III.2 Energy Systems Analysis

Investigators

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Introduction

The Energy Systems Analysis group is a part of the GCEP central assessment effort. The group's main focus is on building 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 under construction are highly detailed and technical in nature. 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 a quantitative understanding of the technological challenges associated with a particular device or technology.

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 as the models are compiled into an integrated framework. The actions of the group serve to train the next generation of energy system engineers (graduate researchers) 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 reversible, or 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 be independently run and verified, and is fully documented with respect to usage, governing equations and reference material. Models can be simple, time invariant, zero-dimensional models as shown for a Molten Carbonate Fuel Cell (MCFC) in Figure 1. However, more detail may be needed, in which case more complex 1-dimensional or quasi 2-dimensional models that track gradients and their associated effects on efficiency will be built. Figure 2 shows a schematic of such a model, used to simulate the MCFC stack.
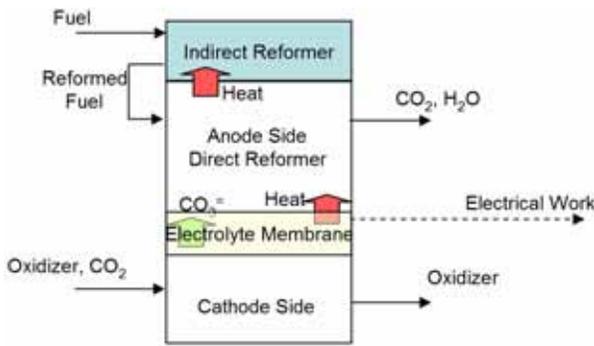
Figure 1: 0-D Fuel Cell Model
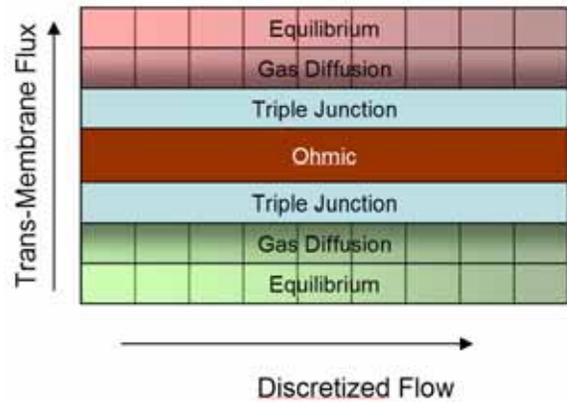
Figure 2: Quasi 2-D Fuel Cell Model

Fuel-Chain Analysis

Subsequently, these individual modules will be put together for fuel-chain-analysis. This first level of integration may be as simple as a gas-turbine model connected to a flue-gas-CO_2-separation model. However, it is anticipated that significantly more complex models will be built, such as a Coal to Hydrogen to Fueling Station to Cryogenic Storage to PEM to Electric Motor model. Such a model would serve to identify mass and energy conversion steps with significant inefficiencies or irreversibilities. A part of such a model, with options for liquid or compressed H_2 and two CO_2 shipment options is shown in Figure 3. These models 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.
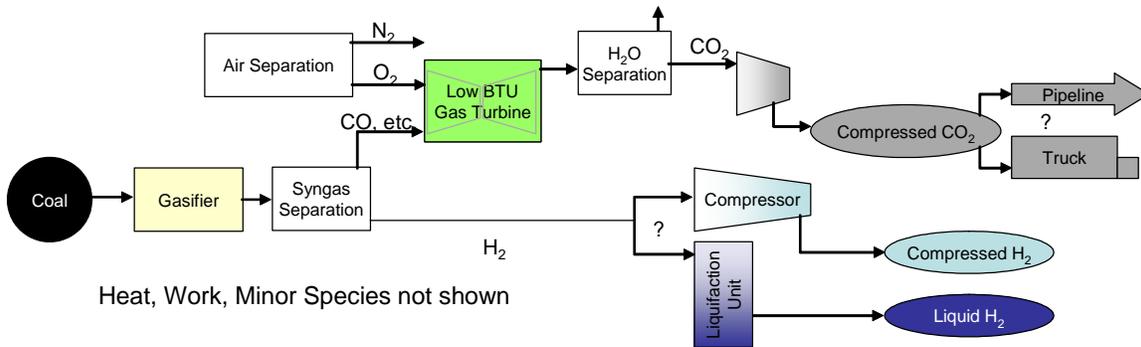
Figure 3: Fuel Chain Analysis Schematic

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. In this way, the effects of real technology development on energy infrastructure can be estimated.

Background

Large reductions in CO_2 emissions will undoubtedly be accompanied by vast changes in infrastructure. The anticipation of such changes has touched off significant activity in the realm of "Systems Analysis." There are two main reasons for this activity:

First, significant innovation is required to move towards a low greenhouse gas (GHG) energy system. This innovation is likely to come from individuals or groups who have a deep understanding of energy issues. Systems Analysis is an effective method of developing such an understanding. Furthermore, candidate solutions to our energy challenges are likely to emerge at the borders of what are traditionally separate systems in the energy world. It is the opinion of this author that waste and inefficiency often occur at boundaries. This phenomenon is certainly true of mechanical systems (composed of mass and energy) where exergy destruction drives transport across component boundaries. However, losses at boundaries occur in economic and political systems as well, where waste, or welfare loss, can be attributed to imperfect communication. Integrated Systems Analysis efforts can pinpoint inefficiencies at boundaries and suggest areas where innovation can improve operation.

Second, in the context of GHG emissions, the energy industry is understandably concerned about adopting large-scale changes in technology. The industry has evolved according to economic principles, and has so far been successful in providing for its customers while remaining profitable. However, a lack of understanding of the consequences (and indeed, the absence of an incentive to discover any unintended consequences) of large scale energy use has placed the industry in a tenuous position. As such, all of the parties concerned with a transition to a low GHG energy system want to fully understand the ramifications of that transition. While the stakeholders would like to resolve the GHG issue, no one wants to trade the challenges we are facing now for another set of *unidentified* challenges. Systems Analysis will help to identify challenges inherent in technologies and policies proposed for a low GHG energy future.

Although Systems Analysis has been recognized as important for the aforementioned reasons, it is still a vaguely defined topic. In the context of energy, the term "Systems Analysis" encompasses (at a bare minimum) 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 Sweeney 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 to the public.

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.

The US National Laboratories have several people working on Systems Analysis. Maggie Mann at NREL is leading a team to analyze various energy technologies associated with hydrogen. 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 made significant progress towards its goal of becoming an integral part of the GCEP assessment process. There are two areas where the group has met its initial targets: identification of software tools capable of handling large-scale system-model integration and building component models of energy conversion technologies.

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.

Because this is research, there is no commercially available software that 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 package that is being developed at Caltech and in the open source community [6]. 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.
- Aspen Plus (from AspenTech) was considered as a development environment due to its highly refined graphical user interface and its vast database of thermodynamic properties. However, the Group eventually decided that the modules in Aspen Plus did not reveal enough of their "inner workings" to develop the fundamental understanding of energy systems that is required.
- Aspen Properties (from AspenTech) is a component of the Aspen Engineering Suite which is comprised of databanks of thermodynamic properties for a vast number of substances. Using an ActiveX interface, it is possible to extract data from Aspen Properties in the Matlab work environment. Development of this interface is currently in progress.
- Multiflash (from InfoChem) is another property data package with a Matlab interface available for immediate purchase. Multiflash is being evaluated as an alternative to Aspen Properties.

Simulations

The Group has produced several internal working documents, each with an associated software module, on various energy-related subjects and technologies. These modules represent the first batch of results ever produced by the GCEP Systems Analysis Group, and 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.

Four modules are described here, and together they cover a significant fraction of a potential fuel-chain. The first module is a *resource analysis* code which returns theoretical values for the exergy content of a very wide range of energy resources. The second module is of a *waste-to-fuel-gas converter*, and the third model is of a *Molten Carbonate Fuel Cell* (MCFC). The final module examines a novel *CO_2 separation* process. While each of these 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.

Summaries of these studies and their key findings are listed below.

Resource Analysis

Exergy is introduced as a tool to assess and compare reservoirs of theoretically extractable work. These reservoirs contain bulk kinetic energy, potential energy due to a restoring field, or chemical potential relative to a reference state. This reference state is derived from the thermal, mechanical and chemical properties of the natural environment. The paper identifies primary exergy reservoirs and their derivative secondary reservoirs we call resources. Different exergy formulas are developed depending on the predominant form of useful energy stored in the material. Resources currently in use or within the realm of our technology are examined for their quality and quantity. The results are useful for scrutinizing current utilization and comparing various energy options independent of technology and cost.

Table I: Exergy Reservoirs by Class

Primary	Secondary (Resources)	Replenishment Time Scale
Celestial Bodies	Tidal	hours
Solar Nuclear	Solar Radiation	millisecond
	Wind	hours
	Wave	hours
	OTEC	days
	Precipitation	days
	Biomass	years
	Fossil Fuels	millions yrs.
Terrestrial Nuclear	Geothermal	days - none
	Fission/Fusion	none

Table I lists the various resources available for harvesting and eventual use. It is clear that solar energy drives almost all of the processes we consider useful for the harvesting of energy. The only comparable resource would be fusible atomic species already present on Earth. The paper does NOT quantify the exergy loss in the transformation from solar energy to the various secondary resources, but it does quantify the exergy content of the secondary resources with respect to the environment.

The software package associated with this paper calculates the exergy content of unit quantities of the various resources from literature data and user input regarding the state

of the resource. For example, the inorganic/hydrocarbon mixture of Tar Sands found in the U.S. has an exergy content of ~6 MJ/kg [7]. This is the absolute upper limit of recoverable work from this resource, and any energy spent harvesting the sands or refining the hydrocarbons will reduce the value.

Armed with estimates of the state and size of each resource, the paper goes on to calculate the exergy content of non-renewable resources and the exergy destruction rate of renewable resources. While the numbers are interesting from a fundamental standpoint, there are enough uncertainties about recoverability factors and environmental consequences of large-scale harvesting that they are not reported here.

Waste-to-Fuel-Gas
A quasi-one dimensional model of a biogasification system has been created based on the anaerobic digestion process. The model analyzes the energy flows and performance of a continuous flow stirred tank bioreactor (CSTR) and a plug-flow bioreactor (PFR) on a thermo-chemical level and predicts the extent of reactions, products formed and other thermodynamic property data. It also measures the inherent performance of the anaerobic digestion process on an energy cum exergy basis. The model is developed for an isothermal reactor (at 25°C) and is flexible with regard to most organic feedstocks. The paper is accompanied by the model code developed in MATLAB and some sample results.
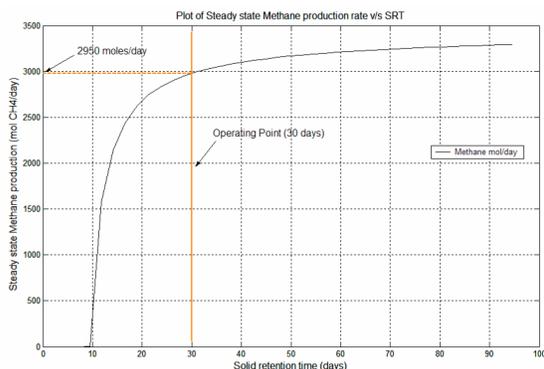
Figure 4: Methane yield for a CSTR
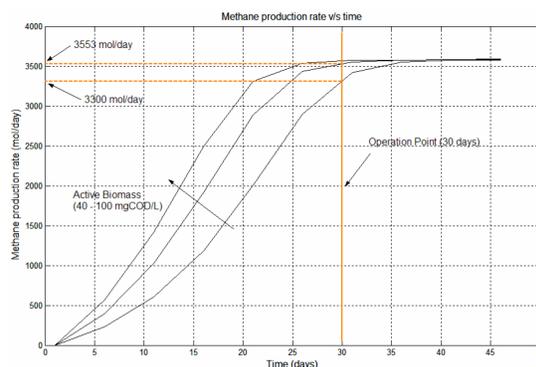
Figure 5: Methane yield for a PFR

While the Methanogenic Efficiencies (total yield per mole of feedstock consumed) are the same between the CSTR and PFR, the Methane Yield from a PFR is significantly higher. Figures 4 and 5 show that a PFR based methane recovery plant will operate considerably faster or with a considerably smaller footprint than a CSTR based plant.

For a mixture of municipal wastewater and fatty acids, methanogenic organisms are able to convert exergy stored in the substrate to methane with an efficiency of about 55%. This efficiency occurs at a solids-retention-time of approximately 30 days, which implies that the volume of the reactor must be 30 times its daily flow-rate to accomplish complete processing of the waste.

Molten Carbonate Fuel Cell

Molten Carbonate Fuel Cells (MCFCs) have many positive characteristics that distinguish them from other energy systems as well as other fuel cells. These features include high temperature operation, carbon dioxide in the oxidant stream, internal reformation, variety of fuel use, potential application to CO_2 separation processes and hybrid system and cogeneration applications. Background information on MCFCs is provided along with a general description of a zero-dimensional representation of the mass and energy flows through a MCFC. Ultimately, an empirically-based, one dimensional molten carbonate fuel cell model is developed.
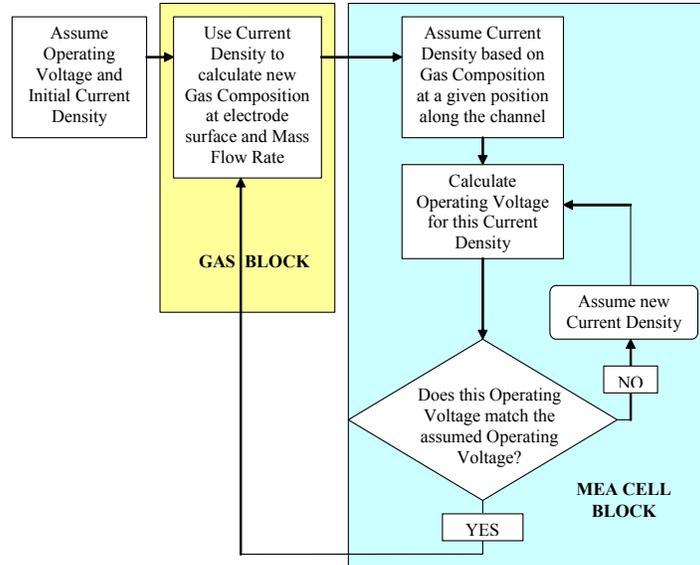
Figure 6: Flow Chart of 1-D MCFC Model

Figure 6 depicts the iterative scheme used to determine the distribution of current density along the length of the gas flow channel. For an overall cell voltage of 0.74 (assumed as an operating in the leftmost block), it is seen that current density varies from ~2800 to ~2000 A/m^2 along a channel with a length of 1 m. The activation, ohmic and concentration overpotentials are calculated for each section of the once the current density at that section is known.

The one-dimensional model is useful for quantifying the performance of the cell in terms of first- and second-law thermodynamic efficiencies, for determining fuel and oxidant utilization, and for examining current-density variation along the length of the gas-flow channel. Current density is a major factor in the local efficiency of the cell, as well as "wear" effects such as carbon deposition and local hot-spots.

CO₂ Separation

Reduction of greenhouse emissions from the use of coal for power is essential to a stable, low GHG future. Current methods of carbon dioxide removal from coal fired power plant exhaust and gasification syngas are summarized, and a new method of carbon dioxide removal from pre-combustion gasification syngas is proposed. A model of hydrate formation is used to determine if this method of separation is chemically feasible in an ideal case.

In the proposed system, CO_2 would be trapped in a solid hydrate form, which can be separated from liquid or gaseous components that do not form hydrates. In principle this technique could be used in many stack-gas situations, but would find immediate application in coal-to-hydrogen plants, where CO_2 and H_2 compose the bulk of the flue-gas.
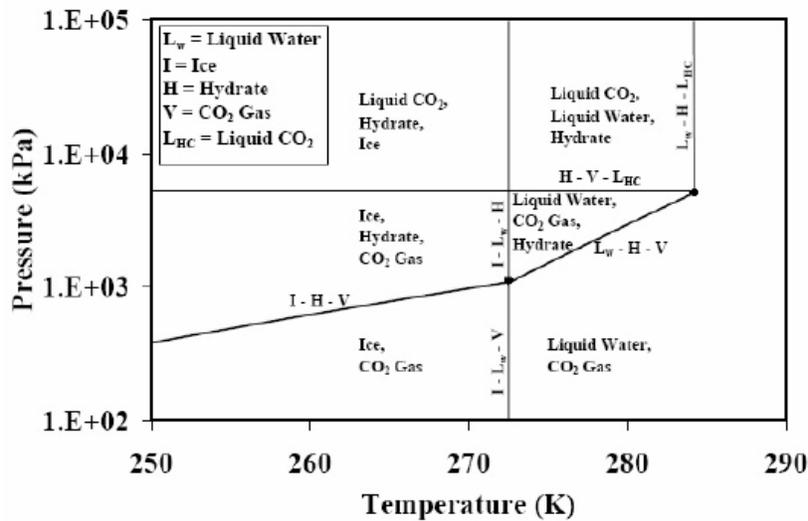
Figure 7: Temperature and Pressure Diagram for CO_2 Hydrate Formation

While there is a stable and predictable region of CO_2 hydrate formation at feasible temperatures and pressures (See Figure 7), it remains to be determined whether or not this method of gas separation can be accomplished more efficiently than more established separation processes (PSA, membrane). Furthermore, the three-phase (H_2 gas, liquid water and CO_2 hydrate) nature of the problem will pose significant challenges in reactor design, and the rate of separation may be limited by mass and heat transport considerations.

Future Plans

Beyond the four modules described above, several more analyses are in progress, including a survey of emerging water electrolysis techniques and a model of a nuclear fission reactor.

The Energy Systems Analysis effort is planned to continue throughout the existence of GCEP. The main focus of the technical effort will be to implement a broad suite of software modules which analyze the performance of energy systems, and to develop a

framework in which these models can be coupled. The coupling will first take the form of fuel-chain analyses, and may evolve from there to encompass energy scenarios.

This scenario modeling cannot take place in the absence of economic data. The Systems Analysis Group will work with the Integrated Assessment Team to build these detailed scenarios. There is already ongoing dialog between the Systems Analyst and John Weyant and Jim Sweeney.

As the energy modeling tools become more refined and efficient, they will find use in the GCEP assessment process. Collaboration between the Systems Analysis Group and the Assessment Analysts will result in more quantitative assessments as well as more refined analysis tools. These tools will find applicability to the broader energy community as they are made public, through internal and external publications and through an interactive web site.

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