Workshop Report on Methods for R&D Portfolio Analysis and Evaluation

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Contract No. DE-AC36-08GO28308

Technical Report
NREL/TP-6A20-75314
September 2020

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Suggested Citation
Bush Brian, Rebecca Hanes, Chad Hunter, Caroline Hughes, Maggie Mann, Emily Newes, et al. 2020. *Workshop Report on Methods for R&D Portfolio Analysis and Evaluation*. Golden, CO: National Renewable Energy Laboratory. NREL/TP-6A20-75314. https://www.nrel.gov/docs/fy20osti/75314.pdf.

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303-275-3000 • www.nrel.gov

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This work was authored in part by the National Renewable Energy Laboratory, operated by Alliance for Sustainable Energy, LLC, for the U.S. Department of Energy (DOE) under Contract No. DE-AC36-08GO28308. Funding provided by U.S. Department of Energy Office of Efficiency and Renewable Energy Strategic Priorities and Impact Analysis Office. The views expressed herein do not necessarily represent the views of the DOE or the U.S. Government.

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List of Acronyms

AAAS	American Association for the Advancement of Science
CILSS	Comité permanent inter-Etats de lutte contre la sécheresse dans le Sahel
CIPDSS	Critical Infrastructure Protection Decision Support System
CSM	Colorado School of Mines
DIW	German Institute for Economic Research
DOE	U.S. Department of Energy
EERE	Office of Energy Efficiency & Renewable Energy
EPA	Environmental Protection Agency
IDSS	Institute for Data, Systems, and Society
IEISS	Interdependent Energy Infrastructure Simulation System
IGERT	Integrative Graduate Education and Research Traineeship
INFORMS	Institute for Operations Research and the Management Sciences
IPCC	Intergovernmental Panel on Climate Change
LANL	Los Alamos National Laboratory
LBD	learning by doing
MIT	Massachusetts Institute of Technology
NOAA	National Atmospheric and Oceanic Administration
NREL	National Renewable Energy Laboratory
NTNU	Norwegian University of Science and Technology
OSTP	Office of Science and Technology Policy
OTA	Office of Technology Assessment
PG&E	Pacific Gas & Electric
R&D	research and development
RAND	Research and Development
STREAM	Systematic Technology Reconnaissance, Evaluation and Adoption Methodology
SEDS	Stochastic Energy Deployment System
TRANSIMS	Transportation Analysis Simulation System
U.S.	United States
UMCP	University of Maryland-College Park
USGCRP	U.S. Global Change Research Program

Executive Summary

Motivation: Risk and uncertainty are core characteristics of research and development (R&D) programs. Attempting to do what has not been done before will sometimes end in failure, just as it will sometimes lead to extraordinary success. The challenge is to identify an optimal mix of R&D investments in pathways that provide the highest returns while reducing the costs of failure. The goal of the R&D Pathway and Portfolio Analysis and Evaluation project is to develop systematic, scalable pathway and portfolio analysis and evaluation methodologies and tools that provide high value to the U.S. Department of Energy (DOE) and its Office of Energy Efficiency & Renewable Energy (EERE). This work aims to assist analysts and decision makers identify and evaluate, quantify and monitor, manage, document, and communicate energy technology R&D pathway and portfolio risks and benefits. The project-level risks typically considered are technology cost and performance (e.g., efficiency and environmental impact), while the portfolio level risks generally include market factors (e.g., competitiveness and consumer preference).

The Workshop: The Workshop on Methods for R&D Portfolio Analysis and Evaluation convened July 17–18, 2019, at the National Renewable Energy Laboratory in Golden, Colorado, and it examined strengths and weaknesses of the various methodologies applicable to R&D portfolio modeling, analysis, and decision support, given pragmatic constraints such as data availability, uncertainties in estimating the impact of R&D spending, and practical operational overheads. Participants employed their deep expertise in approaches such as stochastic optimization, real options, Monte Carlo analysis, Bayesian networks, decision theory, complex systems analysis, deep uncertainty, and technology-evolution modeling to critique the initial example models developed by the project's core team and to conduct thought experiments grounded in real-life technology models, progress data, expert elicitation, and portfolio information. This engagement of participants' methodological expertise with the practical requirements of real-life portfolio decision support yielded ideas for improved approaches, alternative methodological hypotheses, and hybridization of methodologies that are well-grounded theoretically, computationally sound, and realistically executable given data availability and other practical constraints. These ideas will be explored in the subsequent research following this workshop.

Major Challenges: A variety of challenges were identified in work leading up to this workshop, including addressing proprietary and competitiveness concerns; establishing consistent protocols across risk analysts and external experts; assessing and addressing correlations and dependencies within and between technologies; avoiding biases such as overconfidence, confirmation, and motivation; parsing projected costs due to R&D, learning, commodity price changes, etc.; optimizing multiple, sometimes conflicting, criteria such as economic cost, environmental pollution, greenhouse gas emissions, materials use, reliability, robustness, and resiliency; and others. Furthermore, these analyses were and must be done in the context of deep uncertainty about many of the resources, technologies, markets, competitors, and numerous other factors. How risks might be perceived were also of concern: for example, if one R&D investment had only a 10% chance of success and another had 70% but with a smaller potential payoff than the first, how would decision makers respond? If key benefits of a technology are not captured in high-level portfolio evaluations—for instance, if the evaluation considered only cost and not broader metrics such as temporal and spatial availability, economic impact, or consumer

preferences—this could substantially misrepresent the value of particular R&D investments. The following discussion of key findings from the workshop generally confirmed the significance of these challenges, amplified areas of concern, and suggested avenues of research and potential solutions.

Key Issues and Discussion: Many of the major discussion issues raised by the invited participants involved better aligning modeling and analysis activities with requirements for R&D investment decision support. Models should have transparency in their assumptions and structure and treat the major determinants of R&D progress, including non-hardware or "soft" costs. Bottom-up technology-cost models were identified as a useful starting point for the development of more complex (e.g., combined) modeling approaches. Computations should estimate not only the basic economy, technology, and energy metrics, but also encompass market, societal, and qualitative impacts. There exists a pressing need for significantly improved data sources and estimation techniques to better understand the relationships between R&D investment levels and specific technological improvements.

Participants also emphasized the importance of expert elicitation as another primary foundational input to the technology cost and performance modeling. Elicitations require deliberate framing, employment of bias-reduction techniques, and careful synthesis. Advances in expert-elicitation research over the past decade and recent experiments with new elicitation modalities promise substantial improvements in the quality of these difficult elicitations for R&D investment impacts, but further investigation and evaluation of online techniques pre-elicitation interaction of experts, allowance for feedback (for example showing R&D solutions to decision makers, then iterating to adjust the selection of optimal portfolios), aggregation methods, and framing is requisite. In particular, the hypothesis that technology experts may provide better information using learning rates (or individual components of experience curves) and odds ratios rather than current costs and probabilities, especially conditional ones, requires testing. Initial experiments by several of the participants indicate the potential for online expert elicitations to provide results comparable to in-person expert elicitations while reducing costs and logistical challenges, but may require more extensive testing and quality control of the elicitation survey tool (Baker et al. 2019). Further experimentation comparing on-line and in-person expert elicitations in the context of the present study would be useful.

Conscientiously accounting for and communicating uncertainty in R&D project and portfolio evaluation is critical. Expected outcomes, distributional information (e.g., error bars, quantiles, and tornado plots), and measures of regret (via the "minimax" principle) should be estimated using ensemble methods in a real-options and deep-uncertainty context to develop robust strategies that support decision-making. Two-stage stochastic, multi-objective optimization can comprise the primary computational technique used to develop such strategies. Multistage optimization techniques beyond two-stage optimization were deemed by participants as not providing sufficient additional information to justify their increased computational intensity. Scenario-based analysis and techniques for decision-making under deep uncertainty complement stochastic optimization approaches. When probability distributions for the uncertain factors are unavailable, robust optimization is another option.

Any decision-support tool for R&D investment should assist decision makers in discovering and interpreting information that they might otherwise overlook or misinterpret, provide a relatively small set of critical criteria on which decisions can be made, and adapt to the decision-making style and concerns of the users. Presenting decision makers with a set of satisfactory portfolios in optimal risk-informed visualizations comprising both influence diagrams and quantitative plots (including those showing Pareto optimality frontiers), rather than presenting one optimal answer, can assist them in *robust decision-making* that engenders trust through increased transparency and builds intuition over complex dimensional spaces to inform decision-making. This is particularly important to decision makers who might be disinclined towards probabilistic analysis or when specific probability distributions are not readily available. Tools must allow decision-makers to alter input parameters and assumptions interactively and immediately view updated results: this entails having fast-running analytic models.

Supplemental Material: The appendix to this report include biographies of the workshop attendees, revised copies of the material presented at the workshop, fact sheets describing exploratory analyses that raise methodological issues, and an extensive bibliography of portfolio-analysis literature.

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Introduction

This report summarizes the key discussions and ideas generated at the Workshop on Methods for R&D Portfolio Analysis and Evaluation, convened on 17–18 July 2019 at the National Renewable Energy Laboratory in Golden, Colorado. The goal of the R&D Pathway and Portfolio Analysis and Evaluation project is to assist funding decision-making across technology pathways and portfolios by developing methodologies and tools for systematic, scalable pathway and portfolio analysis and evaluation. Such tools will provide high value to the U.S. Department of Energy (DOE) and the Office of Energy Efficiency & Renewable Energy (EERE) by assisting analysts and decision makers in identifying, evaluating, quantifying, monitoring, managing, documenting, and communicating the risks and benefits of prospective energy technology R&D pathways and portfolios. Key questions that these methodologies and tools must help analysts and decision makers address include the following:

- Where should the next dollar of R&D be invested to increase the likelihood of achieving desired returns at the project and portfolio levels?
    - How impactful will specific investments be in advancing a particular technology?
    - What is the likelihood that particular R&D pathways will achieve their goals?
    - At what point should R&D investment be cut or alternative pathways explored?
    - What are the opportunity costs of not investing in a research pathway?
    - What are ideal balances between supporting fewer projects with more resources as opposed to a wider range of projects with fewer resources?
- How should the portfolio be balanced taking into consideration risk, return, time, technology mix, and markets?
- How can risk scoring be made more consistent across projects, portfolios, markets, expert elicitations, and time?
- How can the results of these analyses be quantified and validated? Are the results statistically significant and reproducible, and are they robust when audited by decision makers and external experts?
- What are the most effective mechanisms for communicating these evaluations in different contexts of decision-making?

Addressing these questions can provide significant value by helping decision-makers target R&D opportunities, thereby accelerating the pace of technology development while meeting stakeholder-defined objectives, such as cost, efficiency, environmental impact, etc. They may also help external stakeholders to better understand and assist EERE and DOE R&D decisions and activities.

Challenges

The following issues were emphasized by workshop participants.

Technology modeling: Numerous tradeoffs must be considered and many modeling decisions must be made in constructing appropriately detailed technology models in support of pathway and portfolio analysis. Modeling challenges are exacerbated by the uncertain techno-economic input data (of varied quality) for speculative, nascent, and even established technologies. In order for technology modeling to be tractable, it must focus on the points of leverage for R&D investment—points of leverage which in many cases are poorly known and must be determined in consultation with experts and from exploratory analysis—and on metrics relevant for decision-making stakeholders.

Analysis approaches: Decision support analyses must account for the considerable uncertainties regarding techno-economic input parameters to models, model structure, and the response of the state of technology to R&D investments. A pragmatic method for R&D portfolio decision support must be constructed from the numerous approaches proposed in the academic literature or applied in other practical application areas. It is not obvious whether a single approach adequately meets the requirements for the type of problems considered here or whether a hybridization of techniques can combine the strengths of several methods while avoiding their weaknesses. For instance, some methods rely extensively on propagating probability distributions that originate from expert elicitations whereas other eschew distributional assumptions. The computational resources and runtime of methods vary by orders of magnitude.

Expert elicitation: Past efforts have highlighted both the necessity and challenges of eliciting expert opinions in support of technological forecasts, but there is much active research and differing schools of thought in this area. Primary challenges are the intensity of effort (overhead and resources) required by some elicitation methods, the need to correct experts' cognitive biases such as overconfidence and confirmation, and the selection of precise elicitation questions that yield ranges or distributions. Emerging variations or alternatives to classical expert elicitation such as on-line methods, patent analysis, and historical data may warrant consideration.

Data collection: Techno-economic data on R&D pathways and historical data on those pathways' progress complements the results of expert elicitation but can be similarly difficult to gather and harmonize. In particular, detailed correlations between past R&D investments and progress in specific determinants of technology performance would be invaluable for future technology forecasts. Both timeliness and detail in data pose challenges.

Portfolio analysis: Perhaps inevitably, some technology system or subsystem models may be far more detailed than others, a situation which poses challenges for meaningful consistent comparisons of disparate technologies. There is a risk that lack of information will unfairly bias portfolio decisions towards or away from emerging or high-risk technologies. Portfolio-level decisions may require the simultaneous consideration of a disparate variety of hard and soft metrics, the evaluation of numerous technology models across multiple renewable-energy and energy-efficiency domains, and the treatment of a diversity of levels of maturity.

Communication of results: The variety of decision-making questions, styles, and contexts challenges the creation of tools informing decisions. Complex risk analysis may require complex visualizations and intensive computation, but streamlined, intuitive, and rapid presentation of results may be most effective for decision support. Tools may be designed to be run interactively versus in batch mode, individually versus collectively, for point estimates versus probabilistic ones, on single versus multiple metrics, or prospectively versus retrospectively.

Approaches to Decision Support

Decisions must be framed carefully, with agreement between model-builders, analysts, and decision makers on what question is being asked and what decision is being made. Agreement on and transparency around which basic assumptions are to be used in making the decision is also critical. Any re-framing of decisions must be done carefully and deliberately, with transparency around any changes in assumptions. This clarity is necessary to determine the scope and level of detail required in the modeling effort.

A decision support tool should assist decision makers in discovering and interpreting information that they might otherwise overlook or misinterpret. The tool should provide a relatively small set of critical criteria on which decisions can be made. These criteria can be expressed as *expectations* over probability distributions of uncertain model inputs and parameters or as *regret* representing lost opportunities or opportunity cost. Both types of criteria will aid decision-makers in understanding the long-term consequences, positive and negative, of specific decisions and short-term actions. In addition to the critical criteria, a decision support tool should be able to account for institutional lock-in and be flexible enough to inform decisions made amongst a subset of available options.

Technology Analysis

Model Design

Level of detail: Attendees agreed that models should be computationally tractable and capture the most significant points of leverage for R&D investment and the metrics required for decision-making. There was no explicit agreement regarding the level of detail to include in the models. Model tractability, data availability, and user preferences were discussed as important criteria.

Bottom-up approach: There were some advocates for starting with simple, top-down modeling and perhaps including more detail as the importance of individual components or subcomponents becomes apparent. A predominance of attendees advised bottom-up, cost modeling, whereby models represent the impact of engineering properties and other technology characteristics on the cost of components and subsystems. Both engineering- and physics-based models can serve as starting points for further analysis. The level of technical detail should be adjusted to the availability of data and the metrics relevant to decision makers. Key considerations for this are the synergies between expert elicitation and model building. Workshop discussion advocated exploring how to effectively merge elements of these two approaches using existing work and how to balance these efforts to minimize overhead resources.

Staged decisions: Workshop attendees encouraged focusing on influential components, as represented graphically through tornado diagrams, and removing fixed or non-impactful components from the model in order to more clearly compete potential investments in the more influential components. Decision-making might proceed in stages, with the most impactful portfolio-level decisions being made first.

Experience Curves and Learning by Doing

Experience curves and learning by doing are important to consider in evaluating R&D impacts by setting a baseline for expert elicitation and when evaluating how the cost of a technology will adapt post R&D. Discussion in the workshop examined the importance of these experience curves from many perspectives: the choice of dependent and independent variables for the curves; the availability of data; the techniques and quality of statistical models for experience curves; and uncertainties associated with them.

Soft costs: Soft costs, which can be encompassed in learning curves, include labor such as marketing and sales for customer acquisition, permitting, and installation, and are important to consider. These are more likely to vary regionally when compared with hard costs since learning is local, and information transfers as people move and companies expand (Nemet 2019).

Experience curves and learning by doing (LBD): Some discussion supported directly modeling the impact of investments on experience curves and including this in learning rates. Challenges of this approach include determining the appropriate learning rate baselines for novel technologies and at later stages of R&D and commercialization. Thus, it is practical to include uncertainty bands when examining learning curves, to assign maximum and minimum potential learning based on past measurements along the curve (Lafond, et al., 2018).

Handling Uncertainty

Uncertainty inherent to forecasting future events is a primary source of uncertainty in R&D Pathway and Portfolio Analysis. Representing this uncertainty as probability distributions in technology cost and performance is useful in technology pathway analysis and is similarly useful in considering whether an event will occur when implementing a portfolio model, but such estimates are difficult to elicit from experts. Alternate approaches are further discussed in the Expert Elicitation section. Disagreement among experts regarding probability distributions perhaps could be avoided by techniques such as decision-making under deep uncertainty (situations lacking consensus on system models and probability distributions) and robust decision-making (iterative decision-analytic frameworks for identifying robust strategies), which do not make strong distributional assumptions. It is important to distinguish between uncertainty in the model structure versus uncertainty in the model inputs and parameters and identify which uncertainties can be controlled and by whom.

There was little interest in examining extreme outliers or “black swan” events, but some interest in considering how to incorporate such events into the analysis as low-probability, high-impact incidents.

Sensitivity analyses can assist in understanding how sources of uncertainty can impact predictions. First, the ranges of inputs should be studied to assess the uncertainty surrounding parametric estimates. For instance, can we expect cost or environmental impact estimates to be more accurate? Then, a similar study should be conducted to assess experts' uncertainty in outcomes. Finally, sensitivity analyses can be conducted on the simulation results by studying the predicted outcomes over a range of input parameter combinations.

Analysis Methodology

The models discussed in the workshop drew from fundamentally different methodologies, including Monte Carlo simulation, stochastic optimization, inverse optimization (a blend of statistics and machine learning), direct policy search, real options, robust decision-making, and decision-making under deep uncertainty. Both stochastic and inverse optimization support multistage decision-making, and there was agreement amongst workshop attendees that two stages are sufficient for the purpose of R&D pathway and portfolio decision-making. The first stage represents an optimal (potentially irreversible) decision, and the first and second stages together represent an optimal strategy. For additional details, see the presentations and fact sheets in the appendix. While a single stage is insufficiently flexible for decision-makers, additional stages beyond two quickly become too computationally complex and are thus of limited value in this context. Regardless of the model methodology, methods for dealing with multiple, potentially conflicting objectives are essential. These methods could be "flat" and involve weighting the objectives according to relative importance or be "hierarchical' and involve making successive decisions. Conversely, one objective may be highlighted with the other ones constrained to be at acceptable levels (i.e., the constraint method). Scenario-based analysis and techniques for decision-making under deep uncertainty (i.e., situations lacking consensus on system models and probability distributions) complement the explicitly probabilistic optimization approaches.

There was also agreement amongst attendees that strategies, or longer-term sets of decisions, should be robust across a wide range of scenarios that include a variety of probability distributions or intervals for parameters. A good way to choose strategies is by eliminating strategies that fail to be robust. For instance, if one strategy out-performs another across all scenarios being considered, then the out-performed strategy can be discarded as it is always dominated by the better one. This method enables decisions that avoid the worst outcomes rather than attempting to identify a best possible outcome.

Data Gathering

Data collection poses a major challenge to the R&D Portfolio Analysis modeling effort and was an important focus of the workshop discussion. There is little historical data to relate detailed R&D expenditures and specific technological improvements, so statistically significant correlations between the two are difficult to find. A majority of workshop attendees agreed on expert elicitation as a key data collection methodology for the R&D models, and discussion centered around its associated challenges.

Expert Elicitation

Challenges associated with expert elicitations are the subject of significant research as well as workshop discussion. The toy models developed in preparation for this workshop incorporate probabilities of technological advances, R&D impact on cost, and other relevant parameters. However, these factors are difficult to elicit. Conditional probabilities, such as the probability of an advance in one area enabling a subsequent advance, and branching probabilities are particularly problematic. Odds ratios predicting the relative probability of two events may be easier to elicit. There was a dominant implicit assumption that uncertainty would be represented by probability distributions. However, probability distributions (especially conditional and joint distributions) are challenging to elicit, and instead estimating ranges or moments of the distributions could prove more intuitive to experts. Such interval "ambiguity sets" could then be used in a robust optimization setting.

Elicitation Framing: Clearly and succinctly framing questions is extremely important to guide experts in obtaining pertinent data for model use. For example, the toy models developed prior to the workshop considered impacts on specific parameters affected by R&D, such as component cost. A serious challenge in expert elicitation is anchoring. Elicitations that frame questions around costs may tend to anchor on metrics, such as current costs and linear reductions, but cost reductions over time often go down learning curves which are exponential. Several attendees encouraged focusing expert elicitation on learning curve rates, such as Swanson's law for photovoltaics (Swanson 2006). Assessing experience curves for individual components poses a challenge, since experience curves are typically drawn for technologies as a whole (Lafond et al. 2018); the discussion briefly examined the possibility of combining learning curves for individual components. Workshop attendees recommended presenting experts with background and historical data to help provide context as the experts made their estimates.

Identification and Bias: Expert elicitation can be a two-stage process. A quick screening can help identify the level of knowledge and foresight possessed by each expert in order to focus questions appropriately, with additional follow-up elicitation to gain more detailed predictions if warranted. True experts must be deeply involved with the technology. Elicitations across small sets of experts are acceptable and have demonstrated high performance (Kao and Couzin 2014). Experts are often researchers with a personal and professional interest in the amount of R&D funding a field receives or are optimistic about progress in their fields, which introduce the potential for bias. Such biases need to be assessed and calibrated to make realistic predictions. There was some discussion of the employment of methods from the field of "superforecasting" (see below), which relied on expert generalists rather than on specialists in a particular technology.

Strategy: Interaction between experts can produce more accurate estimations if carefully managed. The Delphi method, for example, introduces iterative expert elicitations, interspersed with feedback from the other experts (Brown 1968). This approach has its drawbacks, particularly groupthink, and alternative approaches were discussed during the workshop, with varying levels of interactivity among experts. At the lowest level, elicitors could present experts with anonymized assessments by other experts. Facilitating discussion between experts prior to or during elicitations can encourage thoughtful engagement and help ensure that important identified information is available to all experts. This informal discussion could take place possibly online or via a wiki, or in the process of a face-to-face elicitation. At the highest level of interactivity, there was brief discussion of group model building, which could produce more accurate results. However, increasing levels of interactivity can, in turn, increase the cost of expert elicitation, which must be considered.

In-person vs. online: Constructing a platform that encourages continuous interaction could improve predictions by addressing discrepancies in assessments by directly questioning experts with differing estimates. Providing long-term feedback to experts has the potential to increase estimation accuracy over time and increase engagement by making the elicitation a more rewarding experience, as described by (Tetlock and Gardner 2016) and cited by participants. However, there are many complexities and conflicting evidence regarding digital versus in-person expert elicitation, which must be addressed (Baker et al. 2019): further experimentation comparing on-line and in-person expert elicitations is warranted.

Data processing: Once estimates have been elicited as raw data, they will need to be aggregated into usable information. Expert opinions can be averaged using Laplace's method or Bayesian techniques, and that pooling may take place either before or after further analysis. Uncertainty absorption (March and Simon 1958) provides a perhaps more qualitative avenue for abstracting expert opinion into actionable forecasts. The data processing may include removal of biases, differentially weighting each expert's estimates, discarding expert estimates determined to be problematic, or other data-cleansing procedures.

Alternatives to Subject Matter Experts: Experts involved deeply in the field do not necessarily have the prescience to predict the economic impact of their research. There was some consideration toward dispensing with experts and using experience-curve models from historical data. Another alternative raised was the use of "superforecasters". Superforecasters have excellent foresight into the likelihood of some categories of near-term future events (Tetlock and Gardner 2016). Superforecasters could prove more adept at predicting "surprise" low-probability, high-payoff technological advances, as well as more steady progress if provided with historical data to aid their predictions.

Portfolio Analysis

Metrics

A variety of metrics can be used to assess the viability of a new technology. The cost of energy and installed capacity were the main metric of interest when discussing investment impact, but investments can impact technical, environmental, and social metrics as well (Wang et al. 2009). It is difficult to combine these into a single objective, particularly since some metrics are not quantifiable, such as absorptive capacity, the ability of a company to understand and apply new information, or the ability of a company or an industry to pivot focus as new information becomes available. The impacts on these areas might be felt on different time scales, necessitating a clearly defined time frame for the evaluation of benefits.

Markets and Policy

Markets and policy influence both the impact of R&D on the cost of energy and the cost of energy itself, irrespective of research advances. As new technologies become possible, policy can be implemented to support and/or regulate their deployment. There was discussion at the workshop as to the importance of considering policy and markets, but no conclusions were drawn as to how to incorporate them into models, other than to leverage the Stochastic Energy Deployment System (SEDS) framework previously developed for EERE.[1] SEDS is an economy-wide energy model of the U.S. that focuses on explicitly simulating uncertainties in energy technology, markets, and policy using a non-equilibrium stochastic methodology that employs system-dynamics modeling techniques and stochasticity in input parameters and system evolution.

Niche markets are beneficial to industries beginning commercialization, and national or international innovative systems can spur technological progress and drive costs down the learning curve, as was the case in the solar industry (Nemet 2019). Policy support for technologies can create constituencies that support a technological program and enable R&D persistence. Conversely, policy might stymie technology deployment and diminish potential investment impact. R&D investment strategies should hedge against policy changes and volatile markets, which add importance to the absorptive capacity of a technology. Skeptical and contrarian investors, issues of consumer response, and other decision factors make cost impact difficult to predict, and more consideration must be taken regarding how to address them in the analysis at the project level and at the portfolio level. Government investment can signal to external investors that a technology has potential and spur additional investment, injecting uncertainty into the total value of R&D investment. The interaction between policy, cost, and R&D progress poses a significant challenge to project evaluation.

Communication and Interaction with Stakeholders

At its core, the R&D Pathway and Portfolio Analysis project strives to aid decision makers in making impactful investments. Communicating results is a key factor in achieving this goal. There was discussion among workshop attendees as to whether a tool that serves this purpose could be standalone or would need to be used by a decision-maker and an analyst collaboratively. However, discussion provided insight into considerations essential to designing such tools to benefit public-sector decision-makers and private-sector investors. The aforementioned SEDS tool is a publicly available example of an uncertainty-aware, energy-system, decision-support model.

Visualization: Elegant interfaces with influence diagrams and limiting information to that necessary and sufficient to answer questions can help clarify the decision options (Oviatt 2006). Presenting decision makers with a set of satisfactory portfolios, rather than one optimal answer, can assist in robust decision-making and provide increased transparency, which is particularly important to decision makers who might be hesitant to embrace probabilistic analysis.

[1] See https://www.nrel.gov/analysis/seds/ for details and for access to the SEDS model.

Interactivity: Elegant models that are only as complex as necessary will compute results more quickly and increase the potential for interactivity. Interactive tools allow decision makers to explore the model by experimenting with, and challenging, assumptions and approaches as they gain insight into the decision landscape. This could also be helpful after priority investment strategies have been selected in order to better understand options for distributing the remainder of the R&D investments across the portfolio.

Additional resources: Decision makers might also benefit from additional information to supplement model results. This could include maps, historical data, current prices, and relevant policies, which might also be provided to experts during the elicitation period. Providing decision makers with similar information, although not directly part of the modeling effort, could encourage model adoption by providing users with the data that influenced model construction and help them make decisions optimized to their own objectives.

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Appendix

Workshop Prospectus

Motivation: The National Renewable Energy Laboratory (NREL) and the U.S. Department of Energy's Office of Energy Efficiency and Renewable Energy (EERE) are pursuing the development of systematic, scalable methodologies and tools for R&D pathway analysis that will assist decision-making across energy research activities. Such methodologies and tools aim to identify and evaluate, quantify and monitor, and document and communicate energy technology R&D pathway risks and benefits, answering questions such as the following:

- Where should the next dollar of R&D be invested to increase the likelihood of achieving specific goals at the project, program, and portfolio levels?
- Under what circumstances is it better to support fewer projects with more resources per project versus a wider range of projects with fewer resources?
- When should R&D investment be redirected to explore alternative pathways?
- What is the likelihood that particular R&D pathways and resourcing will achieve their goals?

To date, the project team has surveyed the literature, evaluated methodologies, and performed computational experiments for several alternative approaches to address these issues. The team believes that the realization of a high-impact R&D portfolio decision-support capability will require carefully crafting a practical approach grounded in state-of-the art methodologies and theories for portfolio modeling, optimization, scenario analysis, and decision under uncertainty.

Goal: The workshop participants will evaluate strengths and weaknesses of the various methodologies applicable to R&D portfolio modeling, analysis, and decision support, given pragmatic constraints such as data availability, uncertainties in estimating the impact of R&D spending, and practical operational overheads. Participants will employ their deep expertise in approaches such as stochastic optimization, real options, Monte Carlo analysis, Bayesian networks, decision theory, complex systems analysis, deep uncertainty, and technology-evolution modeling to critique the initial example models developed by the project's core team and to conduct thought experiments grounded in real-life portfolio information, technology models, and progress data. This engagement of participants' methodological expertise with the practical requirements of real-life portfolio decision support will yield ideas for improved approaches, alternative methodological hypotheses, and hybridization of methodologies that are well grounded theoretically, computationally sound, and realistically executable given data availability and other practical constraints.

Format: This highly interactive one and one-half day workshop emphasizes dialog, exploration, and evaluation of methods for R&D project and portfolio modeling and analysis. It will combine presentations of best practices from multiple methodological points of view and data-informed experimentation to conceptualize hybrid approaches.

Product: Following the workshop, participants will have the opportunity to prepare papers building on the results of the workshop and other information for publication in a special issue of a peer-reviewed journal. These papers will advance efforts to identify, develop, and enable implementation of an R&D portfolio decision-support capability by exploring the strengths, weaknesses, and potential hybridization of methodologies for real-life, risk-aware R&D project and portfolio evaluation and decisions.

Workshop Agenda

July 17		
5:30–7:00	Reception at SpringHill Suites by Marriott Denver West/Golden 1315 Colorado Mills Pkwy, Lakewood, CO 80401	
July 18		
8:00	Breakfast	
8:30	Welcome, goals, and format	Sam Baldwin Brian Bush Maggie Mann
8:40	Introductions	All
9:00	Experiences to date and practical realities	Sam Baldwin
9:15	Participant presentations and Q&A – part I	
	Retrospective: Conclusions from 2010 Workshop on RD&D Planning	Leon Clarke
	Observations on R&D investment from empirical work on technological change	Greg Nemet
	Robust Portfolio Decision Analysis	Erin Baker
	RAND Methods for R&D Portfolio Selection	Steven Popper
10:30	Break	
10:45	Participant presentations and Q&A – part II	
	Real Options and Stochastic Dynamic Programming for Energy R&D Projects	Steve Gabriel
	How accurate were past expert elicitations on energy technologies? How can we do better?	Max Henrion
	Uncertain Clean Energy R&D in Integrated Assessment Models: Expert Elicitation and Approximate Dynamic Programming to the Rescue	Giacomo Marangoni
	Experience curve forecast distributions and applications	Rupert Way
	Technology cost evolution modeling: Lessons learned from photovoltaics and nuclear	Magdalena Klemun
12:15	Lunch	
	Molecules to Markets	Doug Arent
1:00	Exploratory modeling (“toy models”)	
	Stochastic Energy Deployment System (SEDS)	Emily Newes
	Stochastic Optimization for Biorefinery R&D and Process Design	Rebecca Hanes
	Monte Carlo Modeling for Optimization of R&D Investment	Caroline Hughes
	Real Options Applied to a Polysilicon PV Cell Model	Brian Bush

	Summary of Lessons Learned and Puzzles	Brian Bush
2:00	Questions and critique of exploratory modeling	All
2:30	Break	
2:45	Reflections on provisional conclusions/recommendations	Invitees
4:30	Summary and plan for next morning	All
5:00	Adjourn	
6:30	Dinner at Table Mountain Grill 1310 Washington Ave, Golden, CO 80401	
July 19		
8:00	Breakfast	
8:30	Reflections on previous day and areas of general agreement	All
9:00	Thought experiments and comparison/hybridization of approaches	All
10:15	Break	
10:30	Provisional conclusions/recommendations	Invitees
12:00	Lunch	All
12:45	Planning for special issue of journal and follow-up activities	All
1:30	Adjourn	

Biographies of Attendees

Doug Arent

Doug Arent is the Deputy Associate Lab Director of the Scientific Computing and Energy Analysis Directorate at the National Renewable Energy Laboratory (NREL). In addition to his NREL responsibilities, Arent is Senior Visiting Fellow at the Center for Strategic and International Studies, serves on the American Academy of Arts and Sciences Steering Committee on Social Science and the Alternative Energy Future, is a member of the National Research Council Committee to Advise to U.S. Global Change Research Program (USGCRP), and is a Member of the Keystone Energy Board. Arent is the Editor in Chief for *Renewable Energy Focus* and is Associate Editor for the journal *Renewable and Sustainable Energy Reviews*. Arent serves on the World Economic Forum Future of Electricity Working Group and is a member of the International Advisory Board for the journal *Energy Policy* and for Energy Academy Europe.

Arent was a Coordinating Lead Author for the 5th Assessment Report of the Intergovernmental Panel on Climate Change (IPCC). He has been a member of Policy Subcommittee of the National Petroleum Council Study on Prudent Development of North America Natural Gas and Oil Resources, served from 2008 to 2010 on the National Academy of Sciences Panel on Limiting the Magnitude of Future Climate Change, and also served on the Executive Council of the U.S. Association of Energy Economists.

His research interests are centered in energy and sustainability, where he has been active for more than 30 years. He has published extensively on topics of clean energy, renewable energy, power systems, natural gas, and the intersection of science and public policy. Arent has a Ph.D. from Princeton University, an MBA from Regis University, and a Bachelor of Science from Harvey Mudd College in California.

Erin Baker

Erin Baker is Associate Dean for Research at the College of Engineering; the Armstrong Professional Development Professor; and Professor of Industrial Engineering and Operations Research at University of Massachusetts, Amherst. She is the Director of the Wind Energy Fellows, a follow-on from the NSF-funded IGERT: Offshore wind energy engineering, environmental impacts, and policy. She has a Ph.D. in Engineering-Economic Systems & Operations Research from the department of Management Science and Engineering at Stanford University, and a B.A. in Mathematics from U.C. Berkeley. Her research is in decision-making under uncertainty applied to the field of energy and the environment, with a focus on publicly funded energy technology Research and Development portfolios in the face of climate change. She has received grants from the National Science Foundation, the U.S. E.P.A., NOAA, the U.S. Department of Energy, the Sloan Foundation and others. She has given invited keynote talks at WINDFARMS in Madrid and the International Energy Workshop in College Park, Maryland. She is on the editorial boards of Energy Economics, and is an Associate Editor of IISE Transactions and Decision Analysis.

Sam Baldwin

Sam Baldwin is a PhD. Physicist and has served as the Chief Scientist for the Office of Energy Efficiency and Renewable Energy, U.S. Department of Energy (DOE) since 2000. At DOE, he also spent three years on detail to the Office of the Under Secretary for Science and Energy, leading the Quadrennial Technology Review 2015 on R&D opportunities for the Science and Energy programs at DOE, coordinating crosscutting R&D teams, and conducting portfolio analysis. In previous positions he has served with the White House Office of Science and Technology Policy (OSTP), the National Renewable Energy Laboratory (NREL), the Congressional Office of Technology Assessment (OTA), Princeton University, the Sahelian Anti-Drought Committee (CILSS) in West Africa, the U.S. Senate, and elsewhere. He is the author or coauthor of more than a dozen books and monographs at DOE, OSTP, OTA, and elsewhere, and more than 30 papers and technical reports on energy technology and policy, physics, and other issues. He was elected as a Fellow of the American Association for the Advancement of Science in 2007.

Brian Bush

Brian W. Bush is a simulation scientist in the Strategic Energy Analysis Center at the National Renewable Energy Laboratory (NREL) and a member of NREL's Science Advisory Committee. He has led and collaborated on numerous multi-domain energy-infrastructure modeling, simulation, and analysis projects. For eight years he led NREL's Biomass Scenario Model project, a system-dynamics simulation of the cellulosic biomass-to-biofuels supply chain, and its Scenario Evaluation & Regional Analysis project, an optimization tool for regional vehicle-fueling infrastructure. For more than seventeen years prior to his arrival at NREL, he was a technical staff member in the Energy & Infrastructure Analysis Group at Los Alamos National

Laboratory. His work on TRANSIMS (the Transportation Analysis Simulation System) from 1994 to 2000 there focused on leading research on software architecture, the representation of road networks, microsimulation output collection, and data compression. More recently, he also developed computer simulations for complex phenomena such as interacting critical infrastructures and supercomputer hardware architectures. He formerly directed the Interdependent Energy Infrastructure Simulation System (IEISS) and Critical Infrastructure Protection Decision Support System (CIPDSS) projects and held the position of Thrust Area Leader for the U.S. Dept. of Homeland Security's Critical Infrastructure Protection Portfolio in its Science & Technology Directorate. He was a member of LANL's Patent Committee and its Institutional Computing Technical Committee. As a visiting scientist at the National Center for Atmospheric Research, he initiated efforts to connect simulations of weather and climate to impact models for energy and infrastructure networks. He holds a Ph.D. in Physics from Yale University, where he was a National Science Foundation Graduate Fellow, and a B.S. in Physics from the California Institute of Technology.

Leon Clarke

Dr. Leon Clarke is an expert in energy and environmental issues, with a focus on climate change, climate change mitigation strategies, energy technology options, and integrated assessment modeling. He is currently the Research Director at the Center for Global Sustainability and a Research Professor in the School of Public Policy at the University of Maryland. He formerly led the Integrated Human Earth System Science Group and directed a range of integrated assessment modeling activities at the Joint Global Change Research Institute, a collaboration between the Pacific Northwest National Laboratory and the University of Maryland. Dr. Clarke has served as an author and coordinating lead author for the Intergovernmental Panel on Climate Change (IPCC), the National Climate Assessment, and the National Research Council. He has also led a number of multi-institution studies on climate mitigation. Dr. Clarke's professional experience includes his current position, positions in two U.S. national laboratories, in energy consulting, and at an electric and gas utility. Dr. Clarke has a Ph.D. in Management Science and Engineering from Stanford University and Master's degree in Mechanical Engineering from the University of California at Berkeley.

Steve Gabriel

Dr. Steven A. Gabriel is a Full Professor in the Department of Mechanical Engineering, as well as in the Applied Mathematics & Statistics, and Scientific Computation Program at the University of Maryland-College Park (UMCP). He has also been a Co-Director then Director of the Master of Engineering and Public Policy Program. In addition, he is a Research Professor at DIW (German Institute for Economic Research) in Berlin and an Adjunct Professor at the Norwegian University of Science and Technology (NTNU) in Trondheim in the Department of Industrial Economics and Technology Management, as well as a part of the Energy Transition Programme NTNU.

His focus at University of Maryland has been on the modeling and algorithm design for engineering-economic systems combining game theory (one and two-level equilibrium problems), optimization, simulation, and other operations research/decision sciences areas. Application areas have included energy (power and natural gas), environment, transportation, project management, and telecommunications. Selected honors include: being the Gilbert White

Fellow for 2007-2008 at Resources for the Future, analyzing/developing energy equilibrium models, Washington, DC.; the 2014-2015 Professeur Invité Trottier at the Institut de l'Énergie Trottier at Polytechnique Montréal focusing on energy-economic modeling and policy questions, and a Humboldt Fellow from the German Alexander von Humboldt Foundation in cooperation with DIW (2015-2016) in energy market equilibrium modeling. Dr. Gabriel has an M.S. in Operations Research from Stanford University (1984), and an M.A. (1989) and Ph.D. (1992) in Mathematical Sciences from the Johns Hopkins University.

Rebecca Hanes

Rebecca Hanes has been a Modeling and Analysis Engineer in the Strategic Energy Analysis Center at NREL for the past four years. She specializes in supply chain modeling, life cycle assessment, optimization and system dynamics modeling of bioenergy, bioproduct and other renewable energy systems.

Max Henrion

Max Henrion is CEO and Founder of Lumina Decision Systems, in Los Gatos, California. He has 30 years' experience as a professor, decision analyst, software designer, and entrepreneur. He originated Analytica, Lumina's flagship software product about which PC Week said, "Everything that's wrong with the common spreadsheet is fixed in Analytica". Max has led decision analysis and created decision support tools for many clients in the private and public sector, including GE Energy, PG&E, Chevron, California Energy Commission, NREL, US Department of Energy, and the World Bank. He was formerly a Professor at Carnegie Mellon, Department of Engineering and Public Policy, where he continues as Adjunct Professor. He has a BA in Physics from Cambridge University, M. Design from the Royal College of Art in London, and Ph.D. from Carnegie Mellon. He has published three books including Uncertainty: A Guide to Dealing with Uncertainty in Policy and Risk Analysis (Cambridge University Press, 1990), and over 70 articles in decision and risk analysis, energy and environment, and artificial intelligence. He led a project on decommissioning oil platforms that won the 2014 Decision Analysis Practice Award from the Society for Decision Professionals. He was awarded the 2018 Frank Ramsey Medal, the highest honor of the Society for Decision Analysis.

Caroline Hughes

Caroline joined NREL's Strategic Energy Analysis Center in April 2019 after completing her M.S. in Nuclear Engineering at UC Berkeley in 2018. Her research interests include computational modeling, numerical analysis, and research-informed policy. Her current work focuses on R&D portfolio pathway analysis, decision-making under uncertainty, quantum computing, and nuclear innovation with the NICE Future initiative. Caroline earned her B.S. in Engineering Physics with a minor in Applied Math (scientific computing emphasis) from CU Boulder in 2015.

Magdalena Klemun

Magdalena Klemun is a PhD candidate at the Institute for Data, Systems, and Society (IDSS) at MIT. Her research interests are in understanding how the economic and environmental performance of technologies evolves in response to different innovation efforts, with an emphasis on the cost evolution of photovoltaic systems and nuclear power plants, and on the environmental performance evolution of natural gas technologies. Magdalena received her M.S.

in Earth Resources Engineering from Columbia University, where she studied as a Fulbright Scholar, and her B.S. in Electrical Engineering and Information Technology from Vienna University of Technology. In between her studies, she worked as an Analyst for GTM Research, a clean energy market research and consulting company.

Giacomo Marangoni

Giacomo Marangoni is a researcher in the Department of Management, Economics and Industrial Engineering at the Polytechnic University of Milan, Italy. He completed his PhD in 2017 in the same department, developing models for supporting investment decisions in the energy supply and demand sectors under uncertain technical change and sustainability concerns. For his Post-Doc, he moved to Penn State University, USA, to broaden his interests within the field of climate change risk management. There he focused on how to design robust climate policies optimizing conflicting environmental and economic objectives under deep uncertainty. Now he continues this research within Polytechnic of Milan and the RFF-CMCC European Institute on Economics and the Environment.

Margaret Mann

Margaret Mann joined NREL in 1993 and currently leads the transportation infrastructure analysis team in NREL's Transportation and Hydrogen Systems Center, working to develop and coordinate integrated R&D on infrastructure tools, analysis, data, and demonstration projects spanning multiple technology areas such as light- and heavy-duty vehicle electrification, hydrogen fuel cells, and electric vehicle grid integration. Previously she served as technical director for NREL's Clean Energy Manufacturing Analysis Center and as manager for the technology systems and sustainability analysis group in NREL's Strategic Energy Analysis Center.

During her tenure at NREL, she has contributed to the development of systematic methods for credible and objective technology analysis. She has conducted technoeconomic analyses of over fifty energy technologies, including power generation from renewables, distributed generation, battery storage, and transportation. Additionally, she has performed numerous environmental life cycle assessments and supply chain analyses to determine the big-picture impacts of renewable and energy-efficient systems and has developed resource use characterization methodologies for analyzing the various and competing uses of limited resources such as water, land, materials, and installed infrastructure.

Gregory Nemet

Gregory Nemet is a Professor at the University of Wisconsin–Madison in the La Follette School of Public Affairs. He teaches courses in energy systems analysis, policy analysis, and international environmental policy. Nemet's research focuses on understanding the process of technological change and the ways in which public policy can affect it. He received his doctorate in energy and resources from the University of California, Berkeley. His A.B. is in geography and economics from Dartmouth College. He received an Andrew Carnegie Fellowship in 2017 and used it to write a book on how solar PV provides a model for low carbon innovation: "How Solar Energy Became Cheap" Routledge 2019.

Emily Newes

Emily is the Resources and Sustainability Group Manager in the Strategic Energy Analysis Center at NREL and specializes in system dynamics modeling. She has 15+ years of experience in energy modeling, analysis, and data. Emily received a BA in Mathematical Economics from Colgate University and an MS in Mineral Economics with a focus in Operations Research at the Colorado School of Mines. Prior to joining NREL, Emily was the primary research manager at Platts.

Alexandra Newman

Alexandra Newman is a professor in the Mechanical Engineering Department at the Colorado School of Mines (CSM). Prior to joining CSM, she was a research assistant professor at the Naval Postgraduate School in the Operations Research Department. She obtained her BS in applied mathematics at the University of Chicago and her PhD in industrial engineering and operations research at the University of California at Berkeley. She specializes in deterministic optimization modeling, especially as it applies to energy and mining systems, and to logistics, transportation, and routing. She received a Fulbright Fellowship to work with industrial engineers on mining problems at the University of Chile in 2010 and was awarded the Institute for Operations Research and the Management Sciences (INFORMS) Prize for the Teaching of Operations Research and Management Science Practice in 2013.

Mark Paich

Mark Paich has a doctorate degree in System Dynamics from MIT, a master's degree in Economics from the University of Colorado, a BA in Economics from Colorado College, 30+ years of teaching experience at Colorado College and MIT, and is widely recognized as one of the premier practitioners of the System Dynamics approach and leading proponent of its associated simulation tools over the last four decades. Mark has been published in Management Science, Interfaces, and the Sloan Management Review, and his work has been featured prominently in *Business Dynamics: Systems Thinking and Modeling for a Complex World* (Sterman, McGraw-Hill/Irwin, 2000), The Fifth Discipline Field Book (Senge, Currency Press, 1994), and *Surviving Transformation: Lessons from GM's Surprising Turnaround* (Barabba, Oxford University Press, 2004).

Mark has been honored by the System Dynamics Society with both the Applications Award (for his work at General Motors in launching the OnStar project, which also placed 2nd in the Edelman Competition for the best work in operations research and management science) and the Forrester Award (for his authorship of *Pharmaceutical Product Branding Strategies: Simulating Patient Flow and Portfolio Dynamics"* published by Informa Healthcare; 2nd edition March 2009).

In the late 1990s Mark helped build a successful modeling practice as a Senior Specialist at McKinsey & Company, and his leadership at his current position at PWC has resulted in the dramatic expansion of their Analytics and Simulation function to address complex, dynamic issues of strategic interest to PWC clients. In addition, Mark has co-founded two successful boutique System Dynamics consulting firms, and has taught/mentored an inordinate number of practitioners currently utilizing the methodology and leveraging the power of modern simulation approaches.

Steven Popper

Steven W. Popper (PhD, Economics, U. of California, Berkeley) is a RAND Senior Economist and Professor of Science and Technology Policy in the Pardee RAND Graduate School. His work on micro level economic transition focuses on the area of technological change. From 1996 to 2001 he was the Associate Director of RAND's Science and Technology Policy Institute (S&TPI) which provided research and analytic support to the White House Office of Science and Technology Policy and other agencies of the executive branch. His S&TPI work included principal authorship of the Fourth U.S. National Critical Technologies Review, advice on federal R&D portfolio decision-making for the National Science Board, and authorship of Presidential transition documents on S&T issues of national importance. He is a AAAS Fellow and served as the chair of its section on industrial science and technology. Dr. Popper's work on strategy development and foresight has focused on the problem of planning under conditions of deep uncertainty He is co-developer of Robust Decision Making, a methodological framework for analytical decision support under deep uncertainty. He also led the team which developed the Systematic Technology Reconnaissance, Evaluation and Adoption Methodology (STREAM) for the Transportation Research Board of the National Research Council to provide support to local public agencies in making informed, mission-specific adoption decisions over innovative technologies. Among his current projects, he is assisting the US Air Force on systematic methods for identifying potential "game changing" technologies. Dr. Popper is currently the chair for education and training of the international Society for Decision Making under Deep Uncertainty.

Rupert Way

Rupert is a postdoctoral researcher at the Institute for New Economic Thinking at the University of Oxford. He has a background in mathematics, is interested in sustainability, technological change and society, and now works on energy system modelling, technology forecasting and decision-making under uncertainty. His recent work has focused on applying portfolio theory to groups of technologies undergoing progress subject to uncertainty, in order to understand how historical progress trends, technology characteristics and risk aversion affect optimal resource allocation among competing technologies. The methodology developed gives quantitative insight in to the question of when resources should be concentrated in a smaller number of projects rather than spread more thinly over a larger number. He is currently working on applying these tools in the context of the global energy system, investigating how energy technology costs and total system costs are likely to evolve in different scenarios, and exploring the implications regarding which technologies to bet on now to give the best chance of a low cost energy transition.

Workshop Presentations

Selected presentations made at the workshop are available online at <https://bit.ly/3jUj94D>.

- Experiences to Date and Practical Realities—Sam Baldwin
- Retrospective: Conclusions from 2010 Workshop on RD&D Planning—Leon Clarke
- Observations on R&D Investment from Empirical Work on Technological Change—Greg Nemet
- Robust Portfolio Decision Analysis—Erin Baker
- RAND Methods for R&D Portfolio Selection—Steven Popper
- Real Options and Stochastic Dynamic Programming for Energy R&D Projects—Steve Gabriel
- How accurate were past expert elicitations on energy technologies? How can we do better?—Max Henrion
- Uncertain Clean Energy R&D in Integrated Assessment Models: Expert Elicitation and Approximate Dynamic Programming to the Rescue—Giacomo Marangoni
- Experience Curve Forecast Distributions and Applications—Rupert Way
- Technology Cost Evolution Modeling: Lessons Learned from Photovoltaics and Nuclear—Magdalena Klemun
- Stochastic Energy Deployment System (SEDS)—Emily Newes
- Stochastic Optimization for Biorefinery R&D and Process Design—Rebecca Hanes
- Monte Carlo Modeling for Optimization of R&D Investment—Caroline Hughes
- Real Options Applied to a Polysilicon PV Cell Model—Brian Bush
- Summary of Lessons Learned and Puzzles—Brian Bush

Fact Sheets

(See following pages.)

R&D Pathway and Portfolio Analysis and Evaluation: Overview

Risk and uncertainty comprise core characteristics of R&D programs. Attempting to do what no one has done before will sometimes end in failure, just as it will sometimes lead to extraordinary success. The challenge is to identify an optimal mix of R&D investments in pathways that provide the highest return while reducing the costs of failure.

The goal of the R&D Pathway and Portfolio Analysis and Evaluation project is to develop systematic, scalable pathway and portfolio analysis and evaluation methodologies and tools that provide high value to the U.S. Department of Energy (DOE) and its Office of Energy Efficiency & Renewable Energy (EERE) by identifying and evaluating, quantifying and monitoring, managing, documenting, and communicating energy technology R&D pathway and portfolio risks and benefits, thus assisting decision-making across projects and portfolios. The project-level risks typically considered are technology cost and performance (e.g., efficiency, environmental impact, etc.), while the portfolio level risks generally include market factors (e.g., competitiveness, consumer preference). Key questions include:

- Where should the next dollar of R&D be invested to increase returns at the project and portfolio levels?
    - How impactful will specific investments be in advancing a particular technology?
    - What is the likelihood that particular R&D pathways will achieve their goals?
    - When should R&D investment be cut or alternative pathways explored?
    - What are the opportunity costs of *not* investing in a research pathway?
    - When is it better to support fewer projects with more resources or a wider range of projects with fewer resources?
- How should the portfolio be balanced over risk, return, time, technologies, and markets?
- How can scoring of risk be made more consistent across projects, portfolios, markets, experts, and time?
- How can the results of these analyses be assessed and validated? Are the results statistically repeatable and do they hold up to auditing by decision-makers and external experts?
- What are the most effective mechanisms for communicating these evaluations?

Addressing these and related questions could provide significant value by improving the targeting of R&D opportunities, thereby accelerating R&D efforts. They may also help external stakeholders to better understand and assist EERE and DOE R&D decisions and activities.

Background

EERE currently invests almost $1.8 billion annually in R&D. Evaluation of R&D pathways begins with extensive outreach to the broad energy science and technology community—national labs, industry, universities, nonprofits, and others—through workshops and technology roadmapping efforts to gather their inputs on R&D opportunities and challenges. Links to this expert input diminish as decisions progressively move through the EERE and Administration budget-decision process and then Congressional budget appropriations. Developing ways to better link and communicate this genealogy would be useful for decision-making. Following appropriations, EERE widely uses competitive solicitations to select specific proposals for funding. Methods are needed to more effectively evaluate and communicate R&D pathways and portfolios, and to streamline, structure, and better target these processes and to track outcomes over time.

Projects. EERE work on energy R&D pathway and portfolio analysis and evaluation was first done more than a decade ago.[1] Over several years an approach at the R&D project level was developed and tested that: (a) built technoeconomic models of technologies of interest down to the subsystem level and below; (b) elicited expert estimates of the potential impacts of R&D; and (c) conducted Monte Carlo simulation on these models to generate probability distributions of the cost and performance of the technology over time as well as tornado diagrams that indicated which R&D investments could have the most substantial impacts.[2] Toy model examples of such outputs are shown in Figure 1 below. This approach was tested on 36 technologies and involved 167 experts who estimated risk distributions across some 1300 factors. The expert elicitation process faced a variety of challenges—ranging from training, to motivational biases, to social factors. Other complicating factors included: proprietary concerns; handling correlations across subsystems; and parsing costs—such as projections, learning curve impacts, commodity price changes, etc. Results were mixed, with some teams generating key insights and others lesser so. Overall, however, this first experiment showed promise, but highlighted a need to address these and other challenges and to reduce the expense of conducting these expert elicitations and associated activities.

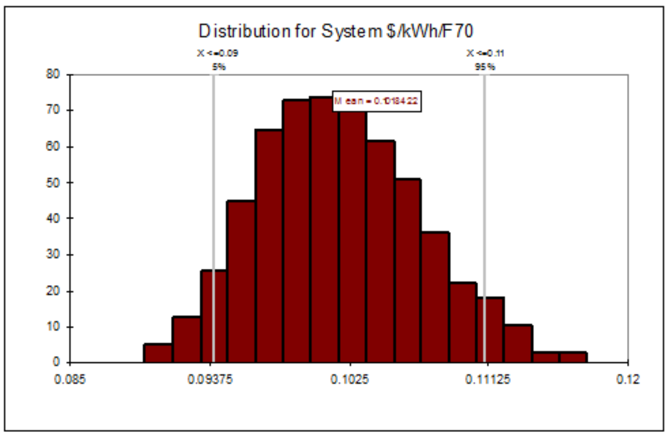
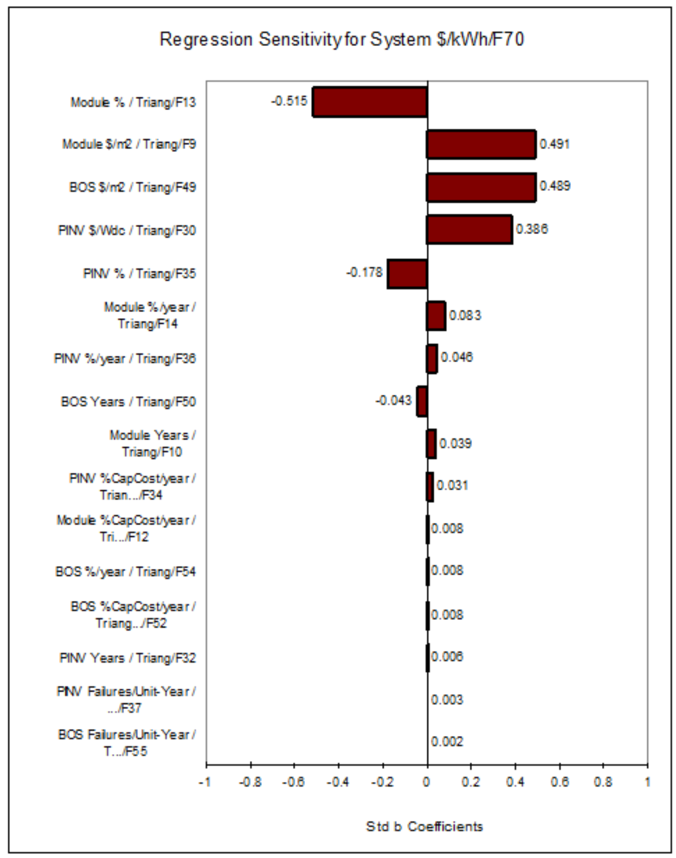


Figure 1. (a) Probability distribution (y-axis) for the cost ($/kWh; x-axis) of a power generation technology using Monte Carlo simulation on a toy model. (b) Tornado diagram showing the R&D investments with the largest impact across module efficiencies (%) and costs, Balance of System (BOS) costs, Inverter costs and efficiencies, etc.



Portfolios. The work at the project level was followed by the development of a portfolio analysis tool to evaluate technologies across programs. The tool developed is the Stochastic Energy Deployment System (SEDS),[3] which is an energy market model that explicitly incorporates risk and uncertainty in its input characterizations of energy technologies, fuel prices, energy policies, and other factors, and then outputs corresponding probability distributions of the market performance of various technologies with R&D. The SEDS tool is discussed in a separate Fact Sheet.

Challenges. A variety of challenges were identified by this work, including: addressing proprietary and competitiveness concerns; establishing consistent protocols across risk analysts and external experts; assessing and addressing correlations and dependencies within and between technologies; avoiding biases such as overconfidence, confirmation, and motivation; parsing projected costs due to R&D, learning, commodity price changes, etc.; optimizing multiple, sometimes conflicting, criteria such as economic cost, environmental pollution, greenhouse gas emissions, materials use, reliability, resiliency, and others. Further, these analyses were and must be done in the context of deep uncertainty about many of the resources, technologies, markets, competitors, and numerous other factors. How risks might be perceived were also of concern: for example, if one R&D investment had only a 10% chance of success and another had 70%, how would decision makers respond? If key benefits of a technology are not captured in high level portfolio evaluations—for instance, if the evaluation considered only cost and not broader metrics such as temporal and spatial availability, or consumer preferences—this could substantially misrepresent the value of particular R&D investments.

Changes. This work concluded approximately ten years ago as EERE budgets substantially shifted from EERE-wide analyses to more program-specific analyses. With this change in focus, work on R&D Pathway and Portfolio Analysis at the EERE-wide level also ended. Presently, EERE and DOE programs have a variety of approaches for R&D pathway analysis, with few relying on quantitative risk analysis,[4] and a similarly reduced emphasis on systematic risk-informed portfolio analysis.

Current Study

Over the past decade much further work has been done by the broad science and technology (S&T) community on R&D analysis and evaluation tools.[5] In addition to Monte Carlo methods, studies have used Real Options, Stochastic Optimization, Bayesian Statistics, Expert Elicitation, Decision Theory, Complex Systems, Deep Uncertainty, Technology Modeling, and other approaches. A key issue for the current study is which of these methodologies or which of their hybrids can best help guide R&D investments for EERE, a public R&D organization. To explore that issue, this study has begun experimenting with a variety of analytical methodologies in highly simplified "toy" models. These explorations aim to efficiently and pragmatically investigate the multiple dimensions involved with modeling and decision-support for investment in R&D portfolios and to identify the particular capabilities, strengths, weaknesses, and insights that each of these different methodologies can contribute.

It is important to distinguish here between R&D Pathways and R&D Portfolios. As used here, R&D Pathways refers to the evaluation of individual technologies, such as solar PV or onshore wind, and their subsystems and components, in order to better target R&D investments to improve that technology as much as possible. For solar PV, this might include consideration of improving module efficiencies (which, drilling down further, might include changing device structures, materials, electrical contacts, etc.), inverter lifetimes, Balance-of-System (BOS) costs, and others.

It is insufficient to simply evaluate the impact of R&D on individual technologies, however; it is also necessary to determine whether the resulting improvement will make a significant difference in meeting national goals and needs. This is the intent of R&D Portfolio evaluation: to evaluate and compare technologies in the overall energy system in order to determine whether R&D investments can help a technology have a significant impact at the regional, national, and/or global scale. In the power sector, for example, this could include evaluating natural gas combined cycle plants, nuclear power, solar PV, onshore wind, and others to determine the impacts of R&D on each to help meet national goals. Across energy sectors, this could include comparing the impact of R&D on high efficiency lighting in buildings, improved batteries for electric vehicles, and more efficient solar PV modules. Conversely, if R&D investments can improve a technology's cost and performance but not sufficiently to ever be able to compete in the market and provide significant benefits, such improvements become moot. SEDS was developed to provide a general energy-economic model for conducting such R&D portfolio evaluations. Ways to improve it or to identify other approaches for evaluating R&D portfolios is a key question which will be explored in detail in a subsequent review.

Summary of Fact Sheets

Stochastic Energy Deployment System (SEDS): SEDS is an economy-wide energy model of the U.S. that focuses on explicitly simulating uncertainties in energy technology, markets, and policy using a non-equilibrium stochastic methodology. The fact sheet describes the model and provides example analysis and uncertainty-visualization results. SEDS is a publicly available example of an uncertainty-aware, energy-system decision-support model.

Polysilicon PV Cost Cell Model: This is a Python reimplementation of a typical, detailed, bottom-up manufacturing model of the sort occasionally developed in support of analysis within EERE technology programs. To avoid issues with proprietary data, the inputs to the model have been "anonymized" through randomization. The fact sheet describes the manufacturing stages embodied in the model, presents cost results, and discusses challenges. This model is used in the analysis of real options (below).

Biorefinery R&D Investment: This is a traditional two-stage stochastic optimization, implemented in Python and using standard optimization software packages (Pyomo, PySP, and IPOPT), applied to R&D investments in biorefinery technologies. The technical model represents the essential influences on technology cost and performance, but taking a "top down" approach (as opposed to the "bottom up" technology approach taken for the aforementioned polysilicon cell model). The fact sheet formulates and solves non-linear and linear optimizations for R&D investment in the face of uncertainties and discusses issues related to discretization, *a priori* probabilities, linearization, and data inputs.

Real Options: This adopts the real-options methods (the Black-Scholes model and binomial lattices) used in financial engineering to the problem of R&D investment in uncertain technologies, comparing closed-form and numerical solutions for R&D investments in polysilicon cells. Results compare investment options and value options such as abandoning (e.g., an American Put option) a line of R&D investment. The fact sheet also discusses limitations and extensions of the method and that it might be combined with other methods.

Monte Carlo Model of Systems/Components: This fact sheet distinguishes the interaction of programs, platforms, systems, and subsystems in R&D investment decisions, particularly exploring the sharing of multiple subsystems and components within different systems and the role of experts with differing types and quality of expertise in estimating the impact of future R&D. The model using a multi-stage optimization where expert opinion is combined and evaluated using Monte Carlo simulations of future outcomes, which are then scored in order to make investment decisions annually. The model interfaces with a standard, annually updated, database of renewable-energy technology cost and performance. Its stochastic simulation results are presented as tornado diagrams showing impacts and uncertainties of investments.

Bayesian Combination of Expert Assessments: This model leverages the subsystem simulation within the Monte Carlo Model in order to grade the performance of subject-matter experts in their predictions of the likely success and subsequent impact of future R&D investments. The grades are translated into weighting factors that evolve over time as more information about the quality of the experts' predictions emerges. Results show conditions under which the effective pool of expertise evolves towards either mixtures of experts or reliance on a single expert.

Petri Nets: Petri nets, which are discrete state-transition models, are used to model two alternative R&D investments in dual-junction photovoltaic cells: either increasing the reuse of parent epi-substrate or replacing chemical-mechanical re-polishing with web-bench surface preparation. Petri nets emphasize discrete transitions between qualitatively different technological states of affairs and allow the modeling of situations where some types of technology advancement may preclude particular future R&D or moot previously undertaken R&D.

Technology Readiness and Performance Levels (TRL/TPL) Model: This stochastic model examines the tradeoffs between R&D investments aimed at moving a technology towards higher readiness for deployment at scale (commercial readiness) versus investments aimed towards more competitiveness in the marketplace (commercial viability).

Autoregressive Models: Our experiments with autoregressive models attempt an empirically driven, statistical approach to complement detailed, bottom-up technology modeling. The fact sheet discusses the formulation and challenges of utilizing empirical/historical data in R&D investment.

Expert Elicitation: This fact sheet summarizes issues and challenges around employing expert elicitation in modeling and decision-support for R&D investment.

Issues and Puzzles

The goal of this work is to provide R&D pathway and portfolio analysis methodologies and tools that are usable and useful to EERE and DOE staff, team leaders, program directors, and Portfolio Managers in systematically identifying, quantifying, evaluating, managing, monitoring, documenting, and communicating technology development risks and benefits, and in assisting project, program, and portfolio decision-making that aligns and balances the portfolio with national goals**.** There are many challenges in achieving this. In addition to the issues noted above, consider the following:

R&D Pathway Analysis Tools

The choice of methodology, level of detail represented, and embodiment in tools poses many considerations for R&D portfolio analysis:

- It is presumably preferable to have analyses linked as closely as possible to the underlying science and engineering of the technology being evaluated, but this can require substantial modeling efforts and may still not answer the core question of how much improvement in cost and performance there can be with a particular level of R&D investment. Experts may be able to estimate these potential technology improvements from R&D investments, but eliciting these estimates can require substantial time and effort. Where is a useful balance between these activities—simulating the physics and eliciting expert estimates—that provides the best possible data at the lowest possible overheads?
- How can these analytical tools best be designed so that they are able to drill down deeply into one technology and shallowly into a second, yet provide useful comparative data across technologies, so that a technology is not represented too favorably or unfavorably as a result of the level of detail of its analytic representation?
- Which methods best handle evaluation of multi-scale, multi-stage analyses?
- What hybrids of Monte Carlo simulation, Real Options, Stochastic Optimization, Bayesian Statistics, Expert Elicitation, Decision Theory, Complex Systems, Deep Uncertainty, Technology Modeling, or other approaches can provide the best combination of capabilities to meet the goals of this work?

Expert Elicitation

Expert elicitation is an essential part of R&D Pathway and Portfolio analysis and is briefly described in a separate fact sheet.

- How can expert elicitation be improved to manage the various difficulties that arise—such as biases of overconfidence, confirmation, or motivation—particularly for this type of technology evaluation?
- How can the costs of expert elicitation be reduced while maintaining the highest possible quality? How well have on-line elicitations worked, and what have been the lessons learned?
- What have been effective approaches for pre-screening experts to select higher performers to participate in elicitations?
- What can be done to evaluate the performance of experts in post-elicitation reviews?
- How might historical data and non-traditional methods (e.g., gamification, online surveys, patent analysis, publication metrics, etc., to sample a larger pool of experts) complement expert elicitation?
- Might adaptive methodologies for expert elicitation streamline and optimize its process and impact?
- How could experts be assessed to assign weights to predictions so that more accurate experts are given higher importance when averaging predictions?

R&D Portfolios

The EERE and DOE R&D portfolios include a wide variety of technologies across every sector of the energy economy and across every stage of development, from early basic research to commercial deployment. These different technologies provide different services with different benefits to end-users. (SEDS, an energy-economy simulation tool, was under development previously—see separate fact sheet—to provide the ability to compare technologies across the R&D portfolio and further work and a separate engagement will examine it and portfolio tools more broadly.)

- How can portfolio analysis tools fairly characterize and compare technologies across the many diverse services they provide, and still be practicable and cost-effective? What approaches should be considered?
- How can potential variations in the objectives of decision-makers at different organizational levels be harmonized into systematic, risk-aware portfolio decisions?

Tracking Data

As R&D Pathway and Portfolio Analysis proceeds, it is essential to analyze and document risks in a manner that is objective, credible, fair, transparent, and auditable with all important assumptions and uncertainties clearly identified. This requires the development of methods to track, monitor, update, and document all appropriate data and analysis, including the ability to track key inputs through the methodology.

- What have been the lessons learned in other such studies for how to do such tracking sufficiently to provide all necessary information without overwhelming the analyst in the process?
- What is the minimum and optimal resolution for tracking data on R&D investment and impact?
- How can the potentially long delays in assessing R&D impact be figured into tracking databases in an actionable and traceable manner?

Communications

Translating the results of the R&D Pathway and Portfolio Analysis into forms useful for many different users and audiences—from program staff to high-level decision-makers, and to diverse external audiences from researchers to stakeholders to the public—raises challenges of communicating complex issues of risk and uncertainty.

- The EERE and DOE decision-making processes currently provide little genealogy on the underlying analysis that led to particular recommendations. How can such genealogy best be communicated?
- What communication tools and approaches, particularly visualization tools, have demonstrated high performance in conveying complex risk issues to various users and audiences with different levels of experience in considering risk issues?
- To assist decision-makers in their efforts to build consensus, characterize technology tradeoffs, and determine potential complementary actions, it may be useful to evaluate multiple metrics across these different technologies and the services they provide. What is the experience with and lessons learned about such efforts and how to communicate the results?

Metrics

Throughout the R&D Pathway and Portfolio Analysis process, it is important to develop and track metrics that can fairly and efficiently evaluate and compare performance at the technology, system, and portfolio levels.

- What has been the experience and lessons learned in determining appropriate metrics, tracking them, and evaluating their effectiveness?
- How can the cost of implementing such metrics be best managed for the issues identified above: staff overhead and training; the cost of modeling and expert elicitation; tracking data; communications; and others?

Tracking

The development of energy technology R&D pathway and portfolio analysis and evaluation methodologies and tools has the potential to significantly support policy maker decision-making and accelerate the realization of national energy-related goals for the economy, environment, and national security. Advancing these capabilities faces substantial methodological and operational challenges, and will strongly depend on capturing the experience and knowledge of the broad science and technology community to be successful; this workshop is a first key step in that process.

[1] See, for example, presentations by Baldwin, Friley, Henrion, and Short at: Joint Global Change Research Institute, "R&D Portfolio Analysis Tools and Methodologies", December 02, 2010, College Park, MD 20740, http://www.globalchange.umd.edu/events/rd-portfolio-analysis-tools-and-methodologies/

[2] See, for example: J. McVeigh, J. Cohen, M. Vorum, G. Porro, G. Nix, "Preliminary Technical Risk Analysis for the Geothermal Technologies Program" Princeton Energy Resources International and National Renewable Energy Laboratory, Technical Report NREL/TP-640-41156, March 2007, https://www.energy.gov/sites/prod/files/2014/02/f7/41156.pdf

[3] See https://openei.org/wiki/Stochastic_Energy_Deployment_System_(SEDS).

[4] As an example of a quantitative tool to examine R&D opportunities, see the Building Technologies Office Scout Tool: https://www.energy.gov/eere/buildings/scout

[5] See bibliography at https://www.zotero.org/groups/2174314.

Stochastic Energy Deployment System (SEDS)

Purpose

SEDS is an economy-wide energy model of the United States; it was developed in part in response to a recommendation by the National Research Council of the National Academies to the Department of Energy to address risk and uncertainty in the DOE's evaluation of technologies and their benefits (National Research Council, 2007). It is a tool to evaluate R&D portfolios, taking the technology-specific risk and uncertainty distributions of the impact of R&D on technology cost and performance and competing them in the SEDS energy-economic model to understand how R&D could impact the market penetration of different technologies and the resulting dynamics between supply, demand, and pricing of the major energy types consumed and produced within the United States.

Methods

SEDS differs from other economy-wide energy models in that it explicitly accounts for uncertainty in technology, markets, and policy. The intent of the model was to be fully open and transparent, well documented, user-friendly, and very fast to enable desktop use and provide real-time response to decision-maker queries. These considerations substantially drove key aspects of model specification, particularly that it is a simulation model rather than an optimization model that solves for equilibrium in order to achieve the necessary speed and ease of use. SEDS focuses on the major drivers within the energy economy and evaluates the impact of uncertainty around those drivers. SEDS uses a Monte Carlo sampling approach to make random draws from the distributions of each input assumption, and then it uses those draws to simulate the evolution of the energy sector to 2050. The end result is a collection of different system evolution pathways from which the likelihood or probability of each pathway can be statistically determined. It is built in Analytica (http://www.lumina.com).

Technology

In particular, SEDS was developed to have much technology representation in the energy conversion and end-use sectors. By modeling a significant number of technology pathways in these sectors, it is possible to simulate the economics-based deployment of new technologies and observe their impacts on the energy and CO_2 intensities of the various sectors. Because new technologies are notoriously shrouded in cost and performance uncertainty, SEDS is uniquely able to explore the deployment and impact of these technologies while specifically addressing the high level of uncertainty surrounding their characterizations.

Biofuels	Electricity	Hydrogen	Liquid Fuels	Buildings	HDV	LDV	Industry
Cellulosic ethanol Corn ethanol	Geothermal (hydrothermal and EGS) Wind Solar (PV, CSP) Conventional fossil fuel IGCC (+ CCS) Combined cycle (+ CCS) Hydro Biomass (+ CCS) Nuclear MSW and Landfill	Central biomass Central SMR Distributed SMR Central wind electrolysis Distributed ethanol reformation Compression, storage, and dispensing (CSD)	CTL Fischer-Tropsch fuels with CCS	Distributed PV Lighting DHW Refrigeration Space Heating Space Cooling Windows	Medium-duty trucks Heavy-duty trucks Aviation Rail	Advanced SI Hybrid electric Plug-in hybrid electric Fuel cell Advanced CI Hybrid electric Plug-in hybrid electric fuel cell Conventional CI Gaseous fuel (CNG/LPG) Hybrid electric	Process heating and refrigeration Electrochemical processes Other primary manufacturing processes Pumps Compressors Motors Boilers Fans Conveyors Lighting Cogeneration

Figure 1 illustrates the impact of various uncertainties on the deployment of a nascent energy technology (NET) by the year 2030. Each chart in Figure 1 adds one more uncertainty to the previous chart.

Chart (A) compares NET capacity from a deterministic business-as-usual (BAU) scenario and a scenario where technology uncertainty is applied. The BAU scenario uses the most-likely value from each input distribution and performs a single simulation over the time horizon using those most-likely values. This results in a deterministic projection of NET capacity, which in this case is the single-point estimate of roughly 1 GW of capacity in 2030. The "Tech" scenario made one hundred random draws (this number was arbitrarily chosen for this example) from every probability distribution defining the cost and performance of various technologies within the SEDS model. Based on those random draws, one hundred unique simulations over the time horizon were performed and the results from each of those simulations were statistically analyzed to produce a distribution that is representative of the underlying one hundred simulations. From chart (A) we see that the inclusion of technology uncertainty gives a range of possible capacity values for NET. This range extends from about 0.2 to 2.1 GW, with the most-likely value being roughly 0.35 GW. Compared to the BAU case, technology uncertainty produces a lower bound of roughly –75% and an upper bound of nearly 110% relative to the 1 GW of capacity projected by the deterministic BAU case.

Chart (B) uses the same draws from the technology cost and performance distributions as was simulated in the "Tech" scenario and adds additional uncertainty by randomly drawing from distributions related to fuel price drivers ("Tech, Fuel" scenario). The "Tech, Fuel" scenario exhibits a wider distribution and the mode or peak of the distribution has shifted somewhat to the left. The relatively small change in the distribution attributable to fuel price uncertainty is due the fact that NET is still high-cost relative to its competitors even when fuel prices are disadvantageous to those competitors.

Chart (C) adds to chart (B) by allowing macroeconomic uncertainty. Macroeconomic uncertainty represents uncertainty in the growth of GDP, manufacturing, population, interest rates, and disposable personal income. Again, for this particular model output, macroeconomic uncertainty does not substantially change the range and mode of the distribution around NET capacity in 2030 because the assumptions used in these simulations project NET to be fairly costly.

In chart (D), we see the distribution widen roughly two-fold and the mode shifts leftward as a result of including R&D uncertainty. Certain draws from the distributions related to improvements in NET costs and performance lead to simulations where NET becomes increasingly more economic and this leads to increased deployment. Given the additional R&D uncertainty, the most-likely outcome is approximately 4 GW of NET capacity compared to the 1 GW that was projected in the "BAU" case.

In chart (E), the R&D uncertainty has been removed and policy uncertainty has been enabled. Here policy uncertainty corresponds to uncertainty around carbon cap regulation, a national renewable electricity standard, and extensions of production and investment tax credits to renewable, electricity-generating technologies. Relative to the "Tech, Fuel, Macro" scenario, the policy scenario has widened significantly although not much mass is skewed towards the higher NET capacity levels. This suggests that only a handful of policy scenarios might lead to increased NET capacity.

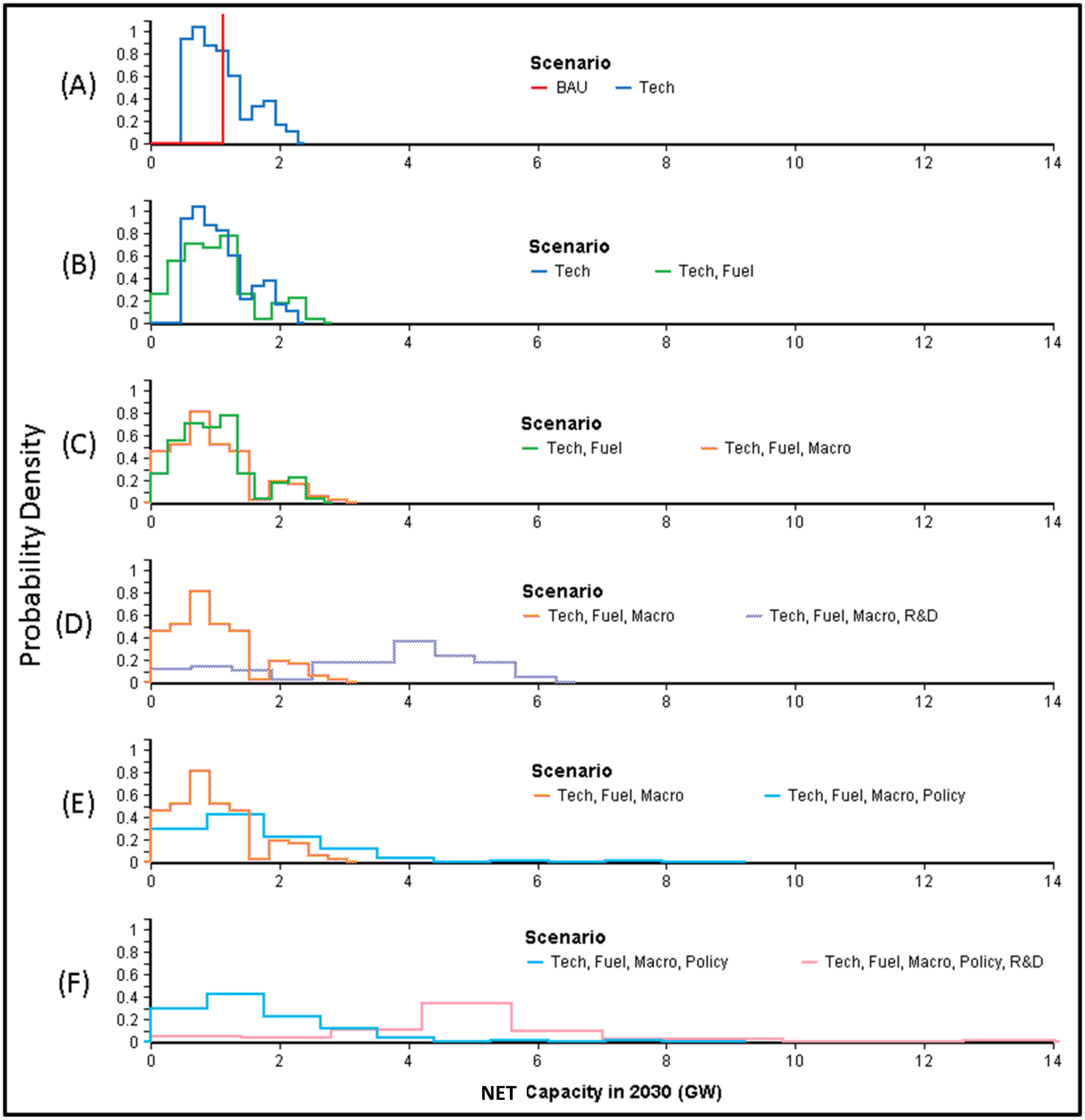


Figure 1: Examples of how various uncertainties might affect the deployment of NET by 2030

Chart (F) shows the impact of including all uncertainties by adding R&D uncertainty to the "Tech, Fuel, Macro, Policy" scenario. The combination of policy and R&D uncertainty leads to a much wider distribution. The NET capacity outcomes under this final scenario range from 0 to 14 GW with the most-likely value being close to 5 GW. Although 5 GW is not significantly more than the 4 GW projected in the 'Tech, Fuel, Macro, R&D" scenario, there is much more mass centered around the 5 GW capacity level in this final scenario, which suggests that the outcome of 5 GW is much more probable than in the scenario that does not consider policy uncertainty.

Lessons Learned and Puzzles

An external review of the initial development of the SEDS model was held on May 7-8, 2009. Overall, the review team felt that development of SEDS had been worthwhile and that after refinement and testing the model was likely to be a useful tool for R&D planning. The reviewers documented a wealth of valuable comments on needed improvements to the model. The following list is a sample taken directly from the report.

Key Criticisms

- *The failure to solve for equilibrium in each period is a serious problem. The non-convergence creates more difficulties in interpretation when the stochastic version is used.*
- *The model is a single region model with average characterization for everything (technologies, prices, etc). Such a regional characterization is poorly positioned to do policy analysis or technology assessments.*
- *SEDS needs a much better market share/market diffusion formulation/technology choice formulation; important non-price factors and consumer preferences are not represented in most, if not all, of the current choice functions.*
- *The model should ensure that more subtle aspects of technology costs are properly accommodated, such as the relative non-dispatchability of some RE sources.*
- *Ensure that expert input considers how Federal R&D funding and policies could impact private R&D investment, and also the impacts of non-U.S. groups doing technology R&D.*
- *The distributions and parameters chosen to represent stochastic variables are themselves uncertain and will influence the model results...the selection of the distributions and their parameters could imply the model contains more information than it really has.*
- *Needs better underlying data on technology and supply chain cost info.*
- *Scope of modeled technologies needs to be more comprehensive.*

SEDS Team Response, Selected

- *We agree that the impact of the absence of equilibrium needs to be measured and, if found to be significant, resolved. We believe it may be possible to construct a special version of the model that iterates within each one-year time step until equilibrium is reached. To quantify the impacts of equilibrium, we will compare the results from this version with results from the existing non-equilibrium version*
- *While regional detail is critical to some aspects of a national energy model, it may be of marginal benefit elsewhere, and added detail always comes at some cost. In addition, data limitations often dictate the level of model detail or impose inconsistent levels among its various parts.*
- *Private and foreign R&D affect benefits from federal R&D in both directions, and the end result may be a "wash".*

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National Research Council. *Prospective Evaluation of Applied Energy Research and Development at DOE (Phase Two)*, 2006. https://doi.org/10.17226/11806.

Link to online data/model

The SEDS model is available at <https://nrel.github.io/portfolio/>.

Toy Biorefinery Model Fact Sheet

Purpose

- Build and solve non-linear two-stage stochastic optimization problems for R&D pathway and portfolio analysis using Pyomo, PySP and IPOPT.
- Explore the impact of linearization on optimal solutions to a non-linear model.
- Compete this toy model with others in a Monte Carlo simulation, to explore whether a less detailed model or its results behave differently than a more detailed model when simulating pathway development.

Methods

- Pyomo: Model building and data management
- PySP: Multi-stage stochastic optimization
- IPOPT: Non-linear solver
- First-order Taylor series expansion: Linearization

Technology

- Two-stage stochastic optimization problem representing R&D on and operation of a biorefinery with two feedstock options, four processing steps, and one product. The biorefinery technology is partially mature but still improvable via targeted R&D on the processing steps. Decision variables are optimized to maximize the biorefinery annual profit. All cost and other equations are reflective of real model behavior but do not contain actual data or input from real-life experts.
- The cost of each processing step is dependent on one process variable x_i (analogous to yield) and one cost variable $c_{max,i}(v_i)$. Costs of different processing steps are independent of each other. The cost variable is a function of the funding received for R&D on that processing step, v_i, and the stochastically selected R&D progress scenario.
- R&D progress scenarios control the extent to which the funded R&D is successful. "Successful" R&D reduces the cost of a processing step.
    - R&D progress scenarios are Failure (no cost reduction), Advance (moderate cost reduction), and Innovation (substantial cost reduction).

<table>
<tr><th></th><th>Sets and Parameters</th><th>Stochastic Variables</th><th>Decision Variables</th><th>Key Equations</th></tr>
<tr><td>Stage One</td><td rowspan="3">$i \in \{p, f, c, s\} = \left\{\begin{matrix}\text{preprocessing,} \\ \text{fermentation,} \\ \text{conversion,} \\ \text{separation}\end{matrix}\right\}$

$j \in \left\{\begin{matrix}\text{stover,} \\ \text{switchgrass}\end{matrix}\right\}$

C_i: Pre-R&D cost parameter

p: Product selling price per short ton

d_j: Feedstock price per dry short ton</td><td>Funding Impact
m</td><td>Funding Amounts
v_i</td><td>Processing Cost Parameter
$c_{max,i}(v_i, m) = C_i\left(1 - m v_i^{0.25}\right)$</td></tr>
<tr><td></td><td></td><td></td><td></td></tr>
<tr><td>Stage Two</td><td></td><td>Process Variables
x_i

Feedstock Amount
s_j</td><td>Processing Cost
$\sum_i \left[c_i\left(x_i, c_{max,i}(v_i, m)\right)\right]\left[\sum_j s_j\right]$

Overall Product Yield
$y = x_p^2 x_f x_c^{0.5} x_s^{0.25}$

Profit
$yp \sum_j s_j - \sum_j d_j s_j - \sum_i \left[c_i\left(x_i, c_{max,i}(v_i, m)\right)\right]\left[\sum_j s_j\right]$</td></tr>
</table>

Results and Discussion

Optimal Results - Original Model

R&D Progress Scenario	Stochastic Variables	Decision Variables								Objective Function Value
		Preprocessing		Fermentation		Conversion		Separation		
		v_p	x_p	v_f	x_f	v_c	x_c	v_s	x_s	
Failure	$m = 0.0$	$9.3M	1.0	$18.1M	1.0	$55.8M	0.47	$16.8M	0.47	$163,500
Advance	$m = 0.05$		1.0		1.0		0.53		0.50	$252,100
Innovation	$m = 0.10$		1.0		1.0		0.59		0.53	$351,800

- For all processing steps, a higher value of x_i equates to higher processing costs and higher processing step yield, although the relationship between x_i, processing cost and yield is different for each processing step.
  - The increase in x_c and x_s under the Advance and Innovation scenarios is due to the increased impact of the R&D funding, which decreased the overall processing costs and enabled higher yields in those processing steps.
  - The preprocessing and fermentation steps were sufficiently low cost that R&D funding had no impact on the optimal process variable values.
- All four processing steps received R&D funding, and the conversion steps received the highest amount by far.
- Annual biorefinery profits (the objective function) increased as the impact of R&D funding increased because the same amount of funding resulted in higher processing cost reductions.

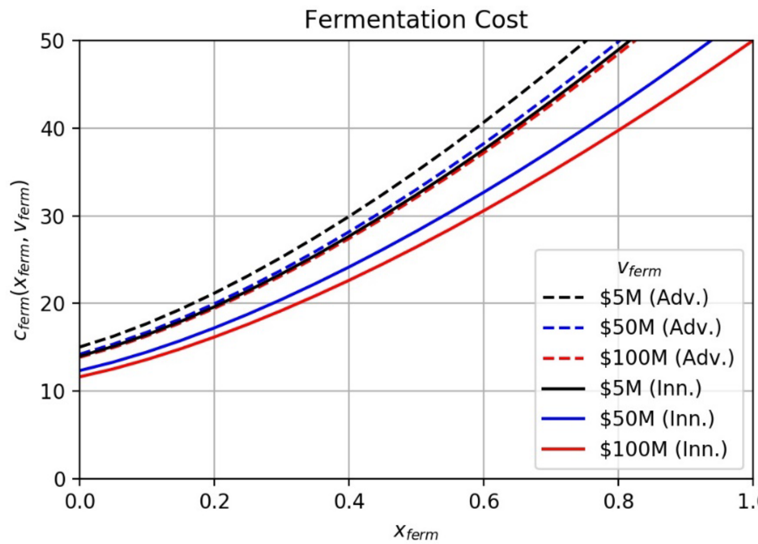
Optimal Results - Linearized Model *(see Impact of Linearization for procedure)*

R&D Progress Scenario	Stochastic Variables	Decision Variables								Objective Function Value
		Preprocessing		Fermentation		Conversion		Separation		
		v_p	x_p	v_f	x_f	v_c	x_c	v_s	x_s	
Failure	$m = 0.0$	$0	1.0	$100M	1.0	$0	0.08	$0	0	$255,100
Advance	$m = 0.05$		1.0		1.0		0.09		0	$252,500
Innovation	$m = 0.10$		1.0		1.0		0.10		0	$254,500

- Under the linearized model, every processing step had a linear relationship between x_i, processing cost and yield, albeit with different slopes and y-intercepts. See page 4 for the linearization procedure.
- Only the conversion process variable changed under R&D progress scenarios, with the magnitude of the change being much less than in the original model.
- The process variable for the separation step remained at zero under all progress scenarios, indicating that under the linearized model it was optimal to sell an unrefined product. This behavior is unrealistic and in future versions of the model could be corrected by linking product selling price to process variables.
- The fermentation step received all available R&D funding.
- Annual biorefinery profits did not increase monotonically with the R&D progress scenario, and the Failure scenario had the highest annual profits.
- Overall the linearized model behavior and optimum are not in good agreement with the original, non-linear model, indicating that for this particular model the reduced model complexity from linearization may not be worth the decrease in modeling accuracy.

Lesson Learned: Optimization with Pyomo and PySP

Discretization. Stochasticity is incorporated into the program by defining a finite number of potential scenarios and assigning each scenario a probability of occurring. In real applications, these probabilities could be determined from expert elicitation or from historical data. The sum of the probabilities over all scenarios defined must be equal to one. Uncertain parameters take on different values in different scenarios, and the probability of the scenario occurring is thus also the probability of the uncertain parameter taking on the value defined in that scenario. The alternative to this discretization is to use continuous probability distributions to capture parameter uncertainty. The stochastic parameter in this problem, m, determined the impact of funded R&D on the biorefinery cost equations:



Progress Scenario	m	Probability of Occurring
Failure *no cost reduction*	0.0	0.4
Advance *some cost reduction*	0.05	0.4
Innovation *significant cost reduction*	0.10	0.2

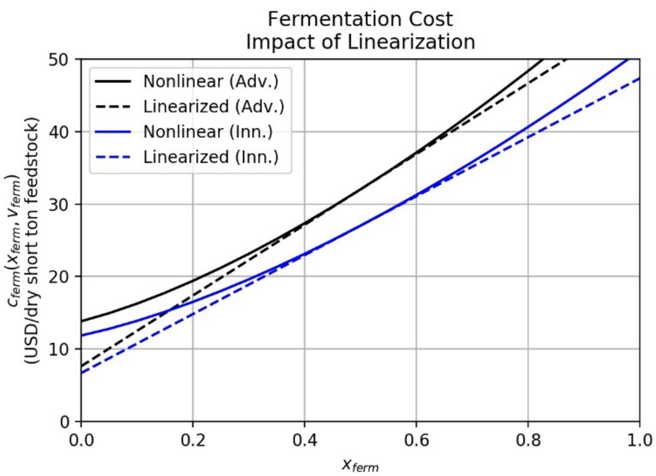
The cost parameter $c_{max,i}$ as well as the overall cost c_i in each processing step is dependent on m as well as on the amount of funding v_i assigned to the processing step. The figure above shows how c_i changes with the amount of funding and the progress scenario for the fermentation processing step.

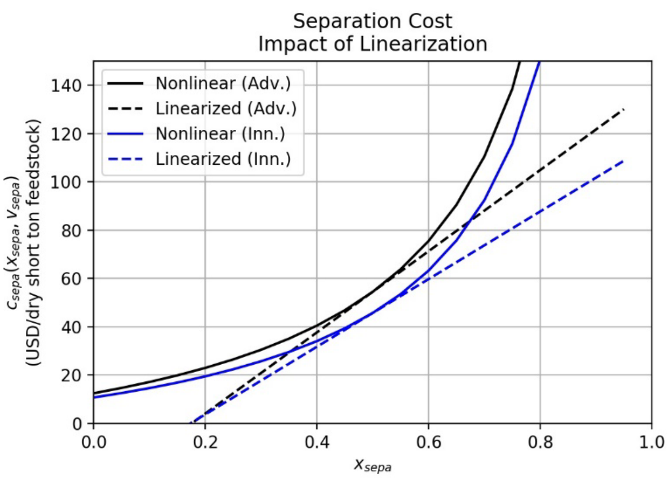
A Priori Probabilities. Probabilities assigned to second-stage scenarios are required to be specified before the problem is solved, and as such must be independent of first-stage decision variables. There is a class of stochastic programs in which scenario probabilities can be dependent on prior stage decision variables as discussed in Jonsbråten et al. (1998) and in Hellemo et al. (2018). In this model, the probability of a particular investment (funding decision) being successful may reasonably be dependent on the amount of funding provided – low or insufficient levels of funding would plausibly lead to Failure more often than high levels of funding.

Model and Scenario Data. Under Pyomo, models can be created as *concrete* models, in which data is hard coded into the model and cannot easily be varied, or *abstract* models, in which the model structure and data is specified separately. The biorefinery model was created as an abstract model to allow different sets of model data to be specified under each progress scenario. This required the creation of three scenario data files which were largely identical save for the parameter that varied according to the progress scenario. Maintaining and updating these data files would quickly become cumbersome and potentially prohibitive for a large-scale model.

Pyomo also utilizes Expressions, symbolic mathematical statements unique to Pyomo models. While Expressions somewhat simplifies model creation, for instance by allowing the definition of a quantity that can be used multiple times in a model, it is relatively easy to define Expressions that cannot be parsed by Pyomo and the solvers used to find optima. There is a small but significant learning curve involved in using Expressions correctly, which presents a barrier for modelers new to Pyomo.

Lesson Learned: Impact of Linearization

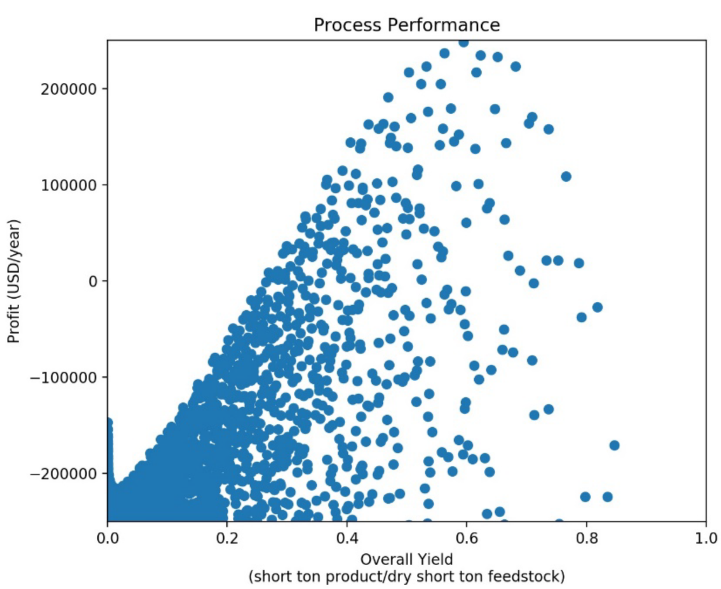


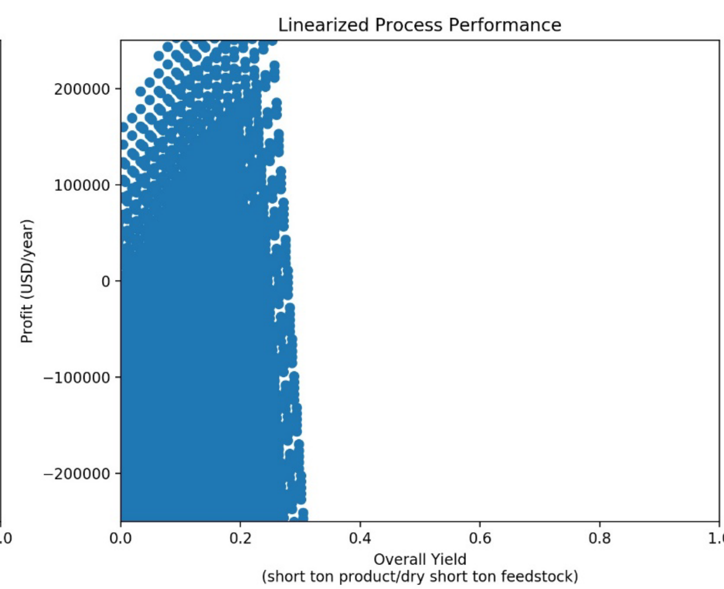


First-order Taylor series expansions around the midpoint of the respective variable ranges were used to linearize model equations.

Cost equations. The agreement between the original and linearized equations depended heavily on the curvature of the original equations. For instance, the linear and non-linear fermentation cost equations are in reasonably good agreement, as shown in the upper figure at left. The linearized fermentation cost equation performs most poorly for $x_f \leq 0.2$. On the other hand, the separation cost equation has an asymptote at $x_{sepa} = 1$, and therefore the agreement between the original and linearized cost equations is poor outside the range $0.4 \leq x_{sepa} \leq 0.6$. This can be seen in the lower figure at left.

Overall model behavior. In the figure below, the subplot on the left shows biorefinery annual profits plotted against overall process yield for the original, fully nonlinear model. On the right are the same values plotted for the linearized model. These results are for the Advance scenario and are a representative sample from the entire solution space. Linearizing the model severely restricts the overall yield values that can be achieved and as a result also constricts the solution space for the biorefinery. Approximately the same range of annual profit values are achieved, and indeed the linearized model appears to have a higher proportion of solutions in the region where annual profits are greater than zero. This is likely due to the linearized cost equations not capturing the exponential growth and asymptotic behavior in the conversion and separation steps, making it so the marginal gains in process variable were the same cost regardless of the process variable value. This leads to heavy cost reductions in those steps and higher profit values, even with lower overall yields.





Polysilicon Cell Cost Model Fact Sheet

Purpose

A detailed, bottom-up polysilicon cell manufacturing cost model was translated from one of the NREL's established Excel manufacturing cost models into a Pythonic version (Woodhouse, 2019). This detailed cost model was developed for two reasons: to test decision making methodologies (e.g., stochastic optimization vs Monte Carlo) and to test different levels of detail in cost models (e.g., simple, new cost model vs a well-established, detailed cost model). Both of these situations are usually present for R&D portfolio managers and the impact of both the decision methodology and the underlying cost model are important to understand when evaluating portfolio allocation approaches.

Methods

This bottom-up cost model evaluates each stage in the manufacturing process sequentially. For this model, the following manufacturing steps are modelled:

- Harvest Chunk – costs associated with harvesting the chunk of polysilicon
- Siemens CVD – costs to obtain the high-grade polycrystalline silicon
- Etch Filaments – cost of process etching the filaments
- Machine Filaments – costs to machine the filaments
- Saw Ingots – costs of sawing process
- Crop Ingots – costs of cropping process
- Anneal Ingots – costs of annealing process
- Grow Ingots – costs of growing the ingots
- TCS – costs of trichlorosilane process

The outputs of the model are a table of levelized cost per kg of polysilicon chunk.

Technology

This is a detailed, bottom-up cost model for the well-established polysilicon cell manufacturing process. As NREL's models contain proprietary costs associated with each process, this analysis has been "anonymized" by using random values that aim to be on the same order of magnitude as the true process, but are not anticipated to be accurate.

Additionally, this model reflects a relatively older manufacturing process technology which has been improved upon since the development of the original Excel model. Importantly, this technology is well-established and has a high degree of certainty around the process design and costs associated with it.

The model follows a direct cost calculation based on the input materials, capital expenditures, operating expenses, and labor expenses. Indirect costs are estimated based on the direct costs. The capital costs are then amortized over the life of the asset.

Results

Inputs:

The model allows the user to select the region for analysis, since the labor costs, financial conditions (e.g. capital recovery), commodity prices, and indirect costs (e.g. installation costs) vary from region to region. For this initial demonstration, the U.S. was selected as the region of analysis.

The model sequentially steps through each of the manufacturing steps. The inputs to each step include information such as specific commodity price, process yield, expected downtime, tooling life and cost, capital cost, process efficiency, etc. From the perspective of the R&D Portfolio manager, each of these inputs could be uncertain and the manager must understand which input parameters are most influential on the resulting cost.

Outputs:

Each manufacturing step has two primary outputs: a financial summary of that step (a Python DataFrame object) and the cumulative material rejection rate (waste). Some steps output additional parameters for future steps to use (e.g., Total Mass of Si per Rod). The final cost summary is the total of all the individual manufacturing step financial summary tables. This model was validated against the original Excel model and matched with machine precision. The financial results from the model validation are shown below.

Cost Component	$/kg Poly Si Chunk	$M/year		%
Material Cost	16.37	$	85.14	52%
Direct Labor Cost	1.93	$	10.01	6%
Utility Cost	4.04	$	21.01	13%
Equipment Cost	3.31	$	17.23	11%
Tooling Cost	0.01	$	0.06	0%
Building Cost	0.16	$	0.81	0%
Maintenance Cost	1.09	$	5.67	3%
Overhead Labor Cost	0.62	$	3.24	2%
Cost of Capital	3.74	$	19.45	12%
Total	**31.27**	**$**	**162.62**	**100%**

Discussion:

A few key elements are very apparent from simply developing this model for future use in other, decision-oriented models. Some of them include:

- Non-linear interactions – some of the manufacturing steps are non-linear.
- Input data quantity and uncertainty – there are on the order of hundreds of input parameters and each could have varying levels of uncertainty associated with them. A sensitivity analysis should be completed to understand which ones are the key cost drivers of the process (e.g., tornado diagrams).
- Upstream process improvements may have a considerable impact due to the effect of compounding at each step in the process (e.g., reducing waste in the Harvest Chunk process percolates through the rest of the model).

Results, continued

Connection to EERE Portfolio Allocation:

Cost models such as this one are used widely across EERE to understand the series of improvements that enable a particular office to meet its technology performance and cost targets. For example, the Solar Energy Technology Office (SETO) sets LCOE targets and tracks progress towards meeting those targets over time, as seen in Figure 1 (Ran, 2018).

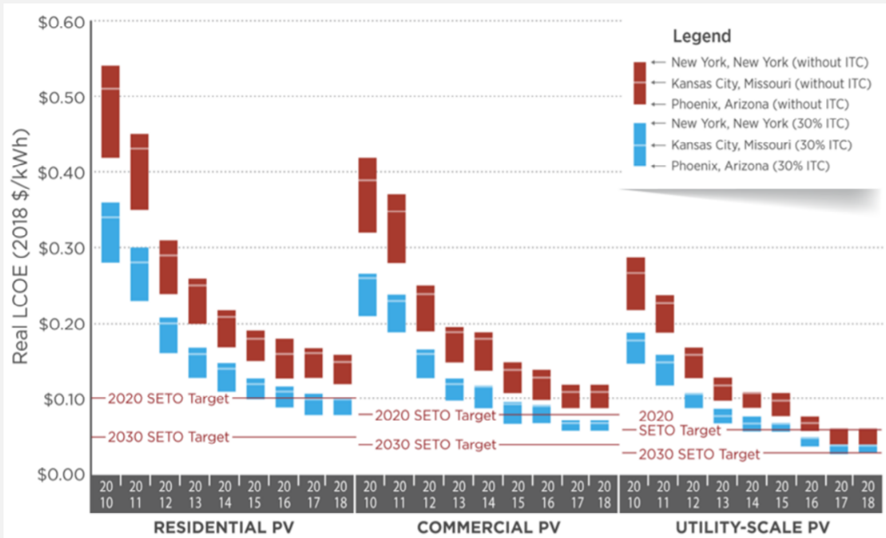


Figure 1. NREL PV LCOE benchmark summary (inflation adjusted), 2010–2018

A techno-economic analysis can then be completed using these manufacturing cost models to develop roadmaps to achieve EERE cost and performance targets, as seen in Figure 2 (Woodhouse, 2019).

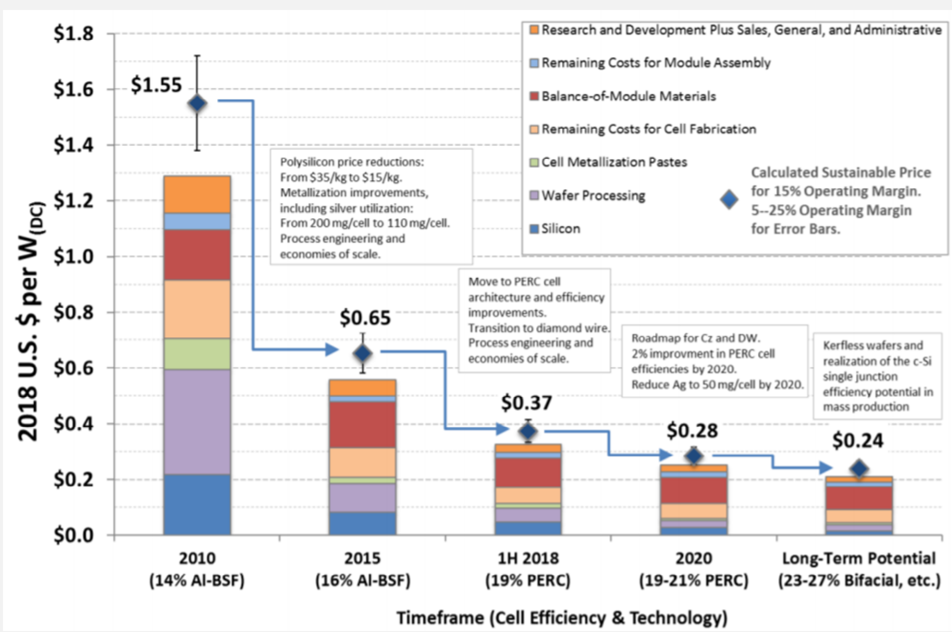


Figure 2. Modeled costs and MSPs for past, present, and projected c-Si modules

Lessons Learned and Puzzles

Lessons Learned:

- Bottom-up, detailed cost models are likely only available for well-established technologies.
- Non-linearities are likely present in detailed cost-models.
- Detailed cost models have significantly more input parameters than simpler cost models and each could have a source of uncertainty.

Puzzles:

- How will two cost models of differing levels of detail / analytical rigor compete fairly for the same R&D dollar?
- Will the additional parameters associated with the detailed cost models increase or decrease the level of certainty of future cost projections?
- If all input parameters have uncertainty associated with them, what is the best process for selecting which ones to focus on? Or should they all be evaluated?
- Are there specific decision making methods that are better for situations with high numbers of uncertain parameters (e.g. Monte Carlo)? Will other methods breakdown with too many uncertain parameters?
- What is the impact of linearizing a cost model? How much information is lost versus how much computational efficiency is gained? Are there specific applications for linear methods (local machine computations) and non-linear methods (high performance computing)?

Conclusions:

A detailed cost model was developed to compare different decision making methodologies and assess the relative importance of the cost-model itself. Developing this model has surfaced a number of puzzles that a real-life R&D program manager must determine how to best approach/solve including non-linearities, number of uncertain parameters, and fair competition across varying detail of cost models.

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Link to online data/model

See <https://nrel.github.io/portfolio/> for further information.

Real Options Toy Model

Purpose

Real options analysis builds upon the conventional discounted cash flow valuation analysis to incorporate aspects of both the ability for management to make decisions while a project is developing as well as uncertainty with respect to the cash flows associated with it. These two aspects make real options analysis a useful tool for decision making under uncertainty.

Two real options models were developed: the classic Black-Scholes model and a binomial lattice model. The Black-Scholes model is a closed-form mathematical model that is capable of valuing European Options (only exercise the option at the end of the holding period, as opposed to American options for which you can exercise them at any time in the holding period). Next, the binomial lattice model is effectively a discretization of the continuous stochastic process underlying the Black-Scholes model and are widely used due to their flexibility and relative ease of implementation. Both models were applied to two scenarios of an organization investing in R&D to reduce the levelized cost of manufacturing a Si PV cell.

By evaluated both a closed-form model and a more flexible binomial lattice model, various insights can be evaluated such as the tradeoff of computation time with accuracy and the power of flexibility in decision making under uncertainty. Additionally, two scenarios were evaluated to show how a R&D Project Manager might decide on how to select input parameters to invest in.

Methods

Black-Scholes

The Black-Scholes model is a closed-form mathematical model that was derived be using stochastic calculus to value European Call or Put options. Mathematically, the Black-Scholes closed-form solution for a European Call is [1, 2]

$$V_C(S,t) = S \cdot \Phi(d_1) - Ke^{-r(T-t)} \cdot \Phi(d_2)$$

$$d_1 = \frac{1}{\sigma\sqrt{T-t}}\left[\ln\left(\frac{S}{K}\right) + \left(r + \frac{\sigma^2}{2}\right)(T-t)\right]$$

$$d_2 = \frac{1}{\sigma\sqrt{T-t}}\left[\ln\left(\frac{S}{K}\right) + \left(r - \frac{\sigma^2}{2}\right)(T-t)\right] = d_1 - \sigma\sqrt{T-t}$$

where

- V_C - Call option value
- S - Current asset value (typically a simple DCF valuation calculation without considering the option value)
- K - Strike price of the option. For real options, can be the implementation cost to execute the strategic option
- r - risk-free interest rate (US Treasury note with duration same as the project timeline)
- σ - volatility of the natural logarithm of the project's free cash flows

- T - time at which option expires
- t - current time
- Φ - is the cumulative distribution function of the standard normal distribution.

The value of the European Put based on the Put-Call parity is [1]

$$V_P(S,t) = \Phi(-d_2) \cdot Ke^{-r(T-t)} - \Phi(-d_1) \cdot S$$

Additionally, closed-form solutions for more complex option valuations have been completed. Below are some of the closed-form approximations that exist [2]:

- Bjerksund Closed-Form Approximation for American Call and Put Options with Dividends
- Barone-Adesi-Whaley Closed-Form Approximation - American Call and Put Options with Dividends

Binomial Lattice

The binomial options model equations are based on the discrete simulation step size as well as an assumption around risk-neutral probability. Mathematically, the formulas are [2, 3, 4]

$$u = e^{\sigma\sqrt{\delta}t}$$
$$d = e^{-\sigma\sqrt{\delta}t} = \frac{1}{u}$$
$$p = \frac{e^{r(\delta t)} - d}{u - d}$$

where:

- u - magnitude of up movement (increase in asset value)
- d - magnitude of down movement (decrease in asset value); usually assumed to be proportional to up movement (recombining tree = reduced nodes in lattice)
- p - risk-neutral probability (discounts probability, or equivalently, cash flows) by risk level to bring back to present value
- σ - volatility of the natural logarithm of the project's free cash flows
- r - risk-free interest rate
- δ - discretized time step

The u and d parameters reflect the simulation step up and down, respectively. The p parameter reflects the risk-neutral probability (adjusted probability rather than adjusting the discount rate). The binomial models typically converge with ~1,000 iterations within each period [2]. As the number of periods increases, the computation expense will increase. Using these formulas, one can calculate the option tree.

Once completed, backwards induction is used to convert these values back to present option values at the time when the value is being considered. Mathematically, this is [3]

- European Call or Put: $V_n = e^{-r\delta t}(pV_u + (1-p)V_d)$
- American Put: $V_n = max\left(K - S_n, e^{-r\delta t}(pV_u + (1-p)V_d)\right)$

- American Call: $V_n = max\left(S_n - K, e^{-r\delta t}(pV_u + (1-p)V_d)\right)$

where:

- V_n- is the value of the option at time-step *n*
- S_n- is the value of the asset at time-step *n*
- V_u- is the value of the option from the upper node at *n+1*
- V_d- is the value of the option from the lower node at *n+1*

The binomial model provides greater flexibility than the closed-form solutions. For example, the binomial model can be readily updated to account for various option valuations (abandon/deploy/continue/expand/contract), multiple options simultaneously, changing volatility values (bushy lattice), and compound options [2]. This increased flexibility can be very useful for real-world projects which exhibit these aspects that cannot be easily included in a closed-form solution such as the Black-Scholes model.

Technology

Real option analysis models can be applied to any investment decision with an expected value and some uncertainty around various future values that affect that expected value.

For this example, a detailed cost model for Si PV cell manufacturing was used as the base model and two R&D investment scenarios were evaluated: investing to improve Metallurgical Grade (MG) Silicon Usage in the trichlorosilane (TCS) formation process or investing in R&D to reduce the MG Silicon waste in the (TCS) formation process. An abandonment option value was estimated assuming that the R&D investment could be reduced at any point in time during the investment time horizon. The total value of each R&D project scenario (asset value [deterministic net present value of the R&D project] plus the abandonment option value) was estimated and compared to determine which is more financially attractive and should receive the R&D investments.

Abandonment Option Valuation Steps/Assumptions

The abandonment option value was estimated via the following steps (summarized in Figure 1):

1. Assume the cash inflows generated by the R&D investment manifested themselves in lower PV cell costs as opposed to no investment (assumed no improvement without R&D investment).
2. The R&D expenditures (cash outflows) were kept constant over the time horizon analyzed. Free cash flows are assumed to be the net difference between lower PV cell costs and R&D expenditures normalized on a $/kg poly Si chunk level.
3. Compute a deterministic improvement over time based on a linear rate of improvement.
4. Compute a stochastic improvement over time based on:
    a. Geometric Brownian Motion (for the R&D investment in MG Usage Rate).
    b. Triangular distribution of improvement over time (for MG Waste Rate)[1].

[1] A triangular distribution was used for illustrative purposes since it is (1) a different distribution than GBM and (2) since that is typically what expert elicitation data results in.

5. Compute 1,000 runs of stochastic progress over time (Monte Carlo) to evaluate the uncertainty in Si PV Cost (resulting values are compared to the deterministic case to determine the uncertainty in free cash flows).
6. Determine the NPV of the deterministic improvement case (base-case).
7. Determine the volatility of the natural log of the returns for the stochastic runs.
8. Compute the salvage value of exercising the option to abandon the R&D investment (NPV of future R&D Expenditures).
9. Input the NPV of the deterministic case (S), salvage value (X), volatility of the stochastic run returns (σ), and other parameters (r, T, t) into the binomial lattice model.
10. Compute the value of the abandon put option.

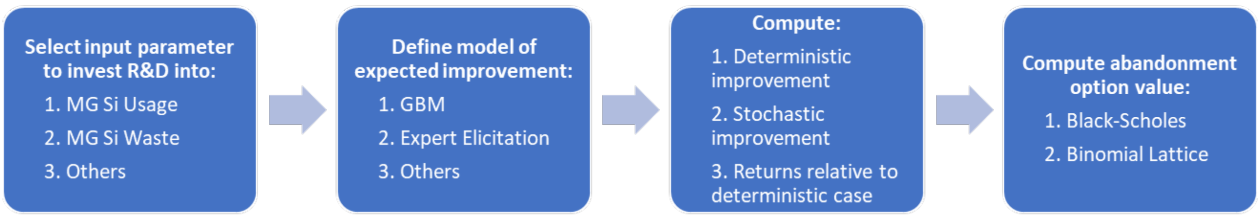

Figure 1. Option value computation flow

Results

Figure 1 shows the results of both R&D investment scenarios. For each scenario, there is a No R&D Case (static Si PV cell cost), Deterministic Case (constant linear improvement over time), and Stochastic Case (Geometric Brownian Motion improvement over time for the MG Usage Improvement scenario, triangular distribution improvement for the MG Waste Reduction scenario). By comparing a world with no R&D investment with that of a constant, deterministic improvement over time, a typical discounted cash flow analysis can be completed to determine the value of the R&D without considering the abandonment option. Similarly, the free cash flows for each stochastic run were computed. Next, the natural log of the returns for each stochastic run were computed and the volatility of the resulting scenarios was determined to be input into the binomial lattice model.

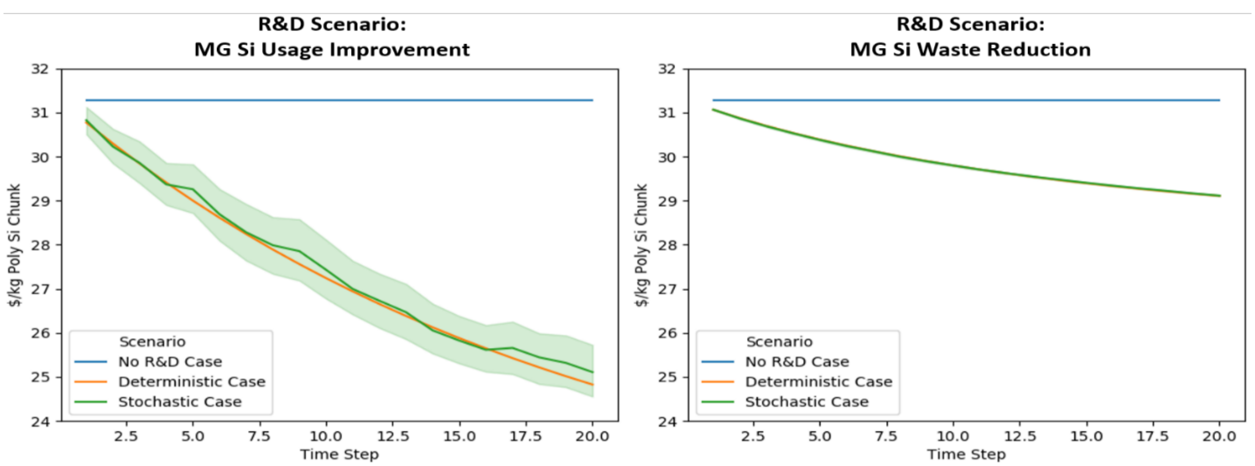

Figure 2. Cost evolution over time (each time step is one quarter of each year) for the three scenarios evaluated. 95% confidence intervals shown in green around the Stochastic Case

Table 1 summarizes the resulting values obtained from the Si PV cost model analysis. The R&D investment required for the MG Si Waste Reduction scenario was assumed to be half that of the MG Si Usage Improvement scenario due to the lower sensitivity on cell cost[2]. Inputting the calculated parameters in Table 1 into the binomial lattice model allows the value of the abandonment put option to be evaluated. Additionally, the inputs were entered into the Black-Scholes model for comparison (although the Black-Scholes model only evaluates a European put option whereas this scenario is an American put option).

Table 1. Binomial lattice model input parameters based on Si PV cell manufacturing cost model

Parameter	MG Si Usage Improvement Scenario	MG Si Waste Reduction Scenario
Deterministic NPV ($/kg-Si)	18.61	3.13
Salvage Value ($/kg-Si)	26.17	13.09
Volatility	0.285	0.14
Risk Free Rate (%)	0.05	0.05
Time (steps)	20	20

The option valuation results are summarized in Table 2 below. The results highlight that the closed-form solution is highly preferable for computation time, however, cannot directly be applied to this example as the option here is an American put.

Table 2. Comparison of R&D investment scenario option values and model computation times

Model	Description	MG Si Usage Option Value ($/kg-Si)	MG Si Waste Option Value ($/kg-Si)	Computation Time (s)
Black-Scholes	European Put	4.40	N/A	<0.001
Binomial Lattice	American Put, 10 steps	7.82	9.95	<0.001
Binomial Lattice	American Put, 100 steps	7.80	9.95	0.03-0.04
Binomial Lattice	American Put, 1000 steps	7.80	9.95	3.51-3.69

To compare R&D investment scenarios against each other, the total value of each R&D project scenario (asset value [deterministic net present value of the R&D Project] plus the abandonment option value) must be computed. These results are summarized in Table 3 which show the MG Si Improvement R&D Project has the superior financial outcome and should be invested in. Interestingly, the R&D Project investing in MG Si Waste Reduction has a very high option price since this is an American Put which means that if the option is exercised, the R&D Project Manager recovers the underlying value of the asset which is likely negative (and thus the option would almost always be exercised).

[2] As mentioned in the Lessons Learned and Puzzles, a generic framework to complete a sensitivity analysis on the combined input parameter and R&D investment should be a first step in determining which aspects of the project could be potential focus areas for R&D investment.

Table 3. Comparison of R&D Projects based on total project value

Scenario	Deterministic NPV ($/kg-Si)	Abandonment Option Value ($/kg-Si)	Total Value ($/kg-Si)	Invest?
Invest in MG Si Usage Improvement	18.61	7.80	26.41	Yes
Invest in MG Si Waste Reduction	3.13	9.95	13.09	No

Lessons Learned and Puzzles

Flexibility versus Computation Time / Resources

- Closed-form partial differential models are much more computationally efficient but are limited in their applicability across various option valuations.

- Binomial lattices are more flexible and can be tailored to handle multiple types of options (abandon/deploy/continue/expand/contract, multiple options simultaneously, changing volatility values, and compound options), but at the cost of computation time (additional examples could be set up for these scenarios).

- Can multiple types of real option analysis techniques (lattice, PDE, Monte Carlo) be combined to flexibly answer questions quickly in a fit-for-purpose manner?

- What happens when there are tens or hundreds of variables that are uncertain? Or multiple real options available at the same time (compound)?

Volatility Estimation

- How should the volatility parameter in the real options valuation (ROV) models be characterized given different forms of volatility in the technology improvement model? E.g. if GBM is used versus a triangular distribution for technology improvement, should the volatility of project returns be estimated differently before being input into the ROV model?

- What is the best way to estimate volatility across different model inputs? Literature seems to be divided on Geometric Brownian Motion and Mean Reversion while expert elicitation results usually result in triangular probability distributions.

- What sources of uncertainty are the most important? Which should be included in the analysis and which ones should not?

What Options to Evaluate

- The real options present (investment timing, to invest, to abandon, technology choice, to switch, to expand, etc.) could be very large. How does one know *a priori* which options (and how many) are the best to value? Why does most literature only analyze ~1-3 options [5]?

- A standard framework is needed to complete a sensitivity analysis to understand which parameters may have the largest impact on system cost before using a real options analysis per dollar of R&D invested.

- How to incorporate non-financial returns into these models such as the value of added services or R&D improvement impacting other Projects?

Conclusions

- Real options analysis presents a powerful tool for evaluating the value of certain options in an uncertain world.

- Real options analysis could be combined with other techniques such as stochastic optimization and Monte Carlo analysis to expand its utility. For example, Monte Carlo is typically needed for volatility analysis which is then input into the real options model while stochastic optimization can take in real options results and be used to select between multiple projects under budget constraints [3].

- The trade-off between model flexibility and computation time need to be evaluated carefully when selecting the purpose for the model.

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Links to online data/model

See <https://nrel.github.io/portfolio/> for further information on the Black-Scholes Model, the Binomial Lattice Model, and the Si PV Manufacturing Cost Model.

Monte Carlo Toy Model

Purpose

Monte Carlo (MC) simulation can be used in R&D Pathway and Portfolio analysis in two key ways. First, it can be used to generate probability distributions of the cost and performance of a technology system using expert estimates of the potential improvements due to R&D investment in the technology's components or subsystems. From this, the relative impact of different R&D investments can also be determined. Second, it can be used to then compete these probability distributions of cost and performance for individual technology systems in an overall market model (see the SEDS Factsheet). This enables one to determine, bottom-up, what difference an R&D investment can make. The focus here is on a toy model of an individual technology. This highlights particular advantages of MC simulation for exploratory modeling—that it is flexible, adaptable to use at many different levels from components to markets (with appropriate model design), and can be run given a variety of input data (Bankes 1993). Future versions of this model will consider the hierarchy, listed with examples, from the bottom up:

Technology System Level	1. **Components:** photovoltaic (PV) poly-silicon (PolySi) wafer, concentrating solar power (CSP) heliostat; inverter electrolytic capacitors 2. **Subsystems:** PV modules, balance-of-systems, inverters 3. **Technology System:** PV System, CSP System
Cross-Technology Systems	4. **Programs:** Solar Energy Technologies Office, Vehicle Technologies Office, Wind Energy Technologies Office
Market-Competition Models	5. **Portfolio:** Electric Power Systems, Transportation Systems, Buildings, … DOE Office of Energy Efficiency and Renewable Energy (EERE)-wide

Research foci within these levels may include improving efficiency and cost. The investment levels can inform funding distributions at the laboratory level when allocating funds within a research area, at the system level, at an EERE program level, or at an EERE-wide level.

Methods

Prediction

This toy model is focused on the technology system, bullets (1) to (3), as listed above. Several scenarios are defined at the component level. Experts are elicited for the probability that a technological advancement can be made at each investment level and how large the particular advancement might be, as modeled by a triangular distribution In addition, the experts are asked the number of times successful R&D on the component can yield improvement; this is used here as a simple way to indicate technical limits in potential advances in a particular area of research, generating declining returns on R&D investment. Experts are also asked for the low, middle, and

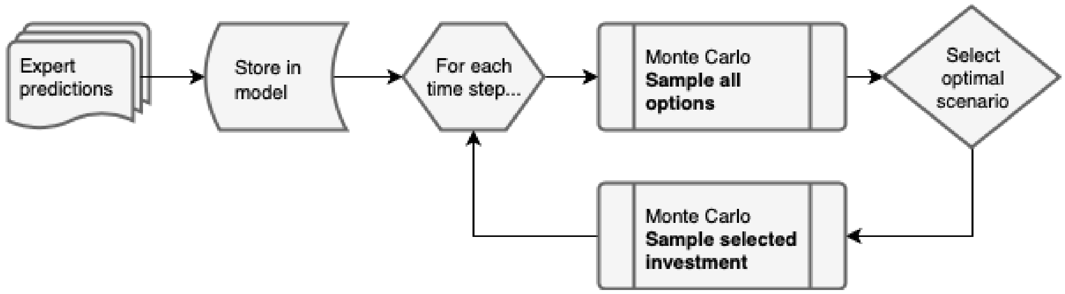

Figure 1. Monte Carlo model flow chart. This is a multistage approach whereby the Monte Carlo sampling Figure 2 is repeated twice. First, every possible permutation of investment scenarios is sampled. These are ranked by a user-determined objective to determine which investment scenario bundle is the best. Next, the Monte Carlo sampling is repeated for the best option, and the results are saved to track the impact of making that investment. This process is repeated to select and make an investment at each timestep.

high impact of an advancement on any parameter that might be affected, such as capital cost or levelized cost of energy or electricity (LCOE). These could also represent the 10^{th}, maximum, and 90^{th} points on a triangular distribution, and the distribution might be modified to adjust weights, as described in the Bayesian Fact Sheet.

Figure 1 shows the overall process that the Monte Carlo model follows. Expert predictions are aggregated by taking averages, either on all requested information *before* the simulation, or on the results of the Monte Carlo simulations *after* all expert predictions have been sampled individually; these averages can be weighted if there is a well-developed basis for doing so. Numerous other schemes for combining expert opinion are also possible but are not explored here (Baker and Olaleye 2012). It is useful to consider tracking expert performance individually, as weights indicating level of expertise can be updated using the technique described in the Bayesian fact sheet; however, developing such weightings is challenging. The model allows for experts to make predictions on one or multiple subsystems, assigning different weights (chosen arbitrarily for the purposes of this model exercise) to their assessment, depending on their familiarity with the subsystems. Monte Carlo sampling is performed for each investment scenario individually. However, when making an investment, decision makers will need to consider bundles of investments: decision makers must consider all permutations of investment options, rather than each investment individually, to suggest a complete investment portfolio. Each bundle has its own combined impact on the considered research foci. These combined impacts are used to determine the score of each investment bundle, which are ranked in a score matrix. This can be ranked based on the impacted parameters, and controlled based on user input to enable multi-objective optimization (Wang et al. 2009). Bundles selected here are based on cost, but other performance characteristics can also be important and could be similarly selected for. The cost and performance distributions for the technologies resulting from the highest-ranking investment bundles can then be used in cross-technology comparisons (bullet (4) above) or used in a market allocation model (bullet (5) above), such as SEDS (see the SEDS factsheet).

Monte Carlo simulation

Thus, an inner MC simulation is used by the decision maker to identify and select the top-ranking R&D investment bundles, and an outer MC is used to generate the probability distributions of the cost and performance for these top-ranking bundles to show the results of the decision process being simulated, and this information can be subsequently used in the steps shown above, bullets (4) and (5).

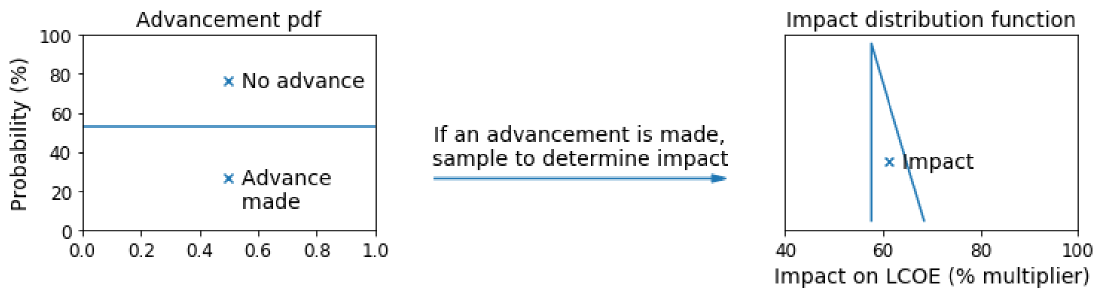

Figure 2. These plots show the Monte Carlo sampling process for the impact of a target investment in balance-of-system cost. First, the advancement pdf is sampled. The probability density function of this discrete event is shown on the interval [0, 1], so that the probability of any event occurring is 100%. If an advancement is made, the triangular distribution is sampled using the Python built-in function.

Monte Carlo Sampling

Figure 2 depicts the sampling process for one combination of subsystem and investment scenario. For each subsystem, the method first samples to determine whether an advancement has been made. If an advancement is possible—the model will first sample to determine whether an investment is made, and then to determine the impact of this investment on improvable parameters, such as LCOE. A maximum number of possible advancements is meant to simulate a theoretical limit on potential research advancements. If an advancement is not possible, no improvement will be observed, affecting the ranking of this investment, deprioritizing it when selecting an optimal investment.

Technology

Data

The Monte Carlo toy model was developed and assessed using hypothetical data. This was informed by two models:

1. The Stochastic Energy Deployment System (SEDS) model informed the improvable parameters considered when applying the Monte Carlo method (see SEDS fact sheet). No SEDS simulations were performed when making this model, but the SEDS input data was used as a reference when constructing the hypothetical data.
2. NREL's Annual Technology Baseline (ATB) database summarizes current power plant financial information, as well as predicted values annually from 2018 until 2050. ATB data was used to approximate the impact of research at the subsystem level at the plant and program levels.

Calculations

A variety of financial, environmental, and social parameters can be considered when making an investment. Here, the LCOE was used to measure the impact; environmental and other factors were not considered. Other factors that were not included in this first toy model – including greenhouse gas emissions, jobs created, and air pollution – will be considered in future iterations of the model.

Levelized Cost of Energy (LCOE). The ATB data is used to assess how the LCOE will be impacted by each investment decision and aid in leveraging subsystem-level simulations to make technology-level and program-level decisions. LCOE (with units of $/MWh) is calculated as follows:

$$\mathrm{LCOE} = \frac{\mathrm{FCR} \cdot \mathrm{CAPEX} + \mathrm{FOM}}{\mathrm{CF} \cdot 8760\ \mathrm{hr/yr}} + \mathrm{VOM} + \mathrm{Fuel}$$

where

- FCR is the fixed charge rate (%),
- CAPEX is capital expenditure ($/kW),
- CF is capacity factor (%),
- FOM is fixed operations and management ($/kW yr), and
- VOM is variable operations and management ($/MWh).

Not all parameters apply to all technologies: the PV portfolio studied here, for instance, does not have an associated fuel cost.

Score. A metric must be defined to rank the investment scenario options and determine which are the best as determined by the desired optimization objective(s). In this instance, the score was calculated as the percent improvement in LCOE per investment dollars spent. Other, more comprehensive, measures, including multi-objective ones, could be incorporated into this framework.

Results

The toy model was applied to potential research on cadmium telluride (CdTe) and poly-silicon (PolySi) subsystems of the PV platform. Balance-of-system cost and inverter lifetime efficiency were components relevant to both subsystems. Each subsystem also had uniquely relevant efficiency parameters that could be improved through R&D. Figure 3 shows how these subsystems and components fit into the overall investment portfolio.

A total of nine experts provided estimates for LCOE improvements. Figure 4 shows the input triangular distributions for each component. The model allows for multiple experts to provide estimates on one or more components, with their estimates weighted by their level of expertise on that specific component.

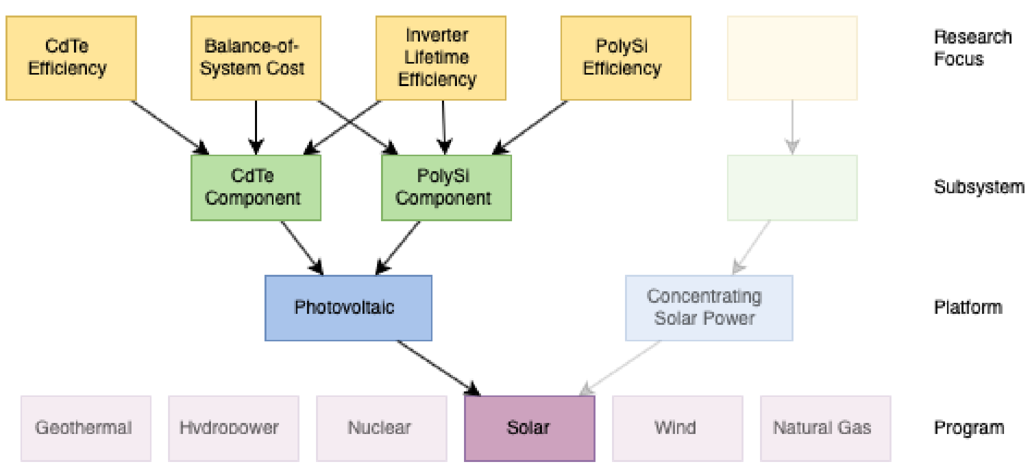

Figure 3. Map of subsystem components to relevant systems included in the toy data to select an investment scenario bundle.

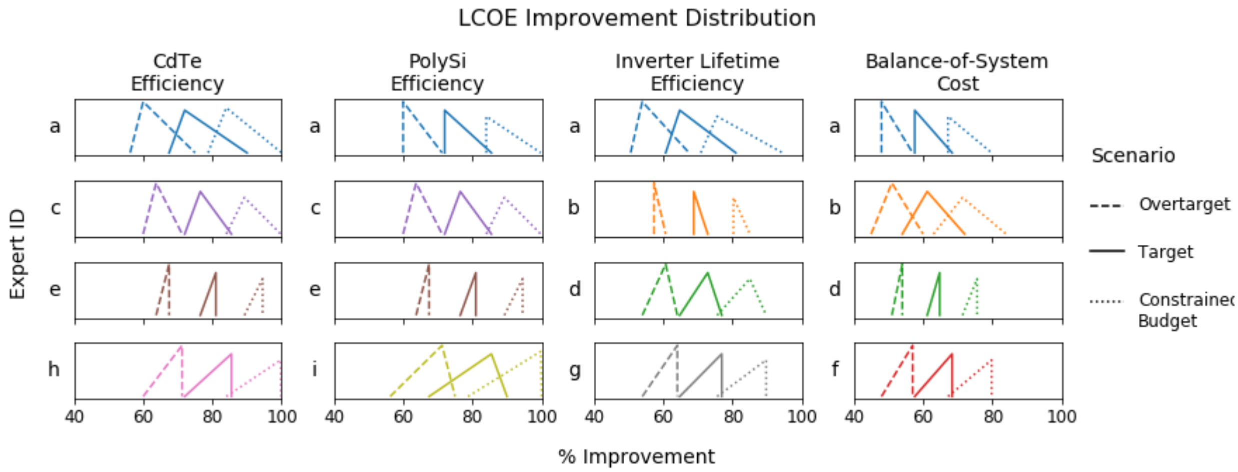

Figure 4. All triangle probability distributions (scaled vertically to have a total probability of 1) for the subsystem components considered by the Monte Carlo model, grouped by expert ID and investment scenario.

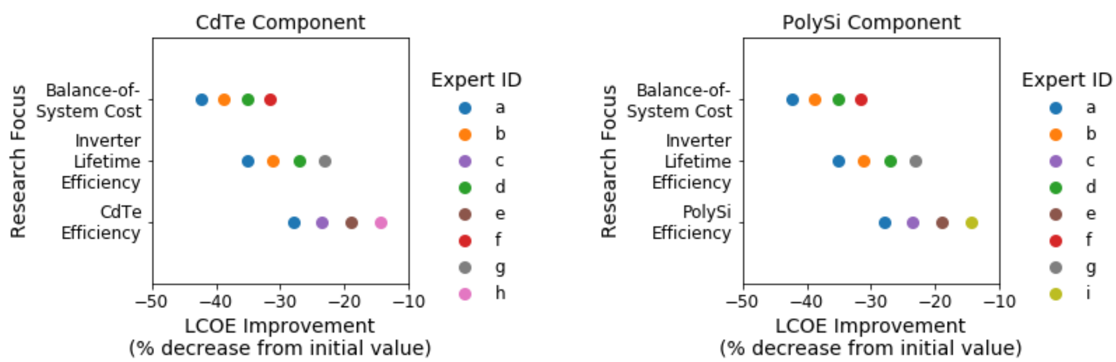

Figure 5. Tornado plots of investment impact on LCOE on the CdTe and PolySi subsystems grouped by expert.

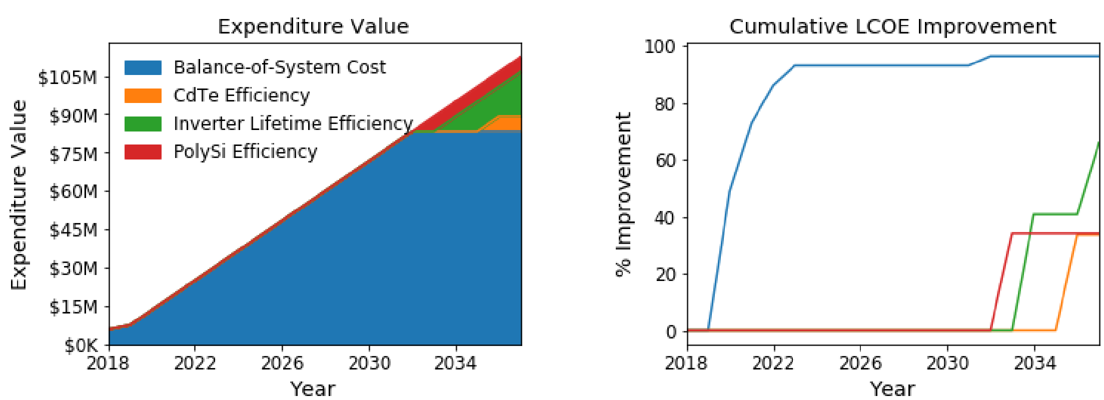

Figure 6. The above plots show the annual investment expenditure by component, as well as the cumulative number of advancements and amount of LCOE improvement made.

Figure 5 shows tornado diagrams separating the contribution to the percent improvement in LCOE by research focus and expert ID. This is meant to serve as a visual aide to decision makers when selecting an investment bundle at each timestep. These plots show that the most beneficial R&D investments in both cases are those that improving the balance-of-system cost. Figure 6 summarizes the results of the entire Monte Carlo simulation. It follows that investments are first made where they will make the most impact: balance-of-system cost, as suggested by the tornado plots in Figure 5. After research has been completed in this focus area, other research foci compete for funding.

Lessons Learned and Puzzles

Lessons Learned

Nested Monte Carlo Models. The Monte Carlo model relies on expert predictions made at various levels of the hierarchy and these can propagate upwards with possibly further nested Monte Carlo simulations to make predictions at higher levels, e.g. the technology system level, based on predictions made at lower levels, e.g. component and subsystem levels.

Runtime. The Monte Carlo method is notoriously slow, requiring a compromise between model fidelity and run time: 500 samples when making predictions were found to produce consistent investment selections in seconds for this small toy model. Scaling it to a much larger, more realistic model may pose a challenge. High performance computers can run the model with little concern over runtime, but we anticipate practical limitations when running in laptop- or desktop-computing environments that may preclude useful application by decision makers.

Close calls. It is possible for there to be several top-ranked investment options whose scores fall within one another's statistical uncertainty, meaning that the selected investment scenario is subject to change between runs. For this reason, it is helpful to display information, such as the tornado plots in Figure 5 to aid decision makers in making more fully informed decisions, including the sensitivities and uncertainties indicated by a broader set of figures.

Puzzles

Correlation. Considering the correlation between components or subsystems may indicate whether an advance in one might lead to a setback or advance in another. For example, significant advancements in heat exchanger efficiency might enable a significant reduction in flow rates and in fan/motor size. At the manufacturing level, a novel manufacturing technique might make another technique obsolete and require the construction of new fabrication centers.

Experience. Technology prices decrease as cumulative production increases, typically with a (Trancik and Zweibel 2006; Kavlak, McNerney, and Trancik 2018). Experts may or may not factor this into their estimations, so adjustments will need to consider this in making adjustments to the model and incorporating consideration of such learning curves in recommendations.

Signaling. How might high government investment inspire private investment or increased interest, which could in turn speed up research progress?

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Modeling Technology Readiness and Performance Levels

Purpose

Technology performance levels (TPLs) complement the commonly used technology readiness levels (TRLs) by distinguishing the economic viability and competitiveness of a technology from its operational scale and commercial maturity [Weber, Costello, and Ringwood, 2013]. Varied definitions and practices for TRLs exist in different industries, with varying levels of precision and rigor, but for the purposes of this example we consider TRLs as a measure of how ready a technology is for commercial deployment, irrespective of its viability in the marketplace [Figueroa, 2011][1]. The TPL, in contrast, assesses how well the technology performs in terms of its economic viability. Both TRLs and TPLs are graded on a 1 to 9 scale. This stochastic model examines the tradeoffs between R&D investments aimed at moving a technology towards a higher TRL for deployment at scale (commercial readiness) versus investments aimed towards higher TPL competitiveness in the marketplace (commercial viability). The model uses purely notional input data and does not represent actual TRL and TPL assessments for real technologies; we have highly idealized TRL and TPL, so the example provided here is purely illustrative. The Appendices to this fact sheet define TRL and TPL levels.

Methods

We begin with a generic description of a technology's cost structure [Connelly, 2019], summarized as its net cost per unit production, N/x, where variables are defined in Table 1 and where

$$N = C/\tau + F + V \cdot x + \sum_{i \in \mathbb{I}} \left(p_i + \sum_{k \in \mathbb{U}} p_k \cdot U_{i,k}\right) \cdot I_i \cdot x - \sum_{j \in \mathbb{O}} p_j \cdot O_j \cdot x \,.$$

The variables C, F, V, I, O, and U, defined in Table 1, depend on the design of the system, which in turn depends upon the history of R&D. The variable C further depends on some commodity prices, labor rates, permitting fees, etc. One might assume that an infinite amount of R&D investment would lead from the present conditions C_0, F_0, V_0, I_0, and O_0 to an optimal design where these attain the values C_∞, F_∞, V_∞, I_∞, and O_∞.

In principle, the parameters C, F, V, I, O, and U depend on both the TRL and TPL levels, though generally not equally. For purposes of the very simple analysis presented here, we model N/x as the simple function $\overline{N} = N/x = f(L_{\text{TRL}}, L_{\text{TPL}})$ of the two technology levels and arbitrarily (for illustrative purposes) choose the following functional form:

$$\overline{N} = f(L_{\text{TRL}}, L_{\text{TPL}}) = -\left(\frac{5}{1+e^{-2(L_{\text{TPL}}-4)\sqrt{L_{\text{TPL}}}/10}} + 1\right)\left(L_{\text{TPL}} + \frac{1}{2}\right).$$

We model the evolution of TRL and TPL as Itô or Stratonovich processes, which are stochastic diffusion processes involving integrals both with respect to time and with respect to Brownian motion. Now consider an R&D investment dr, made over a time period dt, which results in a shift in

[1] Though some DOE programs let marketplace and economic considerations creep into their TRL.

technology readiness or performance level $dL_k = 1_{L_k \leq L_{k,\infty}} \cdot (L_{k,\infty} - L_k) \cdot (\alpha_k \, dt + \beta_k \, dr_k)$, where dr_k is a Gaussian random variable. The α_k represents the drift in TRL and TPL over time due to changing external conditions such as general technological progress, information technology, management expertise, labor rates, raw material prices, etc. The β_k represents the TRL/TPL return on the R&D investment. In the case where we have a detailed technology design model and understand the design's response to R&D investment, these random variables can be expressed more fundamentally in terms of the actual technological process and design. For R&D investment in an individual technology, the policy problem is to select the two β_k as a function of time.

Table 1. Variables in generic cost computation.

Variable	Description	Example Units
C	capital cost	USD
τ^{-1}	capital recovery factor	1/yr
F	fixed operating	USD/yr
V	variable operating costs, excluding feedstock and other commodities	USD/unit
I_i	quantity of inputs (e.g., feedstock, energy, water) i per unit production	kg/unit
$i \in \mathbb{I}$	set of inputs i	-
O_j	quantity of output byproduct/coproduct (e.g., wastewater, GHGs) j per unit production	kg/unit
$j \in \mathbb{O}$	set of outputs j	-
$U_{i,k}$	upstream impact k of production of input i	kg/kg
$k \in \mathbb{U}$	set of upstream inputs k	-
p_i	price of input i, which may be negative in the cases of credits (e.g., RINs, RECs)	USD/kg

For this illustrative model, we choose $L_{\text{TRL},0} = L_{\text{TPL},0} = 1$ $L_{\text{TRL},\infty} = L_{\text{TRL},\infty} = 9$, $\alpha_{\text{TRL}} = \alpha_{\text{TPL}} = 0.02$, $\beta_{\text{TRL}} = 0.4\lambda$, and $\beta_{\text{TPL}} = 0.2(1-\lambda)$, where λ is the fraction of R&D investment in improving TRL and $(1-\lambda)$ is the fraction invested in improving TPL. Thus, TRL has greater responsiveness to investment than does TPL. This reflects the different levels of difficulty in achieving an operational technology at scale versus an economically competitive technology at scale.

We consider the R&D investment optimization problem of adjusting λ on an annual basis in order to minimize $\overline{N}$. We use the following recipe for multi-stage stochastic optimization to estimate $\lambda(t)$:

1. For each year, create an ensemble of potential investments λ and an ensemble of L_k trajectories by integrating the stochastic differential equations using the Python package SDEINT assuming the investment level λ.
2. Select the λ that minimizes the $\overline{N}$ in the final year.
3. Simulate one trajectory to determine L_k for the next year.
4. Repeat the above for that next year.

Note that a more sophisticated optimization would consider all $\lambda(t)$ in step #1, not just considering λ to be a constant from that year onward.

Results

Figure 1 displays an ensemble of TRL/TPL trajectories, each the result of a multi-stage stochastic optimization. These show a general bias towards following the minimum of the function $f(L_{\mathrm{TRL}}, L_{\mathrm{TPL}})$, which has a modestly strong gradient from lower to higher TPL when TRL is in the vicinity of 5.5 and which has stronger gradients from lower to higher TRL when TRL is below 5.5. It is also apparent that the optimization process corrects for advancement that moves the trajectory away from its optimum by emphasizing investment towards that optimum.

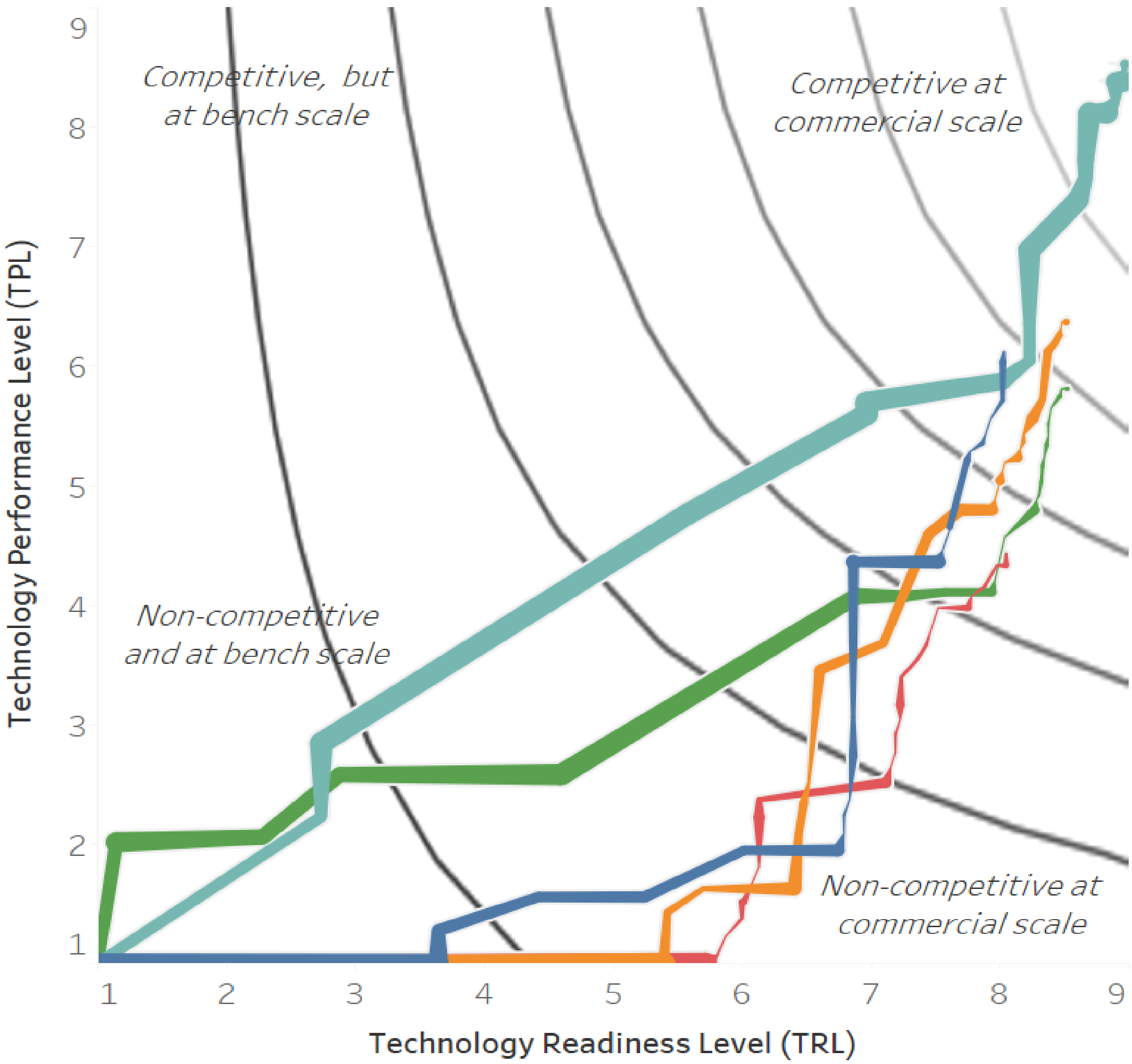

Figure 1. Several thirty-year TRL/TPL trajectories resulting from multi-stage stochastic optimization of technology cost where the relative investment in TRL- and TPL-oriented R&D is optimized each year. Each colored line corresponds to a single ensemble member (i.e., one multi-stage optimization); the thickness of the line reflects the intensity of investment in TRL-oriented R&D. The gray contours in the background represent isolines of constant $\overline{N}$, with lighter lines having lower values. The blue, orange, and red trajectories make fast progress in TRL, but then struggle to increase TPL, resulting in them not reaching the commercial competitiveness achieved by the teal-colored trajectory, which makes balanced, early progress in both TRL and TPL before a final improvement in TPL.

Lessons Learned and Puzzles

- Performing a search over the optimal investment allocation $\lambda(t)$ in a highly stochastic context requires a large number of trajectory evaluations, each of which involves integrating a stochastic differential equation (SDE). The total number of SDE solutions needed equals the product of four factors:
    - number of time steps,
    - size of the ensemble used to compute the expectation of the final-year cost,
    - granularity of the search over λ, and
    - number of optimal trajectories computed.

  Will it be feasible to do this rapidly enough on a laptop computer in order to provide real-time decision support?

- Continuous stochastic models such as Itô or Stratonovich processes do not capture the non-continuous time frames (fiscal quarters and years) over with R&D is bundled, nor do they capture discrete improvements such as a major redesign of part of the technology. What might be done to incorporate these non-continuous factors?

- The model presented here assumes that there is never loss of TRL or TPL. How likely are circumstances where readiness or performance is lost as time progresses?

- TRL and TPL may be too abstract and disconnected from detailed technology models to connect specific R&D investments to improvement in these levels. However, historical data showing the relationship between past R&D investments and changes in TRL/TPL may be relatively obtainable; so might it then be possible to calibrate stochastic models of TRL and TPL?

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Appendix: Technology Readiness Levels [cf. Figueroa, 2011]

TRL 1	TRL1 is the lowest level of technology readiness. Scientific research begins to be translated into applied R&D. Examples might include paper studies of a technology's basic properties or experimental work that consists mainly of observations of the physical world.
TRL2	TRL2 moves ideas from basic to applied research. Applications are speculative; there may be no proof or detailed analysis to support the assumptions. Most work is analytical or paper studies to understand the science better. Experimental work is designed to corroborate the basic scientific observations made during TRL1 work.
TRL3	TRL3 moves to experimental R&D to verify concept works. Includes analytical, laboratory-scale, modeling, and simulation studies to physically validate analytical predictions of separate technology elements. Components of technology are validated, but there is no strong attempt to integrate the components into a complete system.
TRL4	TRL4 is first step in determining individual components will work together as a system. Includes integration of ad hoc hardware in a laboratory and testing them. Supporting information includes results of integrated experiments and estimates of how the experimental components test results differ from system performance goals.
TRL5	TRL5 integrates components so that system configuration is similar to final application. Supporting information includes statistically relevant results from laboratory testing, and analysis of differences between the laboratory and eventual operating system/environment and implications for the eventual operating system/environment.
TRL6	TRL6 steps up to true engineering development/testing of the technology as an operational system in a relevant environment and determines scaling factors that will enable design/production of final system. Includes statistically relevant results from the engineering scale testing. The goal of TRL 6 is to reduce engineering risk.
TRL7	TRL7 demonstrates an actual system prototype in a relevant environment and associated manufacturing scale-up for a relevant time duration. Supporting information includes results from the full-scale testing and manufacturing. Final design is virtually complete. This stage retires engineering and manufacturing risk.
TRL8	The technology has been proven to work in its final form and under expected conditions. In almost all cases, this TRL represents the end of true system development. Product performance delta to plan needs to be highlighted and plans to close the gap will need to be developed.
TRL9	The technology is in its final form and operated under the full range of operating conditions. Emphasis shifts toward statistical process control.

Appendix: Technology Performance Levels [Weber, 2013]

TPL 1	Majority of key performance characteristics and cost drivers do not satisfy and present a barrier to potential economic viability and critical improvements are not regarded as possible within conceptual fundamentals.
TPL2	Some key performance characteristics and cost drivers do not satisfy potential economic viability and critical improvements are not regarded as possible within conceptual fundamentals.
TPL3	Minority of key performance characteristics and cost drivers do not satisfy potential economic viability and critical improvements are not regarded as possible within conceptual fundamentals.
TPL4	To achieve economic viability under distinctive and favourable market and operational conditions, a number of key technology implementation and fundamental conceptual improvements are required and regarded as possible.
TPL5	To achieve economic viability under distinctive and favourable market and operational conditions, some key technology implementation improvements are required and regarded as possible.
TPL6	Majority of key performance characteristics and cost drivers satisfy potential economic viability under distinctive and favourable market and operational conditions.
TPL7	Competitive with other renewable energy sources given favourable (e.g., high feed- in tariff) support mechanism.
TPL8	Competitive with other energy sources given sustainable (e.g., low feed-in tariff) support mechanism.
TPL9	Competitive with other energy sources without any support mechanism.

Simple Petri Net Model for Dual-Junction III-V PV

Purpose

This simple example illustrates the use of Petri nets (state-transition networks) to model the discrete transitions, concurrency, and iteration that can occur in some technology evolution in response to R&D investments. *Discrete transitions* might occur during R&D when research leads to the replacement of one material, procedure, or chemical by another. *Concurrency* occurs when R&D occurs in parallel on multiple aspects of a technology. *Iteration* occurs when R&D repeatedly undertakes to improve the same technological component. Petri nets emphasize discrete transitions between qualitatively different technological states of affairs and allow the modeling of interacting R&D processes that iteratively address concurrent technological issues. Petri nets can also capture situations where some types of technology advancement may preclude specific types of future R&D or render moot previously undertaken R&D.

Methods

Here we apply Petri-net modeling to two subprocesses in the complex sequence for fabricating a dual-junction III-V photovoltaic cell. Figure 1 summarizes the overall process. A key feature of such fabrication is that R&D investments might in principle target any of the myriad processes or materials involved. The R&D objective is to lower the $/W cost and improve the efficiency (η) of the subprocess. The cost of the whole wafer is the sum of the subprocess costs and the product of the subprocess efficiencies. When one year's worth of R&D funds is invested (one "trial"), the impact on cost and efficiency can be modeled with random draws from probability distributions.

This example treats two potential improvements in the first step of Figure 1:

1. *Increased parent epi-substrate reuses:*
   Initially, there are 20 reuses of the epi-substrate. Based on published data [Woodhouse and Goodrich, 2014], we approximate the cost in $/W of this stage of the process as proportional to $e^{3.65-0.98(\ln R)-0.020(\ln R)^2}$ where R is the number of reuses. Each $500K trial has a 90% probability of increasing R; the increase is modeled as the exponential of a Poisson-distributed random variable whose mean is 1.75.
2. *Replacing chemical-mechanical repolishing with wet-bench surface preparation:*
   A wet-bench success replaces chemical-mechanical polishing and has a cost uniformly distributed between zero and $0.1/W. Each $1.5M trial to develop a wet-bench surface-preparation process for the epi-substrate has a 7.5% chance of success.

As shown in Figure 2, where the bottommost portion ("CMP" and "Epi-Substrate") of the "Reference Case" bar changes from almost $6/W to less than $0.1/W in "Mid-Term", these two R&D efforts can result in dramatic reduction in III-V cell cost and modest improvement in efficiency. These are just two of the many potential R&D foci shown in the technology roadmap simulations in Figure 2.

Figure 3 shows the Petri net embodying the above state, transition, and cost assumptions. The left side of the diagram represents the state of the epi-substrate reuse along with the transition

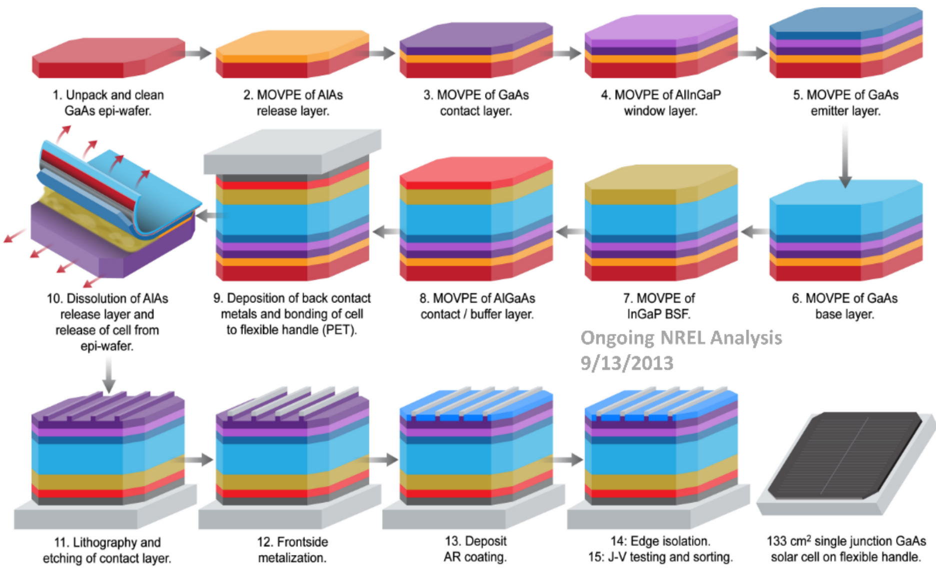

Figure 1. Simplified process flow for fabricating some single-junction III-V solar cells. *(Source: Woodhouse and Goodrich, 2014.)*

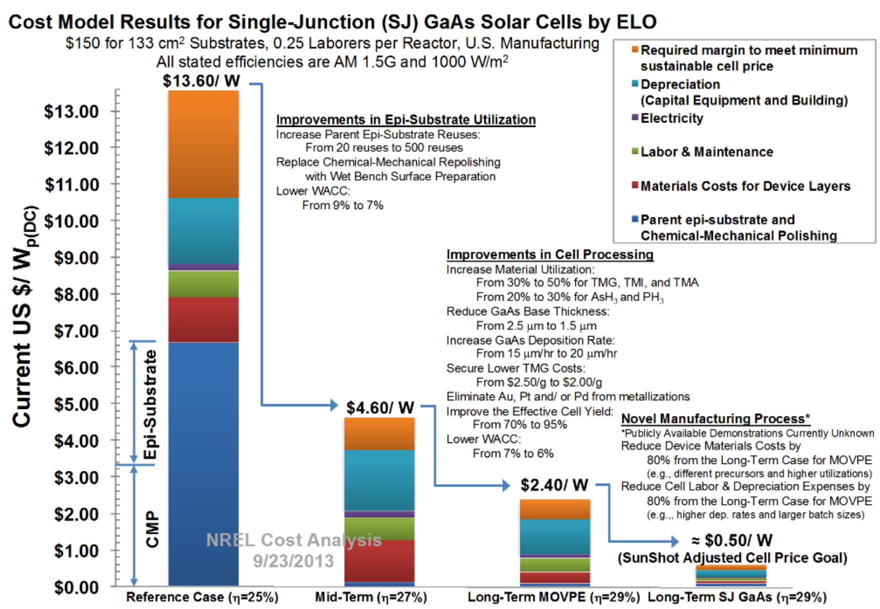

Figure 2. Example R&D opportunities and cost model results for some dual-junction III-V solar cells, based on technology roadmap simulations. *(Source: Woodhouse and Goodrich, 2014.)*

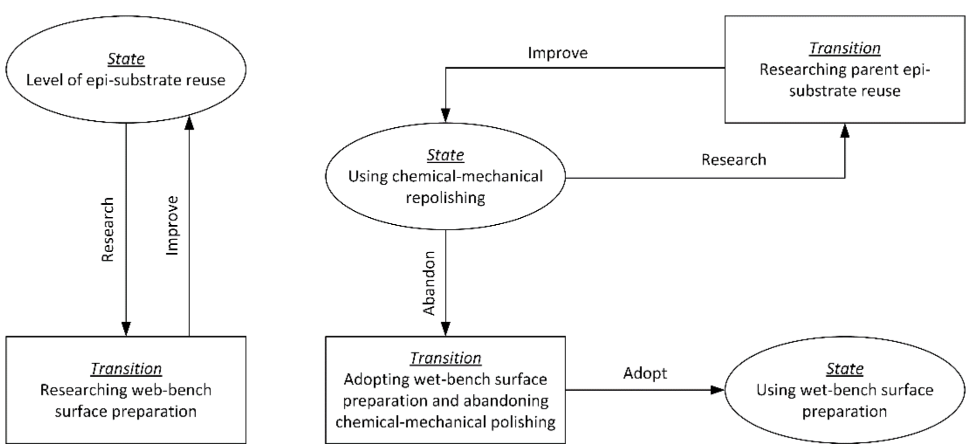

Figure 3. States and transitions in this Petri-net model. The left side shows iteration of research, whereas the right side shows research that results in a design change.

associated with performing R&D to increase the number of reuses. The right side of the diagram shows how the initial state of the design (chemical-mechanical repolishing) can transition to a new design (wet-bench surface preparation) after R&D enables such a transition. We use the SNAKES toolkit [Pommereau, 2015], a Python package, for modeling the Petri nets.

Results

The plots in Figure 4 and the animation in Figure 5 illustrate the trajectories of $/W cost components and the cumulative investment associated with them. Increasing the number of epi-substrate reuses is a repeated process with varied results on each trial and with diminishing returns, whereas transition to wet-bench surface preparation involves repeated attempts and failures until the R&D succeeds and further R&D stops. The simulation trajectories in the upper graph demonstrate gradual, intermittent, and sudden improvements that represent progress made in parallel within a larger system. Note that while the parameters are chosen to mimic the cost analysis of Woodhouse and Goodrich [2014], the investment allocations, rates, and durations are purely notional.

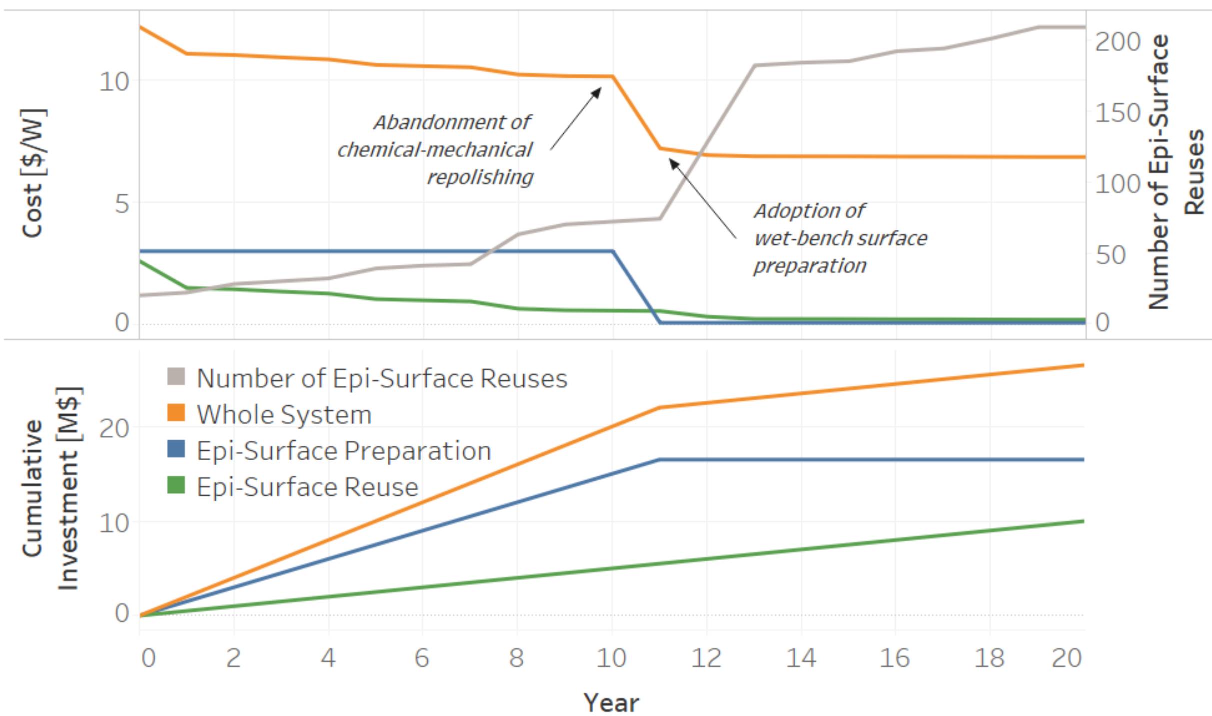

Figure 4. One result of the Petri-net simulation of investments in epi-substrate reuse and surface preparation. Because the simulation is stochastic, each simulation yields a different mix of improvements and costs.

Lessons Learned and Puzzles

1. Petri nets are probably a more general framework than is required for modeling R&D on PV subsystems because the subsystem designs do not have complex enough correlations and dependencies between one another to necessitate use of Petri nets. The overall system can probably be modeled as a cartesian product of state machines

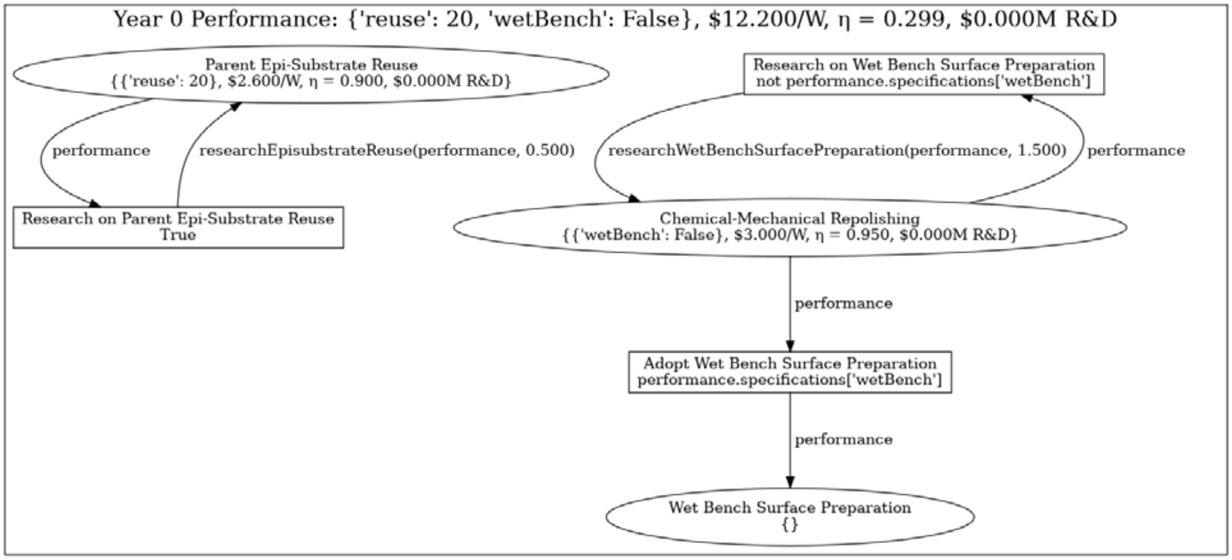

Figure 5. Animation of the state of the petri net for a simple experiment. The title in the animation below shows the overall system cost ($/W), efficiency (η), and spending on R&D for each year. The corresponding data for each subsystem is shown in the ovals.

because most of the PV subprocesses can be researched in parallel, even though they might have different priorities (in terms of R&D investment) and affect overall cost nonlinearly. Might modeling non-PV technologies perhaps benefit from the use of Petri nets?

2. It seems important to be able to represent interdependent R&D processes that have a mixture of continuous improvements versus discrete jumps and where some R&D may block or unblock future R&D activities or make past ones irrelevant. Can this strength of Petri-nets be incorporated in a hybrid model with Monte Carlo simulation, Stochastic Optimization, or others?
3. The Woodhouse & Goodrich publications are nearly sufficient to build simple R&D-focused models that combine PV subprocesses and identify areas of potential improvement, but they do not contain information on how R&D expenditures relate to the actual probabilities and magnitude of improvements. To what extent could historical R&D investment data help determine this or will this need to be determined through expert elicitation?
4. Although the Petri net could be represented as a series of (linear) matrix operations, the investment results are likely nonlinear functions.
5. Graphical representations of parallel R&D progress on technological subsystems seem to be useful for gauging progress.
6. The SNAKES toolkit has several quirks: (a) it requires the programming of functions with no side effects (e.g., on global state or involving input/output) on the Petri nets; (b) it does not report error messages when evaluating which transitions are enabled, so an error in computing enablement results in the transition being marked as not enabled; and (c) it is awkward to represent probabilistic petri nets.

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Bayesian Combination of Expert Assessments

Purpose

This toy model explores the use of Bayesian updating to adjust the weight given to expert estimates of R&D impacts when conducting an analysis of R&D pathways. The aim is to investigate whether a Bayesian approach for combining expert assessments can correct for biases in the experts' opinions relative to "real life", and how rapidly such a correction converges to account for the experts' biases.

Methods

This model leverages the PV balance-of-system cost simulation within the Monte Carlo Model in order to grade the performance of subject-matter experts in their predictions of the likely success and subsequent impact of future R&D investments. The grades are translated into weighting factors that evolve over time as more information about the quality of the experts' predictions emerges. What has been learned about evaluating experts' estimation ability in practice will be examined in subsequent work.

The Monte Carlo Model (see the fact sheet on that model) assigns weights/grades (called *authority* in this Bayesian model) to each expert when combining their assessments into an overall estimate of the impact of particular R&D investments, but those weights are static. The Bayesian approach used here simply updates those authorities after each observation of the impact of an investment. We consider the hypotheses that "authority i" correctly assesses the impact of R&D investment and we then update the prior probability for those hypotheses, $\mathcal{P}(\text{authority } i)$, to a posterior probability, $\mathcal{P}(\text{authority } i|\text{impact data})$, which accounts for the observation of the "impact data" showing the outcome of an R&D investment:

$$\mathcal{P}(\text{authority } i|\text{impact data}) = \frac{\mathcal{P}(\text{impact data} \mid \text{authority } i) \cdot \mathcal{P}(\text{authority } i)}{\mathcal{P}(\text{impact data})}$$

Initially, we give each expert an equal authority. The probability distribution for each expert yields the likelihood function, permitting one to compute $\mathcal{P}(\text{impact data} \mid \text{authority } i)$ for the observed impact of R&D investment. The Bayesian update is applied each time new impact data is observed.

Results

Figure 1 shows the triangular distributions for experts a, b, and c in the Monte Carlo Model. In this study we vary the "real life" distribution to study different possible biases relative to the experts, but start from a "real life" distribution that is approximately unbiased relative to the average of the experts. We leave aside for now the fundamental question of how to determine experts' accuracy or measure biases. In these toy model experiments the bias takes two forms: (i) increasing or decreasing the probability for no advance in the technology (i.e., the point mass of probability on the right side of Figure 1), and (ii) shifting the minimum, apex, and maximum of the triangular distribution to the left or right. Figures 2 and 3 illustrate the evolution of authorities for the case when the experts are collectively approximately unbiased relative to reality (Fig. 2) or collectively biased (Fig. 3). Overall, the results illustrate that the updating scheme makes authorities responsive to the new evidence, taking five or ten updates to fully incorporate it and approximately converge. (Engaging an expert sufficiently to achieve so many updates may be impractical.)

Comparison between bottom panels of Figures 2 and 3 shows that when experts are substantially biased relative to the real-life situation, a hypothetical truly unbiased expert (represented by the fourth, “real life”, expert) captures the total authority. These results hint at the conditions under which the effective pool of expertise evolves towards either mixtures of experts or reliance on a single expert: the authority of experts relatively close to “real life” tend to survive the updating process whereas experts far from “real life” lose authority and may become excluded from the pool of expertise. (This situation raises a concern that an expert with insight into low-probability events might become prematurely and erroneously excluded over time as high probability events are repeatedly observed.) The re-weighting of authorities has implications for the overall quality of predictions: Figure 4 quantifies the extent to which the updating of authorities improves the estimate of reductions in balance-of-system costs relative to statically weight the experts (i.e., not updating their authority weights). The impact of Bayesian updating is not dramatic here.

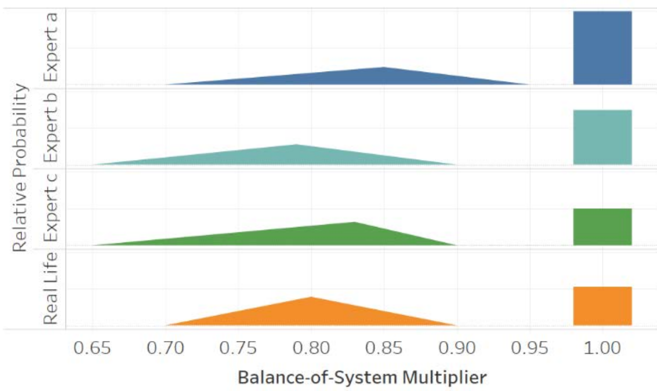

Figure 1. Example triangular probability distributions for R&D investment impact for the three experts (a, b, c) and the “real life” situation. The “multiplier” axis indicates the balance-of-system cost of the technology relative to that cost prior to the investment. The mass of probability at the multiplier being equal to one (shown approximately in the plot as the rectangle on the right side) indicates the chance of an advance not occurring. Expert “a” has a relatively pessimistic bias. “Real life” is unbiased relative to the average of the triplet of experts.

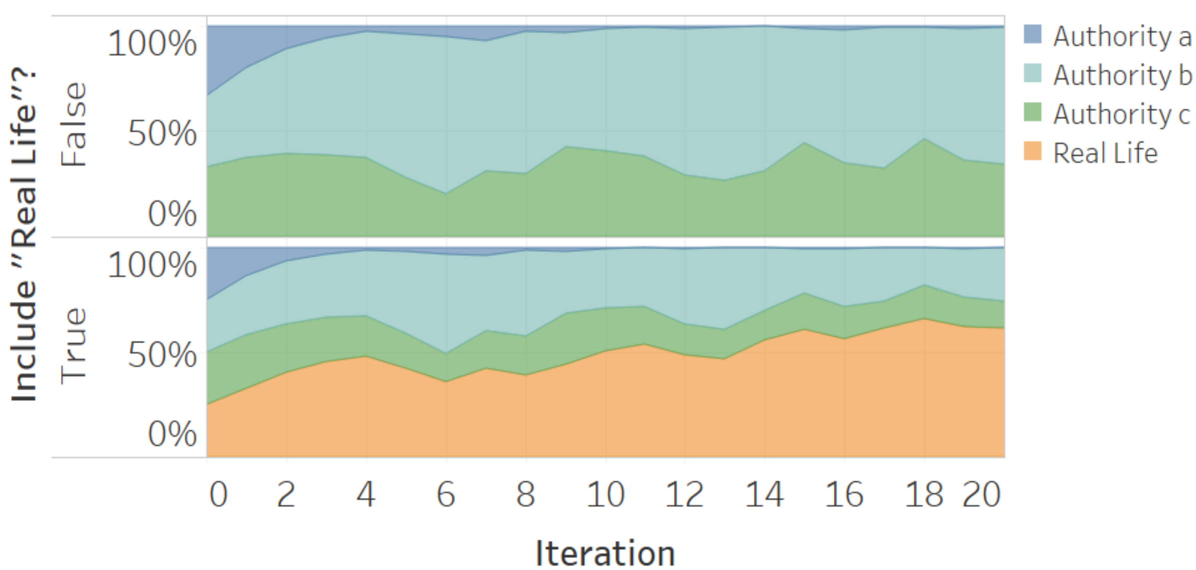

Figure 2. Evolution of authority weights over time as new evidence is received about experts’ performance. As shown in Figure 1, the “real life” situation is approximately unbiased relative to the experts. The upper panel shows the evolution of authorities when they compete among themselves, whereas the lower panel includes a hypothetical fourth expert whose predictions match the real-life situation.

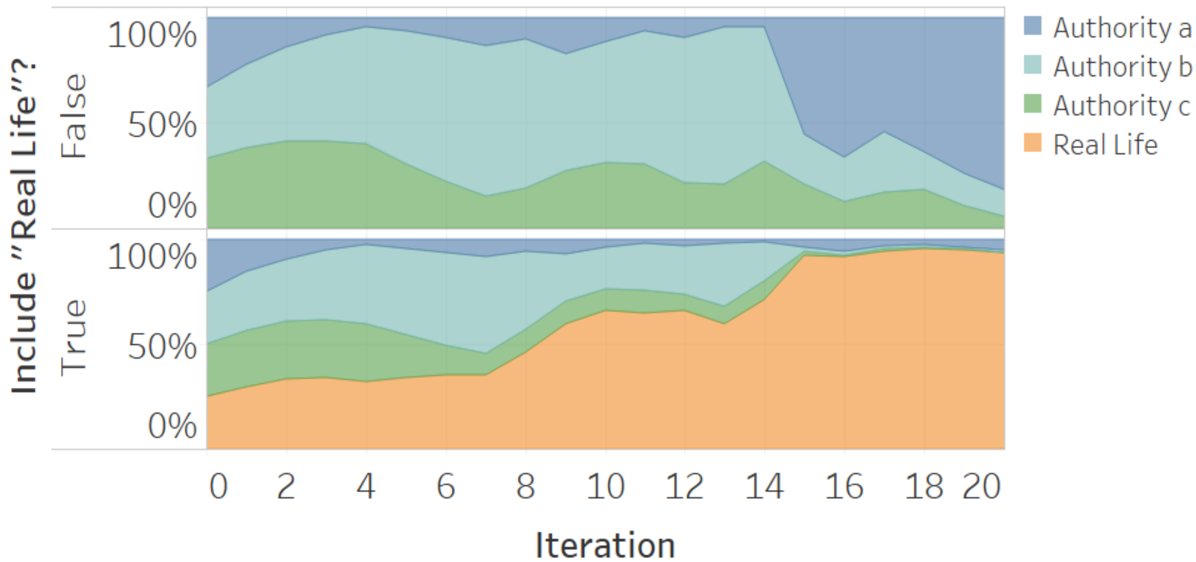

Figure 3. Evolution of authority weights over time as new evidence is received about experts' performance. In contrast to Figures 1 and 2, the "real life" situation is biased relative to the experts, having a lower real-life probability of improvement and a lesser impact when improvement occurs. The upper panel shows the evolution of authorities when they compete among themselves, whereas the lower panel includes a hypothetical fourth expert whose predictions match the real-life situation.

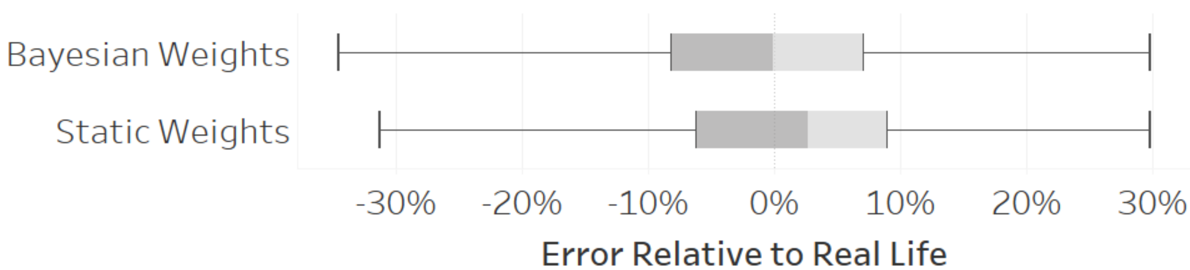

Figure 4. Distribution of errors in estimating PV balance-of-system cost reduction due to R&D investments compared between static authorities versus the Bayesian updating of authorities, as a function of biases towards improvement and towards impact on reducing costs. A one-sided sign test for this 1000-simulation sample accepts the null hypothesis that the Bayesian errors are equally likely to be smaller or larger than the static errors.

Lessons Learned and Puzzles

Lessons Learned

- The Monte Carlo Model's triangular distributions for expert assessments are not generally suitable for this Bayesian updating scheme because triangular distributions have compact support: For instance, if the observed outcome of an R&D investment falls beyond the minimum or maximum of the "triangle", then the likelihood of that observation is zero, resulting in the posterior probability of the expert being zero, too. Thus, a single observation outside of the expert's range of prediction eliminates that expert from having further authority—i.e., they are no longer in the pool of expertise. It is conceivable that, over time, observations falsifying each expert's authority will occur: this will result in all experts being eliminated. Thus, it is desirable for the tails of probability distributions for experts to extend at least as far as the real-life possibilities for observations. Hence, instead of using a triangular distribution, for more robust analysis, one might translate the triangular distributions into a split Gaussian distribution whose right-side and left-side variances match the corresponding variances of a triangular distribution.

- In general, there will be a delay between the making of an investment and the revelation of the impact of that investment. Thus, the Bayesian updates should lag.
- Furthermore, measurements of the impact of R&D investments may be uncertain, too, so measurement error should be convolved with the likelihood functions when estimating the posterior probabilities for the experts.
- A full sensitivity analysis involving different biases in experts, expert pools of different sizes, different investments, and different subsystem/component stacks (i.e., full portfolios, platforms, and projects) is warranted. The simple experiments presented here are too parochial for generalization.
- It appears that the predictive advantage of the Bayesian approach is subtle and that large amounts of experience may be necessary to prove it superior to static weights.

Puzzles

- How does one measure expert performance? How does one distinguish a poorly performing expert from one with keen insight regarding outliers or low-probability events?
- Bayesian updating may tend to gradually eliminate experts that are more biased than the other experts in the pool. Although this might be generally desirable, it might prematurely reduce the overall diversity of expertise and lead to missing rare events (e.g., breakthroughs) that some of the eliminated experts might have better predicted. How should this be managed?
- Should there be separate weights of expertise for the occurrence of an improvement versus the amount of progress once an improvement is made?
- There is an option to finely grade experts. Each expert might be graded on improvements versus amount of advance for each prediction type and scenario for which they make a prediction. One really needs to model correlations of biases in the predictions an expert makes, or sufficient historical data to tease out whether an expert's optimism is confined to an area or whether it is pervasive. How can this be done?
- How does the Bayesian approach compare to a frequentist approach to weighting experts based on their past performance?
- How would Bayesian updating improve if information on an expert's performance is individually feed back to the expert, so they can adjust their future predictions? If experts correct themselves, then weighting them might become moot.

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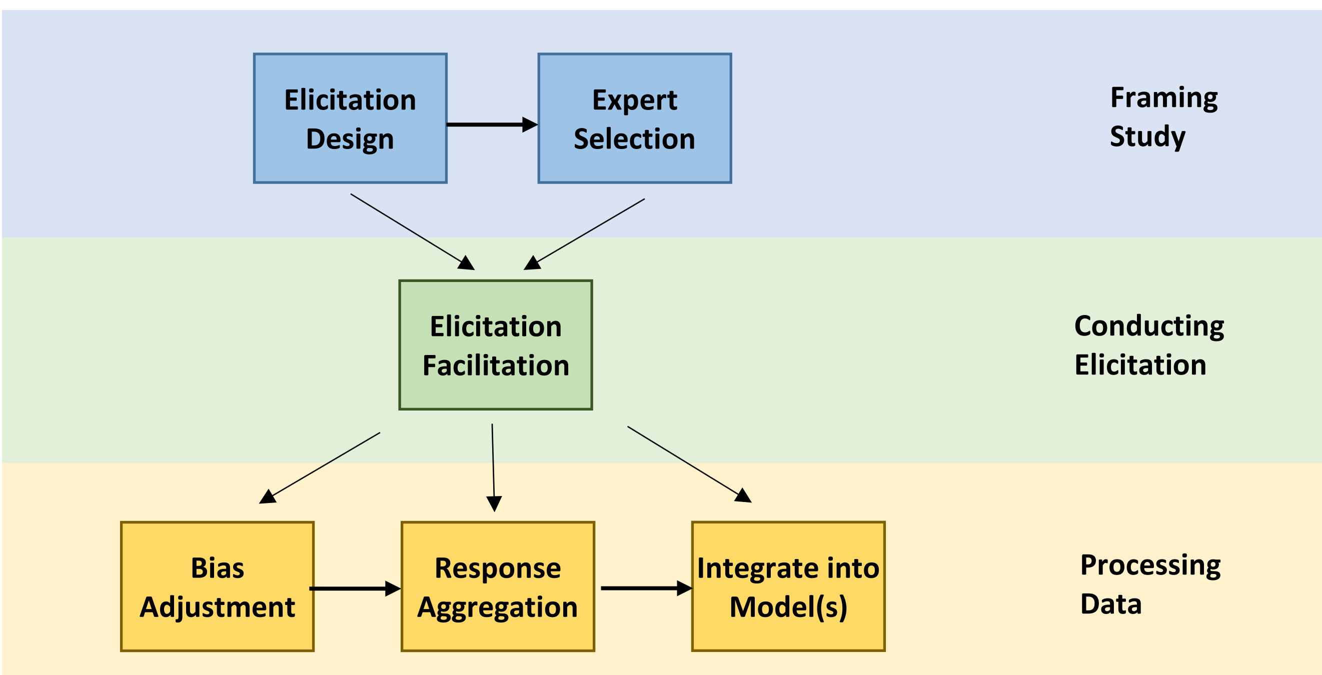
R&D Pathways and Portfolio Analysis and Evaluation
Expert Elicitation Issues Fact Sheet

Context

Expert elicitation has long been used to explore complex domains beyond the reach of available technology and economic models. In the energy sector, one of the first highly visible efforts was that by Rasmussen *et al*. on nuclear power safety. Since then, much has been learned about conducting expert elicitations and the challenges in doing them well, including: the selection of experts; the design of the elicitation; the facilitation of the elicitation; the cognitive biases in responses; the calibration of the individual responses; the methods for aggregating responses; and more.

For this study, the focus is on scientific, engineering, and economic assessments of technology components, subsystems, systems, and portfolios, broken out in logical self-contained technology elements and the impacts of R&D investments on their cost, performance, and other factors of interest. There are no planned assessments of policy, such as valuations for regulatory decisions, which is outside the scope. Experts across industry, universities, national laboratories, and other domains are expected to be tapped for their insights on potential opportunities and impacts of particular research activities on technology advances.

Work on expert elicitation has not yet begun for this study, but it will be an important focus in subsequent activities. This will include a detailed literature review and assessment, a few representative papers reviewed to date are listed below; exploration of issues such as those raised in the next section, possibly including some experiments; and application in pilot project analyses and evaluations. Tapping the experience and expertise of the science and technology community for how to best approach these issues is very important.



Representative Issues

For expert elicitation, the literature review and assessment will evaluate how well issues such as the following can be dealt with for the types of cases that this study targets identify where important gaps remain, and possible approaches for addressing them.

Framing Study	**Initiating Conditions**: What conditions make an expert elicitation worthwhile to undertake or not? Are there conditions (e.g., out-of-sample) that are fundamentally not amenable to such expert elicitation? **Alternatives to Experts**: In situations where no experts exist, are there data-driven, artificial intelligence, causal modeling, or other methods to fill gaps? **Scope of Assessment**: How granular should expert assessment be? Should assessments focus on very specific technological concerns (i.e., improving or replacing a component, material, or process)? What might high-level assessments contribute (e.g., assessments of improvement in overall performance, cost, or readiness)? **Time Frames**: How far into the future are expert assessments actionable? **Target of Assessment**: Should experts solely assess technological aspects of R&D, or should their assessment include other potentially contributing factors? **Number of Experts**: How many experts are necessary and sufficient to evaluate each component or subsystem, before diminishing returns are experienced? **Selection of Experts**: What expertise, experience, or other capabilities should an expert have? Are generalist (i.e., multi-domain) experts useful in specific technological contexts? How can expert self-assessments or other evaluations (literature citations, patents, recommendations) be used? **Design of Elicitation**: What factors should the elicitation assess with what types of questions (e.g., numerical, percentage)? What pre-testing should be done (e.g., for length, clarity, coverage)? **Minimizing Overheads**: How can the cost and time required to produce a high-quality expert elicitation be minimized for both the experts engaged and for the program staff conducting the work? **Cost Effectiveness:** In what situations is the expense and delay due to obtaining expert opinion insufficiently justified by the actionability of the expert-informed results? I.e., when are uncertainties so large as to make expert opinion irrelevant?
Conducting Elicitation	**Background Information and Training**: What background information (technical data, past performance, etc.) should be given to the experts, and what training should be provided (e.g., how to reduce cognitive biases)? **Conduct of Elicitation**: What is the most effective way to conduct an elicitation, such as in-person or on-line, with or without cross-expert discussion, with one-time or iterative engagement, etc.? Can there be benefits of cross-expert interaction without suffering social influences (e.g., peer effects)? **Other Issues**: How can proprietary concerns, competitiveness concerns, and others be minimized?
Processing Data	**Addressing Cognitive Biases**: How can cognitive biases (e.g., anchoring and adjustment, availability, overconfidence, etc.) best be addressed? How can correlations across experts be managed (e.g., particular areas of R&D may have few experts, limited existing literature)? Would it be preferable to create an expert-informed model for making assessments instead of having experts make the assessment directly? **Calibration of Responses**: How can responses be calibrated to address cognitive biases or other factors? How can appropriate weighting of responses be developed and applied, if any—such as by an expert's past performance? **Aggregating Responses**: How can responses to the elicitation best be aggregated and used? Should expertise be pooled prior to evaluating R&D decisions or should multiple expert-based R&D assessments be pooled after the evaluation of potential R&D decisions? **Outliers**: How can one distinguish an insightful outlying response by an expert from a poor response? What diversity of expertise and size of expert pool is needed to ensure that insightful outlying prediction of high-impact actions and events are represented?
Communi-cations	How can the results of expert-informed analysis be accurately and effectively communicated to decision makers, appropriately representing the various risks and uncertainties?
	How might visualizations be made effective use of in communications to decision makers?
	How can the underlying foundational data and analysis be effectively communicated so that the decision maker understands their basis without overburdening the decision maker?

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