

# Energy Systems Analysis

## Investigators

A.J. Simon, Energy Systems Analyst; Rebecca Hunt, Software Engineer; Brooks Moses, Ian Coe, Katie Hoffman, Kelsey Lynn, Adam Simpson, Graduate Researchers

## Introduction

The Energy Systems Analysis group is a part of the GCEP central assessment effort. The group builds quantitative 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: harvesting, 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 all known 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.

These models serve as tools which aid GCEP in identifying areas where technological innovation can increase the efficiency or reduce the emissions of energy conversion devices and systems. The tools may also predict synergies between multiple technologies when the models are compiled into an integrated framework. The group's work with graduate researchers serves to train the next generation of energy system engineers to think critically about energy and material "round-trip" effects.

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:

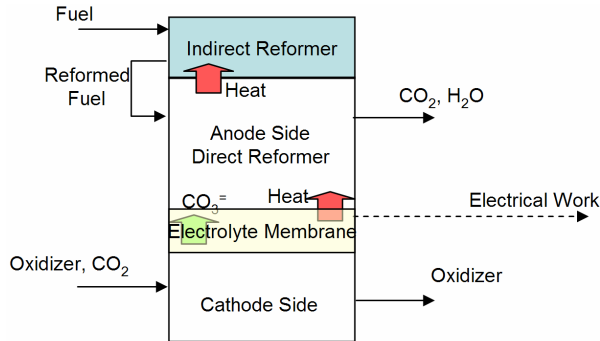
1. Device-Level Modeling
2. Fuel Chain Analysis
3. Energy Network Scenario

### *Device-Level Modeling*

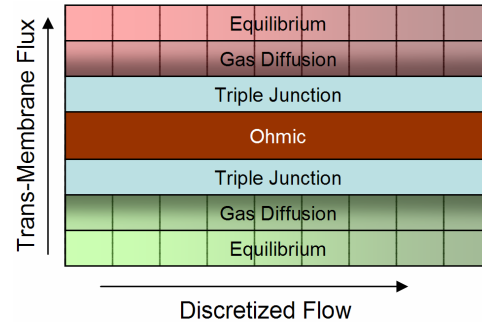
As a first step, individual devices are identified with their associated inputs and outputs. The relationships between the properties of mass and energy as they enter and exit the system are determined by the system model. Model parameters are linked to known state transitions within the system and to 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 2<sup>nd</sup> law efficiencies. The 2<sup>nd</sup> law efficiency number is refined by examining the components inside of the black-box for temporal and spatial gradients where transport and kinetic phenomena cause exergy destruction. For example, a zero-dimensional model of a molten carbonate fuel cell (MCFC) has been built (Figure 1).

The model was then upgraded to a 1+1D study which examines kinetic losses at the electrodes, as well as transport losses in the gas diffusion layer (Figure 2).



**Figure 1:** 0-D Fuel Cell Model



**Figure 2:** 1+1D Fuel Cell Model

### *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 account for inefficiency, 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 effort taking place within GCEP.

### **Background**

In the research community beyond GCEP, the term "Energy Systems Analysis" is used to describe modeling efforts aimed at:

1. quantifying the performance of individual devices.
2. characterizing the interactions between various devices.
3. tracking the fate of resources as they are processed through the energy economy.
4. determining the economic feasibility of various energy use scenarios.
5. predicting the economic outcomes of energy policies.
6. finding the causes of, and solutions to, technological, market or policy failure.

While all of those goals are important to the future direction of the energy industry, the GCEP Energy Systems Analysis Group has chosen to focus on the first two. The Systems Analysis Group and Integrated Assessment team (led by Professors Sweeny and Weyant), will work together on the third. The Integrated Assessment effort focuses on the fourth goal. There are other efforts at Stanford, outside of GCEP, which are directed at the final two goals.

Analysis of energy systems is taking place at numerous organizations across the globe; public and private; governmental, corporate and academic. While the projects are far too numerous and diverse to list here, there are a few efforts that are relatively similar to GCEP's Energy Systems Analysis.

For example, the International Institute for Applied Systems Analysis maintains a computer program called CO2DB (Carbon Dioxide DataBase) [1] which is able to calculate the total GHG emissions from various fuel-chains. The database has a vast number of entries, but not all are functional, and the model is based on "emissions factors" rather than physical device models.

A similar database is being constructed by Commissariat a l'Energie Atomique (CEA), Institut Francais du Petrole (IFP) and Ludwig-Bölkow-Systemtechnik (LBST). This E3 Database [2] is designed to produce analyses for Energy Use, Economics and Emissions from various energy technologies. The E3 Database has not yet been released.

Pacific Northwest National Laboratory (PNNL) and the University of Maryland have established the Global Energy Technology Strategy Program [3], which seeks to model the energy economy from a technology perspective.

The Center for the Management of Environmental Resources (CMER) at the French INSEAD campus is studying the trends of large-scale exergy destruction over time [4, 5]. It is hoped that this study will lead to a better understanding of end-use energy efficiency potential in the future.

Carnegie Mellon University has put together a small suite of energy system models in their "Integrated Environmental Control Model" (IECM). This work has been ongoing since before 1997 [6], and has resulted in a tightly packaged code for analyzing various coal-fired power plant emissions control scenarios.

At Ecole Polytechnique Federale de Lausanne (EPFL), there is a group of students, led by Dr. Favrat, assembling 2<sup>nd</sup> law efficiency models of various energy systems [7].

Dr. Sciubba at University di Roma is also involved in assembling a framework of exergy-related system models [8] which account for energy and material flow through a network of energy technologies.

The US National Laboratories have several people working on Systems Analysis. Maggie Mann at NREL is leading a team to analyze various energy technologies. Andy Lutz at SNL (California) has worked on a "high-level" model for predicting GHG emissions from various hydrogen usage pathways. He has presented some of his

preliminary work to the GCEP Systems Analysis Group, and maintains a dialog with us. Gene Berry at LLNL is working with the energy economists there on hydrogen technologies and has also presented to GCEP.

## **Results**

The Energy Systems Analysis group was established within GCEP in the summer of 2003. Since that time, the group has become an integral part of the GCEP assessment process. The group has built several component models and begun work on integrating them in a software framework.

### *Software*

Several computational tools for the analysis of energy systems have been evaluated and tested for applicability to the Systems Analysis Effort. There are several criteria which the software must meet. It must be easy to program and prototype new models. It should have some thermochemical data embedded. It must be easy to understand how technology sub-components are modeled because new technologies will require modification of simulation parameters. It should be available to the technical community at a reasonable cost so that analysts outside of Stanford can share the models.

There is no commercially available software which satisfies all of the group's needs. Certain tools are undergoing significant in-house enhancements to their functionality. The packages which have been tested are listed here:

- Matlab (from The Mathworks) has been chosen as the programming language of choice for the Systems Analysis Group. Matlab is an extremely flexible programming environment with a wide array of computational tools readily available for adaptation to energy system simulation.
- Cantera (Open Source) is a chemical kinetics and thermodynamics data package that is being developed at Caltech and in the open source community [9]. The Group is using Cantera for chemical equilibrium calculations and kinetics information, while helping to contribute to Cantera's development through feedback to its primary author.
- The Aspen Suite (from AspenTech) is an integrated modeling environment which tracks mass and energy flows and has a wide range of property data. The component models within Aspen are opaque to the user, and are not always suitable for integration into an academic model. However, the property packages are somewhat useful, and are accessible in Matlab via an ActiveX interface.

### *Simulations*

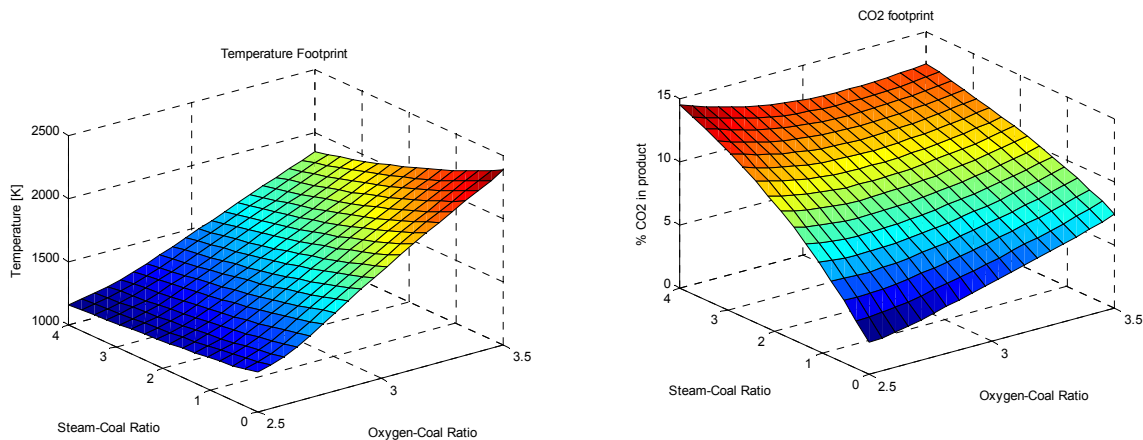
The Group has produced several internal working documents, each with an associated software module, on various energy-related subjects and technologies. These modules are not yet integrated into fuel chains or scenario models. The task of model integration will take place over the next few years, as more modules are developed (see the Future Plans section below). However, these initial modules lay the groundwork for a much larger model "fleet" which will serve GCEP's ultimate goal of technology assessment.

In addition to last year's models [10] (*resource analysis, waste-to-fuel-gas conversion, molten carbonate fuel cell, hydrate-based CO<sub>2</sub> separation*), several new models are in progress. While each of the completed and developing modules currently stands on its own and is fairly specific in device performance prediction, the range of models spans resource harvesting, fuel processing, electricity generation and product-gas treatment. The models in progress are as follows:

### *Coal Gasification and IGCC*

A zero-dimensional model of a coal gasification plant has been built to analyze exergy flows through various power cycle configurations. Oxygen separation, gasification, gas-turbine and steam-turbine cycles have been modeled with varying degrees of detail. As expected, it is found that a high degree of heat integration is required to reach acceptable thermal efficiency.

This model exemplifies the difficulty of working with coal in an integrated thermodynamic modeling framework. Because coal is a highly complex chemical substance, a priori enthalpies and entropies are impossible to determine. Because of the existence of trace species not found in the standard reference environment (chlorine, sulfur, and ash components such as silicon and aluminum), precise exergy values are difficult to obtain. However, even with an ideal-gas-only modeling tool such as Cantera, the group was able to obtain a reasonable gasification footprint [11] while accounting for both sulfur and bulk ash impurities (Figure 3).



**Figure 3:** Temperature and CO<sub>2</sub> Gasification Footprints

### *Solar Photovoltaic*

Solar energy represents the largest constant exergy flux through our sphere of influence. With current technology and at steady state, photovoltaic cells are the most efficient way of turning solar exergy into electrical work. This model explores some of the fundamental limits of solar photovoltaics.

Factors that influence the ability of a panel to harvest sunlight are the panel's orientation towards the sun, the panel's material and its temperature. Semiconductors with a single bandgap are limited to harvesting 31% of the energy in sunlight. This

corresponds to ~40% of the exergy available, however, there is still some debate on how to appropriately calculate photon exergy.

### *Energy Storage for Grid Load Leveling*

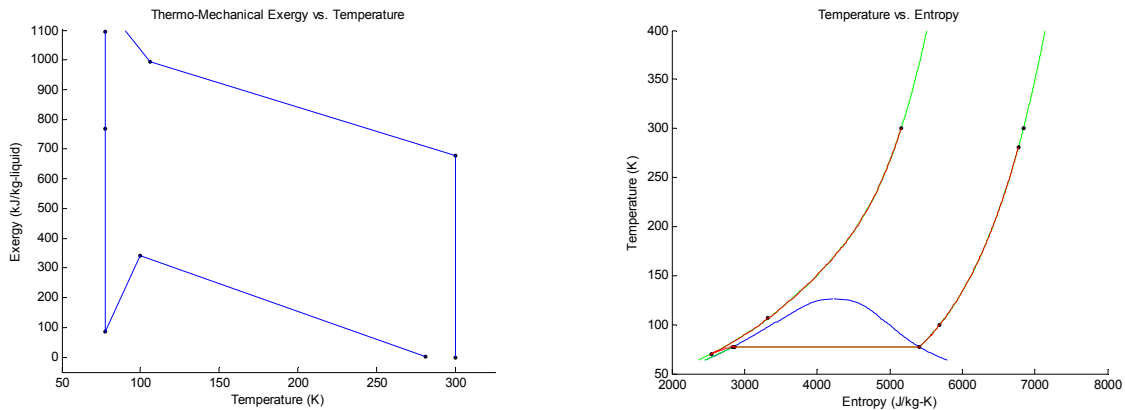
Large-scale energy storage encompasses a class of energy technologies that have immediate application to smoothing out short-time and diurnal fluctuations in electricity demand on the grid and longer term application to intermittent renewable energy resources. One key component to the efficiency of the grid is the constant matching between electricity demand and electricity supply. Use of energy storage to offset inefficient or CO<sub>2</sub>-intensive "peaking" electricity generators could be beneficial. However, actual fuel savings and emissions reduction depend on the round-trip efficiency of the storage mechanism as well as the relative efficiency and emissions of the base-load power used to charge the storage system.

This project examines pumped hydroelectricity and compressed air energy storage as large-scale reservoirs, flywheels as intermediate reservoirs, and supercapacitors and superconducting magnetic energy storage as fast-response devices. Their influence on total fuel usage and CO<sub>2</sub> emissions are examined for various baseload, intermediate and peaking scenarios.

### *Fuel Gas Liquefaction*

Liquid hydrocarbon fuels are prized for their gravimetric and volumetric exergy density. Normally gaseous hydrocarbons may have higher gravimetric energy density than their liquid counterparts, but they have volumetric energy densities which are orders of magnitude lower. Cryogenic liquefaction of these fuels is one means by which to increase their volumetric energy density. The minimum energy needed to liquefy a gaseous fuel from its standard state represents the physical exergy of the liquid fuel. Whether or not this exergy is recovered when the fuel is consumed, an investigation into the exergy investment in fuel liquefaction reveals that the process is highly inefficient

A numerical model of a Heylandt liquefier for a pure substance reveals significant exergy destruction in the expansion valve and in the heat exchangers. Heat leaks into the cold section of the device would increase these irreversibilities to the level normally seen in industrial processes.



**Figure 4:** Process diagrams for a Helandt Liquefier

### *CO<sub>2</sub> Separation Technologies*

In conjunction with other internal assessments at GCEP, the systems analysis group is building a suite of models of CO<sub>2</sub> separation techniques. The literature tends to organize various capture technologies via configuration: post-combustion, pre-combustion, and oxyfuel. However, it is sometimes useful to differentiate strategies based on separation phenomena: chemical solution, physical solution and adsorption, chemical adsorption, phase separation, and mineralization. Five technologies, representative of all three plant configurations and four separation phenomena, have been chosen for numerical analysis in an integrated framework (Table 1).

**Table 1:** CO<sub>2</sub> Capture Technologies

Technology	Phenomenon	Configuration
Amine Solvent	Chemical Solution	Post-Combustion
Ion-Transport Membranes	Chemical Adsorption/Solution	Oxyfuel
Pressure-Swing Adsorption	Physical Adsorption	Oxyfuel or Post-Combustion
Hydrate Separation	Phase Separation	Pre-Combustion
Chemical Looping	Physical Adsorption	Oxyfuel or Other

### **Future Plans**

In the short term, the Systems Analysis Group will finish building and integrate the CO<sub>2</sub> separation models discussed in the previous section. In order for the integration to be successful, a well defined framework must be built that can interconnect and compare various system models. An Application Programming Interface is currently being designed to handle this task. The interface will consist of the ability to link energy conversion devices via different streams of matter and energy. While this approach is similar to that of commercially available flowsheet solvers, our framework will be far more amenable to customized energy conversion "blocks" and masked or "black-box" type subsystems.

In order to facilitate property data calculation, GCEP will continue to work with Cantera and extensions of Cantera. Last year, an interface/extension was developed for Cantera that allows researchers to track and record multiple states of a particular substance in the Matlab workspace. This year, that interface will be extended to encompass an arbitrary number of property data files, and upgraded to an object-oriented code base. Further development on the Matlab/Aspen interface will take place as material properties are needed from Aspen.

In the long term, the group will continue its discussions with other groups engaged in energy systems analysis. First and foremost, energy systems analysis fills the space between the broad-based Energy Assessment Group within GCEP and the Integrated Assessment Group run by John Weyant. The group is already in open dialogue with the Hydrogen Systems Modeling group at Sandia National Laboratories, and has discussions scheduled with Lawrence Livermore National Laboratory and Ecole Polytechnique Federale de Lausanne. The group will continue to build its model code base and recruit and educate the best and brightest thermodynamics students.

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## Contacts

A.J. Simon: [ajsimon@stanford.edu](mailto:ajsimon@stanford.edu)  
Rebecca Hunt: [rahunt@stanford.edu](mailto:rahunt@stanford.edu)