert assessment of the proportion of available reservoir storage likely to be suitable, thereby obtaining a constraint on storage.

Scenarios
A set of scenarios will form the basis for the quantification of risks. Assuming a structurally sound storage site is selected free of any known fractures and faults, a scenario for leakage could be that a fault remained undetected during the site characterization process, CO₂ contacts this fault, the fault turns out to be active, serving as a conduit for the CO₂ that migrates to adjacent zones and seeps to the surface through the overburden.

External events
External events can include natural events like earthquakes, the movement of old faults, the creation of new fractures and geochemical changes that destabilize the reservoir. Manmade changes include wellhead failures, pipeline ruptures and leakage through wells. The injection of large volumes of CO₂ at high pressures can induce micro-seismicity and subsidence due to dissolution (for example in carbonate aquifers).

Evidence
Evidence selected for the assessment will include:
1) Evidence from analogues such as naturally occurring CO₂ reservoirs and natural gas reservoirs.
2) The results of experiments, analytical models and simulations.
3) Results from demonstration projects. A set of 3-6 cases that span the range of reservoir types could be selected for review. These could be for proposed sites such as the Ohio River Valley
reservoir; and ongoing demonstration projects such as Weyburn and Sleipner. Results from the Weyburn risk assessment (IEA GHG 2004) estimate that after 5000 years, the average cumulative release of CO₂ to the atmosphere is predicted to be 0.2% of initial CO₂ in place with a 95% confidence interval of 0.005% to 1.3% of initial CO₂ in place.

Extensions and Future Work

The assessment meeting at Stanford is tentatively scheduled for mid to late summer depending on the level of preparation and availability of the participants. After this stage, the assessment will be extended to external participants. The results will serve to integrate the current state of knowledge regarding the long-term viability of CO₂ storage, and provide insights into the relative magnitudes of uncertainty in different parts of the system. This will be important from a risk monitoring and control perspective for which there are many potential applications of our work.

A natural next step is to determine the impact on the future evolution of Carbon Capture and Storage. The treatment of risk in global economic models will need to be carefully considered in the light of risk-cost tradeoffs, mitigation options and future technological change. Future researchers should look at:

1) The interplay between risk and the regulatory framework - In most countries, the lack of regulatory framework may delay the application of CO₂ capture and storage. It is expected however that the regulatory framework will evolve through cooperation between government, industry, and other stakeholders as the number of demonstration and commercial projects increases. (Opinion of Carbon Capture Project policy team, personal communication, 2004)

2) Public perception and risk communication - A study conducted by Howard Herzog and Tim Curry of the MIT Laboratory for Energy and the Environment on “Public Opinions on Carbon Capture and Storage”, concludes that public awareness of CO₂ capture and storage technology is low to non-existent; therefore gaining public acceptance is likely to be challenging and will depend on how the benefits and risks of Carbon Capture and Storage are communicated to the public.
References


IEA GHG Weyburn CO₂ & Storage Project Summary Report 2000-2004


Appendix D: Quantifying the Leakage Rate Associated with Carbon Storage

Investigators
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Introduction
Sequestering carbon dioxide geologically in depleted oil and gas reservoirs, saline aquifers and coal seams is one of several strategies in an arsenal of techniques to mitigate the potential disasters of global warming and climate change. Carbon dioxide from point sources like power plants is captured, transported and stored in geological storage locations beneath the Earth’s surface, thereby reducing the level of anthropogenic greenhouse gases in the atmosphere. Geological CO$_2$ storage, particularly in saline aquifers, has garnered a lot of attention over the last few years. This is evident from the large number of recent publications in the field [van der Meer, 2002]. Cost-effective monitoring of the storage site both during the time of CO$_2$ injection and after operations are complete, is crucial to prevent seepage to the biosphere and to make geological sequestration an acceptable solution.

To design a monitoring program for a geological CO$_2$ storage site one must select appropriate measurement tools. Some of the current methods include geophysical and geochemical techniques, sensors and transducers, well-logs, land surface deformation methods and satellite-based technologies [Benson and Myer, 2002]. Other important design considerations include determining where to locate these tools and how long and how often one should monitor the sequestration site. We focus on analyzing how often time-lapse seismic surveys should be performed for monitoring sequestration sites.

Time-lapse seismic provides good spatial coverage and resolution for monitoring geological CO$_2$ storage sites [Myer et al, 2002]. It is an established technique in the oil and gas industry and initial results from Sleipner (Norway) have demonstrated that time-lapse surveys can effectively track the CO$_2$ plume movement in the subsurface. An average of one million tonnes of CO$_2$ have been pumped into the Utsira formation at Sleipner annually since operations began in 1996 [Herzog, 2001]. There have been four time-lapse surveys performed till 2002 and results have shown that there is no sign of leakage till date [Arts et al, 2004]. However, time-lapse is an expensive monitoring technique and may account for over half of the total monitoring costs [Benson et al, 2004]. These costs may be lower than carbon capture and storage costs but can be significant when accumulated over the entire lifetime of a CO$_2$ storage project. We examine the trade-off between the survey costs and the harmful consequences associated with CO$_2$ seepage to the biosphere using a dynamic programming formulation for a finite horizon model. We also formulate an infinite horizon model to compare the results. The model assumptions and features are explained in the next section. Results from a base case are analyzed using single-parameter sensitivity analysis to understand the effects of
critical model parameters on the mean optimal interval between surveys and the total expected costs. More complex multi-dimensional sensitivity analysis is handled through the Monte Carlo simulation approach. We conclude with the potential benefits that regulators and sequestration project managers can gain from the formulated mathematical model and policy implications of the presented results. Finally, we discuss further extensions to the work and some open-ended questions about monitoring storage sites.

**Model Formulation**

*An Finite Horizon Dynamic Programming Model*

The dynamics of the CO₂ sequestration process are simplified and modeled as a four state Markov decision process with transition probabilities. The states are based on definitions of the different types of CO₂ plume movement adopted by Chalaturnyk and Gunter (2004). The states are described as follows –

M (migration): injected CO₂ safely migrating within the target zone.

L (leakage): significant leakage from the target zone to the adjacent geosphere.

R (recovered migration): safe migration after recovery from the leakage state.

S (seepage): seepage from geosphere to the biosphere.

The states are observed only when a monitoring survey is performed. Each state is a simplification of the sequestration dynamics and the actual condition of the reservoir. The states summarize the overall reservoir characteristics regarding the location and movement of the CO₂ plume, thus enabling a simple dynamic programming formulation. The possible state transitions are depicted in Figure 1.

![Figure 3: States of the dynamic program and all possible transitions](image)

**Model Assumptions**

The general model contains several assumptions, mostly for the sake of analytical tractability and compact formulation. The major assumptions are listed below –

1. We assume that the system may go to state S only from state L. This is realistic because a seep to the biosphere cannot physically occur before a leak from the reservoir to the overburden or other parts of the geosphere outside the target zone.
2. We assume that once observed to be in state L, remedial measures (like changing the pressure gradient) are always taken to immediately bring it to state R. Some remedial measures are listed in Benson and Hepple (2004).

3. Once in state L we can not go back to state M. Thus whenever a leak occurs and we are able to detect it by the timely use of seismic testing, we go to state R and not back to state M. The reservoir has possibly changed due to the remedial measures.

4. If state L is not detected in time it will result in the occurrence of state S (seepage). S is assumed to be a stopping state and there is no decision formulation once state S is observed. S is associated with a penalty cost representing the harmful consequences of seepage to the biosphere.

5. Costs are incurred only through the following means: survey costs, cost of remediation to convert state L to state R, and the cost of being in state S. S is associated with the harmful consequences of CO$_2$ seepage: possible damage to the soil and terrain, health effects for humans, dissolution of CO$_2$ into the water table, and others [Wilson and Keith, 2002].

6. We assume that when the seismic survey is performed the state is observed perfectly. Seismic has good resolution and this may be a reasonable assumption based on the broad sense in which we have defined our states. Also, an initial 3D seismic is assumed to have been performed in the beginning before injection, and the geology is assumed to be more or less known.

7. The time to transition to another state is assumed to be exponentially distributed because the memory-less property of the exponential distribution allows the Markov formulation. Another advantage of the exponential time assumption is that it allows an easy and intuitive conversion from expert opinion to the single parameter of the exponential distribution in the mathematical model. The expected time to leak (or seep) is the reciprocal of the parameter - the leakage (or seepage) rate. and may be obtained from expert opinion or simulation results.

A Dynamic Program
The states of the Markov decision process have been described in detail in the previous section. The decision involves choosing the next time to perform the seismic survey, given that a survey has just been performed. The optimal time can be determined by the method of backward recursion. Let $\theta$ be the observed state at the current time $t$. $C(\theta, t)$ is the total expected cost from time $t$ till the end of the horizon, if the seismic survey was performed at time $t$ and state $\theta$ was observed. The goal is to choose the optimal ‘$T$’ (from the set $\tau$), or time till the next survey, such that costs are minimized. $\beta$ is the discount factor and $N$ is the number of years in the horizon. The finite-horizon dynamic programming formulation is given by:

$$C(\theta, t) = \min_{T \in \tau} \left(f(\theta, T) + \beta T \sum_{\phi} C(\phi, t + T)P(\phi | \theta, T) \right) ; \quad (t = 1, 2, \ldots N-1)$$

$$C(\theta, N) = h(\theta) ; \quad \theta \in \{M, L, R\}$$
\[ C(S, t) = c_2 + y(t) \; ; \; S \text{ is a stopping state; } (t = 1, 2, \ldots N) \] (3)

Equation (1) includes \( f(0, T) \), or what we will call the cost function. This is defined as the expected cost incurred from the decision-epoch at time \( t \) to the next epoch at time \( t+T \). It comprises of survey and possible remediation costs as well as expected costs of harmful consequences of undetected seepage. Other important terms in the equation are the probability of transitioning from state \( \theta \) to state \( \Phi \) \( [P(\Phi|\theta, T)] \) (which we will denote the probability function) and the future costs \([C(\Phi,t+T)]\). Equation (2) is the boundary condition. For the model we assume that seismic testing is not performed after year \( N \). The boundary condition takes care of the cost associated with ending in state \( L \) with the function \( h(\theta) \). Equations (1) and (2) are invalid for state \( S \) as it is a stopping state, so equation (3) is used for state \( S \). The cost is assumed to be linear in time and it includes both a fixed component \( c_2 \) and a time-dependent component \( y(t) \). The fixed part of the cost ensures that there is a cost incurred even if the reservoir reaches state \( S \) towards the end of the horizon. The cost function and the probability function in equation (1) are modeled using the exponential time between state transitions.

The Probability Function \( P(\Phi|\theta, T) \)
From the memory-less property of the exponential distribution, if the reservoir is in a certain state, the distribution function for the time taken till the next transition is not affected by \( \text{how long} \) it has already been in that state. Let us say that a survey is performed anytime in the horizon and the observed state is \( M \), i.e. the entire CO\textsubscript{2} plume is migrating safely in the target zone. Now we can reset the time to zero by the property above. For the reservoir to remain in state \( M \) after time \( T \), a leak must not have happened during this time period. The probability is:

\[ P(M | M, T) = 1 - \int_0^T p_1 e^{-p_1 t} dt \] (4)

For the state to change to \( L \) after time \( T \), a leak happened at any time \( t \) during this time period and a seep did not happen after the leak, at any time \( t' \) between \( t \) and \( T \).

\[ P(L | M, T) = \int_0^T p_1 e^{-p_1 t}(1 - \int_t^T q e^{-q t'} dt') dt \] (5)

For the state to become \( S \) after time \( T \), both the leak and subsequent seep occurred.

\[ P(S | M, T) = \int_0^T p_1 e^{-p_1 t}(\int_t^T q e^{-q t'} dt') dt \] (6)

The transitions from state \( R \) to states \( R, L \) and \( S \) have similar expressions; \( p_1 \) (the rate of leakage given state \( M \)) is to be replaced by \( p_2 \). Thus,

\[ P(R | R, T) = 1 - \int_0^T p_2 e^{-p_2 t} dt \] (7)

\[ P(L | R, T) = \int_0^T p_2 e^{-p_2 t}(1 - \int_t^T q e^{-q t'} dt') dt \] (8)

\[ P(S | R, T) = \int_0^T p_2 e^{-p_2 t}(\int_t^T q e^{-q t'} dt') dt \] (9)

The chance of a future leak is different from normal migration as the reservoir conditions have been altered. The equations for transition from state \( L \) are exactly the same as those for state \( R \) because of the model assumption that remedial measures are taken to convert \( L \) to \( R \) immediately whenever \( L \) is observed.

\[ P(\phi | L, T) = P(\phi | R, T) ; \; \phi \in \{R, L, S\} \] (10)
The Cost Function $f(\theta, T)$

If the state is observed to be M after a survey is performed, then the cost from the current decision-epoch to the next includes the cost of the next survey (denoted as c) and the cost of seepage if the state moves from M to S during time T. Both costs are paid after time T and hence they are discounted by $\beta^T$. The probability of going from state M to S in time T has been derived in equation (6). If seepage occurs at a constant rate $r$ tonnes per year at time $t'$ then the total amount of CO$_2$ that enters the biosphere is $(T-t')^r$. This seepage may possibly be undetected but that is not a necessary model assumption. If $x$ is the tax per tonne of CO$_2$ that seeps to the biosphere, then the cost of seepage is $(T-t')^r x$. The tax accounts for both the local and the global consequences. This is explained in greater detail later in the manuscript. We can derive the expected cost as:

$$f(M, T) = \beta^T c + \beta^T \int_0^T p_1 e^{-p_1} \left(\int_{t'}^T q e^{-q(T-t')}r x dt'dt\right)$$

Similarly, if the observed state is R,

$$f(R, T) = \beta^T c + \beta^T \int_0^T p_2 e^{-p_2} \left(\int_{t'}^T q e^{-q(T-t')}r x dt'dt\right)$$

If L is observed, an extra cost $c_1$ must be paid immediately for recovery to R.

$$f(L, T) = c_1 + \beta^T c + \beta^T \int_0^T p_2 e^{-p_2} \left(\int_{t'}^T q e^{-q(T-t')}r x dt'dt\right) = c_1 + f(R, T)$$

The probability and cost functions can be replaced in equation (1) to complete the formulation. For the analysis, we estimate model parameters according to a hypothetical base case.

A Base Case

The base case for our model is a hypothetical saline aquifer. We generally choose model parameters on the conservative side to represent a sequestration project that is of a high-risk nature. There is some uncertainty about the leakage and seepage risks in the aquifer but we only consider one major pathway, such as a fault in the caprock that may lead to leakage to the overburden and subsequent seepage to the biosphere. We assume that the frequency of seismic surveys can be anywhere between once a year and once every seven years. The lower bound of one year is based on the observation that seismic may not be beneficial if the plume has not moved substantially. The upper bound of seven years is an estimate of the frequency that may be necessary from the perspective of regulations. We choose a horizon of one hundred years to incorporate seismic testing for the operational period (during injection) and the closure period (post injection). These are two out of the four distinct phases for the life cycle of a sequestration project: pre-operational, operational, closure and post-closure [Benson et al, 2004]. The number of years in the horizon can be easily increased to accommodate a longer time-frame and more phases incorporating seismic testing.

The cost of seepage includes not only the cost of the carbon tax arising from an ineffective sequestration project, but also the consequences of damage to the soil and ecology, water table contamination and human health effects. Typical values of the imposed carbon tax alone may be $25-$30. For the base case we assume that the cost of seepage is double that amount, $60 per tonne of seepage, which includes the harmful local consequences. A more detailed study should calibrate the tax according to the specific conditions near the surface of the geological site. It is critical to include both the
global risk of ineffective sequestration and the local risks associated with environmental
damage [Wilson and Keith, 2002] in these costs. The cost of the seismic survey and
remediation costs are assumed to be $1 million each. Once a seep is detected, we assume
that a fixed cost of $60 million is spent owing to remediation action to control the
seepage and the cost of the consequences themselves. We choose this number as it
signifies that the tax is applicable for 1 million tonnes of CO₂. This is 5% of 20 million
tonnes, which is the estimated total volume to be injected in Sleipner Field, Norway
[Herzog, 2001]. Another way of looking at it is that the CO₂ may seep for a certain time
period (the seepage time) at a constant rate (seepage rate) after S is detected. To calculate
the seepage cost we must multiply this volume with the tax. To capture the time-
dependent component of the seepage cost, we assume that seismic must be performed
annually after seepage is detected, to satisfy regulatory bodies. Many policy problems use
a discount rate of 2-6%; the higher value in the range was used was discounting in this
case.
The parameters for time to leakage and seepage are on the conservative side. We assume
that the expected time to leakage is 10 years and the expected time to seepage is 10 years,
given that the leak occurred. As previously discussed, we assume that if and when the
leak is detected, the new state becomes recovered migration through remediation action.
We assume that now the expected time to leak is 5 years, or in other words the rate of
leakage is twice as frequent as it was previously. Note that from our definition of the
states, leakage and seepage signify movement of any amount of CO₂, not the movement
of the entire plume. The parameter notation, description and base case values are
summarized in table 1.

Table 1: Parameters of the model and base-case values

<table>
<thead>
<tr>
<th>PARAMETER SYMBOL</th>
<th>DESCRIPTION</th>
<th>BASE-CASE VALUE</th>
</tr>
</thead>
<tbody>
<tr>
<td>p₁</td>
<td>Rate of leakage given state M</td>
<td>0.1</td>
</tr>
<tr>
<td>p₂</td>
<td>Rate of leakage given state R</td>
<td>0.2</td>
</tr>
<tr>
<td>q</td>
<td>Rate of seepage given state L</td>
<td>0.2</td>
</tr>
<tr>
<td>β</td>
<td>Discount Factor</td>
<td>0.94</td>
</tr>
<tr>
<td>c</td>
<td>Cost of the seismic survey</td>
<td>$1 million</td>
</tr>
<tr>
<td>c₁</td>
<td>Cost spent on remediation to bring state L to state R immediately</td>
<td>$1 million</td>
</tr>
<tr>
<td>c₂</td>
<td>Fixed cost spent after detection of seepage</td>
<td>$60 million</td>
</tr>
<tr>
<td>x</td>
<td>Cost of undetected seepage per ton CO₂</td>
<td>$60</td>
</tr>
<tr>
<td>seep_time</td>
<td>Total time taken for CO₂ to seep, after it has been spotted</td>
<td>10 years</td>
</tr>
<tr>
<td>seep_rate</td>
<td>Rate at which CO₂ seeps to the biosphere (assumed constant)</td>
<td>0.1 million tonnes per yr</td>
</tr>
<tr>
<td>N</td>
<td>Number of years in horizon</td>
<td>100 years</td>
</tr>
<tr>
<td>τ</td>
<td>Constraint set for possible values</td>
<td>{1,2,3,4,5,6,7}</td>
</tr>
</tbody>
</table>
**An Infinite Horizon Model**

Another model was formulated to incorporate the possibility of an infinite horizon, i.e. seismic testing of geological storage sites long after operations are complete and indefinitely into the future. The main advantages of the infinite horizon formulation are: 1) the simplicity of the formulation and calculations, and 2) the uncomplicated optimal policy. For the finite horizon dynamic program, the optimal policy is the optimal time until the next seismic should be performed and this is a function of both the state and the time. In the infinite horizon case, the optimal time before the next seismic does not depend on time, i.e. it is a stationary policy.

**Model Assumptions**

Many of the model assumptions in the finite horizon case also hold for the infinite horizon model. The main differences are –

1. We assume that once remediation occurs, the reservoir goes back to state M immediately. Hence, there is no separate state R as in the finite horizon model. This assumption allows for evaluating T by solving a single equation.

2. To gauge the effect of the expected costs through seepage during the current interval, we present and compare two models – the approximate infinite horizon model (henceforth called the AIH model) and the exact infinite horizon model (called the EIH model). In the AIH model, we neglect the costs of seepage associated with the interval between the current decision epoch to the next epoch. Presumably, these costs may be small when compared to the overall seepage costs if the next seismic test is performed soon. This assumption will be made more precise later in this section.

3. The major assumption is that the cost-to-go from a particular state does not depend on the time. This is the critical difference between the two models and is a consequence of the infinite horizon assumption, i.e. testing will proceed indefinitely into the future. Infinite horizon models may not be realistic, but often they act as a good approximation to decision problems where the horizon length is not known.

The notation for the infinite horizon model is similar to that of the finite horizon model. Let $c$ be the cost of the seismic test, $c_1$ the cost of remediation action and $\beta$ the discount factor. These parameters and others have already been summarized in table 1 previously. We now define some of the new variables of interest. $V_m$ is the cost-to-go from state M (excluding the cost of the test just performed), $T$ is the time until the next test and $V_s$ is the cost of seepage (this includes the fixed cost of seepage and the cost from frequent seismic after seepage). As before, the possible actions are the choice of the next time to perform the seismic survey, given that a survey has just been performed. Thus the goal again is to find the optimal ‘$T$’ (from the set $\tau$) such that the cost $V_m$ is minimized. $g(T)$ is...
the expected cost of seepage if a seep occurs before the next decision epoch (equation 14). Recall that this expression was also a component of the cost function in the finite horizon model (see equation (11) and the brief explanation before that, for instance).

\[ g(T) = \int_0^T p_i e^{-\rho_i t} \left( \int_t^T q e^{-\gamma(T-t')}r xdt' \right) dt \]  

(14)

Figure 2 shows a graphical depiction of the EIH model in the form of a tree. This is possible only because of the infinite horizon assumption and by recognizing that after a certain time \( T \), if the state remains as state M, then the cost-to-go is exactly the same as previously. If we are currently in state M and we perform the next test at time \( T \), we may be in any of the 3 states after time \( T \): M, L or S. We will incur costs at the next epoch depending on what state we land up in. These costs are shown on the leaves (end-points) of the tree, and the probabilities of arriving at each state are shown above the branches of the tree (in bold). Note that all costs are paid after time \( T \) and hence they are discounted by \( \beta^T \). The tree denotes the EIH model which includes the \( g(T) \) terms; for the AIH model we should set \( g(T) \) equal to 0.

\[
\begin{align*}
V_m & \quad \beta^T (c + V_m + g(T)) \\
P(M | M,T) & \quad \beta^T (c + V_m + g(T)) \\
P(L | M,T) & \quad \beta^T (c + c_1 + V_m + g(T)) \\
P(S | M,T) & \quad \beta^T (V_s + g(T)) \\
\end{align*}
\]

Figure 2. Exact infinite horizon (EIH) model

We observe that the infinite horizon formulation can be expressed by relating the cost-to-go, \( V_m \), with the time till the next seismic test, \( T \). This is written by equating the cost-to-go at the current epoch with the total expected cost-to-go for the next epoch, and manipulating the terms to obtain the following equation:

\[ V_m = \beta^T \left[ \frac{c(1-P_s) + P_L c_1 + P_S V_s + g(T)}{1 - \beta^T (1 - P_s)} \right] \]  

(15)

In equation (15), \( P_L \) and \( P_S \) are abbreviations for \( P(L | M,T) \) and \( P(S | M,T) \). They have been derived previously in equations (5) and (6) respectively, whereas the formula for \( g(T) \) was presented in equation (14). Equation (16) shows the equation for the AIH model, i.e. when \( g(T) \) is assumed to be negligible as compared to other costs. Note that \( P_L, P_S \) and \( g(T) \) are all functions of \( T \). The integrals are for the special case of exponentially distributed transition times and they can be simplified further. The optimal value of \( T \), or the optimal time to perform the next seismic test, is the value of \( T \) that minimizes \( V_m \).
The base case values chosen were those from the finite horizon model, so that results from all the models could be compared. Even though the finite horizon model allows for a different state (R) after remedial action is taken when a leak is observed, for our analysis we assumed that state R is in fact just the same as state M. This is because the infinite horizon model assumes that the same migration state M is recovered after remediation and therefore a comparison between the models makes more sense with this consistency. Please see table 1 to review the base case values for all the parameters.

**Results**

A numerical method incorporating Bellman’s optimality principal was used to solve the finite horizon model. As mentioned earlier, the solution to the dynamic program is a policy of optimal actions, i.e. optimal time to perform the next survey given the current state and the current time. The infinite horizon models were also evaluated numerically by minimizing $V_m$ in equations (15) and (16). In all cases, the two summary results that are presented are the mean interval between tests given that the plume is in state M (normal migration) and the total expected costs. The finite horizon model gives the most conservative results (in terms of frequency of testing) whereas the approximate infinite horizon method gives the least conservative results. This is because the approximate method neglects the expected costs of seepage of the current interval and thus predicts that frequent seismic monitoring may not be necessary. The finite horizon model indicates that more frequent testing is required due to the boundary effects, i.e. effects towards the end of the horizon. Results from a one-way sensitivity analysis on the base case for all models are discussed below:

**Single-parameter Sensitivity Analysis**

By changing one model parameter at a time, we can evaluate the individual effect of that parameter on base case values. Figure 3 displays the relationship between the cost of the seismic survey and the optimal time until the next test for all the models. A discount rate of 6% was used for the analysis; the implication of higher discounting is that the cost of a seepage in the future is less disconcerting. A survey performed earlier would spot the
leakage earlier and remediation methods would have been utilized earlier, resulting in savings in costs attributed to excessive seepage. This is the essence of the trade-off between choosing the time to perform the next survey. The obvious result that a cheaper survey allows for more frequent testing is also evident from figure 3. Figure 4 depicts a monotonic increase in total costs with the cost of the survey, as expected. Note that for a seismic survey of $5 million, the total expected cost can be more than $40 million over a hundred year period. All three models have similar trends for the total expected cost but the optimal time is drastically different for each of them. The AIH model suggests that testing should not be very frequent because it ignores certain costs of seepage.

Figure 3. Base-case sensitivity plot for optimal time interval between surveys vs. survey costs

Figure 4. Base-case sensitivity plot for total expected costs vs. survey costs
In figure 5 we observe that when the risk of seepage is low, it is generally optimal to schedule a larger interval between tests. Counter-intuitively, frequent seismic testing is not cost-effective even when the risk of seepage is very high, above a certain threshold. This is as a result of our model assumptions as well as the fact that seismic testing does not alter the risk of seepage. If the risk is too high then the seepage is likely to occur anyway, so testing is in vain. Such a high risk may never be a practical problem because presumably sites will be selected carefully. The total expected costs are highest for a certain range of the expected time to seep (figure 6). When the rate of seepage is very high, then a seepage is likely to occur earlier and it is optimal to save on operational costs of seismic monitoring. Perhaps surface monitoring techniques that alleviate the seepage consequences should be the focus of monitoring programs in this case.

Figure 5. Base-case sensitivity plot for optimal time interval between surveys vs. rate of seepage

Figure 6. Base-case sensitivity plot for total expected costs vs. rate of seepage

Figures 5 and 7 reflect similar trends. In figure 7 though, all the models show very different trends. For the finite horizon model, frequent testing is ideal whenever the rate
of leakage is high. In the case of the EIH model, for the very high risk scenario of a high leakage rate, it is best to perform the survey after a longer interval as the transitions from M to L and R to L happen quickly and even a survey performed sooner would not be cost-effective for an infinite horizon. The AIH model is unable to capture any of these trade-offs and appears to be too simplistic. The total costs in figure 8 monotonically increase unlike those in figure 6. This is a more intuitive result: the total expected costs increase as reservoir leakage becomes more frequent or more ‘risky’.

![Figure 7. Base-case sensitivity plot for optimal time interval between surveys vs. rate of leakage](image7)

![Figure 8. Base-case sensitivity plot for total expected costs vs. rate of leakage](image8)

**Monte Carlo Sensitivity Analysis**

To perform multi-dimensional sensitivity analysis, we used the Monte Carlo simulation approach. For this analysis, we only used the finite horizon model as it was shown to be the model most sensitive to changes in the parameter values. Our results from this section would not be very different for the other models. 100,000
simulation runs were carried out over plausible ranges for all model parameters and summary statistics were obtained for all the selected combinations of input variables. The power of this technique lies in the fact that different hyper-planes of the simulated data can be investigated separately to check for interesting patterns and insights.

Figure 9 is a scatter plot of all the simulation runs and accounts for all variable model parameters on the 3 axes. The x and y-axes represent the seepage and leakage factors respectively. The seepage factor accounts for seepage risks and consequences by incorporating Monte Carlo simulated seepage rates, times, probabilities, and seepage penalties. The leakage factor accounts for leakage risks and consequences by combining the time to leak and the remediation cost. The z-axis shows the product of the remaining parameters: the discount factor and the survey cost. The simulated data points are colour coded with the optimal mean interval between surveys. Note the shape of the data shell and the distinct pattern in the mean interval. A low seepage factor and low survey cost imply that seismic need not be too frequent. Figure 10 contours mean optimal survey interval as a function of survey cost and seepage factor. Monte Carlo sensitivity analysis helps to understand interlinked trade-offs between critical model parameters. Some of the figures have also been presented in Bhattacharjya et al, 2006.
Conclusions

Seismic monitoring aids in determining the overall condition of the reservoir. The optimal frequency of seismic surveys balances survey costs and the risk of seepage. Frequent seismic surveys ensure that timely intervention is possible, and remediation action can prevent or at least delay seepage to the biosphere. Numerical results from the mathematical model and sensitivity analysis can be useful inputs for designing cost-effective monitoring programs and determining regulations. We have shown that some models can capture the trade-offs more effectively and that costs for a mid-interval seepage should not be neglected. The results indicate that site-specific monitoring schedules are essential for sequestration policy and planning since the optimal schedule is sensitive to model parameters, and these will vary across different geological storage sites. Quantitative models such as the one presented support qualitative analysis regarding decisions in sequestration monitoring.

Discussion

Monitoring of geological storage sites and particularly seismic testing has several benefits. These can be classified into the following categories, the 3 R’s: research, regulations and remediation. Sequestration is still in the exploration stage, hence seismic surveys provide essential information about how the CO$_2$ plume would move in the subsurface. For instance, observations from the Sleipner Field demonstrate a “pinching
effect” due to the thin layers of shale in the Utsira sands [Arts et al, 2002; Arts et al, 2004]. The most important aspect from the regulations point of view is that seismic and other such monitoring techniques can verify that everything is going as planned. Although ‘verification’ may be hard to model in a decision-theoretic approach, it is essential from a policy perspective. In this paper, we assume that regulations is a constraint that is fed into the model. The remediation benefits of monitoring may be the most important as project managers can take important decisions that can alter the existing scenario and rectify or mitigate possibly disastrous consequences.

Future work may involve repeating the numerical results and the sensitivity analysis for a more realistic site, like the Weyburn site. The dynamic programming model can be extended by introducing lognormal distributions for leakage and seepage based on the effects of trapping mechanisms. Different trapping mechanisms evolve in different ways over time and storage security should typically increase with time at an effective site [Benson and Cook, 2004; Gale, 2002]. The lognormal distribution with suitable parameters may capture this temporal evolution. One can also implement the model with more states, depicting different kinds of leakage and seepage pathways. Another possible extension is the inclusion of different monitoring approaches and finding the optimal portfolio of monitoring tools over time.

References


Workshop on Carbon Sequestration, November 18-22, 2002, Regina, Saskatchewan, Canada.


Appendix E: A “Chicken and Egg Problem” That Could Impede the Development of a Hydrogen Economy

Investigators
James Sweeney, Professor of Management Science and Engineering; Katherine Calvin, Graduate Researcher.

CEP has three main objectives: (1) “identify promising opportunities on technologies for low emissions, high-efficiency energy supply,” (2) “identify barriers to the application of these new technologies at large scale,” and (3) “conduct research into technologies that will help to overcome barriers and accelerate global applications.” (GCEP, 2007) Thus far, hydrogen vehicles have been identified as a low emission, high-efficiency energy option. Fuel cell vehicles are more energy efficient than conventional automobiles and emit only water vapor. The hydrogen that fuels the vehicle can be produced from clean, domestically available, renewable sources. However, barriers exist hindering the adoption of hydrogen vehicles. A commonly identified barrier is the “chicken and egg” problem. This research project aims to determine whether or not the chicken and egg barrier exists, and thus fits with the second goal of the GCEP project.

The hydrogen economy has been classified as a chicken and egg problem. Car manufacturers do not want to alter their production facilities and mass produce hydrogen fuel cell vehicles until hydrogen fuel is widely available at a reasonable cost for fear that consumers will not purchase the vehicles. Consumers cannot purchase vehicles until they are produced, and will be unwilling to purchase vehicles in the absence of fueling stations selling competitively priced fuel. Should fuel suppliers invest in a fueling station infrastructure, these fueling stations would operate well below capacity in the early years due to insufficient demand. This excess capacity would lead suppliers to want to charge a higher price for hydrogen in order to prevent a profit loss. However, consumers will be unwilling to pay such a price. Thus, fuel suppliers would rather wait until enough vehicles are in the market to warrant operating at full capacity. As Daniel Sperling explains, “fuel suppliers condition their investment decisions on the existence of a fuel market, and automakers condition their investment decisions on the supply of fuel with the combined result of investment paralysis; no one is willing to make the initial commitment.” (Sperling, 1988)

Currently, efforts are underway to spur investment and end the paralysis through the creation of both national and statewide programs. Many of these programs rely on public-private partnerships and government funding to encourage the adoption of hydrogen technologies and speed the transition to a hydrogen economy. For example, the recently released blueprint for the California Hydrogen Highway calls for a $10,000 per vehicle subsidy and 50/50 cost sharing on hydrogen fueling infrastructure. (Cal-EPA, 2005). The goal of this research is to determine whether such government intervention is necessary. The specific question asked is whether a fuel supplier can economically justify undertaking the burden of building a hydrogen fueling infrastructure and offering hydrogen at a cost comparable to that of gasoline. In the California Hydrogen Highway Net Blueprint, the economy team found that the cost of the hydrogen infrastructure was too large to be economically justified by the private sector without government funding.
Their analysis assumes a short time frame during which all hydrogen suppliers charge a price equivalent to the prevailing gasoline price. The analysis conducted for this research extends the time frame and explores higher hydrogen price in future years. The idea is that if a fuel supplier can differentiate its product and build a loyal customer base, it can charge a higher price in later years and earn a positive economic profit. In this research, several questions are raised: (1) can suppliers differentiate their products, (2) will the purchasers of hydrogen exhibit brand loyal behavior, (3) can hydrogen fuel suppliers charge a price above cost for hydrogen, (4) what profit is necessary to offset the short-term subsidy, and (5) is it possible for a supplier to earn this needed profit?

Can suppliers differentiate their products?

While the hydrogen itself may be a homogenous commodity, suppliers can potentially differentiate their product through differences in the fueling station itself – e.g. better customer service, cleaner restrooms, convenience stores, etc. In the US gasoline industry, firms often partner with other companies (e.g. Subway, Dairy Queen, etc.) to help distinguish themselves. Furthermore, the US gasoline industry spends millions on advertising to create brand recognition. In 1999, eighteen firms spent a combined total of $179 million on advertising. (EIA, 2001).

Will the purchasers of hydrogen exhibit brand loyal behavior?

The concept of brand loyalty arises when consumers have a decision to make between purchasing a product from several different firms. Brand loyalty is a conscious choice to purchase of a particular brand as opposed to other brands over a period time (Jacoby and Kyner, 1973). Product differentiation, whether perceived or actual, tends to increase brand loyalty. Furthermore, brand loyal buyers are not easily influenced by price oscillations and are “committed to the value and price appeal of the brand.” (Daly, 1970). Several factors can lead to brand loyalty. In some cases, consumers may not want to spend time searching for a better alternative and instead continue to purchase from the brand from which they initially bought the product. In other cases, switching costs deter customers from trying a new product. Consumers must learn new information to gain the same experience from the product and are thus reluctant to switch brands. These costs are more significant in new and emerging product markets. (Gabszewicz, et al., 1992). The hydrogen economy is an emerging market with the potential for product differentiation and therefore has the factors affiliated with brand loyal markets. However, whether or not customers in the hydrogen fuel market will exhibit brand loyalty is unknown. Thus, this research project explores differing degrees of brand loyalty and compares the findings to a base case that assumes no brand loyalty.

Can hydrogen fuel suppliers charge a price above cost for hydrogen?

Because the hydrogen economy is not yet established, the answer to this question is unknown. The ability to price above cost depends on the market power a particular firm exhibits. Determining market power depends on the industry structure, pricing behavior of the firms in the market, and brand loyalty. Industry structure and with it pricing behavior are the most important determinants of market power. For example, if the hydrogen fueling station industry develops into a perfectly competitive industry without product differentiation or brand loyalty, in equilibrium, all fuel suppliers will be forced to
price hydrogen at cost. The presence of entry barriers, limiting the number of firms in the industry, however, may allow firms to charge a price above cost. Furthermore, the presence of product differentiation and brand loyalty will accentuate a firm’s market power and allow it to charge an even higher price.

What profit is necessary to offset the short-term subsidy?

The answer to this question depends on how many years gasoline needs to be subsidized and how many firms are in the market. For example, using the National Research Council’s hydrogen cost and demand estimates (NRC, 2004), a 7% discount factor, and assuming that two firms will supply the expected hydrogen demand of the United States at gasoline prices for a period of 10 years starting in 2015 leads to a subsidy of approximately $3.6 billion. Assuming that ten firms are in the market, a subsidy of approximately $721 million is necessary. In both cases, a firm will need to expect to earn at least the subsidy amount in future years in order to justify investing in the hydrogen economy.

Is it possible for a supplier to earn this needed profit?

The ability to earn a substantial profit depends on the ability to price above cost. For instance, to earn enough profit to justify paying the subsidy in the ten firm example ($721 million), each firm would need to set the hydrogen price 1.2% above the average cost of hydrogen. As before, these estimates use the NRC costs and demand, a 7% discount rate, and assume that the ten firms evenly divide the market. The price markup is for the years 2015 to 2050. Whether or not firms can charge the prescribed markup depends on the characteristics of the industry.

Precisely how the hydrogen fueling station industry will develop is unknown. One could assume that the hydrogen fuel supply market will develop much like that of gasoline, into an oligopoly, dominated by a few firms. Game theory is often used to determine production and pricing decisions in an oligopoly. This method is invoked in this research project. Specifically, equilibrium behavior is found by making an assumption about one’s rivals’ behavior, and then choosing a best response given that assumption. Two classic oligopoly models, Bertrand and Cournot, are implemented for this problem.

In the Bertrand model, a firm assumes that its rivals face an infinitely elastic demand curve (i.e. the rival charges the same price regardless of the decision firm’s action). Without product differentiation, the Bertrand model leads to a surprising result; with only two firms, a competitive pricing scheme arises. In this competitive pricing scheme, a firm earns a long-run profit of zero. Thus, if a fuel supplier expects a homogenous product Bertrand scenario to arise, a hydrogen subsidy is not economically justified. However, the presence of product differentiation, allows firms in a Bertrand competition to exude some market power, the extent of which depends on the number of rivals and degree of substitutability among products.

In the Cournot model, a firm assumes that its rivals face an inelastic demand curve (i.e. the rival produces a particular quantity regardless of price). In such a model, the
price elasticity of demand becomes important. Assuming a demand elasticity of zero (i.e. consumers by a particular quantity regardless of price) allows a firm to charge an infinite price. The inclusion of a non-zero price elasticity reigns prices in to a more reasonable level.

A Cournot competition will lead to higher prices than those of Bertrand Competition. For instance, in the ten firm example without brand loyalty, the Bertrand model results in an equilibrium price of $3.23 in 2025. This price is equivalent to the cost per unit of hydrogen in that period. The Cournot model, however, results in an equilibrium price of $5.78. Thus, while the Bertrand model has zero long-term economic profits, the Cournot model leads to positive profits.

As is shown in the examples above, the belief a firm forms about its rivals heavily influences the resulting decision. Thus, a variety of beliefs are explored and the resulting pricing and production decisions compared.

Thus far, the research conducted has been focused on the United States as a whole, taking information and assumptions from the NRC’s Hydrogen Report. However, with the recent release of the California Hydrogen Highway Blueprint, the project will be altered to concentrate on California specifically. The Blueprint concludes that state funding is necessary to spur investment in hydrogen infrastructure. This research project explores whether or not that conclusion is true. Is government funding needed or will fuel suppliers have incentives to finance the investment on their own?

Sources
http://www.hydrogenhighway.ca.gov/plan/reports/volume1_050505.pdf


http://www.eia.doe.gov/emeu/finance/sptopics/downstrm00/index.html


Appendix F: Knowledge Stock and Cost Curves: A Firm Based Approach

Investigators
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1 Introduction

The cost of producing a good typically declines as the knowledge stock or equivalently the ‘technology’ associated with the production of that good increases. This phenomenon was first described in literature by Wright (1936), who reported that unit labor costs in airframe manufacturing declined significantly with accumulated experience of the workers. Although Wright’s (1936) work focussed on learning-by-doing and related experiential phenomenon in the production of a good (one of the factors which affect knowledge stock), his work has now been extended to incorporate the effects of R&D investment as well as spillovers from related areas and has been applied widely within the energy technology realm. Recent examples are PV modules (Harmon, 2000; Watanabe, 2000), combined cycle gas turbines (Claeson et al., 2002), fuel cells (Tsuchiya, 2002), ethanol production (Goldemberg, 1996), carbon sequestration technologies (Riahi et al., 2002), wind energy sector for Denmark (Neij, 1999 a, b), Germany (Durstewitz & Hoppe-Kilpper, 1999), United States (Mackay & Probert, 1998), and other countries (Lund, 1995; Ibenholt, 2002; Klaassen et al., 2002; Soderholm & Sundqvist, 2003).

In general, the knowledge stock \( (H) \) associated with producing a good, refers to the broad set of processes covering know-how, methodology, equipment and experience, used by humans for production (Clarke et al., 2005). We discuss below a comprehensive list of sources which influence \( H \).

(1) Autonomous Innovation - Autonomous innovation refers to the development of new technologies (or increase in knowledge) through innovation, which occurs naturally, independent of the influence of external factors (Goulder & Mathai, 2000). Nakicenovic (1997), describes autonomous innovation as ‘manna from heaven’, which occurs without any R&D investment and without the risk entrepreneurs usually face.

(2) R&D Investment - R&D investment refers to expenditures aimed at increasing the knowledge stock. It includes both basic scientific as well as applied research expenditures. Further, it also includes induced innovation - innovations, which are influenced by a change in policy. R&D is funded by both the government and the private sector and is conducted by industry, government, universities, and research organizations.

(3) Learning-by-Doing (LBD) and related experiential phenomenon - LBD represents the notion that the more an agent or an organization repeats a task, the more adept or efficient the organization becomes at that task (Clarke et al., 2005).
LBD thus refers to an increase in $H$, which occurs as the agents become more efficient at utilizing and managing the existing $H$. It is a natural process and is free, though it can be influenced by policy. LBD does not describe just one phenomenon but a range of experiential phenomena. In its purest form, LBD related to manufacturing labor productivity for a single product and production line. Workers on an assembly line become more and more efficient over time with repetition of their individual tasks. The concept of LBD can be further extended to incorporate design and material input improvements in production that may arise from the feedback of workers or while diffusing the product to end-users. This latter experience effect is referred to as Learning-by-Using (Clarke et al., 2005). A range of activities take place at the boundary between experiential phenomenon and R&D. For example, the day-to-day design improvements that companies make arise from information gained from learning and from R&D, but are not exclusively one or the other (Clarke et al., 2005).

Traditionally, LBD has been estimated by the statistical correlation between the declining cost of production in time period $t$ ($CP_t$) and cumulative industrial output till time period $t$ ($CO_t$). As production increases it will represent an increase in the utilization of the resources being used by the industry and hence an increase in $H$ without additional cost which is essentially the notion of LBD. These are referred to as ‘learning curves’, ‘experience curves’ or the so called 1 factor models (1FMs). If $Q_t$ is the industrial output and $UCP_t$ ($UCP_t = CP_t/Q_t$) the unit cost of production in time period $t$ then 1FMs can be mathematically represented as $UCP_t = B(CO_t)^{-\alpha}$, where $B$ and $\alpha$ are constants which can be determined econometrically. While LBD may be one of the factors underlying these curves, 1FMs also reflect the effects of autonomous innovation, R&D investment, spillovers, and economies of scale that arise in response to demand or the expectation of demand for a product, unless they are statistically controlled for these other factors. 1FMs also suffer from issues of simultaneous causality bias and omitted variable bias which are discussed later. Thus, while 1FMs may be an efficient way of representing the effect of declining cost of production due to all the above factors, they are extremely crude in isolating the effect of LBD.

(4) Spillover Effects - Spillover effects can be divided into extra-industry spillovers and own-industry spillovers.

(i) Extra-Industry Spillovers: The effect of increasing $H$ for the industry un-
der consideration due to an increase of H undertaken in another industry, research organization or university is referred to as an extra-industry spillover. For example, the development of advanced turbine designs in the aerospace industry made the high efficiency natural gas combined cycle turbine in the electricity generation industry possible. It is important to note that extra-industry spillover effects make technological advance possible, but often require alterations to deploy in the receiving sector (Cohen & Levinthal, 1989). Much of the change in technologies relevant in an energy context arise through extra-industry spillovers from largely unrelated sectors (Clark et al., 2005).

We can categorize extra-industry spillover effects into two types: direct extra-industry spillover effects and indirect extra-industry spillover effects. Direct extra-industry spillovers are those that improve technology in industry i with no effort required within industry i. For example, R&D into silicon wafers may directly reduce the costs of PV cells. Indirect extra-industry spillovers, on the other hand, do not directly improve technology in industry i, but create a pool of knowledge that can be exploited by own-industry activities such as R&D and LBD (Cohen & Levinthal, 1989). For example, developing new silicon wafers is simply not a matter of placing them in PV panels, the PV cells and silicon wafers have to be customized, to take advantage of the advances in nanotechnology.

(ii) Own-Industry Spillovers: The effect of increasing H for the firm under consideration due to an increase of H undertaken in another firm in the same industry is referred to as an own-industry spillovers.

In recent literature (Miketa & Schrattenholzer, 2004; Barreto & Kyperos, 2003; Klaassen et al., 2003; Soderholm & Sundqvist, 2003; Kouvaritakis et al., 2000) the 1FM has been extended to a so called 2 Factor Model (2FM). The 2FM, first proposed by (Kouvaritakis et al., 2000) stipulates that the cost of producing a good at time \( t \) \((CP_t)\) declines as a function of two factors: ‘cumulative industrial output’ of that good \((CO_t)\) and ‘cumulative R&D expenditures’ \(^2(RD_t)\) till time \( t \) instead of just ‘cumulative industrial output’ as is the case in the 1FM. Appendix A of (Miketa & Schrattenholzer, 2004) gives the underlying economic theory of deriving the 2FM, which has been used by all the above mentioned studies. 2FMs can be mathematically represented as \( UCP_t = B(CO_t)^{-\alpha}(RD_t)^{-\beta} \), where \( B, \alpha \) and \( \beta \)

\(^2\)R&D expenditures typically do not include extra-industry R&D expenditures. They include own-industry R&D expenditures (i.e., the total R&D expenditure in the industry) as well as direct R&D aid provided by the government to the industry.
are constants. These constants can be estimated by linear regression after transforming the equation by taking logarithms. Three serious econometric problems arise while following this approach: (i) omitted variable bias \(^4\) (ii) simultaneous causality bias \(^5\) and (iii) multi-collinearity between independent variables \(^6\).

Omitted variable bias could be a major problem in the 2FM since the cost of production is clearly influenced by variables other than cumulative industrial capacity and cumulative R&D expenditure; most notably by economies of scale and extra-industry spillover effects which are correlated with these two independent variables, particularly with cumulative industrial output. Simultaneous causality bias may also be a serious issue as the cost of production of a good may decrease as its cumulative industrial output increases, and at the same time cumulative industrial output may increase as the cost of production decreases. Since cumulative industrial output and cumulative R&D expenditure are highly correlated, multicollinearity of independent variables may also pose a serious threat to the analysis. To address these problems, studies such as (Soderholm & Sundqvist, 2003), attempt to employ instrumental variable techniques; however they claim that it is extremely difficult to find the appropriate instruments for cumulative industrial output and cumulative R&D expenditure.

(Clark et al., 2005) note that in the context of estimating H for energy technologies: (i) the effect of LBD and related experiential phenomena is small, and (ii) the dominant driver for increasing H are spillovers, largely from other sectors. All studies mentioned above, except for Watanabe (2000), focus on factor models for the industry as a whole. Instead of having a 2FM based on ‘cumulative industrial output’ and ‘cumulative R&D expenditures’, which very roughly differentiates the effect of LBD and R&D expenditure, we propose a new 2FM based on ‘cumulative R&D expenditures’ and time. The definition of cumulative R&D expenditures would now include own-industry R&D expenditure, direct aid given by the government

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\(^3\)UCP\(_t\) is typically adjusted for changes in the prices of inputs. Please see (Berndt, 1991) for details.

\(^4\)An omitted variable bias arises if an independent variable whose true regression coefficient is nonzero is excluded from the model. If this happens, the estimated values of all the regression coefficients will be biased unless the excluded variable is uncorrelated with every included variable (Wooldridge, 2002).

\(^5\)Simultaneous causality bias occurs when the dependent variable is caused by all the independent variables as well as one or more of the independent variables is caused by the dependent variable (Wooldridge, 2002).

\(^6\)Multicollinearity occurs when independent variables are so highly correlated that it becomes difficult or impossible to distinguish their individual influences on the dependent variable (Greene, 1993).
to the industry as before and extra-industry R&D expenditure, the effect of which this industry can absorb directly, without any effort. We discuss the underlying economic theory behind this in section 2.4. In this 2FM, the effect of changing the cost of production due to R&D expenditure would be a better approximation than the previous 2FM as this incorporates extra-industry spillover effects. The effects of all other factors such as LBD and related experiential phenomena (this effect is small and was captured crudely in the previous 2FM), autonomous innovation and economies of scale would be captured in the coefficient of time. The new 2FM would reduce the problems of multi-collinearity (as the correlation between R&D expenditure and time would be less) and reduce simultaneous causality (as it is likely that the reverse causality between cost of production and R&D expenditure is also less). However, the problem of omitted variable bias would still persist as R&D expenditure would be influenced by omitted variables such as economies of scale and extra-industry effects which are not captured. We would have to employ instrumental variable regression with appropriate instruments to overcome this.

All studies mentioned above focus on empirically estimating how the cost of producing a good would decline as $H$ increases for the entire industry. The distinction in the studies arise primarily because different studies consider different sources which influence $H$. The table below shows some of the different sources considered in the most recent studies.

<table>
<thead>
<tr>
<th>Study</th>
<th>AI</th>
<th>R&amp;D</th>
<th>LBD</th>
<th>El SpOv</th>
<th>OI SpOv</th>
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<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>Pure LBD</td>
<td>LBU</td>
<td>R&amp;D &amp; LBD</td>
</tr>
<tr>
<td>Berndt, 1991</td>
<td>no</td>
<td>no</td>
<td>yes</td>
<td>no</td>
<td>no</td>
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<tr>
<td>Watanabe, 2000</td>
<td>no</td>
<td>yes</td>
<td>no</td>
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<td>no</td>
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<tr>
<td>Isoard &amp; Isoaria, 2001</td>
<td>no</td>
<td>no</td>
<td>yes</td>
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<tr>
<td>Soderholm &amp; Sundqvist, 2003</td>
<td>no</td>
<td>yes</td>
<td>yes</td>
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<td>This paper</td>
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In this paper, we develop a theoretical firm-based model. Although the model is theoretical all its parameters may be estimated econometrically, if we had the required data, through the new 2FM discussed above and in section 2.4. However, for our purposes we shall simply assume the value of the parameters for the theoretical model. The theoretical model focuses on the strategic interaction between firms.

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their optimal R&D investment, the relationship between optimal R&D, profits and absorptivity (defined in section 2-2) of firms and finally how the cost of production decreases as $H$ increases. Our model will compare these issues for firms which are operating at their "nash equilibrium" to when they are operating at their "collusive optimal." We consider initially a two-period model which we extend to T-periods. Our analysis is general, but will focus on energy technologies in which the effect of LBD and related experiential phenomena is small and hence can be neglected, and the dominant driver for increasing $H$ is R&D expenditure and spillovers. The PV generation industry is an excellent example.

2 Theoretical Model

2.1 General Assumptions

(i) There are $N \geq 2$ firms. These firms form the PV industry and are involved in the design and manufacture of PV cells or equivalently in the generation of solar electricity (see Appendix A-2 for definition of solar electricity).

(ii) This is a $T \geq 2$ period model. We first consider a two period model (i.e., $T = 2$) and later extend it to a larger number of periods.

(iii) We assume all firms in the industry are identical and behave similarly. This implies that all firms have identical capital ($K_i^t$) and labor ($L_i^t$) input requirements, output of solar electricity ($q_i^t$), R&D expenditure ($RD_i^t$) and knowledge stock ($H_i^t$) for any time period. The $t$ subscript refers to the time period. This may seem a strong assumption; however it is not a very distorted representation of the PV cell industry structure. It also greatly simplifies our analysis. See Appendix A-3 for a brief overview of the firms in the PV industry. Almost all PV cell manufacturing firms are comparable in size, organization and ability of the labor they employ. Further, they either use 2nd generation technologies or are in the process of transitioning to them.

(iv) We assume that there is no entry or exit of firms during any time period. This restricts our analysis to the short run and hence we shall not assume $T$ to be very large (i.e., assume $T \leq 5$). In the long run this assumption would have to be relaxed.

(v) We assume each firm faces constant returns to scale with respect to its inputs: capital and labor. This is consistent with the assumptions of the afore mentioned

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8Please see section 3 (ii) for the case when we can extend $T$ till $\infty$.

9Economies of scale have often been cited as a source of decreasing technology costs, and therefore as a justification for policies that might increase deployment of emerging technologies such as PV cells. While economies of scale are undoubtedly important in bringing down the costs of emerging technologies, they are not a source of increasing knowledge stock. Economies of scale pertain to
empirical studies such as Miketa & Schrattenholzer (2004). Further, we assume that the returns to scale do not change in any period \(^{10}\).

(vi) We assume that each firm faces the same linear demand curve, given exogenously, for all periods given by \( p = a - b \cdot Q \), where \( a > 0, b > 0 \), \( p \) is the market price of a unit of solar electricity and \( Q \) is the total industry output of solar electricity.

### 2.2 Knowledge Stock for a firm

We define knowledge stock of a firm \( i \) in the beginning of period \( t \) \((H_i^t)\) as the cumulative scientific and technological knowledge gained by this firm through its own R&D expenditures, spillovers from other firms in the industry (i.e., own-industry spillovers) and direct extra-industry spillovers in previous periods.

Absorptivity of a firm \((0 \leq \lambda \leq 1)\) is the fraction of knowledge in the public domain that a firm can exploit and assimilate. \( \lambda = 0 \) implies no spillover effects whereas \( \lambda = 1 \) implies complete spillover effects. \( \lambda \) depends on the firm’s managerial and organizational capabilities and the skill of the labor it employs among other things. We make the following assumptions about the knowledge stock of a firm:

(i) The increase in knowledge stock of a firm is *discrete* in time, not continuous.

(ii) At the beginning of a period \( t \) all firms will decide their optimal R&D investment \((RD_i^t)\) for *that period simultaneously*.

(iii) The R&D decision of any firm in the beginning of period \( t \) will only bear fruit at the beginning of period \( t+1 \). Hence, the R&D decision of a firm in the beginning of period \( t \) will *not* affect its knowledge stock in period \( t \), but for all subsequent periods (including \( t+1 \)). It thus follows that in a \( T \) period model firms will invest in R&D in the first \( T-1 \) periods and not in the last period.

(iv) We assume that an R&D investment decision of \( RD_i^t \) by a firm \( i \) in period \( t \) will create new knowledge worth \( RD_i^t \) at the beginning of period \( t+1 \). We call this the deterministic case. We can relax this assumption by assuming an R&D investment decision of \( RD_i^t \) by a firm \( i \) in period \( t \) will create new knowledge worth \( RD_i^t \cdot X \) at the beginning of period \( t+1 \) where \( X \) is any discrete random variable between 0 and 1. We call this the stochastic case \(^{11}\).

\(^{10}\)The model is solved numerically; hence we can study the effect of changing returns to scale and this assumption maybe relaxed.

\(^{11}\)In this study we do not discuss the stochastic case, leaving it for future work. If we assume \( X \) to be a discrete random variable between 0 and \( \infty \), we could partially model Autonomous Innovation.
(v) Each firm shall absorb knowledge from other sources only at the beginning of a new period not during the course of a period. It follows from (iii) and (v) that the knowledge stock of a firm can only change at the beginning of a new period. Hence, $H_1^i = 1 \forall i = 1$ to N.

(vi) Since all firms are identical, it follows that each firm will have the same knowledge stock at the beginning of period 1. We normalize this knowledge stock to 1.

$$H_1^i = 1 \forall i = 1$$

(vii) Since all firms are identical, it also follows that each firm will have the same absorptivity ($\lambda$). We assume $\lambda$ does not change in any period. It is imposed exogenously on each firm at the beginning of the first period.

We can represent the knowledge stock of a firm $i$ ($\forall i = 1 - N$) in the beginning of period $t$ ($\forall t = 2 - T$) ($H_t^i$) mathematically for the deterministic case as equation (1) and for the stochastic case as equation (2).

$$H_t^i = H_{t-1}^i + RD_{t-1}^i + \lambda(RD_{t-1}^i + T_{t-1})$$

$$H_t^i = H_{t-1}^i + RD_{t-1}^i \cdot X + \lambda(RD_{t-1}^i \cdot X + T_{t-1})$$

where $T_{t-1}$ represents the direct extra-industry spillovers in period $t-1$. Cohen & Levinthal (1989), have used a similar functional form for a single period model.

### 2.3 Cost Function for a firm

We assume each firm faces a Cobb-Douglas production function given by $q_t^i = A_t(K_t^i)^{\alpha_K} (L_t^i)^{\alpha_L}$ in any period $t$. This is consistent with the assumptions of the afore mentioned empirical studies such as (Miketa & Schrattenholzer, 2004). $A_t$ represents the knowledge stock of period $t$. Following vast empirical studies by (Griliches, 1979) we assume $A_t = B(H_t^i)^{\alpha_H}$, where $B$ is a constant. Further, if a firm decides to invest $RD_t^i$ in R&D for period $t$, it will face a cost of $(1-\nu) \cdot RD_t^i$ where $0 \leq \nu < 1$ is the fraction of R&D subsidy provided by the government. Prices of capital ($r_t$) and labor ($w_t$), $\alpha_K$, $\alpha_L$, $\alpha_H$ and $B$ are given exogenously. To determine its (variable) cost of production for period $t$ ($CP_t^i$) (not total cost) each firm will solve for period $t$

$$CP_t^i = \min_{K_t^i, L_t^i} \begin{cases} \hat{K}_t^i \cdot r_t + \hat{L}_t^i \cdot w_t \\ B(H_t^i)^{\alpha_H} (K_t^i)^{\alpha_K} (L_t^i)^{\alpha_L} \geq q_t^i \\ q_t^i > 0 \end{cases}$$

8
Following (Berndt, 1991) we can solve the above minimization problem to determine \((CP^i_t)\).

\[
CP^i_t(q^i_t) = D_t \cdot (B)^{-1} \cdot (H^i_t)^{-\alpha_H/s} \cdot s \cdot (q^i_t)^{1/2}
\]

\[
D_t = d \cdot (r^i_t)^{\alpha_K} \cdot (w^i_t)^{\alpha_L/s}
\]

\[
d = (\alpha_K)^{-\alpha_K/s} \cdot (\alpha_L)^{-\alpha_L/s}
\]

\[
s = \alpha_K + \alpha_L
\]

The total cost of firm \(i\) for period \(t\) is then (assuming fixed cost to be zero):

\[
TC^i_t(q^i_t) = D_t \cdot (B)^{-1} \cdot (H^i_t)^{-\alpha_H/s} \cdot s \cdot (q^i_t)^{1/2} + (1 - \nu) \cdot RD^i_t
\]  (3)

Since we have assumed constant returns to scale with respect to capital and labor inputs \((s = 1)\) equation (3) reduces to

\[
TC^i_t(q^i_t) = D_t \cdot (B)^{-1} \cdot (H^i_t)^{-\alpha_H} \cdot q^i_t + (1 - \nu) \cdot RD^i_t
\]  (4)

### 2.4 Estimating Parameters

We now outline a procedure for estimating the parameters of the cost curve econometrically. These parameters shall be needed in our theoretical model. We change the Cobb-Douglas production function each firm faces given in section 2.3 by adding a time factor as follows: \(q^i_t = A_t(K^i_t)^{\alpha_K}(L^i_t)^{\alpha_L}\) where \(A_t = B(e^{ct+\varepsilon_t})(H^i_t)^{\alpha_H}\), \(c\) is a constant, \(t\) is the time period and \(\varepsilon_t\) is the stochastic disturbance. The solution to the previous minimization problem will then become

\[
CP^i_t(q^i_t) = D_t \cdot (B \cdot e^{ct+\varepsilon_t})^{-1/2} \cdot (H^i_t)^{-\alpha_H/s} \cdot s \cdot (q^i_t)^{1/2}
\]

\(D_t\) is the same as defined in the previous section. We shall conduct our analysis over a time period range for which \(s\) remains constant. Taking logarithms on both sides we get

\[
\ln(CP^i_t) = L + \frac{\alpha_K}{s} \ln(r^i_t) + \frac{\alpha_L}{s} \ln(w^i_t) - \frac{\alpha_H}{s} \ln(H^i_t) - \frac{c}{s} \ln(t) + \mu^i_t
\]  (5)

where \(\mu^i_t\) is the transformed stochastic disturbance, \(L\) is a constant, \(r^i_t\) and \(w^i_t\) are the real prices of capital and labor respectively. We may estimate \(L, \alpha_K, \alpha_L, \alpha_H\) by running an ordinary least squares regression. Once these constants have been estimated we can easily determine \(D_t\) and \(B\). As discussed earlier in section 1, in (5) the independent variables are not highly correlated and hence multicollinearity may not be a serious problem. Further, as discussed earlier, simultaneous causality
may be present and can be checked using the Hausman specification test (Hausman, 1978). It is also likely that there maybe a problem of omitted variable bias as $H_t$ maybe correlated to omitted variables such as extra-industry spillovers, LBD and economies of scale effects. If this is the case (which would be dependent on our data set) we would have to resort to IV regression by finding the appropriate instrumental variables for $H_t$.

The functional form of $H_t$ given in (1) and (2) is not the most general. A more general representation of $H_t$ is as follows

$$H_t = (1 - \gamma)H_{t-1} + RD_{t-1} + \lambda(\theta \cdot RD_{t-1} + T_{t-1})$$

(6)

This form is not used in our simple theoretical model because it adds no additional insights. However, if we were estimating all the parameters econometrically we would have used this. Here, $\theta$ (Cohen & Levinthal, 1989) is the degree to which the research effort of a firm may spillovers to the pool of knowledge in the public domain. $\theta$ is determined by exogenous factors such as patent policy, which is similar for all firms, and hence its value is the same for all firms. $\gamma$ (Griliches, 1995) is the rate of depreciation of the knowledge stock as the past knowledge becomes outdated. $\gamma = 0$ and $\theta = 1$ in our analysis. Further, it is important to note, that the duration of a time period in our model is the time it takes for an R&D investment made at the beginning of the period to bear fruit. Studies by (Klaassen et al., 2003), (Watanabe, 2000) and others generally suggest a depreciation rate ($\gamma$) of 3 percent per year and time lag ($t$) for R&D to bear results as 2 years for PV generation technologies. $H_t$ and $RD_t$ are measured in dollars. Estimation (although crude) of the initial knowledge stock ($H_1$) and absorptivity ($\lambda$) of a firm has been discussed in detail in (Miketa & Schrattenholzer, 2004) and (Schmidt, 2004) respectively. (Miketa & Schrattenholzer, 2004) have estimated $H_t$ to be roughly around $15 billion dollars for the PV industry.

We next consider the estimation of direct extra-industry spillovers effects in period $t$ ($T_t$). We modify the methodology suggested by (Jaffe, 1988). Let there be N areas of patents related to the PV generation industry. Each industry or research organization $j$ which is somehow related to the PV industry will have a certain positive number of cumulative patents in at least one of these N areas till the beginning of period $t$. Hence, we can calculate the fraction of cumulative patents in each area for industry $j$ till period $t$. Let $F^j_t$ denote the vector for industry $j$, whose components are the fraction of the cumulative patents in each of the N areas till period $t$. It is, therefore, a $N \times 1$ vector. We then define the ‘technical proximity’ of the PV
industry with industry $j$ for period $t$ as

$$w_t^{PV,j} = \frac{F_t^{PV'} \cdot F_t^j}{\| F_t^{PV} \| \cdot \| F_t^j \|}$$

If industry $j$ invests in total R&D of $RD_t^j$ in period $t$ then $T_t$ (in dollars) is approximated as

$$T_t = \sum_{j \neq PV} w_t^{PV,j} \cdot RD_t^j$$

Once we have estimated $H_t^j$ we can normalize this to 1 and correspondingly change our values for $RD_t^i$ and $T_t$. Having estimated $\alpha_K$, $\alpha_L$, $\alpha_H$, $D_t$ and $B$ we would have to estimate $a$ and $b$ to get the demand function $p = a - b \cdot Q$ for the PV industry; this is a standard econometric problem.

For our theoretical model we normalize $H_t^j$ to 1 and assume the real prices of capital ($r_t$) and labor ($w_t$) are each equal to 1 $\forall t$. Further, we assume $\alpha_K = 0.5$ and $\alpha_L = 0.5$ which ensures that there are constant returns to scale with respect to capital and labor inputs (our initial assumption). Hence $D_t = 2 \forall t$. For all calculations we assume $B = 2$, $\alpha_H = 2$, $a = 12$, $b = 1.5$, $\rho$ (discount factor) = 0.05, $N = 2$, $T_t = 0 \forall t$ (i.e., no extra-industry spill-over effects), arbitrarily, such that $RD_t^j$ and $q_t^j$ of all firms come out to be non-negative $\forall t \leq 5$, $\forall \lambda (0 \leq \lambda \leq 1)$, and $\forall \nu (0 \leq \nu < 1)$.

2.5 Two-Period Models

We consider two two-period models. In each model, firm $i$ will choose the following in the beginning of period 1: optimal output for period 1 ($q_t^i$), optimal R&D investment for period 1 ($RD_t^i$) and optimal output for period 2 ($q_t^2$). It will do so by maximizing its profits over the two-period horizon using backward induction. We have assumed that in any period all firms will choose their optimal output and R&D investment for that period simultaneously in the beginning of the period. For reasons discussed earlier (section 2.2) firms will not invest in R&D in period 2. Hence, this setup has a one-time R&D investment by firms. The two models we discuss are: (i) Nash Equilibrium Model and (ii) Collusive Optimal Model.

\footnote{It is inconsequential whether output or R&D is chosen first for a given period. This is because optimal output for any period will depend on the level of knowledge stock in that period. An R&D decision for this period will bear fruit only in the next period and hence will influence the knowledge stock and optimal output decision of subsequent periods and not of this period.}
2.5.1 Nash Equilibrium (NE) Model

In the Nash Equilibrium Model each firm will choose $q_i^*, RD_i^*$ and $q_i^*$ ($\forall i = 1 - N$) such that $q_i^*$ is a best response to $q_i^{-i*}$, $RD_i^*$ is a best response to $RD_i^{-i*}$ and $q_i^*$ is a best response to $q_i^{i*}$ $\forall i = 1 - N$. This will thus constitute a pure strategy nash equilibrium.

(i) **Beginning of period 2:** In the beginning of period 2 firm $i$ will choose its optimal output ($q_i^*$), by maximizing its profit in period 2 given that: its knowledge stock at the beginning of period 2 is $H_2$ and that all other firms are choosing their optimal output simultaneously. Firm $i$ will solve the following maximization problem

$$
\max_{q_i^* \geq 0} \left[ a - b(q_i^* + Q_2^{-i*}) \right] \cdot q_i^* - D_2 \cdot (H_2^i)^{-\alpha_H} \cdot q_i^*
$$

Differentiating this with respect to $q_i^*$ and setting the differential to 0 we get

$$
a - b(2 \cdot q_i^{i*} + Q_2^{-i*}) - D_2 \cdot (H_2^i)^{-\alpha_H} = 0
$$

Replacing $Q_2^{-i*} = (N-1) \cdot q_i^*$ (identical firms) in the above expression we get

$$
q_i^{i*} = \frac{a - D_2(H_2^i)^{-\alpha_H}}{b(N + 1)} \tag{7}
$$

(ii) **Beginning of period 1:** In the beginning of period 1 firm $i$ will choose its optimal output ($q_i^{i*}$) and its optimal R&D ($RD_i^{i*}$), by maximizing its profit in period 1 and discounted profit in period 2 given that: all other firms are choosing their optimal output simultaneously and that all other firms are choosing their optimal R&D simultaneously. Firm $i$ will solve the following maximization problem

$$
\max_{q_i^{i*} \geq 0, RD_i^{i*} \geq 0} \left( a - b(q_1^{i*} + Q_1^{-i*}) \right) \cdot q_1^{i*} - D_1 \cdot (H_1^i)^{-\alpha_H} \cdot q_1^{i*} - (1 - \nu) \cdot RD_1^{i*}
$$

$$
+ e^{-\rho} \left( a - b(q_2^{i*} + Q_2^{-i*}) \right) \cdot q_2^{i*} - D_2 \cdot (H_2^i)^{-\alpha_H} \cdot q_2^{i*}
$$

subject to

$$
H_2^i = H_1^i + RD_1^{i*} + \lambda(RD_1^{-i*} + T_1)
$$

Differentiating this with respect to $RD_1^{i*}$ and setting the differential to 0 we get

$$
- (1 - \nu) + e^{-\rho} \left( a - 2b(q_2^{i*}) - bQ_2^{-i*} - D_2(H_2^{i*})^{-\alpha_H} \right) \frac{dq_2^{i*}}{dRD_1^{i*}} - e^{-\rho} b(q_2^{i*}) \frac{dQ_2^{-i*}}{dRD_1^{i*}}
$$

$$
+ e^{-\rho} \alpha_H D_2(q_2^{i*}) (H_2^{i*})^{-\alpha_H - 1} \frac{dH_2^i}{dRD_1^{i*}} = 0
$$
Further we have
\[
\frac{dH_j^2}{dR_i^1} = 1 \\
\frac{dq_{j^*}}{dR_i^1} = \frac{\alpha H D_2 (H_j^{*})^{-\alpha H - 1}}{b(N + 1)} \\
\frac{dQ_{j^*}}{dR_i^1} = \sum_{j=1,j\neq i}^{N} \frac{dq_{j^*}}{dR_i^1} = \frac{\alpha H D_2 \lambda}{b(N + 1)} \sum_{j=1,j\neq i}^{N} (H_j^{*})^{-\alpha H - 1}
\]

Since firms are identical we have, \(H_j^{*} = H_i^{*} (\forall j = 1 - N)\), \(R_i^* = R_i^* (\forall j = 1 - N)\) and \(Q_j^{*} = (N-1) \cdot q_j^{*}\). We can simplify the above equation to get
\[
\frac{b(N + 1)(1 - \nu)e^\rho}{\alpha H} (H_j^{*})^{2\alpha H + 1} - D_2 a \left( 1 - \frac{\lambda(N - 1)}{N + 1} \right) (H_j^{*})^{\alpha H} + (D_2)^2 \left( 1 - \frac{\lambda(N - 1)}{N + 1} \right) = 0 \tag{8}
\]

We shall solve this equation numerically to determine the optimal value of \(H_j^{*}\). We can then determine \(R_i^*\) from \(H_j^{*} = H_i^{*} + \lambda T_1 + R_i^*(1 + \lambda(N - 1))\) easily. Further, differentiating the objective function with respect to \(q_i^1\), setting the differential to 0 and proceeding as earlier we get
\[
q_i^{1*} = \frac{a - D_1 (H_i^{*})^{-\alpha H}}{b(N + 1)} \tag{9}
\]

The choice of \(q_i^{1*}\) (or \(q_i^{1NE}\)), \(R_i^*\) (or \(R_i^{1NE}\)) and \(q_i^{2*}\) (or \(q_i^{2NE}\)) determined in this way constitutes a pure strategy Nash equilibrium for firm \(i\). Note that \(\lambda = 0\) implies no spillover effects whereas \(\lambda = 1\) implies complete spillover effects. We have solved this model numerically for values of the exogenous variables indicated at the end of section 2.4. Sample calculation and second order conditions are in Appendix A-4. Figure 1 shows the plot of the optimal discounted profit of firm \(i\) (\(\pi_i^{1NE}\)) with respect to its absorptivity (\(\lambda\)). Figure 2 shows the plot of the optimal R&D investment of firm \(i\) (\(R_i^{1NE}\)) with respect to its absorptivity (\(\lambda\)). Explanations are given in section 3.

### 2.5.2 Collusive Optimal (CO) Model

In the Collusive Optimal Model, firms shall collude to decide their optimal output and their optimal R&D investment. For deciding optimal (collusive) output each firm will choose \(q_i^{1*}\) and \(q_i^{2*} (\forall i = 1 - N)\) such that it maximizes the profit for
the entire industry. The collusive output \((q_1^*, q_2^*)\) can be thought equivalent to having only one firm in the industry which chooses its optimal output to maximize its monopoly profit and then dividing this optimal output equally among all firms (since firms are identical). Firms shall always collude in this way while choosing their optimal output. Simultaneously, each firm will choose its optimal R&D investment, \(RD_1^*\), by maximizing the profit of the entire industry. There will be monopoly-like collusion between firms to choose R&D only when \(\lambda = 1\) (i.e., the industry shall decide its monopoly optimal R&D investment which will be divided equally among the firms), no collusion when \(\lambda = 0\) (firms behave as separate entities while deciding optimal R&D investment) and partial collusion when \(0 < \lambda < 1\).

(i) **Beginning of period 2:** In the beginning of period 2 each firm \(i\) will choose its optimal output \((q_2^i)\), such that it maximizes the total profit of the industry in period 2 given that: its knowledge stock at the beginning of period 2 is \(H_2^i\). Since firms are identical \(q_2^i\) will be the same for all firms. Firm \(i\) will solve the following maximization problem

\[
\max_{q_2^i \geq 0} N \cdot [a - bNq_2^i] \cdot q_2^i - N \cdot D_2 \cdot (H_2^i)^{-\alpha_H} \cdot q_2^i
\]

Differentiating this with respect to \(q_2^i\) and setting the differential to 0 we get

\[
Na - 2bN^2 \cdot q_2^i - ND_2 \cdot (H_2^i)^{-\alpha_H} = 0
\]

This can be simply written as

\[
q_2^i = \frac{a - D_2(H_2^i)^{-\alpha_H}}{2bN}
\]

(ii) **Beginning of period 1:** In the beginning of period 1 each firm \(i\) will choose its optimal output \((q_1^i)\) and its optimal R&D \((RD_1^i)\), such that it maximizes the total profit of the industry in period 1 and discounted profit in period 2. Since firms are identical \(q_2^i\) and \(RD_1^i\) will be the same for all firms. Firm \(i\) will solve the following maximization problem

\[
\max_{q_1^i \geq 0, RD_1^i \geq 0} N \cdot \left( [a - bNq_1^i] \cdot q_1^i - D_1 \cdot (H_1^i)^{-\alpha_H} \cdot q_1^i - (1 - \nu) \cdot RD_1^i \right)
\]

\[
+ e^{-\rho N} \cdot \left( [a - bNq_2^i] \cdot q_2^i - D_2 \cdot (H_2^i)^{-\alpha_H} \cdot q_2^i \right)
\]

subject to

\[
H_2^i = H_1^i + RD_1^i + \lambda((N - 1)RD_1^i + T_1)
\]
Differentiating this with respect to $RD_i^1$ and setting the differential to 0 we get

$$- N(1 - \nu) + e^{-\rho t} N\left( a - 2bN(q_2^i)^* - D_2(H_2^i)^{-\alpha_H}\right) \frac{dq_2^i}{dRD_i^1} + e^{-\rho t} N\alpha_H D_2(q_2^i)^*(H_2^i)^{-\alpha_H-1} \frac{dH_2^i}{dRD_i^1} = 0$$

Further we have

$$\frac{dH_2^i}{dRD_i^1} = 1 + \lambda(N - 1)$$

$$\frac{dq_2^i}{dRD_i^1} = \frac{\alpha_H D_2(1 + \lambda(N - 1))(H_2^i)^{-\alpha_H-1}}{2bN}$$

We can simplify the above equation to get

$$\frac{2bN(1 - \nu)e^\rho}{\alpha_H(1 + \lambda(N - 1))} (H_2^i)^{2\alpha_H+1} - D_2a(H_2^i)^{\alpha_H} + (D_2)^2 = 0 \quad (11)$$

We shall solve this equation numerically to determine the optimal value of $H_2^i$. We can then determine $RD_i^1$ from $H_2^i = H_i^1 + \lambda T_i^1 + RD_i^1(1 + \lambda(N - 1))$ easily. Further, differentiating the objective function with respect to $q_1^i$, setting the differential to 0 and proceeding as earlier we get

$$q_1^i = \frac{a - D_1(H_1^i)^{-\alpha_H}}{2bN} \quad (12)$$

The choice of $q_1^i$ (or $q_1^{CO}$), $RD_i^1$ (or $RD_i^{CO}$) and $q_2^i$ (or $q_2^{CO}$) determined in this way constitutes the collusive optimal for firm $i$. We have solved this model numerically for values of the exogenous variables indicated at the end of section 2-4. Sample calculation and second order conditions are in Appendix A-4. Figure 3 shows the plot of the optimal discounted profit of firm $i$ ($\pi_i^{CO}$) with respect to its absorptivity ($\lambda$). Figure 4 shows the plot of the optimal R&D investment of firm $i$ ($RD_i^{CO}$) with respect to its absorptivity ($\lambda$). Figure 5 and Figure 6 compare the Nash equilibrium and collusive optimal cases. Explanations are given in section 3.

### 2.6 T-Period Models

In this section we extend the 2-period model discussed above to a T-period model. We use a finite horizon, discrete-time, dynamic programming approach to solve the resulting model. At the beginning of period $t$ each firm $i$ will simultaneously choose
its optimal output \((q_t^i)\) and optimal R&D investment \((RD_t^i)\) for period \(t\). Thus, \(q_t^i\) and \(RD_t^i\) will be the choice variables for firm \(i\) for period \(t\). Moreover, since all the information at the beginning of period \(t\) that bears on current and future decisions for firm \(i\) is summarized by its knowledge stock at the beginning of period \(t\) \((H_t^i)\), \(H_t^i\) is the state variable for firm \(i\) for period \(t\). We shall have two different dynamic programs depending on whether we are solving the: (i) Collusive Optimal Model or the (ii) Nash Equilibrium Model.

2.6.1 Collusive Optimal (CO) Model

The DP for the Collusive Model is given as follows

\[
V_t^i(H_t^i) = \max_{q_t^i \geq 0, RD_t^i \geq 0} \left[ N \cdot \left( (a - bNq_t^i) \cdot q_t^i - D_t \cdot (H_t^i)^{-\alpha_H} \cdot q_t^i - (1 - \nu) \cdot RD_t^i \right) + e^{-\rho} \cdot V_{t+1}^i(H_{t+1}^i) \right] \quad \forall t = 1 - (T - 1)
\]

\[
V_T^i(H_T^i) = \max_{q_T^i \geq 0} \left[ N \cdot (a - bNq_T^i) \cdot q_T^i - N \cdot D_T \cdot (H_T^i)^{-\alpha_H} \cdot q_T^i \right]
\]

\[H_t^i = H_1^i + RD_t^i + \lambda((N - 1)RD_1^i + T_1) \quad \forall t = 2 - T \text{ and } H_1^i = 1\]

In any period \(t\) the choice of the collusive optimal output \(q_t^i\) will have no influence on the current or future state of knowledge stock, and hence no effect on the profit for firm \(i\). It depends only on the current state of knowledge stock and is calculated simply by differentiating the objective function with respect to \(q_t^i\), which is

\[
q_t^i = \frac{a - D_t(H_t^i)^{-\alpha_H}}{2bN} \quad \forall t = 1 - T
\]

In any period \(t\) the choice of R&D, however, will influence the future state of knowledge stock and hence affect the firm’s profit. We assume that a firm can invest in R&D only between \([0, 0.5]\) for any period. We make this assumption to decrease computations and also to take into account another realistic scenario that a firm cannot invest too large an amount in R&D at any one time. For a given

13This is true for all periods except the last period for which the firm will only choose its optimal output. Further, for reasons discussed earlier, it is inconsequential whether output or R&D is chosen first for a given period.

14A 0.5 R&D investment is also a very large amount for a single period by a firm keeping in mind that the initial knowledge stock of a firm is \(H_1^i = 1\). However, in this study our purpose is demonstrative rather than getting a good approximation on any value.
value of $\lambda$ and the possible R&D range the state variable $H_t^i$ will have a different range for different periods. For each period and each $H_t^i$ we shall calculate the collusive optimal $RD_t^i$ through recursion, using backward induction. Since all firms are identical they invest the same in R&D. Proceeding backwards in time we can determine the collusive optimal R&D in period 1 (since $H_1^i=1$), and consequently the collusive optimal R&D policy in each period.

We solve this model for values of the exogenous variables indicated at the end of section 2.4 using MATLAB for $T=5$ (i.e., a four time R&D investment). Sample calculation are in Appendix A.5. Figure 8 shows the plot of the collusive optimal discounted profit of firm $i$ ($\pi_t^{CO}$) with respect to its absorptivity ($\lambda$). Figure 9 shows the plot of the collusive optimal total R&D investment of firm $i$ ($RD_t^{CO}$) with respect to its absorptivity ($\lambda$). Explanations are given in section 3.

### 2.6.2 Nash Equilibrium (NE) Model

The DP for the Nash Equilibrium Model is given as follows

$$V_{t}^{i**}(H_{t}^{i}) = \max_{q_{t}^{i} \geq 0, RD_{t}^{i} \geq 0} \left( [a - b(q_{t}^{i} + Q_{t-1}^{i})] \cdot q_{t}^{i} - D_{t} \cdot (H_{t}^{i})^{-\alpha H} \cdot q_{t}^{i} - (1 - \nu) \cdot RD_{t}^{i} \right) + e^{-\rho \cdot V_{t+1}^{i**}(H_{t+1}^{i})} \forall t = 1 - (T - 1)$$

$$V_{T}^{i**}(H_{T}^{i}) = \max_{q_{T}^{i} \geq 0} \left( a - b(q_{T}^{i} + Q_{T}^{i}) \cdot q_{T}^{i} - D_{T} \cdot (H_{T}^{i})^{-\alpha H} \cdot q_{T}^{i} \right)$$

$$H_{2}^{i} = H_{1}^{i} + RD_{1}^{i} + \lambda(RD_{1}^{i} + T_{1}) \forall t = 2 - T \text{ and } H_{1}^{i} = 1$$

As in the collusive model, the nash equilibrium optimal $q_{t}^{i*}$ will depend only on the current state of the knowledge stock and can be calculated by differentiating the objective function with respect to $q_{t}^{i*}$, and replacing $Q_{T}^{i*} = (N-1) \cdot q_{2}^{i*}$ (identical firms), as in the two period model, to get

$$q_{t}^{i*} = \frac{a - D_{t}(H_{t}^{i})^{-\alpha H}}{b(N + 1)} \forall t = 1 - T$$

(14)

As earlier, for a given value of $\lambda$ and the possible R&D range the state variable $H_{t}^{i}$ will have a different range for different periods. To calculate the nash equilibrium R&D choice (which is sub optimal) for firm $i$, we have to first calculate the best
response R&D profile for firm i, for all possible values of $H_t^i$ for a period $t$. We do this by keeping the R&D level of all other firms fixed and then calculating the optimal R&D for firm $i$ through recursion, using backward induction. We repeat this for all possible R&D values of the other firms. For each $H_t^i$, we then choose the R&D level which is equal to all other firms’ R&D.\textsuperscript{15} We thus will have the nash equilibrium R&D for all possible values of $H_t^i$ for a period $t$. Proceeding backwards in time we can determine the nash equilibrium R&D in period 1 (since $H_1^i=1$), and consequently the optimal nash equilibrium R&D policy in each period.

We solve this model for values of the exogenous variables indicated at the end of section 2-4 using MATLAB for $T=5$ (and hence a four time R&D investment). Sample calculations are in Appendix A-5. Figure 10 shows the plot of the nash equilibrium discounted profit of firm $i$ ($\pi_{1NE}^i$) with respect to its absorptivity ($\lambda$). Figure 11 shows the plot of the nash equilibrium total R&D investment of firm $i$ ($RD_{1NE}^i$) with respect to its absorptivity ($\lambda$). Figure 12 compares the nash equilibrium and collusive optimal cases. It is important to note that in the T-period DP problem, solved above, the maximum R&D that a firm can choose is constrained to 0-5. In the 2-period problem, discussed earlier, there was no constraint on the choice of R&D. If the DP is solved for $T=2$, but with no constraint on the choice of R&D, it would lead to the same results as the 2-period problem.

3 Conclusions

Almost all studies attempting to estimate the decrease in the cost of a good due to an increase in its knowledge stock (particularly in an energy context) have been empirical and industry-based. The distinction in the studies arise primarily because different studies consider different sources which influence $H$. In this paper, we develop a theoretical model which is firm-based and hence can also capture strategic interactions between firms. Although the model is theoretical its parameters may be estimated econometrically, if we had the required data. The theoretical model can incorporate a wide variety of sources which influence $H$ such as autonomous innovation and uncertainty concerning the impact of R&D expenditures which are very difficult to model through empirical studies. Moreover, our model incorporates direct extra-industry spillovers which are vital in an energy technology context. The model is solved using a finite horizon, discrete-time, dynamic programming approach. Following are some of the conclusions from the the 2-

\textsuperscript{15}The nash equilibrium of firms will be the intersection of their best response functions. Since firms are indentical, at their nash equilibrium all firms shall invest in the same R&D.
period model:

(i) In both the NE and CO models (Figures 1 and 3) it is evident that the higher the absorptivity, greater will be the optimal profit earned by a firm. If increasing absorptivity came free then a firm given a choice would choose the highest absorptivity available. However, in reality absorptivity is not free. It depends on the firms managerial and organizational capabilities and the skill of the labor it employs among other things. If each firm has one dollar to spend it can either invest it in R&D effort or in increasing absorptivity. Suppose $C(\lambda)$ (an increasing and convex function) is the hypothetical cost of increasing absorptivity for each firm, then a firm will invest in increasing absorptivity as long as $\frac{d\pi^*_i}{d\lambda} = \frac{d\pi^*_i}{dRD^*_i}$. Although not shown here, it can be proven analytically also (using the envelope theorem), that $\frac{d\pi^*_i}{d\lambda} > 0$.

(ii) The profit earned by a firm producing at its CO is always greater than the profit earned by it, if it is producing at its NE (Figure 5) for all absorptivities. The NE output and NE R&D investment is thus not pareto optimal in this setting as a change in the allocation of these resources would increase profit for all firms. From a firm’s perspective it will always be beneficial to collude. However, for collusion to be sustainable (otherwise the firms will revert to their nash equilibrium and the collusion will break) either this ‘game’ (i.e., the game of deciding R&D and output in each period) has to be repeated an infinite number of times or there has to be an element of uncertainty in the number of times it will be repeated. Further, a credible punishment strategy would have to be devised which ensures that no firm will deviate from the collusive action. To study this, we would have to solve the DP given in section 2.5 for an infinite horizon and attempt to get analytical expressions (which is easier for the finite horizon problem) for the NE and CO cases. This would be an interesting future extension of the work.

(iii) In both the NE and CO models (Figures 2 and 4) it is evident that, the higher the absorptivity lower will be the optimal R&D investment by the firm. A higher absorptivity implies higher spillovers. In the NE model, with higher spillovers, a firm can increase its profits by increasing its knowledge stock, from the research effort of its rival firms, for free, without having to put the same effort in its own R&D. Hence, each firm will choose to invest less in R&D and will ‘free-ride’ on the R&D effort of other firms. In the CO model, with higher spillovers, each firm will need to invest less in R&D to increase the profit of the industry as compared to when there were lesser spillovers. There are no free-riding effects in the CO
model. A higher absorptivity for each firm thus implies that the total pool of R&D decreases but the accessibility of that pool to each firm increases. This is consistent with the work of (Cohen & Levinthal, 1989), who have done a similar analysis for a single period model.

(iv) It is inconclusive whether the optimal R&D spending by firms is higher in the CO model or the NE model (Figure 6). According to the stylized case analyzed in this study, if the absorptivity of firms is low \( \lambda < 0.23 \) then firms tend to invest more in R&D when they are operating at their NE as compared to if they are colluding. However, if the absorptivity of firms is high \( \lambda > 0.23 \) then firms invest more in R&D when they are colluding as compared to operating at their NE. Figure 7 shows the relationship between knowledge stock at the end of period 2 and absorptivity; which is similar to Figure 6.

The optimal R&D investment (and knowledge stock) for the NE and CO model become equal when equations (8) and (11) are identical or equivalently \( \lambda = \lambda^* \). \( \lambda^* \) is calculated as follows

\[
\frac{N + 1}{1 - \frac{\lambda^*(N-1)}{N+1}} = \frac{2N}{1 + \lambda^*(N-1)} \quad \text{or} \quad \lambda^* = \frac{N + 1}{(N + 1)^2 + 2N} \quad \text{for} \quad N \geq 2
\]

It follows that firms invest in greater R&D in the NE model as compared to the CO model when \( \lambda < \lambda^* \) and invest in greater R&D in the CO model as compared to the NE model when \( \lambda > \lambda^* \). We leave the analytical proof of this claim for future work.

In the NE model, as \( N \to \infty \), \( q_{1}^{NE} \to 0 \), \( q_{2}^{NE} \to 0 \), \( \pi_{1}^{NE} \to 0 \). Further, \( RD_{1}^{NE} \) will become 0 and the knowledge stock stable (i.e., \( H_{2}^{NE} = H_{1}^{NE} = 1 \)) for a finitely large N (before \( N \to \infty \)) which can be calculated by replacing \( H_{2}^{NE} = 1 \) in equation (8). In the CO model, as \( N \to \infty \), \( q_{1}^{CO} \to 0 \), \( q_{2}^{CO} \to 0 \), \( \pi_{1}^{CO} \to 0 \). Although, \( RD_{1}^{CO} \to 0 \) also, each firm will invest in R&D and the knowledge stock will increase (i.e., \( H_{2}^{CO} \geq H_{1}^{CO} = 1 \)) for \( 0 < \lambda \leq 1 \). The \( H_{2}^{CO} \) can be calculated by taking the limit \( N \to \infty \) in equation (11) for \( 0 < \lambda \leq 1 \). This gives

\[
\frac{2b(1 - \nu)e^{\beta}}{\lambda a H} (H_{2}^{CO})^{2 \alpha H + 1} - D_2 a (H_{2}^{CO})^{\alpha H} + (D_2)^2 = 0
\]

(v) The above conclusions are important from a government policy perspective. To spur R&D investment (and hence increase knowledge stock) in the industry the government may attempt to: (a) Provide R&D subsidies to firms, which clearly

\[\text{consistent with the work of (Cohen & Levinthal, 1989), who have done a similar analysis for a single period model.}\]

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\[\text{consistent with the work of (Cohen & Levinthal, 1989), who have done a similar analysis for a single period model.}\]
increases the R&D investment of firms as shown in Figures 2, 4, 6. (b) Attempt to appropriately influence firm interactions (i.e., either prevent or promote collusion based on the absorptivities of firms and other relevant factors). (c) Although not shown numerically, controlling direct extra-industry spillovers ($T_t$) would have an impact on the optimal R&D investment of firms; an increase in $T_t$ would decrease optimal R&D investment for that period. Among other things $T_t$ represents research done by universities and research organizations which depend on government funding. If we had the required data, this analysis could be extended to determine whether the government would be better off increasing $T_t$ or providing R&D subsidies, to increase the total knowledge pool for the PV industry.

(vi) The T-period model offers similar insights as the 2-period model. Firms invest in their maximum R&D in the first few periods; this decreases subsequently as the knowledge stock increases. The increase in knowledge stock implies that the unit cost of production ($U_C P_t^t = D_t (B)^{-1} (H_t^2)^{-\alpha_H}$) decreases with time, which is represented in a so-called ‘cost curve’. The nature of the cost curve, will depend on whether firms are operating at their nash equilibrium or collusive optimal as well as their absorptivity. Figure 13 shows the ‘cost curve’ for firms operating at their collusive optimal for different absorptivities.

It follows (Figure 13) that if the firms operate at their collusive optimal the cost of production decreases the most if the absorptivity of firms is 1. In contrast, an extension of the 2-period model to T periods would show that if firms are operating at their nash equilibrium then the cost of production decreases the most if the absorptivity of the firms is 0. The intuition behind this follows from Figure 7 (which can be conceptually extended to T periods). Figure 7 shows that in the NE model $H_t^{2NE}$ decreases (and hence production cost increases) with an increase in absorptivity, while in the CO model $H_t^{2CO}$ increases (and hence production cost decreases) with an increase in absorptivity. We leave the analytical proof of these claims for future work and give an intuitive explanation below.

For high absorptivity (say $\lambda = 1$) $H_t^{2NE} < H_t^{2CO}$. This is because, in the NE model, at such a high absorptivity the free-riding effect is significant among firms. Thus, all firms tend to invest much less in their own R&D by free-riding on their rivals R&D, and consequently have a smaller $H_t^{2NE}$. In contrast, the CO model has no free-riding effect. It has a set of firms behaving completely collusively like a monopoly (or under partial collusion if $\lambda < 1$) while choosing their optimal R&D investment; with the objective of maximizing industry profits. Hence, these firms tend to invest much more in their own R&D than the NE model firms, and consequently have a higher $H_t^{2CO}$. For $\lambda = 0$, $H_t^{2NE} > H_t^{2CO}$. First note that, for $\lambda = 0$,
there is no free-riding effect in both the NE and CO models (the CO model never has free-riding effect anyway). Hence, in both situations, firms are not dependent on each other for R&D investment. However, in the CO model, firms are choosing (as always) their collusive output, which is a monopoly output for the entire industry. By the very nature of a monopoly, the prices are higher and the quantity produced lower (see equations (7), (10) for comparison). Since, in the CO model, firms produce less than the NE model, their cost of production is lesser. Further, since the purpose of R&D is to reduce the cost of production, the CO model firms require a lesser R&D; consequently the CO model firms invest in lesser R&D than the NE model firms and hence $H_2^{CO} < H_2^{NE}$ for $\lambda = 0$. As $\lambda$ increases, the increase in the collusive nature of choosing R&D for CO model firms tends to increase $H_2^{CO}$ (which captures the effect of $RD_1^*$ as well as $\lambda RD_1^{-i*}$). Further, as $\lambda$ increases, the increase in the free-riding nature of choosing R&D for NE model firms tends to decrease $H_2^{NE}$. This gives the intuitive explanations for Figure 6, Figure 7 and hence Figure 13.

4 Further Work

We believe that this work can be extended to provide real insights to the PV Industry. Following are suggestions which can be potential extensions:

(1) Determine the exogenous parameters econometrically.

(2) Instead of just having one set of identical firms, we can divide the firms into two groups. All firms in one group will have identical characteristics, however each group will be different from the other. We may use a statistical technique such as cluster analysis to categorize the firms into groups. Possible classifications could be based on: firms that were established in the 1970s as compared to the ones started in the late 1990s, or firms which use 1st generation technologies as compared to those which use 2nd generation technologies (Appendix A.1 and A.3), or some other distinctive features. This approach would be a data intensive task. Once divided into two groups we could then easily work out the NE and CO interaction among the groups. This is equivalent to working with two asymmetric firms.

(3) Perform sensitivity analysis for all the assumed exogenous parameters. Even if we estimate these parameters econometrically, sensitivity analysis would still be useful, as it would provide insights as to how a change in these parameters would affect knowledge stock.
(4) Attempting to get a closed form solution for the infinite horizon problem (discussed in section 3) and analytic proofs for the claims made in the conclusions.

(5) Extending this model to the stochastic case for T periods and then infinite periods.

5 References

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Appendix G: A Stochastic Programming Framework for the Valuation of Electricity Storage

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1 Introduction

Electricity, which is generated, purchased and distributed in its own unique market, currently plays a far more significant role in the fundamental aspects of daily life than ever before. As industrialized and developing countries alike thirst for more and more power, there will be a strong need for innovation in energy efficiency and generation and transmission asset utilization to keep up with the ever increasing energy demands. The U.S. alone will require an additional 80GW of new generation capacity by 2015. This anticipated increase in the generation capacity must be addressed by taking into account increasing fuel costs, tighter environmental restrictions, and an aging transmission and distribution system, which already causes losses of some $100 billion annually due to reliability issues.

The electricity market is often regarded as one of the few industrial sectors that is far behind its expected level of technical modernism when considering its influence on economic prosperity, environmental sustainability and human development. According to the Electric Power Research Institute (EPRI) electricity technology roadmap, modernizing the electricity infrastructure could increase economic productivity by 0.7% per year over business-as-usual conditions. In the United States alone, this translates into about $3 trillion per year in additional GDP by 2025 [1].

The future of the power industry’s generation portfolio will inevitably include a strong mix of renewable technologies. The recent trends in new renewable generation facilities have shown positive growth, especially in the wind sector, where over the past six years alone, installed capacity within the U.S. has grown by over 300%. One of the significant drawbacks of wind technology is the intermittency of the generation due to the variability of wind. This variability leads to increased procurement costs for various reliability services, increased transmission congestion costs, and additional strain on the remaining generation units that must be called upon in the generation voids created by wind [3]. This problem may be minor for a penetration of 5% of wind, but will be more drastic as penetration approaches 20% [2].

Energy storage may help mitigate all of the listed problems, and in many cases may be a complete solution. This helps motivate the fact that currently 2.5% of the total electric power delivered within the U.S. is cycled
through a storage facility. Although this number may appear significant at first, it pales in comparison to the 10% and 15% of total power cycled through storage facilities in Europe and Japan respectively [4]. Drivers for the energy storage market range from the increasing energy demand to the need for improved energy security and reliability [5].

Irrespective of the market structure, pricing within power markets is a very complex process marred by price spikes, jumps, high volatility, and seasonal effects, having the combined effect of making the market incomplete from a financial standpoint. Prices determined in electricity spot markets are extremely volatile and are highly dependent on time of day and seasonal effects. The daily fluctuations provide a clear potential for arbitrage profits by purchasing electricity during off peak hours (typically at night) when the price is low, storing that power, and then selling the stored power during peak hours at a significantly higher price.

It is claimed, however, that the inexistence of electricity as a tangible, storable asset, and the inadequate relationship between markets eradicates almost all arbitrage arguments. This is a conclusion that we will specifically address within this paper.

This paper focuses on the valuation of energy storage technologies through arbitrage profits within large scale power markets. Although there are countless storage applications in fields such as distributed generation and on-site reliability, they will not be considered in this analysis. However, several results may easily be extended to these areas. We begin with a brief overview of storage technologies and their applications, and present a mathematical model for such facilities. From there, we incorporate the storage model into a series of mathematical programs that seek to optimize the operation policy of a given storage plant by maximizing intraday arbitrage profits. We conclude with a summary of the findings and the arbitrage valuation results from the analysis.

2 Overview of Energy Storage Systems

Energy storage technologies enable an offset in time between power generation and power consumption. This ability to store energy has a profound impact on not only the physical characteristics of the power grid,
but also on the financial and investment strategies of power market participants. Energy can be stored in potential, pneumatic, kinetic, electrochemical, electromagnetic, electrical, chemical or thermal form. The appropriate technology is very much dependent on the application due to the range in characteristics of the different technologies. For high-quality (non-thermal), large-scale energy storage, the most prevalent energy storage technologies are pumped hydro, compressed air energy storage, flywheels and batteries.

In this section, we briefly introduce the various applications of electricity storage within power markets, and outline several value opportunities for such systems. We begin with a figure from the Electricity Storage Association summarizing the various storage technologies and their applications.

Figure 1: Summary chart of electricity storage technologies

2.1 Applications of Energy Storage Systems

2.1.1 Load Leveling

The term “load leveling” refers to the balancing of nighttime troughs and afternoon peaks for a more level generation curve, making use of unused off-peak capacity while decreasing the need for peaking capacity. Thus a reduction in high-cost peak generation is met with an increase in the level of low-cost baseload
generation, as depicted in Figure 2. In addition to the apparent economic advantage, load leveling also
increases generation flexibility, allowing for the use of technologies with greater fuel efficiency and lower
emissions.

![Figure 2: Demand profile with electricity storage](image)

**2.1.2 Arbitrage**

As the load profile fluctuates throughout the day, so too does the spot price of electricity, consistent with
economic principles for a constrained or limited resource. Arbitrage capitalizes on this economic opportunity
through the purchase of inexpensive off-peak power that is sold during peak hours for a net profit. Alter-
atively, a company who consumes peak power could use a storage system to purchase inexpensive off-peak
power for their own use during peaking hours, thereby reducing their electricity costs.

**2.1.3 Spinning Reserve**

Spinning reserve is the primary subcategory of reserve power and generally refers to partially loaded plants
that can ramp up (or down) to provide additional (or remove excess) generation capacity in order to meet
sudden and unpredictable demands or contingencies. Spinning reserve plants have extremely low utilization
and quick startup times, which are also characteristics of most types of energy storage systems, thus making
energy storage systems a natural candidate for such ancillary services.
2.1.4 System Regulation

System regulation refers to the constant balancing of load fluctuations on the grid to account for power reliability, power quality and transmission and distribution problems. Power reliability refers to the frequency of extended power failures, during which the end-user is completely disconnected from utility power generation for more than about two minutes. Power quality refers to either a very short outage (zero voltage for less than two minutes) or to a non-zero voltage interruption, including voltage inconsistencies and harmonics. Energy storage can increase both power quality and reliability through its use as an uninterruptible power supply (UPS) system in case of power failure, whether caused in generation or transmission, and also through its use as an onsite power generator in remote or isolated distributed generation systems.

In areas where demand has increased beyond the capability of the T&D system, energy storage can store electricity during periods of inadequate transmission capacity to alleviate transmission and distribution overloads down-line of the congested area. Used in this manner, energy storage can defer necessary T&D upgrades for several years.

2.1.5 Storage with Intermittent Renewable Generation

Renewable generation technologies, such as solar and wind, are intermittent in nature and in general provide a stochastic generation curve dictated by the environmental conditions. A storage facility can be used to match generation with demand, and smooth the generation profile accordingly. With regard to utility load leveling, discussed above, energy storage allows constant generation to meet a variable demand; conversely in this application, energy storage provides the capability for an intermittent (variable) power generator to serve a constant demand, or for a variable generator to meet a different variable demand. Combined with energy storage, renewable generation systems are more flexible and self-sustaining, allowing them to serve remote users and/or break-away sections of the grid.

Energy storage can also aid in transmission and distribution for renewable generation. Many renewable systems are located in rural areas where the electric grid is weak and unable to handle large amounts of
Energy. Energy storage can transform the intermittent large bursts of energy to a smaller, constant amount of energy that the grid can handle. This is one specific example of the potential transmission and distribution applications discussed in the previous subsection on system regulation.

2.2 Value Opportunities for Energy Storage Systems

Through its various applications, energy storage can be beneficial for all of the stakeholders within the power market structure. In this section of the paper, we examine only a few of these potential benefits. The obvious value opportunity for storage systems from a financial viewpoint is through arbitrage profits from time-differentiated pricing of electricity across peak and off-peak hours. We will briefly discuss the economic value of storage from three other perspectives: the value of storage as a peak generation technology, the value of storage as an ancillary service, and finally the value of storage in terms of the environmental benefits it provides.

2.2.1 Peak Generation

Aside from the time-differentiated profit opportunities, there are several additional benefits of storing power and regenerating it during peak hours when the system is deficient. The most significant impact is through the reduction in the need for peak generation from high marginal cost plants having large fuel costs, such as natural gas facilities, which result in higher average electricity rates for the end user. Fuel cost reductions occur as a result of load leveling, namely using storage during off peak hours to offset a portion of the generation requirements during peak hours.

2.2.2 Ancillary Markets and Reliability Services

Although it is difficult to evaluate the impact of storage services on reliability without taking into account concepts like value of lost load (VOLL), it is clear that any contribution towards system reliability, however marginal, will have a significant impact on social surplus. EPRI has estimated that the annual lost produc-
tivity due to short duration power quality events and service disruptions is at least $53 billion per year, and the total losses from all adverse quality events accounts for $119 billion per year [5]. Thus an increase in grid reliability, even by only a few percentage points at times when the system is already constrained, can result in a national social benefit on the order of billions of dollars.

The primary approach to establishing the monetary value of the reliability services that are offered by storage facilities, as summarized in the previous section, is through their market value in the ancillary markets. Generalizations from these valuations for the assessment of storage systems within this context may provide no clear insights into their true value. Storage systems are in general deemed to be highly dependent on location, and the valuation of particular ancillary services will depend on the local market structure and both the need for and value placed on such reliability services.

2.2.3 Environmental Impacts

With increasing concerns regarding global climate change and $CO_2$ emissions, the movement toward clean technologies is gathering momentum. Unfortunately, many of these technologies, like nuclear, integrated gasification combined cycle (IGCC), and large hydro cannot easily be ramped to meet a variable load, limiting such technologies to baseload generation. Energy storage will become essential in enabling these non-emitting baseload generators to meet peak demand as well, thus significantly reducing $CO_2$ emissions in regions where baseload generation is primarily a low emission technology.

Similar to the valuation of the reliability services that a storage system can provide, the environmental gains may be assessed from the current market prices of various emissions permits. With the belief that the permits reflect the fair value of emissions as determined by the market and governed by extensive field research, the use of pre-existing market instruments is deemed to be a sufficient valuation measure for the environmental impacts of storage systems.
3 Modeling Electricity Storage

We will now motivate the valuation of a storage facility strictly through arbitrage arguments and discuss the optimal arbitrage policies under uncertainty. In the valuation framework, we seek an optimal operation policy in a power market once a storage plant has been constructed. We begin by presenting a mathematical abstraction of the storage system, and the parameters that govern an energy storage model, including all costs.

3.1 Electricity Storage Model

All energy storage systems can be modeled in the same fashion regardless of the form in which the system stores energy. A schematic generalizing the structure of this storage system model is presented in Figure 3, illustrating the basic components of power input, the storage medium, and power output.

![Figure 3: A generalized schematic of a storage system](image)

Energy storage technologies are characterized by four distinguishing physical attributes:

- **Power Rating** [MW]: the maximum power output. The maximum power input is assumed to be equal to the maximum power output unless otherwise stated; if different, the maximum power input is the **Conversion Rate**.

- **Energy Capacity** [Joules or MWh]: the amount of energy that can be stored within the system. The amount of time a storage system can output at a given power is the **Discharge Time** and is directly

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1 The issues surrounding optimal sizing of plants and plant location are beyond the scope of this paper.
proportional to the energy capacity for a constant power output.

- **Efficiency**: the ratio of energy discharged by the system to energy input into the system, and can be split into: **Conversion Efficiency** refers to losses experienced when converting the power input into a storage medium. **Storage Efficiency** refers to time-based losses during storage.

- **Reaction Time**: the time necessary for a system to “turn on” and begin charging or discharging or to switch between charging/discharging modes.

Using these physical characteristics, we can define the following set of variables:

**Storage Constraints**

- \( t \) period of time under consideration (hours)
- \( q^D_t \) maximum quantity that can be sold (Discharged) in a single period (MWh)
- \( q^R_t \) maximum quantity that can be bought (Recharged) in a single period (MWh)
- \( S^t \) maximum storage capacity as determined by the system’s energy capacity (MWh)
- \( \gamma_S \) storage efficiency (fraction of stored electricity maintained over one period)
- \( \gamma_C \) conversion efficiency (fraction of purchased electricity that gets stored)

### 3.2 Dynamic Model for Operations

We now assume that an energy storage facility exists and that the objective of the firm owning this facility is to maximize profits simply by exploiting arbitrage opportunities in the real-time electricity spot market. The decision of the plant operator in each period is simply to choose a quantity of energy that it will either purchase and put into storage, or discharge to the grid:

**Decision Variables**

- \( q^D_t \) quantity of electricity sold (Discharged) at time \( t \) (MWh)
- \( q^R_t \) quantity of electricity purchased (Recharged) at time \( t \) (MWh)
- \( S_t \) amount of electricity in storage at time \( t \) (MWh)

The basic operation of the plant may now be described by the storage dynamics:
Storage Dynamics

\[ S_t \leq \gamma_S \cdot S_{t-1} + \gamma_C \cdot q_t^R - q_t^D \quad \forall \ t \]

Prior to establishing any financial models, several additional exogenous parameters must be defined:

**Additional Parameters**

- \( p_t \): price of electricity at time \( t \)
- \( r \): interest rate
- \( T \): number of time periods

The time parameter, \( t \), in this model appears subtle, yet significant complexity arises with the discretization of time into distinct time periods, and decision periods (or stages). Each time period may be on the order of minutes, hours, days or weeks, with the total number of periods summing to an hour, a day, a week or month, respectively. In general, electricity market prices are provided with an hourly increment, and due to the periodic nature of prices, a daily or weekly total decision horizon is typically sufficient. The estimation challenges will be further discussed when we examine price processes in the next major section.

With the time period specified, the next issue to be addressed is the length and frequency of decision stages. The time period represents the discretization of the samples of the prices, however each decision stage may be a duration of time that involves several time periods. With hourly prices, the decision stage may be hourly, whereby the operator makes a storage decision for each hour in a day, or it may be several hours, where a day is broken into say 3 or 4 stages of 8 or 6 hours each respectively. The decision would be to specify a storage policy over the duration of each stage.

The market structure typically restricts the decision stage; for example, in a fixed day ahead market, the storage facility would need to forecast its operation policy for the entire 24 hour period of the following day without any realizations of actual prices to update the policy. This issue will be further addressed when we discuss the optimal policies in a stochastic setting.
3.3 Arbitrage Model for Profits

We are interested in determining precisely how much profit can be earned by following an arbitrage strategy. The firm must choose how much power to buy or sell over time at the prevailing prices, subject to a variety of costs and constraints that are related to the physical aspects of the storage facility:

**Storage Costs**

- $C_D(q^D_t)$: cost of discharging $q^D_t$ units
- $C_R(q^R_t)$: cost of recharging $q^R_t$ units
- $C_S(S_t)$: cost of storing $S_t$ units for one period

Such costs arise when we consider the physical nature of the charging and generation costs, or costs associated with maintaining the energy within the storage facility. A simple example of this is the fuel generation costs of a CAES facility, where the plant must use a natural gas turbine to convert the compressed air back into electricity. Given these variables and parameters, we can now establish the storage plant’s profit maximizing objective function:

$$
\sum_{t=1}^{T} \left[ p_t(q^D_t - q^R_t) - C_D(q^D_t) - C_R(q^R_t) - C_S(S_t) \right] \cdot e^{-rt}
$$

This objective as stated is nonlinear, since the cost functions have not been described and are unrestricted. The problem is easily made linear if the cost functions are restricted to being linear with zero intercept. The resultant linear program is:

- **maximize**
  $$
  \sum_{t=1}^{T} \left[ (p_t - C_D) \cdot q^D_t - (p_t + C_R) \cdot q^R_t - C_S \cdot S_t \right] \cdot e^{-rt}
  $$

- **subject to**
  $$
  0 \leq q^D_t \leq \bar{q}^D, \quad \forall \ t
  $$

  $$
  0 \leq q^R_t \leq \bar{q}^R, \quad \forall \ t
  $$

  $$
  0 \leq S_t \leq \bar{S}, \quad \forall \ t
  $$

  $$
  S_t \leq \gamma_S \cdot S_{t-1} + \gamma_C \cdot q^R_t - q^D_t, \quad \forall \ t
  $$

Here $C_D$, $C_R$ and $C_S$ represent the slopes of the respective cost functions. Since most available cost data is presented as a variable cost, this linear cost assumption is reasonable.
One of the main drawbacks of the linear programming model is that it assumes that all future prices are known with certainty, which is clearly unrealistic considering the volatility of electricity spot prices. In fact, it would be a significant mistake to use the LP model as a means of estimating the expected profits of a storage facility by looking back on realized prices since what is optimal in hindsight is not the same as what is optimal looking forward.

The LP model does, however, provide the absolute highest achievable profit which may then be used as a benchmark for other models, and may be used as a means of assessing the value of information for the uncertainties. To deal with the uncertainty in prices, we will introduce stochastic programming and dynamic programming models.

4 Stochastic Profit Models

The linear programming model (LP) has been introduced as a means of finding the optimal solution to a deterministic storage problem. For any particular price path, this solution is an upper bound of achievable profits given perfect information. Under particular market structures it may be possible to come close to achieving this upper bound in day ahead markets using LP’s on very accurate forecasts. However, in general, the real time price for the spot rate of electricity exhibits significant volatility and is therefore difficult, if not impossible, to predict accurately.

This motivates the use of probabilistic models for the derivation of arbitrage value, in particular the use of dynamic programming and stochastic programming. The LP approach can also be used in a stochastic setting by setting the prices equal to the expected values of the price realizations over time. This approach to the storage problem with uncertainty can be used to quickly find a lower bound on profits, but otherwise it is unsophisticated and performs poorly relative to the alternative techniques that we will now discuss.
4.1 The Dynamic Programming Model

In general, a dynamic programming (DP) approach to a problem discretizes the problem’s state space and uses a backwards recursion to derive the optimal value and optimal policy at every state. The state variable describing the problem at a particular stage is defined in such a way that it completely describes the process. Given the state of the process at the beginning of a stage, we make a decision which transforms the process to the ending state at the end of the stage. The objective is to maximize (or minimize) the expected objective over all stages.

Dynamic programming algorithms are often limited in their application due to the “curse of dimensionality”, which describes the rapid expansion in model size with the number of states. To maintain a tractable formulation, the dimension of the state space must stay small (typically no more than 3 or 4 dimensions) and the discretization of each dimension must be relatively coarse. This rules out the use of processes that track past histories (e.g. ARMA processes) and limits the ability of a DP to properly address continuous state and action spaces without great computational expense. For this reason, we restrict ourselves to a Markovian price process for the DP model.

Nevertheless, the solution to a DP is quite useful in that it provides an optimal contingency plan for every realizable state of a system, requiring only one pass through the DP to obtain the optimal policy for all possible realizations of the random process. The DP approach also allows for the consideration of many decision stages, since the problem size grows linearly in the number of stages. This makes dynamic programs particularly useful for solving problems in which many decisions must be made.

The storage problem involves determining the optimal profit maximizing policy depending on both the current storage level and the realized price throughout the hours of the day. Thus we are dealing with a 24-stage, 2-dimensional model with a state space that spans all possible storage levels and all possible spot prices. The action space is simply the amount of electricity to be charged or recharged and is subject to the standard capacity constraints. At each stage, every action generates an immediate profit or loss and determines the storage level that will be obtained in the subsequent stage. The expected profit of each action
is therefore the sum of the immediate profit or loss and the expected value of the next state, which we can compute since we have already established the expected values for all future states. The optimal choice at each stage is clearly the action that yields the highest expected profit.

We will now apply this dynamic programming routine to the linear programming model. We begin by defining the parameters of the general Markov decision process (MDP) with specifications particular to the storage problem given in parentheses:

**MDP Parameters**

- **$T$** number of stages (each stage $t = 1, \ldots, T$ is assumed to be one hour)
- **$P$** discrete space of realizable electricity prices ($p_t \in P \subseteq [10, 200]$)
- **$S$** discrete space of storage levels ($s_t \in S \subseteq [0, \bar{S}]$)
- **$\Omega$** finite state space ($\omega_t \in \Omega = P \times S$)
- **$X$** finite action space ($x_t \in X \subseteq [\bar{q}^D, \bar{q}^R]$)

where $x_t$ is the quantity charged or discharged from storage in stage $t$.

**$Pr(\omega'_{t+1}|\omega_t, x_t)$** conditional probabilities of state transitions

**$\Pi(\omega_t, x_t)$** profit function for all $\omega_t \in \Omega, x_t \in X$

Within the DP, the profit function is defined as:

$$\Pi(\omega_t, x_t) = [p_t \cdot (q^D_t - q^R_t) - C_D \cdot q^D_t - C_R \cdot q^R_t - C_S \cdot s_t] \cdot e^{-rt} \quad \forall \omega_t \in \Omega, x_t \in X$$

where $q^D_t = -[x_t]^- \quad \text{and} \quad q^R_t = [x_t]^+$.  

The conditional transition probability distributions reflect the uncertainty in the MDP, and since the only uncertainty here is the price, we can represent these distributions as:

$$Pr(\omega'_{t+1}|\omega_t, x_t) = Pr((p'_{t+1}, s'_{t+1})|(p_t, s_t), x_t) = Pr(p'_{t+1}|p_t) \cdot I_{s'_{t+1} = s_t - x_t}$$

where $I$ is a standard indicator function. That is, the only states we can transition to with positive probability are those with storage levels equal to the current storage level minus (plus) the amount currently discharged (recharged). The positive probabilities are given by the Markov price process and are dependent on both the current price and the current time.
The Bellman equation for the defined MDP becomes:

\[ V_t(\omega_t) = \max_{x_t \in X} \left[ \Pi(\omega_t, x_t) + \sum_{\omega_{t+1} \in \Omega} P_r(\omega_{t+1} | \omega_t, x_t) V_{t+1}(\omega'_{t+1}) \right] \]

When we use the same deterministic prices, we get the same storage policy and optimal profit as before, which is of course expected. However, this model allows the additional flexibility of considering uncertain prices through the use of the transition probabilities function, making the second term in the Bellman equation nothing more than the conditional expectation of the value in the next stage given the current state.

The drawbacks of this approach include the necessary discretizations of the price, storage and action spaces, and the fact that only basic (essentially Markov) price processes can be modeled. The discretizations are particularly problematic when storage and conversion inefficiencies are present in the model. When these parameters are present, it is frequently necessary to round to the nearest state. This encourages the algorithm to optimize over this rounding process, which is clearly undesirable. As evidence of the scope of this problem, situations have been observed in which the profits from the dynamic program exceed those of the linear program over the same price path, which is clearly erroneous since the LP provides an upper bound on profits.

4.2 The Stochastic Programming Model

The stochastic programming (SP) approach is quite different from the dynamic programming approach and can be used to solve an entirely different class of problems. Whereas the DP is useful for solving problems with multiple decision stages and limited state spaces, the SP performs best on problems with just a few decision stages (e.g. three or four), but can handle very large state spaces.

We implement several versions of a stochastic programming approach to solving the storage problem. One of the main advantages of the SP is that its ability to handle large spaces allows it to deal with random processes that keep track of historical values. Thus we can use an ARMA or a non-Markovian stochastic process to model prices. Both a three-stage model and four-stage model have been implemented. The three-stage model has the following formulation:
Three-stage SP Formulation:

\[
\max_{\bar{q}_t^D, \bar{q}_t^R, S_t} \quad \frac{1}{N} \sum_{i=1}^{N} \sum_{t=1}^{8} \left[ (\tilde{p}_i^t - C_D) \cdot q_t^D - (\tilde{p}_i^t + C_R) \cdot q_t^R - C_S \cdot S_t \right] \\
+ \frac{1}{MN} \sum_{i=1}^{N} \sum_{j=1}^{M} \sum_{t=1}^{16} \left[ (\tilde{p}_{ij}^t - C_D) \cdot q_t^{D^{ij}} - (\tilde{p}_{ij}^t + C_R) \cdot q_t^{R^{ij}} - C_S \cdot S_t^{ij} \right] \\
+ \frac{1}{LMN} \sum_{i=1}^{N} \sum_{j=1}^{M} \sum_{k=1}^{L} \sum_{t=1}^{24} \left[ (\tilde{p}_{ijk}^t - C_D) \cdot q_t^{D^{ijk}} - (\tilde{p}_{ijk}^t + C_R) \cdot q_t^{R^{ijk}} - C_S \cdot S_t^{ijk} \right]
\]

subject to

\[
0 \leq q_t^D \leq \bar{q}_t^D \quad \forall \ t \\
0 \leq q_t^R \leq \bar{q}_t^R \quad \forall \ t \\
0 \leq S_t \leq \bar{S} \quad \forall \ t \\
S_t \leq \gamma_S \cdot S_{t-1} + \gamma_C \cdot q_t^R - q_t^D \quad \forall \ t \\
0 \leq q_t^{D^{ij}} \leq \bar{q}_t^D \quad \forall \ t, i \\
0 \leq q_t^{R^{ij}} \leq \bar{q}_t^R \quad \forall \ t, i \\
0 \leq S_t^{ij} \leq \bar{S} \quad \forall \ t, i, j \\
S_t^{ij} \leq \gamma_S \cdot S_{t-1}^{ij} + \gamma_C \cdot q_t^{R^{ij}} - q_t^{D^{ij}} \quad \forall \ t, i, j
\]

The models return a single optimal policy for the first eight or six hours respectively, and the optimal policies for the next stages are dependent on the simulated price paths. In order to implement these models in practice on actual observed price paths, we use the observed prices in previous stages and solve the reduced problem going forward. For example, in the three-stage problem, the optimal policy that is returned for the first eight hours is carried out. Then the actual prices observed during the first eight hours are used to generate correlated price paths for the two-stage problem going forward. Solving the two-stage problem gives the optimal policy for the hours 9 through 16, and then the prices observed over that period are used to simulate prices for the final one-stage problem.
For most actual implementations of these models, parameters \( L = M = N = 50 \) and \( K = L = M = N = 20 \) were used, respectively. With these values, the problems could be solved in about thirty seconds on a standard laptop. Figure 4 shows the tree structure of sample price paths that are generated, where for clarity we show an example with \( L = M = N = 3 \). The price process used in the simulations is the topic of the upcoming section.

![Realizations of Stochastic Price Paths](image)

Figure 4: A sample set of random price scenarios for a 3 stage model

5 Treatment of Electricity Prices

In this section we explore the characteristics of electricity prices, and the corresponding price models which may be used to capture these unique features. Several of the distinguishing features of electricity price processes include high volatility, large spikes, mean reversion to a daily pattern and seasonality.

There are a variety of reasons for the high volatilities, but the fundamental drivers include fuel prices, hydrological conditions, seasonal effects, weather dependence, new generators and transmission upgrades. The biggest drivers are the inelasticity of demand and the “hockey stick” nature of the supply curve. This fundamental nature of the supply versus demand creates an environment that is prone to large electricity price spikes.

Another reoccurring theme among most electricity price models is mean reversion. Typically, the electricity market exhibits extremely high mean reverting tendencies, where spikes generally last for only brief periods.
An important caveat regarding this reversion property is that the mean value for electricity prices varies on an hourly basis in a quasi-predictable manner that is correlated with the demand. Hence a model that uses a constant mean value across all hours of a day will overestimate the actual volatility of prices, and will lose the trends that are necessary for temporal arbitrage.

Similar to the predictable pattern of price movements throughout a day, electricity prices fluctuate on a seasonal basis as well according to the local demand profile. This seasonality must be taken into account when modeling the price process in order to achieve proper estimates of the mean and the variance of the hourly prices for each month. Failure to account for the seasonality will affect the true mean of the hourly prices and will introduce an overestimation of the variance of the prices.

5.1 Mathematical Models of Electricity Prices

In light of the characteristics of electricity described thus far, we will introduce several methods for representing the electricity price process. We begin with a very simple process using empirical values, and move from there to more complex financial engineering methodologies.

5.1.1 Correlated Random Variables with Gaussian Noise

We begin by describing a very simple Gaussian noise price process. Due to the predictable patterns that electricity prices exhibit throughout a day, the mean varies on an hourly basis, and so our mean value, $\mu_t$, exhibits a time dependency. In its most trivial form such a process may be simulated by:

$$\vec{P} = E(\vec{P}) + \sigma \cdot \vec{\epsilon}$$

where $\vec{P}$ is a 24x1 vector of hourly prices, $E(\vec{P})$ is the vector of the hourly mean prices, $\sigma$ is a diagonal matrix of discrete hourly volatility, and $\vec{\epsilon}$ is a 24x1 vector of realizations of a standard normal random variable.

In order to alleviate the independence assumption of hourly prices, the cross correlations of hourly prices must be incorporated into the volatility term, $\sigma$. Using a Cholesky decomposition, the positive definite
covariance matrix of the original hourly prices is decomposed into $C = LL'$, where $L$ is a lower triangular matrix with positive diagonal elements. Thus the price process may now be simulated using:

$$\bar{P} = E(\bar{P}) + L \cdot \bar{\epsilon}$$

It can be shown that simulation of the price process using this approach preserves all of the statistical properties of the original distribution of prices.

5.1.2 Advanced Financial Engineering Techniques using Brownian Motion

The empirical framework may be generalized to a stochastic process that describes the price as a Brownian motion process. Although this methodology has its shortcomings for the modeling of electricity price dynamics as described above, it is a good general starting point to build from. With this assumption in mind, the general framework for the modeling of electricity spot rates will be consistent with models found in interest rate derivatives.

We begin the modeling framework with the simple case of single factor equilibrium models. In the world of financial assets, we refer to the standard geometric Brownian motion (GBM) model of short rates, otherwise known as the Rendleman and Bartter model of the risk neutral process for the short rate. In this case the spot price $P$ follows:

$$dP = \mu P dt + \sigma P dz$$

where $dP$ is the change in price over the time interval $dt$, $\mu$ is the expected drift of the price over this interval, $\sigma$ is the volatility of the price, and $dz$ is a standard Brownian motion. The discrete time representation of this model is:

$$\Delta P = \mu P \Delta t + \sigma P \epsilon \sqrt{\Delta t}$$

where $\epsilon$ is a standard normal random variable.

Commodity price structures often exhibit strong mean reversion, as is the case with electricity prices. We refer back to the geometric Brownian motion model and modify it by introducing mean reversion, to arrive
at the classic Vasicek model:

\[ dP = a(\mu - P)dt + \sigma dz \]

where \( a \) is the mean reversion coefficient. A more generalized mean reversion model using time dependent mean values, \( \mu(t) \), has been introduced by Hull and White:

\[ dP = a \left( \frac{\mu(t)}{a} - P \right) dt + \sigma dz \]

The models introduced thus far do not account for the spikes that are evident in electricity prices. For this, we may refer to the jump diffusion framework first presented by Merton, and later extended to the electricity price process framework by Deng [10]:

\[ \frac{dP}{P} = a(\mu - \ln P)dt + \sigma(t)dz + \kappa Pdq \]

The downfall to this model is the difficulty in characterizing the required parameters. In effect, we have four static parameters to calculate, in addition to two parameters, namely the volatility and the drift, which are functions of time and underlying price. If we further assume that the volatility is not a deterministic function, but that it is in fact stochastic in nature, then the complexity of the model in itself becomes far too difficult to manage, or parameterize in a meaningful manner. For this reason we will limit our model to the mean reverting model based on the Hull-White approach.

### 6 Profit Maximization Through Arbitrage Models

Our analysis of arbitrage has been focused, thus far, on the development of the necessary models for the stochastic price process, and the physical operation of storage facility, given that it is already available. We will now calibrate the generalized models and test the stochastic models under different price processes and compare the resulting profit with the best case control profits (perfect information).
6.1 Storage Model Calibration

The analysis will contrast two storage technologies, compressed air energy storage (CAES) and the Sodium Sulfur (NaS) battery. Of the available storage technologies, pumped hydro and CAES are the two most suitable for exploiting arbitrage opportunities; however, in the United States, there are very few suitable geographic locations remaining for pumped hydro, if any. On the other hand, the Electric Power Research Institute estimates that more than 85% of the U.S. has geological characteristics that will accommodate an underground CAES reservoir [4], making CAES the logical choice for assessment.

Smaller scale storage technologies will be limited to the NaS battery, since storage losses and capital costs of the other technologies render them virtually useless in such applications. We refer the reader back to Figure 1 contrasting the various storage technologies. We begin the analysis by introducing the physical constraints and parameters that are consistent with our two target storage facilities.

<table>
<thead>
<tr>
<th>Characteristic</th>
<th>NaS Battery</th>
<th>CAES</th>
</tr>
</thead>
<tbody>
<tr>
<td>Power recharge capacity</td>
<td>10 MW</td>
<td>300 MW</td>
</tr>
<tr>
<td>Power discharge capacity</td>
<td>10 MW</td>
<td>300 MW</td>
</tr>
<tr>
<td>Energy capacity</td>
<td>100 MWh</td>
<td>3000 MWh</td>
</tr>
<tr>
<td>Storage efficiency</td>
<td>0.97</td>
<td>1.00</td>
</tr>
<tr>
<td>Conversion efficiency</td>
<td>0.85</td>
<td>0.85</td>
</tr>
<tr>
<td>Discharge Cost</td>
<td>0</td>
<td>$3/MWh + $7/MBtu \times 4.1 \frac{MBtu}{MWh} = $31.7/MWh</td>
</tr>
<tr>
<td>Recharge Cost</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Storage Cost</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

6.2 Calibration of Price Processes

To develop policies from our calibrated models, two price processes will be introduced, and the optimization programs will be assessed for each of the developed price routines. The data used for the development of
the price processes is hourly marginal locational prices obtained from the New England ISO power market.

6.2.1 Correlated Brownian Motion

The first price process will be based on correlated Gaussian noise using the Cholesky decomposition of the covariance matrix of hourly price data as described in the previous section. This process will be the basis of the main SP model and the Gaussian noise process. In each stage, the random prices are generated using the knowledge of all previous prices; thus, all realizations of hourly prices have the desired mean, variance and correlation characteristics.

6.2.2 Mean-Reverting Markov Stochastic Process

In order to do away with the complete path dependence of the previous method, we generalize the model to a Markovian stochastic process which may easily be used in a DP framework. The chosen mean reverting process is described by a simple modification to the standard Hull-White model:

$$dP = a(\mu_t - P)dt + \sigma dz$$

Here, the drift terms, $\mu_t$, are time dependent parameters that vary according to the hour of the day. This enables the described Markov process to be free from serial correlations with the previous realizations of the hourly prices, while maintaining the familiar daily trends that are prevalent in electricity market prices.

This price process has been calibrated through a maximum likelihood estimation approach using the same NE-ISO price data. The details of the formulation of the MLE equations and their results will not be provided here, however it is important to note that a significant issue with this approach is the large number of parameters that must be estimated, 24 hourly mean values, the volatility, and the mean reversion coefficient.

A second version of the stochastic program has been implemented using this mean-reverting Markov process to model prices. This version is generally less accurate than the correlated Gaussian noise approach, since it sacrifices the ability to correlate current prices with historical prices. However, this approach has the
advantage that it can sensibly be compared with the dynamic program, since the DP uses this same Markov process.

6.3 Model Results of Arbitrage Profits

6.3.1 LP Optimal Storage Policies

In order to examine the effect of both the technological parameters as well as the hourly price path, we begin by examining the policies dictated by the linear program on a deterministic price path in Figure 5. The significance of this result lies in the contrast between the two policies given storage efficiency. recall that the CAES system is assumed to have loss-less storage over time, whereas the storage efficiency of the NaS battery is assumed to be 0.97 [4]. Consequently the battery cannot take full advantage of the low prices during off-peak periods since its time dependent losses will negate any profit opportunity by the time the prices increase.

![CAES - Price vs. Storage Policy](image_url)

![NaS - Price vs. Storage Policy](image_url)

Figure 5: Optimal storage policies for the CAES and NaS battery systems

We now examine the optimal deterministic LP storage policies under a set of three sample price paths denoted by path (a), (b) and (c). The paths, depicted in Figure 6, corresponds to three typical price scenarios:

- **Price Path (a)** - portrays a typical price path throughout a day with the expected low off-peak prices and a significant rise in prices during peak periods.

- **Price Path (b)** - portrays an unusual day in the electricity markets where prices remain relatively
low for the duration of the day.

- **Price Path (c)** - portrays the standard low off-peak prices and higher peak-prices; however there is no significant peak in prices. This two tiered price path is typical to the standard model of price paths used in most power market analyses, including the storage valuation study conducted by EPRI [4]. We will shortly demonstrate that this price path has a tendency of undervaluing the arbitrage profit opportunities.

![Sample Price Paths](image)

**Figure 6: The three different electricity price paths**

The second series of plots in Figure 7 provide the optimal deterministic LP policy for a CAES system for each of the three described paths. The resultant arbitrage profits under these scenarios for the CAES facility are $89,354, $1,726 and $22,985 for paths (a), (b) and (c) respectively. It is clear that if prices follow a typical path having low prices and a marked price peak (such as in path (a)), then the opportunities for profits are significant. Moreover, such a scenario may result in profits that are 4 times greater than a standard two tiered price approach.
Figure 7: Optimal deterministic LP storage policies for the CAES system under different price paths. From top to bottom: path (a), path (b) and path (c)

6.3.2 SP and DP Optimal Storage Policies

The same three price paths may be used to give us an interesting perspective on the operation of the optimal policy from the stochastic program. Figure 8 provides a comparison of the optimal policies from a 3 stage and a 4 stage stochastic program. Note that the policy is the same irrespective of the price path within the first stage (the first 8 hours for the 3 stage SP, and the first 6 hours for the 4 stage SP).
Figure 8: Optimal SP storage policies for the CAES system under the different price paths

Finally, we have the dynamic programming solution for the CAES system under the three different paths (Figure 9). The DP formulation has the following characteristics:

**Dynamic Program Parameters**

\[ T \] stages in hourly increments (24 hours)

\[ P \] discretized hourly prices in $1 increments, \( P \subseteq [10, 200] \Rightarrow 191 \text{ Prices} \)

\[ S \] discretized storage levels:

- CAES: discretized in 10MWh increments \( S \subseteq [0, 3000] \Rightarrow 301 \text{ Levels} \)
- NaS Battery: discretized in 0.5MWh increments \( S \subseteq [0, 100] \Rightarrow 201 \text{ Levels} \)

\[ X \] finite action space of the quantity charged/discharged (MWh)

- CAES: discretized in 10MWh increments \( X \subseteq [-300, 300] \Rightarrow 61 \text{ Levels} \)
- NaS Battery: discretized in 0.5MWh increments \( X \subseteq [-10, 10] \Rightarrow 21 \text{ Levels} \)

\[ Pr(\omega_{t+1} | \omega_t, x_t) \] conditional probabilities of state transitions (191x191x24 matrix)

Although the policies here are not as extreme as the ones given by the deterministic solution, the DP does provide notably different policies for the different price paths. This is a result of the more frequent decision stages that the DP uses in determining the optimal policy. For example, in the case of price path (b), the DP solution takes a very modest position in the storage level, and does not purchase a large quantity of electricity during off-peak periods since it repeatedly updates its state and realizes that the price is not following the standard trend. As a result, the profit levels for the three paths under the different optimization policies reflects the significance of the additional decision stages. A comparison of the policies and their resulting
profits for each price path is provided in Figure 10.

Although the previous analysis helps in observing the behavior of the different policies under quite distinct price paths, it is necessary to carry out the policies in a general setting in order to determine the expected arbitrage profits. To do this, we have determined the expected profits under five different policies:

(i) The linear program on the expectation of the price path

(ii) The 3 stage SP using a sample of 125,000 scenarios using the Gaussian noise price process

(iii) The 4 stage SP using a sample of 160,000 scenarios using the Gaussian noise price process

(iv) The 3 stage SP using a sample of 125,000 scenarios using the mean-reverting price process

(v) The dynamic program using the mean-reverting price process

Models (ii) and (iii) demonstrate the effect of introducing an additional decision stage, while the purpose of model (iv) is to provide a comparison between the SP and the DP policies under a single price process, in order to prevent any further discrepancies between the models. The arbitrage profits from these models for the CAES and NaS battery systems are summarized in Figure 11.
Figure 10: Optimal storage policies for the CAES system using the different optimization schemes for price paths (a), (b) and (c)
Figure 11: Expected daily arbitrage profits for the CAES and NaS battery systems using the different optimization schemes

6.4 Sensitivity Analysis

We now use the models at our disposal to examine the sensitivity of the profits to the model parameters. For the sake of brevity, we provide only the sensitivity observations of significance. We contrast both the stochastic solution in addition to the linear program over the expected prices in each case, and observe that the stochastic program consistently dominates the simple expected LP solution.

We begin by varying the physical parameters of the CAES system, namely the conversion efficiency, the maximum discharge rate (the generator size) and the energy capacity (storage size). As expected, we have relatively linear increases with increases in both the recharge/discharge size and conversion efficiency. The critical observation here is that there is a finite useful size for the storage itself. Here we can see that for the 300MW CAES facility, approximately 3 hours of storage is sufficient to extract all arbitrage profit opportunities. The bottleneck is the generator size, where an increase in the discharge/recharge rate provides greater profit opportunities than a larger storage tank.

The profit opportunities of the CAES system are also highly susceptible to the prevailing fuel costs. As shown in the sensitivity graph, a 30% increase in the discharge cost leads to a 50% decrease in arbitrage profits. Thus fears of an impending rise in fuel costs may have a detrimental effect on the arbitrage opportunities of CAES facilities.
Finally, we examine the effects of storage efficiency on arbitrage profits. Beginning with the base case of 97% efficiency for the NaS battery [4], we note that there are significant incentives in decreasing the time dependent losses of storage systems, since a modest increase in storage efficiency yields gains of 50% or more in arbitrage profits.

7 Summary and Conclusions

7.1 Cost Benefit Analysis

We conclude this paper by first summarizing the cost-benefit analysis of storage facilities using the results of our arbitrage profit models. For the two storage facilities under consideration, the cost breakdown is:
Figure 13: Sensitivity of arbitrage profits to discharge costs of the CAES system

Figure 14: Sensitivity of arbitrage profits to storage efficiency of the NaS battery system

<table>
<thead>
<tr>
<th>Cost Component</th>
<th>NaS Battery</th>
<th>CAES</th>
</tr>
</thead>
<tbody>
<tr>
<td>Power Conversion Cost</td>
<td>$2270/kW</td>
<td>$450/kW</td>
</tr>
<tr>
<td>Storage Cost</td>
<td>$200/kWh</td>
<td>$1/kWh</td>
</tr>
<tr>
<td>Total Cost</td>
<td>$43 million</td>
<td>$138 million</td>
</tr>
<tr>
<td>O&amp;M Fixed Cost</td>
<td>$50/kWyear = $500,000/year</td>
<td>$13/kWyear = $3.9 million/year</td>
</tr>
<tr>
<td>Disposal Cost</td>
<td>$43/kW = $430,000</td>
<td>0</td>
</tr>
<tr>
<td>Life</td>
<td>15 years</td>
<td>30 years</td>
</tr>
</tbody>
</table>

Using these costs we can summarize the profits as:
<table>
<thead>
<tr>
<th>CAES Plant</th>
<th>Daily Profit</th>
<th>Annual Profit ($M)</th>
<th>Fixed Costs ($M)</th>
<th>Net Profit ($M)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stochastic Program</td>
<td>$22,500</td>
<td>$5.63</td>
<td>$3.90</td>
<td>$1.73</td>
</tr>
<tr>
<td>Dynamic Program</td>
<td>$37,280</td>
<td>$9.32</td>
<td>$3.90</td>
<td>$5.42</td>
</tr>
<tr>
<td>Wind (DP)</td>
<td>$39,000</td>
<td>$9.75</td>
<td>$3.90</td>
<td>$5.85</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>NaS Battery Plant</th>
<th>Daily Profit</th>
<th>Annual Profit</th>
<th>Fixed Costs</th>
<th>Net Profit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stochastic Program</td>
<td>$1,147</td>
<td>$286,750</td>
<td>$500,000</td>
<td>-$213,250</td>
</tr>
<tr>
<td>Dynamic Program</td>
<td>$1,625</td>
<td>$406,250</td>
<td>$500,000</td>
<td>-$93,750</td>
</tr>
</tbody>
</table>

The NaS Battery has a negative net profit, and so is not a feasible solution for arbitrage profit schemes. The CAES facility yields positive net profits; however, when one considers the roughly $138 million price tag for the construction of such a plant, the finances do not bode well. Nevertheless, we have only considered arbitrage profits alone in this valuation. When coupled with additional revenue and value sources, such as participation in ancillary service markets and reliability services, the CAES facility has the potential of becoming economically viable.

### 7.2 General Results

The primary difference in our models (LP vs. DP vs. SP) stems from the number of decision stages used in the optimization. Profit gains of 45-55% were realized from upgrading from the 1 stage LP to 3 stage SP, and an additional 10-25% of gains when switching from the 3 stage to the 4 stage SP. The dynamic program outperformed all models by a factor of 66-120% simply due to the fact that the optimization was carried out over 24 stages. Although, the dynamic programming approach is amenable to multi-stage decision problems (eg. 24 hours), and provides an exact solution without simulation requirements, the state-space problem limits the price/wind model choice, and further limitations on the problem size within each dimension make the DP susceptible to discretization errors.

The stochastic programming approach provides flexibility in the choice of price and wind models, allowing
for a richer modeling framework for representing such stochastic processes. This flexibility extends to the alleviation of discretization errors within the process. Moreover, the framework allows for the ability to deal with a large number of uncertainties, coming at the expense of a limited number of decision stages. Nevertheless, the structure of the problem within specified stages is often appropriate for power markets where participation in the market often occurs hours in advance, rendering most dynamic programming solutions virtually useless.

The selection of a single day (24 hour period) for the optimization has proven to be an accurate reflection of the overall system dynamics. A separate test was conducted using an optimization over five separate days vs. a single consecutive five-day period, and the results gave little difference; thus, a daily approach is a sensible time frame. There is, however, a significant difference when considering the starting point within the 24 hour period. A final test was carried out using different endpoints for the 24-hour interval for the optimization problem, and as expected the results displayed significant discrepancies. The standard practice of starting around midnight was shown to be optimal, once again not affecting the results of the analysis provided in this paper.

Finally, sensitivity analysis results have shown that 5 hours of storage capacity is more than sufficient to capture the majority of arbitrage profits. The limitation in most storage systems from an arbitrage perspective is the discharge/recharge rate, namely the size of the generator. When dealing with storage plants in general, the storage efficiency is a very important parameter to consider for daily arbitrage applications. It has been shown, via the analysis of the NaS battery, that even a small storage loss will almost eliminate all arbitrage profit opportunities.

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References


Appendix H: The Value of Information in Spatial Decision Making

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The Value of Information in Spatial Decision Making

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Abstract

Decisions involving selection of sites over a lateral domain with a spatially correlated distinction of interest are common in several realms. In this paper we use the decision-analytic notion of value of information on models common to spatial statistics. We formulate methods to evaluate monetary values associated with experiments performed in the spatial decision making context, including the prior value, the value of perfect information, and the value of the experiment. The prior for the spatial distinction of interest is assumed to be a Markov random field where the value at each spatial site belongs to a finite set of states. The likelihood distribution can take any form depending on the experiment one decides to acquire. Typical experiment types are binary registration or a Gaussian measurement at selected spatial sites. We demonstrate how to efficiently compute the value of an experiment for Markov random fields of moderate size. The most computationally demanding task is solving an integral over the result of the experiment under evaluation, which we accomplish using Monte Carlo integration. We explore and compare some measures for the worth of an experiment in our problem context. Our methods are illustrated on two examples. One is relevant to conservation biology, where the downstream decision is the spatial allocation of reserve sites. The other application is motivated by seismic exploration in the petroleum industry. These simple examples demonstrate the complex interplay between the likelihood of the experiment, spatial interaction and the nature of the downstream decision and its associated values. The approach naturally fosters a multi-disciplinary outlook for valuing information in spatial decision making, and stimulates ideas for creative alternatives in decisions related to experimentation.

Keywords: value of information, Markov random field, spatial decision making, experimental design.
1. Introduction

Gathering the right kind and right amount of information is crucial for any decision making process. Auxiliary decision opportunities regarding information gathering are often created when an important decision is to be made in the future. This downstream decision may have a lot at stake and it may be worthwhile to obtain more information before the decision is actually taken, i.e. before an irrevocable allocation of resources. A crucial question to answer is - how much information should one purchase? This is a decision which is related to the well-established concept of value of information, also known as value of clairvoyance, in decision analysis (Howard, 1966; Raiffa, 1968; Matheson, 1990). The value of information (VOI) for a particular information gathering scheme is the maximum monetary amount that a decision maker should be willing to pay to acquire it. The VOI depends on several factors, including the prior probabilities, the “quality” of the test and the decision maker’s utility curve.

In this paper we present models that compute the value of information for experiments performed in the context of spatial decision making. We use the phrase spatial decision making to refer to decision problems with two important characteristics: 1) the decision generally involves a choice of alternatives over space, for instance, selecting sites; and 2) the distinction of interest is typically spatially correlated. There are several applications that are relevant within this context. Petroleum exploration and production is a natural contender as a possible application: here the distinction of interest is the presence or absence of oil; the presence of oil is spatially correlated in a reservoir, and the decision maker must decide where to drill wells to recover oil and maximize profits. Another application is conservation biology where decisions are made regarding the number of reserve sites and their spatial location. Here the distinction of interest is the presence or absence of a particular species. We illustrate our methods on examples from both these applications.

We briefly discuss some recent work that can be viewed as spatial decision making, but none of which include the full generality that we adopt in this paper. Polasky and Solow (2001) present issues regarding the value of information in conservation biology. They use decision-analytic concepts to investigate the value of information of surveys in the reserve site selection problem. Reserve site selection refers to the selection of sites for establishing biological reserves with the purpose of conserving and nurturing certain species. In their paper, Polasky and Solow show that inferences about value of information in such a setting can often be counter-intuitive. However, they assume that the species incidences are independent and use a value criterion that is not associated with monetary units. Houck and Pavlov (2006) estimate the value of information for electromagnetic surveys in petroleum exploration using the decision-analytic approach. Although their case study is illustrative, they work at the global level of the reservoir by using a simple decision tree formulation. Diggle and Lophaven (2006) describe a Bayesian hierarchical model for geostatistical design of monitoring sites for salinity at sea. Their goal is to minimize spatial prediction variance. With their philosophy it is hard to relate the statistical model to the downstream decision and its associated values, and therefore to compare the worth of an experiment with its cost. In fact, downstream decisions are rarely treated directly in geostatistical situations; the focus is mostly on prediction variance and parameter estimation, see e.g. Müller (2001).

We introduce a decision-analytic formulation to situations that naturally exhibit spatial dependence. We use a categorical Markov random field (MRF) model (Besag, 1974) for the distinction of interest. Other Bayesian prior models can also be used. An advantage with moderate size
MRFs is that recursive assessment of such categorical MRFs (Reeves and Pettitt, 2004) allows us to calculate the marginal probabilities and to sample directly from these models. We are interested in evaluating experiments that are performed to obtain more information about the distinction of interest. We use a monetary value measure to ensure that the value of information corresponds directly to the maximum a decision maker should be willing to spend to purchase an experiment. Our models can easily be extended to deal with other measures of value. For the sake of clarity, we assume throughout the paper that the decision maker is risk-neutral (Raiffa, 1968). In other words, the decision maker is indifferent between a lottery of uncertain monetary prospects and the expected value of the lottery. Our models can incorporate risk aversion or risk seeking behavior if required.

Section 2 develops basic notation for the rest of the paper. In Section 3 we present the model assumptions and equations. This section explains how we integrate spatial statistics with different approaches to valuing information; it is our main contribution in this work. Our focus is on the decision-analytic philosophy but we also mention a formulation using entropy as a measure for valuing information in spatial decision making. In Section 4 we describe an algorithm that couples Monte Carlo simulation and a recursive method for computing the value of information of an experiment. This computational method is crucial for assessing the value of information in practice. The algorithm is demonstrated on several examples in Section 5 to develop critical insights. We begin with a simple hypothetical example from the domain of conservation biology and graduate to a more realistic example from petroleum exploration, motivated by data collected at a reservoir in the North Sea. Finally, we discuss our conclusions and directions for further research in Section 6.

2. Basic Notation

In this section we introduce notation and basic terminology. The word field is used to denote the spatial system under consideration. The field lies on a lateral 2-dimensional grid composed of \( n_1 \times n_2 \) cells, i.e. the grid has \( n_1 \) rows and \( n_2 \) columns with a total of \( N \) cells, where \( N = n_1 n_2 \). Each cell may have identical length and width but this is not essential; the size of the cell is determined by the application and the scale of the study. Besag (1974) refers to this kind of setting as a lattice system. We can index the cells in the grid from top to bottom and left to right as \( i = 1, 2, \ldots N \). This will enable us to refer to a particular cell by using a single index.

Let \( x \) be the random variable over the entire field for the distinction of interest, or in other words, the latent variable which is of interest to the decision maker. Letters with a subscript \( i \) denote the outcome at cell number \( i \), while letters without any subscript refer to the set of outcomes over the entire field. Thus \( x = \{ x_i : i = 1, 2, \ldots N \} \). Furthermore, we assume that \( x_i \) is a categorical random variable that equals any one out of \( d \) possible colors (or states). When \( d = 2 \), \( x_i \) is a Bernoulli random variable. For this work, we will choose \( x_i = 1 \) as the favorable outcome at cell \( i \). The joint prior probability of an outcome \( x \) is denoted by \( p(x) \), while the marginal probability of an outcome \( x_i \) is denoted by \( p_i(x_i) \). The marginal prior probability of the favorable outcome \( x_i = 1 \) is then \( p_i(1) \).

Let \( y \) be the random variable for the result of an experiment, which may be conducted in the future to obtain more information about \( x \). The experiment is to be performed in cells with indices in the set \( J \), a subset of \( \{1, 2, \ldots N\} \). Therefore, \( y = \{ y_j : j \in J \} \). The experiment need not be
performed at all the cells in the grid. In fact, it may be optimal to perform the experiment only at a few cells, depending on all the parameters and the cost of the experiment. The likelihood for the experimental result \( y \) given the outcome of the distinction of interest \( x \) is \( p(y|x) \). For a continuous random variable \( y \), \( p(y|x) \) is a density function; it is a probability function if \( y \) is a discrete random variable. We inspect both cases with the help of examples, but for presenting our methods we treat \( y \) as continuous. The marginal likelihood of the experimental outcome can be obtained by summing out all possible configurations of \( x \), i.e. \( p(y) = \sum x p(y|x)p(x) \). For \( d \)-colored categorical fields \( x \) of size \( N \), this is a summation over \( d^N \) terms and can be computationally demanding.

The posterior probability of the outcome of the distinction of interest \( x \) given an experimental result \( y \) is \( p(x|y) \). The marginal posterior probability of an outcome \( x_i \) at cell \( i \) given an experimental result \( y \) is written as \( p_i(x_i|y) \). As the favorable outcome we use \( x_i = 1 \), which has marginal posterior probability \( p_i(1|y) \). In this paper, we analyze the value of such an experiment \( y \) and present insights using examples motivated by different types of possible experiments.

3. Model Formulation

We now expand on the terminology and specify model assumptions regarding the probability distributions for \( x \) and \( y \). The conceptual equations that determine measures for the value of an experiment are also explained in this section. The actual computational issues are postponed until Section 4.

3.1 Prior spatial model for the distinction of interest

Spatial dependence in the distinction of interest \( x \) is incorporated through the use of a categorical first-order MRF formulation (Besag, 1974). This implies that the probability for a certain outcome in a given cell, given the outcome in the entire field, depends only on the outcome in the four neighboring cells. The spatial field is thus represented as an Ising model with \( \beta \) as the interaction parameter:

\[
p(x) = \frac{\exp[\beta \sum_{i\sim j} I(x_i = x_j) + \sum_{i=1}^{N} \alpha_i(x_i) \]}{z}.
\]

\( I(A) \) is an indicator function taking value 1 if \( A \) is true and 0 otherwise. The first summation in equation (1) is over all pairs \( x_i \) and \( x_j \) that are closest neighbors in the grid, and \( z \) is a normalizing constant. The point-wise prior function \( \alpha_i(x_i) \) is a function of the outcome at every cell. It provides the mechanism for including prior information about the outcome at a particular cell, based on expert opinion or previous data. On the other hand \( \beta \) controls the spatial dependence of the latent variable. We assume that \( \beta \) and \( \alpha_i(x_i) \) are known a-priori. The special case when \( \alpha_i(x_i) = 0 \), \( \forall x_i, i \) is known as the uninformative prior case. In this situation, the marginal probabilities are such that each color is equally likely at every cell.

3.2 Likelihood model for the experiment

The random variable \( y \) is the result of an experiment performed in cells with indices in the set \( J \). The decision maker will purchase the experiment only if it is worthwhile to do so. Conducting
the experiment should increase the profitability of the decision by more than its cost. We are ultimately interested in some measures of the worth of this experiment.

We assume that \( y_j \), the result for the experiment at cell \( j \), given the outcome over the entire field \( x \), depends only on the marginal outcome \( x_j \). The experimental result at a particular cell is hence conditionally independent of the outcome of the latent variable at other cells, given the outcome at its own cell. This is a reasonable assumption because several experiments and surveys in spatial decision making satisfy this property in practice by providing only local information about sites. From conditional independence, we get:

\[
p(y|x) = \prod_{j \in J} p(y_j|x_j).
\] (2)

Each local likelihood distribution \( p(y_j|x_j) \) can be any probability distribution - discrete or continuous, depending on the kind of experiment being performed. We discuss the particular likelihood function used in the context of examples. We show results from a binary experiment (Section 5.1) and a Gaussian experiment (Section 5.2).

### 3.3 A simple decision-analytic framework

In this section we present a simple decision-analytic framework so that we can explain the concepts easily, and create a framework that is not completely guided by case-specific issues. We make some critical assumptions about the nature of the downstream decision:

i) We assume that the main decision specifically involves a one-time selection of cells from the field. Sequential decisions regarding cell-selection are not considered.

ii) The decision maker’s goal is to obtain value from the individual cells. It is thus possible to alienate each cell and think about costs and revenues for each cell separately. In this way we are only concerned with the marginal probabilities of the favorable outcome at each cell. This may not be the case in practice - for instance, value from the main decision may involve joint (global) properties of the entire field, or it may depend on interactions between cells. Crucially, this assumption ensures that the value from the field is equal to the sum of the values from the cells.

iii) The decision for selection of cells is an unconstrained decision problem. The decision maker may choose as many cells as is profitable. The introduction of constraints would entail that the decision at a particular cell could not be made independently of those at other cells.

We present a more general formulation in Section 3.4, where we relax the second and third assumptions.

Say that the cost of selecting cell \( i \) is \( C_i \) and the revenue gained from observing the favorable outcome at that cell is \( R_i \). No revenue is gained if any other outcome is observed. Note that the outcome for a cell is not ascertained until and unless the cell is selected. As an example, \( C_i \) may be the cost associated with drilling a well at cell \( i \) and \( R_i \) is the corresponding revenue obtained from discovering oil at that cell. We are now equipped with all the notation and assumptions necessary to calculate the value of information and other related measures for an experiment. Firstly, the decision maker can take his/her decision without purchasing the experiment. In that case the expected value from the \( i^{th} \) cell \( V_i \) is given by:

\[
V_i = \max\{0, [R_i \cdot p_i(1) - C_i]\},
\] (3)

where \( p_i(1) \), as mentioned earlier, denotes the prior marginal probability of the favorable outcome \( x_i = 1 \). It is optimal for the risk neutral decision maker to choose the \( i^{th} \) cell only if the expected
profit is positive. Hence the value is the maximum of 0 (for the case where the cell is not selected) and the expected profit expression $R_i p_i(1) - C_i$ (for the case where the cell is selected). The favorable outcome is seen when $x_i = 1$ and all other outcomes result in zero revenue. With the assumptions we have described, the prior value ($PV$) or the total value from the field based on the prior alone is the sum of the expected value from the cells:

$$PV = \sum_{i=1}^{N} V_i = \sum_{i=1}^{N} \max\{0, [R_i \cdot p_i(1) - C_i]\}. \quad (4)$$

What if the decision maker had perfect information about the latent variable? In other words, what if a clairvoyant would be willing to reveal the outcome of the latent variable? How much should the decision maker pay for this information? The $i^{th}$ cell has a favorable outcome with probability $p_i(1)$. If it is indeed favorable, the value obtained is the maximum of 0 (cell is not selected) and $R_i - C_i$ (cell is selected). The decision maker will choose not to select a cell if it is known that the outcome is not favorable, thereby making zero profit.

The value with free clairvoyance (VFC) (see e.g. Howard and Abbas, 2006) on the distinction of interest over the whole field is the sum of the expected value (with free clairvoyance on the distinction of interest) obtained at the individual cells. Hence,

$$VFC = \sum_{i=1}^{N} p_i(1) \cdot \max[0, (R_i - C_i)]. \quad (5)$$

In most situations, presumably the revenues outweigh the costs throughout the field. Therefore $R_i > C_i \forall i$. This implies that equation (5) can be reduced to $V FC = \sum_{i=1}^{N} p_i(1) \cdot (R_i - C_i)$.

The value of perfect information (VOPI) on the distinction of interest, which is the most that the decision maker should pay for perfect information on the distinction of interest, is the increase in profitability from the prior situation to the one where clairvoyance is obtained without cost. Note that this is only true for people who follow the delta property (Howard and Abbas, 2006). The delta property is a popular assumption in the decision analysis literature since it enables an analytically tractable method for calculating value of information. The property is satisfied by people who have an exponential or straight-line utility-curve, and since a risk-neutral decision maker has a straight-line utility-curve, s/he satisfies the delta property. Therefore,

$$VOPI = VFC - PV. \quad (6)$$

In both PV and VOPI calculations, the value depends only on the marginal probabilities of observing the favorable outcome since the value from a particular cell does not depend directly on other cells. We call the set created by these marginal probabilities over the grid, the prior probability map. The prior probability map is $\{p_i(1) : i = 1, 2, \ldots , N\}$. If the experiment is performed, a result $y$ is observed before the main decision is made. The marginal posterior probability of a favorable outcome $x_i = 1$ in the $i^{th}$ cell is $p_i(1|y)$. The computation for the conditional value of the $i^{th}$ cell is along the same lines as in equation (3), replacing the prior with the posterior. The expected value $V_i'$ is evaluated with the expectation over the experimental result $y$:

$$V_i' = \int_y \max[0, R_i \cdot p_i(1|y) - C_i] p(y) dy. \quad (7)$$
With the assumptions we have described, the value with the free experiment (VFE) is the sum of the expected value $V'_i$ over all cells:

$$VFE = \sum_{i=1}^{N} V'_i = \sum_{i=1}^{N} \int \max[0, R_i \cdot p_i(1|y) - C_i] p(y) dy. \quad (8)$$

As in the case of clairvoyance on the distinction of interest for a delta person, the value of information for the experiment (or for short, the value of the experiment (VOE)) can be computed as the difference between value with the free experiment and value from the prior.

$$VOE = VFE - PV. \quad (9)$$

This is the gain in profitability from performing the experiment and hence this is the maximum that should be spent on purchasing the experiment. In our opinion the VOE is the best measure for the worth of an experiment because, by definition, it indicates how valuable the experiment is to the decision maker in monetary units. However poor the experiment is, one can always choose to ignore the results and end up being as well off as before. For a worthless experiment $VOE = 0$. Also, no matter how good the experiment is, it cannot be better than directly obtaining information about the latent variable since this is the variable that is of ultimate interest to the decision maker. In this way, the VOPI acts as an upper bound on the VOE.

This naturally leads to another measure of the experiment: the chance of knowing (COK) (Howard and Abbas, 2006). It can be shown that for a risk-neutral decision maker, \[ COK = \frac{VOE}{VOPI}, \quad 0 \leq COK \leq 1. \quad (10) \]

The chance of knowing can be explained as follows: Consider a lottery where with a probability $p$, a clairvoyant will provide perfect information on the distinction of interest for no charge and with probability $1 - p$ will provide no information. The probability $p$ that makes the decision maker indifferent between obtaining the experiment for free and playing this lottery is the chance of knowing for that experiment. A good experiment would require a higher probability for a person to be indifferent, whereas for a poor experiment a smaller value of $p$ would suffice. To summarize, the COK is a number between 0 and 1 that rates the worth of an experiment in a certain context.

VOE provides an actual monetary value on information, and COK presents a quick and intuitive way to compare different experiments with each other and also with information on the distinction of interest. In Section 4 we describe how the equations presented in this section can be solved.

3.4 A general decision-analytic framework

We will now show a more general framework where we relax two of the assumptions presented in Section 3.3. Rather than treating cells separately, the joint distribution of the distinction of interest is considered. Furthermore, the constrained case needs special attention since the action (where to select sites) depends on the outcome of the distinction of interest.

Let $f(a, x)$ be the value derived from a realization of the field $x$ when action $a$ is taken. $a$ is one of the actions in the set of alternatives $A$, or $a \in A$. The prior value, before any information is revealed, is the value derived from the optimal course of action based on the prior on $x$. It is
optimal for the risk-neutral decision maker to choose the action that maximizes the expected value. Thus,
\[
PV = \max_{a \in A} \left[ \sum_{x} f(a, x) \cdot p(x) \right].
\] (11)

For the case of perfect information on the distinction of interest, the realization \(x\) is known to the decision maker before the optimal action is chosen. The value of perfect information is given by the difference between the expected value with free clairvoyance on the distinction of interest and the prior value:
\[
VOPI = \sum_{x} \max_{a \in A} [f(a, x)] \cdot p(x) - PV.
\] (12)

Note that the order of summation and maximization is reversed for the VOPI equation. As before, the value of the experiment is the difference between the expected value given result \(y\) and the prior value:
\[
VOE = \int y \max_{a \in A} \left[ \sum_{x} f(a, x) \cdot p(x|y) \right] p(y) dy - PV.
\] (13)

The COK can be obtained from equation (10).

To motivate how this general formulation might be preferred to our simplified version presented in Section 3.3, consider the petroleum example again. For a comprehensive study at a suitable scale, the area of each cell would not be large. Deviated wells could drain oil from adjacent cells and therefore the cost for an adjacent cell would be less if its neighbor is already selected. Value from the field would also depend on interaction factors such as permeability and the flow of oil in the reservoir. Another issue is that of constraints in selecting sites; the budget for a field puts a limit on the number of wells that can be drilled. All these aspects must be modeled intelligently in the spatial decision making context, because the price we pay for generality is a severe increase in computational intensity. For the simple framework presented in Section 3.3, the VOE calculation of equation (7) involves an integral over the experiment which is approximated and summed over all \(N\) cells. In addition to this calculation, the general framework also requires a summation over \(x\), as seen in equations (11) and (13). It is hard to provide general guidelines for the value function and the actions as they would remain case-specific.

### 3.5 Another criterion: Entropy

In this section we discuss entropy as another criterion for evaluating experiments. We do not provide numerical examples, but merely define the concept and compare it with our decision-analytic approach. The notion of entropy, introduced from *information theory*, see e.g. Ash (1965), has been used to measure the reduction in uncertainty of \(x\) on observing the outcome \(y\) of an experiment. The entropy is defined by
\[
H(x) = - \sum_{x} p(x) \log p(x),
\] (14)

which can be constructed sequentially as
\[
H(x) = H(x_N) + H(x_{N-1}|x_N) + \ldots + H(x_1|x_2, \ldots, x_N).
\] (15)
This sequential formulation is used when computing entropy, see Appendix A. The expected reduction in entropy from the experiment \( y \) is

\[
EMI = H(x) - \int y H(x|y)p(y)dy,
\]

where EMI is the expected mutual information between \( x \) and \( y \).

Both VOE and EMI can be used as measures for valuing information. However, there is a wide gulf between the philosophies of the two measures. For instance, EMI provides a sense of how much uncertainty can be reduced by performing an experiment, but it cannot directly imply how much the decision maker should pay for it. It is hardly surprising that the decision-analytic notion of VOE is tied inexorably with decisions and the preferences of the decision maker. VOE is a more complete measure for valuing information and also more difficult to obtain. According to Howard and Abbas (2006), an experiment should be conducted when it is: (i) relevant to the distinction of interest, (ii) material to the decision that brings value and (iii) economic for the decision maker. A material experiment is one that can affect the decision, i.e. the action chosen by the decision maker is not identical for different outcomes of the experiment. By the decision-analytic philosophy, information from experimentation may reduce uncertainty but is not valuable until it can change the decision. An economic experiment in our context is one that costs less than the VOE. Entropy based parameters such as EMI only address aspects of relevancy of the experiment, without addressing the other two requirements. An experiment with zero mutual information will be irrelevant for the distinction of interest. Mutual information measures may be used as a guide in designing the most relevant experiment (e.g. Mukerji et al, 2001). The three requirements of an experiment being relevant, material and economic are intertwined - for example, an immaterial experiment will not be economic because its value is 0. Ascertaining the value from a decision to be made in the future is often a difficult task; yet it is crucial if measures like VOE are to be estimated.

4. Computational Issues

The joint distributions for the distinction of interest and for the experimental result are over the entire field with \( N \) cells and are likely to be high dimensional. Solving equation (7) analytically may not be possible in general, so we use Monte Carlo simulation by generating realizations of the experimental result. The same holds for several of the expressions in Section 3. The Monte Carlo simulation is shortly described as follows: We generate \( M \) independent and identically distributed (i.i.d.) random samples \( y^1, y^2, \ldots, y^M \) from \( p(y) \). For the \( m^{th} \) sample, let \( w(y^m) = \max[0, R_i \cdot p_i(1|y^m) - C_i] \). Now we can approximate equation (7) as

\[
V_i' \approx \frac{1}{M} \sum_{m=1}^{M} w(y^m).
\]

An exposition on Monte Carlo methods can be found in Liu (2001). In general, a high dimensional integral of a function \( w(y) \) over a region \( D \), can be approximated as follows:

\[
\int_D w(y)p(y)dy \approx \frac{1}{M} \sum_{m=1}^{M} w(y^m), \quad y^m \sim p(y), \quad m = 1, \ldots, M, \quad \text{i.i.d.}
\]

10
The Monte Carlo error is not large if a sufficient number of realizations are generated.

In our simple framework from Section 3.3 we first generate i.i.d. realizations $x^1, x^2, \ldots, x^M$ of MRFs in equation (1). We next draw realizations of the experiment $y^1, y^2, \ldots, y^M$. These are marginally from the distribution $p(y)$. For each of these conceptual datasets $y^m$ we compute the marginal posterior for the favorable outcome denoted by $p_i(1|y^m)$. We use the recursive forward and backward techniques to 1) draw realizations $x^m$, and 2) compute the marginal $p_i(1|y^m)$. We will refer to the two methods as RecGenerate and RecCompute respectively, to specify where exactly they are used in the main algorithm. The recursive method itself is based on Reeves and Pettitt (2004) and outlined in Appendix A.

The algorithm for computing the value of an experiment is as follows:

1. Find the marginal prior probability for $x$ using RecCompute.
2. Solve equations (3) through (6) to find the PV and the VOPI.
3. Generate a realization $x$ from the prior with RecGenerate.
4. Generate a conditional realization $y$ of the experimental result from the likelihood of the experiment, given the realization $x$. The general form of the likelihood is depicted in equation (2).
5. With the current realization of the experiment $y$, use RecCompute to evaluate the marginal posterior probability of the favorable outcome $x_i = 1$, denoted as $p_i(1|y)$, and compute the associated value. This is done for all cells $i = 1, \ldots, N$.
6. Repeat steps 3. - 5. a total of $M$ times, and approximate the integral for $V'_i, i = 1, \ldots, N$, in equation (7) with the average value from the simulations, shown in equation (17).
7. Solve equations (8) through (10) to get VOE and COK.

Crucial tasks in steps 1. - 7. of the algorithm are RecGenerate and RecCompute, using recursive computing on the field of size $n_1 n_2 = N$. The recursive method presented in Appendix A is of order $O(N)$, but for each step of the recursion we need to evaluate and store terms of size $d^{n_1}$; this is the computer memory intensive part of the algorithm. Therefore the smallest grid dimension $n_1$ should not be too large (say not more than $n_1 = 10$ for $d = 3$). In our case, with only one favorable outcome, the most efficient way is to use $d = 2$ and marginalize over all non-favorable categories. However, such a marginalization would not be natural from a modeling perspective. For example, in the petroleum exploration case, it is easier for experts to consider three categories: oil sand, brine sand and shale, and assign prior probabilities and likelihoods for each class. Also, more than one outcome can be favorable in general.

Note that the algorithm above only applies to the simple framework of Section 3.3. The computational advantage of this model is that the marginal posterior probability $p_i(1|y)$ of the favorable outcome is easily calculated by the recursive algorithm. For the more general setting of Section 3.4, one may require a function of the joint distribution over the entire field $p(x|y)$, and this is not easy to obtain in general. A more complicated and time consuming Monte Carlo method would be necessary for the general case. The algorithm of choice would typically depend on the particular situation.
5. Examples

5.1 Example from conservation biology

Consider a region of land under scrutiny in a conservation biology project, modeled as a 3 by 3 grid. The decision maker is interested in selecting sites from the grid to set up natural wildlife reserves with the goal of conserving an endangered species. However, there is uncertainty regarding the presence of the species. If the decision maker selects a cell, she must pay the cost $C$ (assumed to be the same across cells) for construction of the natural reserve. If the species is present at a cell that she chooses, she obtains revenue $R$ (again assumed to be the same across cells). The decision maker will not know for sure whether the species is present or not until the cell has been selected. Let $x$ be a random variable for the presence or absence ($d = 2$) of the species at all cells in the grid. The categorical outcome $x_i$ is 1 if the species is present at cell $i$ and 0 if the species is absent. The decision maker is interested in the value of information for different kinds of surveys.

In this example we analyze experiments that have binary results. We also assume for now that if the experiment is purchased, it will be performed at all cells in the grid. One can imagine a survey where a team explores every cell and indicates whether they believe the species is present or not, for each cell. The survey result $y_i = 1$ implies that the team believes the species is present at cell $i$ and $y_i = 0$ suggests otherwise. The experimental results need not be accurate. Say that the accuracy of the test at every cell is the same and is denoted by $\gamma$. This accuracy is defined by the following likelihood equation:

$$p(y_i = k|x_i = k) = \gamma; \forall i. \quad (19)$$

The likelihood may be different conditioned on whether the latent variable $x_i$ is 1 or 0. Sensitivity and specificity have been the terms used in the literature to denote these likelihoods. For simplicity we will combine these such that there is only one parameter. A value of $\gamma$ close to 1 indicates a good test, i.e. a test with high accuracy. We choose to model the field’s spatial prior as an uninformative prior, i.e. we have no prior point-wise information on the field, and believe that there is an equal chance of species presence or absence in every cell. There is some spatial correlation for $x$, determined by the interaction parameter $\beta$. Furthermore, $C = 1$ monetary unit (so that revenue can now be written in units of $C$).

First we assume that the cell-selection is unconstrained, i.e. the decision maker can select as many cells as is profitable. Sensitivity analysis on the parameters $\beta$ and $\gamma$ can provide insights into general trends. Figure 1 shows VOE as a function of these parameters in three plots, for revenue $R = 2, 5$ and 10 monetary units from left to right respectively. Let us analyze trends within each plot to begin with. Firstly, the accuracy is a critical parameter. The curve for $\gamma = 0.9$ shows the highest VOE. In all three graphs, $\gamma = 0.5$ has $VOE = 0$ as the experiment provides no information about the distinction of interest. The VOPI is a horizontal line and has the same value (4.5 units in this case) for all $\beta$ and for all $R \geq 2$. It only depends on the marginal probability of success in each cell, which is 0.5 in the case of the uninformative prior, and does not depend on $\beta$. Note that the VOE increases as $\beta$ increases. This is because the chance that the entire grid will either contain the species at all cells or in no cells becomes higher as $\beta$ increases. The experiment becomes more valuable as $\beta$ increases because it can tell you about a possible jackpot (all cells favorable) or prevent a huge loss (all cells unfavorable). As there are no constraints on the number of cells...
that can be selected, the decision maker is free to choose all the cells or none; for large values of \( \beta \), this all-or-nothing policy is optimal. Therefore in the unconstrained case for the uninformative prior, the experiment can really make a difference for large \( \beta \). The spikes in the curves are due to Monte Carlo error, and are most notable for the plot of \( R = 10 \). We use \( M = 25000 \) Monte Carlo simulations in this example. VOE is not very sensitive to \( \beta \) for lower values, which is useful to know if one is unsure about the interaction parameter or cannot spare much time for estimating it.

Now observe the differences between each of the plots in Figure 1. Consider the case of \( \gamma = 0.7 \) and \( \beta = 0 \) in the graphs for \( R = 2 \) and \( R = 5 \), and compare them. For this choice of \( \gamma \) and \( \beta \), \( VOE = 0 \) for \( R = 5 \) whereas for \( R = 2 \) VOE is almost 2 units. Experiments do not automatically become more valuable when the decision situation is more lucrative. When \( R = 2 \), there is a chance for the experimental result to change the main decision, and in this way the experiment is valuable as it is able to affect the decision. On the other hand if \( R = 5 \) (and \( \beta = 0 \)), it is worthwhile to select all cells no matter what the experiment has to say. This is a fundamental issue in the decision-analytic approach to valuing information.

What if there are constraints on the number of reserve sites that can be selected? We use ideas from both Section 3.3 and Section 3.4 to solve the equations for the situation of constraints in cell-selection. We retain the assumption that the cells act as separate units, while introducing another parameter: \( k \), or the maximum number of cells that can be selected (based on a budget). Once we have a particular probability map (prior or posterior), we can maximize profits from the field by choosing the best \( k \) prospects, if profitable. Even in a simple example with only 9 cells, trends in VOE when the problem involves both spatial dependence and constraints in cell-selection can be
counter-intuitive. Figure 2 demonstrates results from sensitivity analysis on $\beta$ for a test with an accuracy of $\gamma = 0.9$. We compare the VOE for $k = 1, 5$ and $9$ for $R = 2$ (left) and $R = 5$ (right) in Figure 2.

The graph on the left is more in accordance with our initial reaction; VOE is highest when $k = 9$ and lowest when $k = 1$. The case with $k = 9$ corresponds to the unconstrained case as there are $N = 9$ cells in the field. As we observed in Figure 1, VOE appears to increase in the unconstrained situation. However, for $k = 5$ and to some extent also for $k = 1$, VOE seems to decrease as $\beta$ increases. This is even more prominent in the graph on the right. We explain this tendency as follows. The experiment conducted over the entire field has a certain facet that can be relatively more valuable when there is both low spatial dependence and a limit on the number of cells that can be selected. It tells you which cells are likely to be favorable, thereby guiding the decision maker about the choice of site location. There is a little more leeway for the decision maker regarding selection of an appropriate location when there is high spatial dependence. Thus VOE can be relatively smaller when $\beta$ is high. There are other seemingly unusual trends in the plot for $R = 5$. The VOE for curve $k = 5$ appears to be much higher than the other two curves for smaller $\beta$. It is indeed possible for the experiment to be more valuable in the situation when there are constraints, as opposed to when there are none. In the realistic situation of an informative prior on a large grid, the interaction between the parameters can become even trickier to understand. Simple examples can highlight some of the ideas that should be kept in mind while gathering information. High likelihood experiments are useful, but they should be able to affect the downstream decision.

Figure 2: Sensitivity analysis in the constrained case. The accuracy of the experiment is $\gamma = 0.9$. Two plots of VOE vs. $\beta$: (left) revenue $= 2$ units; and (right) revenue $= 5$ units. Each plot shows VOE for 3 values of $k$ (the maximum number of cells that can be selected): $k = 1$ (dotted line), $k = 5$ (solid line) and $k = 9$ (dashed line).
5.2 Example from petroleum exploration

We next use an example from the petroleum industry to demonstrate how our formulation can be employed for real-world applications. It is not a detailed case study by itself, but can give a sense of how an actual case study would be performed. The case we are considering is a lateral two dimensional reservoir domain that is a candidate for oil exploration. Decisions have to be made regarding which data attributes to analyze and over which spatial area. More specifically we evaluate the value of different attributes obtained from seismic reflection data (Avseth et al, 2005). We are interested in analyzing the value of information for two attributes of amplitude versus offset (AVO) seismic data. If these attributes are purchased, the decision maker will have to pay to conduct AVO processing and analyses. The example is motivated by previous work on AVO seismic data from the Glitne field in the North Sea, for example Eidsvik et al. (2004) and Avseth et al. (2005). These studies predicted the spatial distribution of oil sands based on AVO seismic attributes. The results obtained using just one of the AVO attributes (called \( R_0 \), normal-incidence reflectivity) were quite different from using both (called \((R_0, G)\), normal-incidence reflectivity and gradient with offset), and it is hence of interest to study the value of different seismic attributes following the decision-analytic framework outlined earlier. Furthermore, we compare the value of partial tests to that of acquiring AVO attributes along the entire field. We have chosen to postpone details regarding the model and implementation of this rather complex seismic example to Appendix B.

The focus of attention is a \( n_1 = 5 \) by \( n_2 = 20 \) grid \((N = 100)\); a part of a reservoir that may be the lobe of a turbidite system and hence of main interest for exploration. The distinction of interest is the rock and fluid composition which takes on any one of \( d = 3 \) colors: oil sand \( (x_i = 1) \), brine sand \( (x_i = 2) \) or shale \( (x_i = 3) \). The only profitable outcome is that of oil sand. For the MRF prior model in equation (1) we use \( \alpha_i(x_i) \neq 0 \), representing an informed prior based on previous knowledge and expert geologic opinion. The experimental result \( y_j, j \in J \) is a continuously distributed random variable. With an experiment that measures only one AVO attribute, \( R_0 \), the measurement at site \( j \) is \( y_j = R_{0,j} \in \mathcal{R} \), whereas a situation where both AVO attributes are acquired is indicated by \( y_j = (R_{0,j}, G_j)' \in \mathcal{R}^2 \). The experimental results are assumed to be Gaussian distributed with likelihoods given in Appendix B.

Figure 3 shows the AVO seismic data from a \( 5 \times 20 \) grid from the North Sea (Eidsvik et al, 2004). This data is somewhat upscaled from the original dataset and each gridcell is of size \( 100^2 \text{m}^2 \). The domain in Figure 3 is hence of size \( 500\text{m} \times 2000\text{m} \). For parameter estimation of interaction parameter \( \beta \) we assume that this field is similar to the one under consideration and use the data for this purpose. We estimate \( \beta \) in equation (1) based on these AVO seismic data and fixed values of \( \alpha_i(x_i) \). The maximum likelihood estimate of \( \beta \) is computed by evaluating the marginal likelihood \( p(y) \) for a set of \( \beta \) values, see Appendix A. In Figure 4 we display \( p(y) \) as a function of \( \beta \), and see that the maximum likelihood estimate is about 0.9. In the following calculations we treat this parameter as fixed.

Now recall that we do not have the extracted AVO attributes for the reservoir. We will compute the value of information for some experimental configurations to identify which attribute(s) to extract. We do, however, suppose that geologic knowledge is present. We assess a realization of the field from a hypothetical geologist, along with the confidence in the assessment using a likelihood function at all cells. We obtain the point-wise function \( \alpha_i(x_i) \) from geologic expert opinion. This knowledge assigns high \( \alpha_i(1) \) for central cells and the South-East flank, larger \( \alpha_i(2) \)
Figure 3: Seismic data from the Glitne reservoir in the North Sea. The display shows two seismic attributes $R_0$ (top) and $G$ (below). Each grid cell is $100\text{m} \times 100\text{m}$ and the domain covers an area of $500\text{m} \times 2000\text{m}$.

Figure 4: Maximum likelihood estimation of $\beta$. The graph is obtained by evaluating the marginal likelihood $p(y)$ using the Glitne dataset for several $\beta$ values between 0 and 1.5. The maximum is near 0.9.

and $\alpha_i(3)$ in other areas. In Figure 5 we show the marginal prior probabilities of the favorable oil sand.

We demonstrate the value of information for the full test, i.e. extracting seismic attributes at every grid cell $i = 1, \ldots, N$, and for two partial tests covering only parts of the domain. The
Figure 5: Prior probability of oil sand. The image shows \( p_i(1), i = 1, \ldots, 100 \). Note that oil sand is more likely in the central parts and in the South-East where the pointwise prior terms \( \alpha_i(1) \) are larger.

Figure 6: Cell locations for two kinds of partial tests. Partial test 1 covers 12 cells in the central part (shaded blue), while partial test 2 covers 15 cells in the South-East (shaded red). In comparison the full test covers all 100 cells.

two partial tests are shown in Figure 6. Partial test 1 covers the central parts of the domain, while partial test 2 mostly covers the south-eastern parts. These two spatial domains are believed to be the most likely candidate areas for oil, as specified by the informative prior. For each of the tests we consider using only the \( R_0 \) seismic attribute, or both \( (R_0, G) \) seismic attributes. Altogether this entails six testing configurations.

For evaluating the decision-analytic expressions we use the algorithm at the end of Section 4. We briefly illustrate how we compute the VFE for this example. First we generate \( M = 10000 \) realizations of the MRF \( x \), two of these realizations are illustrated in Figure 7 (top). Next, test results are generated for each realization of the MRF. For each of the six configurations the test result will be generated from different likelihood functions depending on the particular spatial design and on the seismic attributes. In Figure 7 (middle) we illustrate the test results of \( R_0 \) for a full test conditional on the MRF realizations in Figure 7 (top). Finally, based on the test results, we compute the marginal posterior probability of the favorable state oil at each gridcell. These marginals are used when computing the VFE in equation (17). In Figure 7 (bottom) we show the marginal probabilities of oil for each of the two test results in Figure 7 (middle). Note that the
The marginal probability of oil sand in Figure 7 (left, bottom) is small in the North-West, even though the realization Figure 7 (left, top) shows oil sand in that part. This occurs since oil sand and shales are almost indistinguishable based on $R_0$ data alone (see Appendix B), and because the shale in this region of the field is more likely a priori.

We assume a cost of $C = $2 million for drilling a well at a cell, and a revenue of $R = $5 million if a well discovers oil sand at a cell. Note that these are costs and revenues per cell and are obtained from back-of-the-envelope calculations. They would be obtained from management and petroleum engineers in a real-world case study. We use the volume of a cell, the assumed porosity and fraction of recoverable oil and the price of oil to estimate the revenue.

Results of the tests and attribute selection schemes are displayed in Table 1. The specific course of action regarding experimentation depends on the cost of each configuration, which would depend on factors such as whether the reservoir is offshore or not, etc. It seems likely that in this case, purchasing both attributes over the entire field may be most beneficial. The VOE and COK values are high in our example, particularly when both the attributes $(R_0, G)$ are acquired over the
Table 1: Value of experiment (VOE) and chance of knowing (COK) for seismic AVO attributes $R_0$ and $(R_0, G)$ and for different experimental configurations; complete test, partial tests 1 and 2.

<table>
<thead>
<tr>
<th></th>
<th>Complete test</th>
<th>Partial test 1</th>
<th>Partial test 2</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>VOE (million $)</td>
<td>COK</td>
<td>VOE (million $)</td>
</tr>
<tr>
<td>$R_0</td>
<td>4.91</td>
<td>0.07</td>
<td>0.48</td>
</tr>
<tr>
<td>$(R_0, G)$</td>
<td>35.94</td>
<td>0.51</td>
<td>1.93</td>
</tr>
</tbody>
</table>

entire field. This is because decisions regarding several cells in the field can be strongly affected by the experimental result. The field itself seems to be very lucrative, and has a prior value of around $12 million. We would expect COK values to be much lower in practice because the magnitude of revenues and costs typically result in a very high VOPI in the petroleum industry. In our example, VOPI is around $70 million. Depending on the costs involved, partial test 2 may be preferred over partial test 1 - the numbers indicate that intelligent experimental positioning can be extremely valuable. Also, again depending on the costs, a partial test with both attributes can be better than a complete test with only one attribute. The decision-analytic approach naturally encourages creative alternatives for decisions related to experimentation. There are often several alternatives regarding the kind and specific location of the experiment, and these can be discussed at length by the stakeholders.

6. Conclusions and Future Research

In this paper, we propose a decision-analytic approach to valuing experiments performed in situations that naturally exhibit spatial dependence. We incorporate dependence by modeling the system as a two dimensional grid, and by treating the joint prior distribution of the distinction of interest as a Markov random field. The experimental decision is based on the value of information in our framework. We illustrate our methodology with the help of two examples. Our example from conservation biology indicates that spatial dependence can play a significant role in determining the value of an experiment. The petroleum exploration example is a demonstration of how our framework can be applied in real-world case studies. The results suggest that intelligent experimental design can add substantial value to the decision situation. Moreover, decisions regarding the choice and location of experiments should be analyzed by a multi-disciplinary task-force. Our methodology inspires a collaborative effort by aggregating the experimental likelihood, prior spatial model and downstream decisions and associated values into a single meta-model.

Decision trees and similar tools have previously been used to compute the monetary value of information in spatial decision making. These techniques aggregate distinctions to a global level and therefore excessively simplify several important aspects of the decision problem, including the alternatives, experimental likelihood and value assessments. Employing a formulation with a grid incorporates spatial dependence, manoeuvres the spatial decision making problem to a more realistic front, and encourages creative alternatives for experimental design.

There are several possible directions for further research. One direction involves statistical issues. For instance, other prior models like Gaussian models can be investigated. Hierarchical Bayesian models could also be captured within our framework, such as a prior on $\beta$, but we have
not pursued this idea here. From the computational point of view, algorithms for larger grid sizes should be explored. In our framework the recursive method works best for moderate size grids, say $n_1 < 10$. Block updating using Gibbs sampling is a possible way to estimate value of information for larger grids. Other simulation techniques could also be considered; specific techniques may possibly be suitable for specific models. Finally, the decision-analytic assumptions can be relaxed or modified in future work. We currently focus on the marginal probabilities in our simple framework. In general, the value from the field can depend on the joint distribution of the distinction of interest. Sequential decisions and even sequential experimentation are other avenues that can be examined. Decisions regarding experimentation should be subjected to intensive analysis in all domains, particularly in realms where there is the additional complexity of spatial dependence.

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Appendix A: Recursive computations for Markov random fields (MRFs).

Let \( \mathbf{x} = (x_1, \ldots, x_N) \) be a categorical MRF on the two dimensional regular grid. Here, \( N = n_1n_2 \) is the total number of grid nodes, \( n_1 \) is the shorter direction (say North) and \( n_2 \) is the longer direction (say East). Assume that each \( x_i \in \{1, \ldots, d\}, \ i = 1, \ldots, N \), i.e. the categorical values can take \( d \) possible colors. Suppose the grid nodes are numbered sequentially from North-West so that \( x_1 \) is the categorical value in the North-West, \( x_{n_1} \) in the South-West, \( x_{n_1(n_2-1)+1} \) in the North-East, and \( x_N \) in the South-East. See Figure 8 for an example of a grid and the indexing of cells.

![Grid and Indexing](image)

Figure 8: Illustration of a \( 3 \times 3 \) grid and the indexing of cells. For an Ising model the full conditional probabilities at cell 5 depend only on the outcomes at the four nearest neighbors (shaded colors).

The MRF probability function is written as

\[
p(\mathbf{x}) = \frac{\exp[\beta \sum_{i \sim j} I(x_i = x_j) + \sum_i \alpha_i(x_i)]}{z} = \frac{h(\mathbf{x})}{z},
\]

(20)

where \( i \sim j \) means all neighboring pairs, \( \beta \) and \( \alpha_i(l), \ i = 1, \ldots, N, \ l = 1, \ldots, d \) are model parameters. This is the simplest MRF and is known as the Ising model, where the neighbors of an interior node \( i \) are defined by \( i + 1, i - 1, i - n_1, \) and \( i + n_1 \), see Figure 8. If node \( i \) is on the edge or is a corner node, some of these neighbors vanish. The normalizing constant \( z \) is given by

\[
z = \sum_{x_1=1}^{d} \cdots \sum_{x_n=1}^{d} h(\mathbf{x}).
\]

(21)

Note that this normalizing constant is a function of the model parameters. Location specific parameters \( \alpha_i(l) \) can be functions of data \( y_i \) via the likelihood term, i.e. \( \alpha_i(x_i) = \log p(y_i|x_i) \),
\[ x_i \in \{1, \ldots, d\}. \] The density in equation (20) is then a posterior \( p(x|y) \), and the normalizing constant depends both on parameters and the data. The marginal likelihood of data is given by

\[
p(y) = \frac{p(y|x)p(x)}{p(x|y)} = \frac{\prod_j p(y_j|x_j)h^1(x)/z^1}{h^2(x)/z^2} = \frac{z^2}{z^1},
\]

(22)

where \( h^1(x) \) and \( z^1 \) are defined by \( \alpha_i(x_i) \) terms including only prior information, while \( h^2(x) \) and \( z^2 \) are defined by both prior information and the \( \log p(y_j|x_i) \) likelihood terms. Hence, the functional expressions depending on \( x \) cancel and the marginal likelihood equals the ratio of the normalizing constants in posterior and prior. For parameter estimation of \( \beta \) we evaluate the marginal likelihood for a set of parameter values and find the maximum likelihood over this set.

The probability function for \( x \) in equation (20) can be written sequentially as:

\[
p(x) = p(x_1|x_2, \ldots, x_n)p(x_2|x_3, \ldots, x_N) \ldots p(x_{N-1}|x_N)p(x_N)
= p(x_1|x_2, \ldots, x_{1+n_1})p(x_2|x_3, \ldots, x_{2+n_1}) \ldots p(x_{N-1}|x_N)p(x_N)
= \frac{h(x_1|x_2, \ldots, x_{1+n_1})h(x_2|x_3, \ldots, x_{2+n_1}) \ldots h(x_{N-1}|x_N)h(x_N)}{z},
\]

(23)

where we use the Markov property, but choose to condition on all buffer variables in the sequential line up. The buffer is of length \( n_1 \) in this case. It gets shorter in the last (easternmost) column. The terms in expression (23) are defined by

\[
h(x_1|x_2, \ldots, x_{1+n_1}) = \exp\{\beta[I(x_1 = x_2) + I(x_1 = x_{1+n_1})] + \alpha_1(x_1)\} \quad \text{for the first location,}
\]

then goes on for \( x_2, x_3 \) and so on, until \( h(x_{N-1}|x_N) = \exp\{\beta[I(x_{N-1} = x_N) + \alpha_{N-1}(x_{N-1})]\} \) and \( h(x_N) = \exp\{\alpha_N(x_N)\} \).

We first illustrate a method for recursive forward computation of the normalizing constant \( z \) in equation (21). This method follows Reeves and Pettitt (2004), and \( z \) is computed by summing out one variable at a time. The recursion starts by

\[
z_1(x_2, \ldots, x_{n_1+1}) = \sum_{x_1=1}^d h(x_1|x_2, \ldots, x_{1+n_1}),
\]

(24)

since \( x_1 \) is only involved in the first term of the sequential formulation in equation (23). The recursive calculation continues by using the equation that for general \( i \leq N - n_1 \)

\[
z_i(x_{i+1}, \ldots, x_{i+n_1}) = \sum_{x_i=1}^d h(x_i|x_{i+1}, \ldots, x_{i+n_1})z_{i-1}(x_i, \ldots, x_{i+n_1-i}).
\]

(25)

The terms in \( (x_{i+1}, \ldots, x_{i+n_1}) \) takes one value for every buffer configuration, and with \( d \) colors we have \( d^{n_1} \) possible configurations. As the buffer length gradually decreases in the last column, the number of possible configurations gets smaller, and at the final step \( N \) we calculate

\[
z = z_N = \sum_{x_N=1}^d h(x_N)z_{N-1}(x_N),
\]

(26)

which is the normalizing constant in equation (21).
We next demonstrate a recursive backward sampling algorithm for drawing $x$ from the probability function in equation (20). The value of $x_N$ is sampled from probability vector

$$p_N(x_N) = \frac{1}{z} \sum_{x_1=1}^{d} \ldots \sum_{x_{N-1}=1}^{d} h(x)$$

$$= \frac{1}{z} h(x_N) z_{N-1}(x_N), \quad x_N \in \{1, \ldots, d\}.$$  \hspace{1cm} (27)

where the sequential normalizing constants evaluated in equation (25) and (26) are used. We continue in this manner; generating $x_{N-1}$ conditional on the sample of $x_N$ from probability vector

$$p(x_{N-1}|x_N) = \frac{\sum_{x_1=1}^{d} \ldots \sum_{x_{N-2}=1}^{d} h(x)}{zp(x_N)}$$

$$= \frac{h(x_{N-1}|x_N) z_{N-2}(x_N, x_{N-1})}{z_{N-1}(x_N)}, \quad x_{N-1} \in \{1, \ldots, d\},$$  \hspace{1cm} (28)

and so on for all $i = N - 2, \ldots, 1$.

We finally present a backward evaluation scheme for the marginal probabilities $p_i(x_i), i = N, \ldots, 1$. The marginal for $x_N$ is given directly in equation (27). For $N - 1$ we first arrange the joint density $p(x_{N-1}, x_N)$ and then sum out $x_N$:

$$p_{N-1}(x_{N-1}) = \frac{\sum_{x_1=1}^{d} \ldots \sum_{x_{N-2}=1}^{d} \sum_{x_{N-1}=1}^{d} h(x)}{z}$$

$$= \frac{\sum_{x_{N-1}=1}^{d} h(x_N) h(x_{N-1}|x_N) z_{N-2}(x_N, x_{N-1})}{z}, \quad x_{N-1} \in \{1, \ldots, d\}. \hspace{1cm} (29)$$

For general node $i$ this evaluation consists of a backward construction of the joint probability for the buffer of length $n_i$. The marginal for node $i$ is then evaluated by summing over all buffer configurations $x_{i+1}, \ldots, x_{i+n_i}$ for each possible value of $x_i \in \{1, \ldots, d\}$. A similar backward formula is used when computing the entropy defined by the sequential formula in equation (15).

**Appendix B: Implementation issues for the petroleum exploration example**

The two amplitude versus offset (AVO) seismic attributes that are used here are denoted as $R_0$ and $G$. The first attribute relates to the reflectivity of a seismic wave at zero angle, while the latter is associated with the reflectivity of a seismic wave as a function of angle (offset angle between emitted and received signal). If one acquires only $R_0$, there is no information about the variation of the reflected response as a function of angle. The seismic reflectivity is connected to the rock and fluid composition of the subsurface. These relationships are quite well known in rock physics, see e.g. Avseth et al. (2005), and are typically modeled as a hierarchy of physical attributes such as pressure and shear wave velocity and density.

In Eidsvik et al. (2004) statistical relationships for each level of the hierarchy of physical attributes was specified. We use these statistical relationships in a Monte Carlo setting to fit a Gaussian likelihood model to the AVO seismic data, conditional on oil sand, brine sand and shale. For the case with only $R_0$ the likelihood equals

$$p(y_j|x_j) = \text{Normal}[\mu_1(x_j), 0.06^2], \quad y_j = R_{0,j}, \quad j \in J,$$  \hspace{1cm} (30)
where $\mu_1 = (0.03, 0.08, 0.02)$. For the case with both attributes $R_0$ and $G$, the likelihood equals

$$p(y_j|x_j) = \text{Normal} \left\{ [\mu_1(x_j), \mu_2(x_j)], \begin{bmatrix} 0.06^2 & -0.007 \\ -0.007 & 0.17^2 \end{bmatrix} \right\} 
\begin{bmatrix} R_{0,j} \\ G_j \end{bmatrix}, \quad j \in J, \quad (31)$$

where $\mu_2 = (-0.21, -0.15, 0)$. The off-diagonal entry in the covariance matrix in equation (31) corresponds to a correlation between $R_0$ and $G$ of about $-0.7$. In these equations we use $x_j \in \{1, 2, 3\}$; 1 corresponds to oil sand, 2 is brine sand, and 3 is shale.