Energy Systems Analysis

Investigators

A.J. Simon, GCEP Energy Systems Analyst; Rebecca Hunt, GCEP Software Engineer; Karen Law, Kelsey Lynn, Brooks Moses, Jodie Prud'homme, Ben Reineman, Adam Simpson, Graduate Researchers, Stanford University

Introduction

The goal of Energy Systems Analysis is to develop a methodology for measuring the impact of technologies from an energy- and materials-usage standpoint. The Energy Systems Analysis team supports GCEP's missions of building a technical portfolio and assessing the impact of research by developing software models that allow quantitative comparisons of energy technologies. As part of the GCEP Central Assessment effort, the analysis team's work allows GCEP members to better understand where opportunities exist to reduce the emissions or increase the efficiency of energy systems and devices.

The Analysis group builds models of mass and energy flow through existing and proposed energy technologies. The technologies under study encompass the same range of subjects that GCEP is investigating: harvest, storage, distribution, conversion and use of energy. The models are designed to encompass varying levels of technical detail. Each model tracks the inputs and outputs as well as intermediate states for the material and energy streams used by a device. Such models can pinpoint the most efficient and least efficient steps of device operation, and provide the researcher with an in-depth understanding of the technological challenges faced by engineers and scientists. This work will help GCEP locate promising research opportunities for low-emissions, high-efficiency energy technologies and identify barriers to the large-scale application of these new technologies.

The basis of the models is exergy analysis, whereby the irreversible steps in energy conversion processes are identified, quantified and compared to ideal models of energy conversion. The Energy Systems Analysis Group is taking a bottom-up approach to energy system modeling, composed of three phases:

1.   Device-Level Modeling

2.   Fuel Chain Analysis

3.   Energy Network Scenario

Device-Level Modeling

As a first step, individual devices are identified with their associated inputs and outputs. The relationships between the properties of mass and energy as they enter and exit the system are determined by the system model. Model parameters are linked to know state transitions within the system and to material and kinetic constraints. Each model is a self-contained module which can stand on its own, and is fully documented with respect to usage, governing equations and reference material.

Models start out as simple, time-invariant "black-box" representations of an energy

system with assigned 2nd law efficiencies. The 2nd law efficiency value is refined by examining the components inside of the black-box for temporal and spatial gradients where transport and kinetic phenomena cause exergy destruction.

Fuel-Chain Analysis

Subsequently, these individual models will be integrated into a fuel-chain-analysis framework. The framework that links together individual components inside of a single device model will be extensible such that it can link devices together into a fuel chain. The fuel chain model will be built on a "well-to-waste" philosophy, which tracks the resources needed to run all of the internal components, and follows the energy and mass until it is returned to a state in equilibrium with the environment. A sequential chain of devices can be used to explain any inefficiencies, while a branched model can be used to compare various fuel chains and explore device synergies.

Energy Network Scenario

Eventually, energy network models will be built from individual components, chains and distribution scenarios. It is important to note that the component models will not lose any fidelity during this scale-up process. The effects of real technology development on energy infrastructure can be estimated and incorporated into the Integrated Assessment and Technology Assessment efforts taking place within GCEP.

Background

The term "Energy Systems Analysis" at GCEP is used to describe modeling efforts aimed at:
1. quantifying the performance of individual devices and
2. characterizing the interactions between various devices.

The tools, process, and results from the Systems Analysis work towards these goals is described in the next section.

Analysis of energy systems is taking place at numerous organizations across the globe. In these groups, energy systems analysis work may focus on different goals than those GCEP is working towards. These goals may include:
- tracking the fate of resources as they are processed through the energy economy;
- determining the economic feasibility of various energy use scenarios;
- predicting the economic outcomes of energy policies;
- finding the causes of, and solutions to, technological, market or policy failure.

The GCEP Assessment team focuses on the first option in the list above, tracking the fate of resources as they are processed through the energy economy. Other "Energy Analysis" systems are being developed at numerous organizations elsewhere: public and private; governmental, corporate and academic. For a more detailed list of these systems, please see the 2005 GCEP Technical Report.[1]

Results

The Energy Systems Analysis team was established in 2003. Since that time, the group has become an integral part of the GCEP assessment process. The group has developed several component models and also has built multiple tools which facilitate model development.

Software Tools

The Analysis Team has taken advantage of commercially available and open source software to facilitate the development of thermodynamic system models. Each software package has been selected based on its ease of use and development, its ability to provide the technical components required, and its reasonable cost. There is not a single tool that provides all of the features required for successful energy system analysis, therefore several packages are required. The following list describes the main tools used by the Analysis Team and how they are being adapted for thermodynamic analysis.

1. Matlab (from The Mathworks) has been chosen as the programming language of choice for the Systems Analysis Group[2]. Matlab is an extremely flexible programming environment with a wide array of computational tools readily available for adaptation to energy system simulation. All of the models and tools described in the next section are written in MATLAB.

2. Cantera (Open Source) is a chemical kinetics and thermodynamics data package that is being developed at Caltech and is released under an open source license.[3] The Analysis Group is using Cantera for chemical equilibrium calculations and kinetics information. The Systems Analysis Team has worked with the developer of the Cantera code base to expand the Pure Component chemical calculations by writing a Carbon Dioxide module and submitting a Heptane module. Additionally, the team has worked to enhance the functionality of the MATLAB interface.

3. The Aspen Suite (from AspenTech) is an integrated modeling environment which tracks mass and energy flows and has a wide range of property data not available in other tools.[4] The Analysis team accesses the property packages in Matlab via an ActiveX interface.

Modeling Tools

In order to build the energy models in a productive and streamlined manner, the GCEP Energy Systems Analysis team has developed a number of software tools. These tools provide a number of functions. First, they provide a consistent interface to programmatically access the different packages described above. This reduces the learning curve and allows more efficient development. Second, a framework has been developed that allows the interchange of information between these packages and between system models, allowing developers to work with multiple underlying tools within one model in a clear, consistent, and realistic manner.

One tool, titled "State Toolbox for Cantera" provides an object oriented interface to Cantera chemical state properties. Written in MATLAB, the State Toolbox was written specifically to enable the tracking of multiple thermodynamic states. Additionally, this package fixes some of the shortcomings of the Cantera property and equilibrium

calculations and extends the property calculations. The State Toolbox also adds the ability to calculate the exergy of given states.
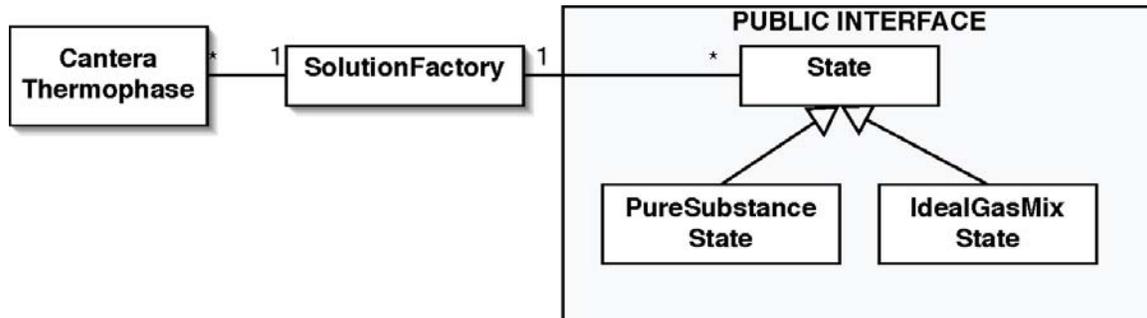

Figure 1: This Unified Modeling Language (UML) diagram shows the object relationship developed for the State Toolbox for Cantera. The Cantera ThermoPhase represents the Cantera object available in Cantera, while the SolutionFactory stores the relationships between Cantera Thermophases and State Toolbox representations of chemical states.

The State Toolbox for Cantera is available to the open source coding community.[5] By making this code available to the wider community, the Analysis team hopes to foster development of and with the model. Providing a shared framework is one step toward integrating our models with those at other institutions.

Aspen is accessed through a tool titled "Stanford Aspen Matlab Interface" (SAMI). This tool provides an object oriented MATLAB interface that accesses Aspen property packages. The Application Programming Interface (API) developed for SAMI is consistent with that of the State Toolbox for Cantera. This provides greater ease of use for researchers familiar with Cantera or the State Toolbox for Cantera. Since Aspen does not have the same distinction between pure substances and mixes that Cantera does, SAMI has an interface that, while similar to the State Toolbox, is simpler.
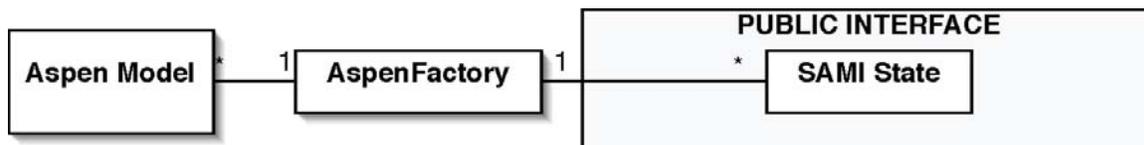

Figure 2*: This UML State diagram of SAMI demonstrates how Aspen Models are managed in a manner similar to that in the State Toolbox for Cantera.

The SAMI package is one part of the work done with Aspen in the GCEP Energy Analysis Team. Additionally, Aspen property packages developed at other institutions have been integrated and enhanced by the Analysis student-researchers

A major component of the tool framework is GCEP Streams. The GCEP Streams package not only provides a representation of physical systems, but also assists the

energy systems modeler in integrating multiple models and tools used in their work. GCEP Streams are used in device level modeling to represent different streams of matter or energy. This software package can integrate tools developed with the State Toolbox, SAMI, and Cantera, allowing the programmer to access the chemical calculations or property packages while building a higher-level model. GCEP Streams enable the connection of device level models to build a Fuel Chain Analysis model, providing a mechanism to appropriately model multiple technologies.

Models

The Energy Systems Analysis team works to build software models of energy systems. These models perform thermodynamic analysis of energy systems, allowing comparative studies of various technologies. This is done by looking at the theoretical efficiencies of systems and varying parameters.

The Energy Systems Analysis team worked with student researches in 2005-2006. This work served to train the next generation of energy systems engineers to think critically about energy and materials. Additionally, the students' work and models provided new insights into specific technologies. The results of some of these models are described below.

CO$_2$ Separation and Capture

Post-combustion carbon dioxide separation was compared with oxy-fuel combustion on a 2nd law basis. The State Toolbox for Cantera was used as the basis of this model, and provided the framework in which to analyze the exergy of all of the material states in each system configuration. The goal of the model was to identify the greatest opportunity for improved technology to impact the energy cost of CO$_2$ capture. Technology is represented in the model by each separation unit's second law efficiency. Baseline efficiencies were chosen to reflect the most widely used separation technologies on the market: 13% for an amine unit used for flue gas CO$_2$ separation and 22% for a cryogenic unit needed for O$_2$ separation from air.

It was found that there is a greater opportunity for improvement in post-combustion systems, and that there is often a need for post-combustion separation in oxy-fuel systems anyway. However, under certain conditions of high fuel carbon content, high equivalence ratio, and high oxygen purity, oxy-fuel systems can be more efficient than post-combustion separation systems.
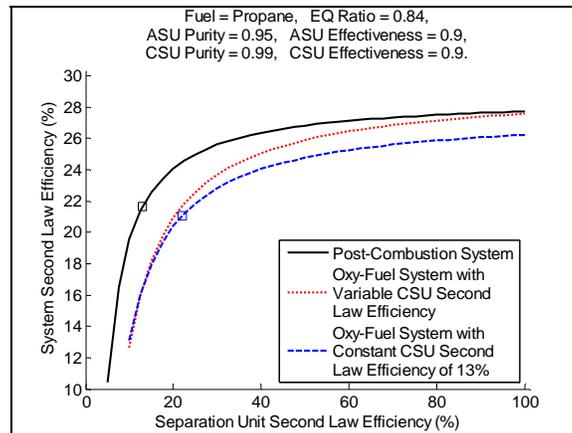
Figure 3: There is more room for improvement in Post-Combustion capture than in Oxy-Fuel combustion given today's technology.
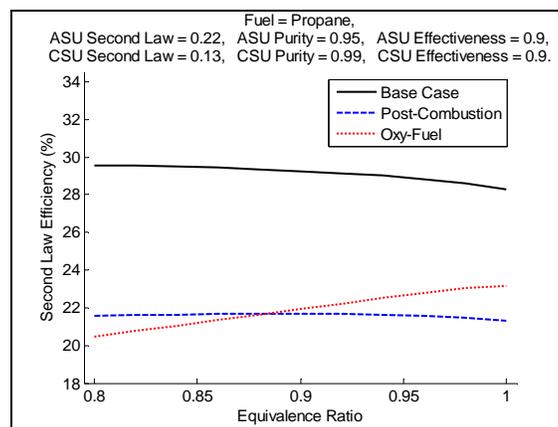

Figure 4*:* At very high equivalence ratios, Oxy-Fuel combustion can surpass Post Combustion Separation

A paper based on these results has been accepted for presentation at the Efficiency, Cost, Optimization and Simulation Conference (ECOS 2006).

Solar Hydrocarbon Reforming

One concern about the deployment of solar collectors is their relatively low efficiency in turning sunlight into an exergy carrier. During a transition from a fossil-energy based system to a renewable system, it may be advantageous to combine energy from two resources and thereby improve the efficiency of the use of each resource. Solar-driven hydrocarbon reformation is an example of such a system.

In this system, concentrated solar energy is used to drive the steam-reforming of a hydrocarbon (fossil) energy resource. Such a system would be advantageous in that it would:

1) Avoid the need for air separation or post-reformation syngas separation.
2) Avoid excess CO_2 release from combustion-driven vessel heating.
3) Use proven infrastructure to convert fuel energy to electricity.

It is clear that such a system would be more costly than a typical autothermal hydrocarbon reformer. However, the system does have the potential to be competitive with other forms of solar collection.
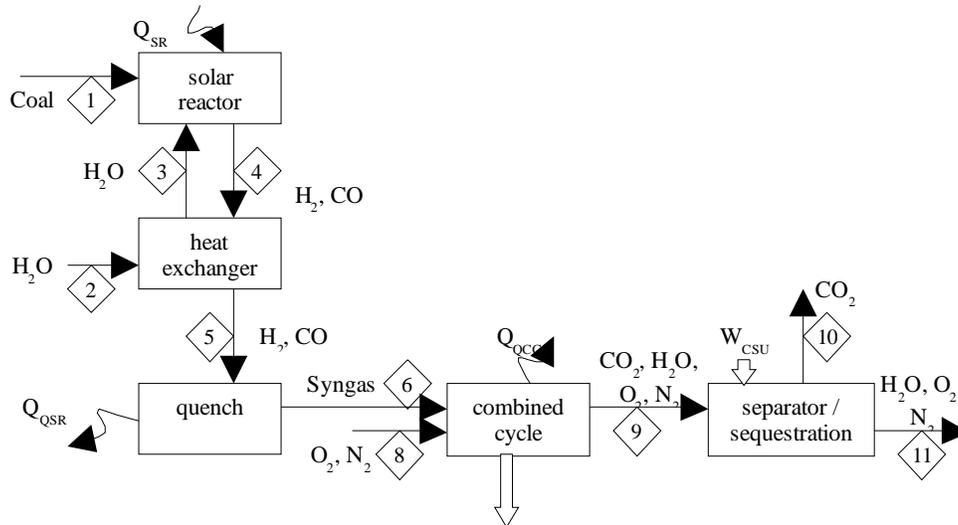

Figure 5: Conceptual layout of the solar-hydrocarbon reformer

The efficiency of only the solar part of the system can be viewed as the "exergy upgrade" of the hydrocarbon fuel.

$$\eta_{II,Solar} = \frac{Ex_{syngas,out} - Ex_{fuel,in}}{Ex_{solar,in}}$$

Analysis has shown that this efficiency can be high enough such that when syngas is converted to electricity (in a standard combustion-fired turbine), the overall solar efficiency significantly exceeds that of photovoltaic cells.

Energy Storage

A model that links emissions and efficiency to electricity generation and storage technologies was built in order to quantify potential resource and CO_2 savings that might result from deployment of storage technologies to the grid. As expected, it was found that emissions reductions are tied directly to the makeup of primary generation technologies, and that storage alone does not significantly impact greenhouse gas emissions.

Under a scenario with a high percentage of low-emissions baseload power (nuclear), it is possible to offset some CO_2 emissions by reducing the need for intermediate and peaking generation through time-shifting demand via storage.   However, in a scenario where baseload power is generated with high emissions equipment (coal), peak-shaving with storage can actually increase emissions.

As intermittent renewables (particularly wind) penetrate into the market represented by a particular grid, they will naturally offset CO_2 emissions. However, it is only under a

scenario where the displacement of large fractions of CO_2-emitting baseload power is assured that augmenting the intermittents with storage can actually reduce overall GHG emissions.
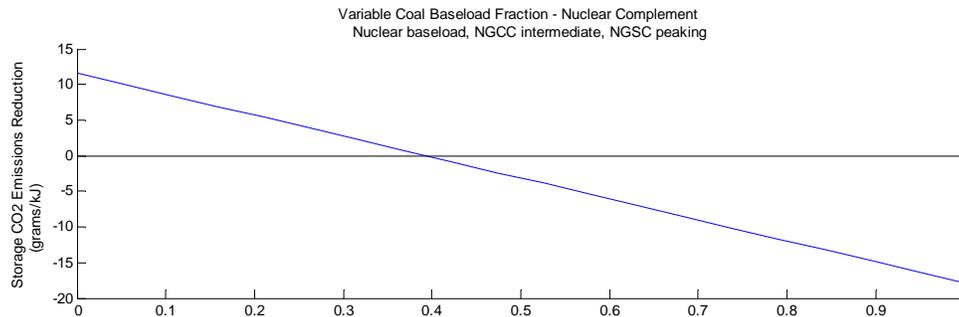

Figure 6: Emissions reduction due to electrical storage as a function of fraction of baseload power that is coal-based.

Future Plans

The Energy Analysis Team will continue to support GCEP's mission of identifying opportunities for research and breakthrough technologies by providing informative tools, models and analysis of energy technologies.

The Energy Analysis Team is continually investigating and maintaining communication with other analysis groups. Our communication with other groups has included an open dialogue with the Hydrogen Systems Modeling group at Sandia National Laboratories. We have met with and look forward to future communication with a group at Ecole Polytechnique Federale de Lausanne that is working on a multi-university thermodynamic programming framework. Discussions are also taking place with Lawrence Livermore National Laboratory. We are evaluating available software such as that written at TU Delft. By fostering open communication, we hope that shared insights will inform our decisions, and we will remain on the forefront of thermodynamic modeling technologies and options.

We will develop tools and models for energy systems analysis to inform the proposal review process. We will continue to share and support the tools we have developed to facilitate the modeling of energy systems. The tools will be used to develop new device level models and fuel chain analysis, which will eventually incorporated into Energy Network Scenario.

Future work on tools includes more development on Cantera, the open source chemical kinetics and thermodynamics package. We are actively involved in the development process and have been granted developer access to the code repository, allowing us to contribute to the growth and utility of this software package.

We also plan to investigate thermodynamics software in development at universities such as TU Delft. We will examine the feasibility and benefits of using new software, possibly developing a MATLAB API consistent with that developed for other tools used at GCEP.

Future models developed will be tightly integrated with the needs of GCEP, with the goal of identifying opportunities for research and breakthrough technologies.

References

[1] "2005 GCEP Technical Report" available online at
   http://gcep.stanford.edu/research/technical_report/2005.html
[2] MALTAB produced by Mathworks
   http://www.mathworks.com
[3] Cantera, hosted by the California Institute of Technology
   http://www.cantera.org
[4] Aspen, produced by AspenTech
   http://www.aspentech.com
[5] State Toolbox for Cantera package available at
   http://project.sourceforge.org/sct-cantera

Contacts
A.J. Simon: ajsimon@stanford.edu
Rebecca Hunt: rahunt@stanford.edu