41623R02

Conceptual Design of Optimized Fossil Energy Systems with Capture and Sequestration of Carbon Dioxide

Semi-Annual Technical Progress Report No. 2

Reporting Start Date: March 23, 2003
Reporting End Date: September 22, 2003

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Date Report Issued: December 2003

DOE Award Number: DE-FC26-02NT41623

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Conceptual Design of Optimized Fossil Energy Systems with Capture and Sequestration of Carbon Dioxide

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ABSTRACT

In this second semi-annual progress report, we describe research results from an ongoing study of fossil hydrogen energy systems with CO_2 sequestration. This work was performed under NETL Award No. DE-FC26-02NT41623, during the six-month period March 2003 through September 2003.

The primary objective of the study is to better understand system design issues and economics for a large-scale fossil energy system co-producing H_2 and electricity with CO_2 sequestration. This is accomplished by developing analytic and simulation methods for studying the entire system in an integrated way. We examine the relationships among the different parts of a hydrogen energy system, and attempt to identify which variables are the most important in determining both the disposal cost of CO_2 and the delivered cost of H_2.

A second objective is to examine possible transition strategies from today's energy system toward one based on fossil-derived H_2 and electricity with CO_2 sequestration. We are carrying out a geographically specific case study of development of a fossil H_2 system with CO_2 sequestration, for the Midwestern United States, where there is presently substantial coal conversion capacity in place, coal resources are plentiful and potential sequestration sites in deep saline aquifers are widespread.

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EXECUTIVE SUMMARY

In this second semi-annual progress report, we describe research results from an ongoing study of fossil hydrogen energy systems with CO_2 sequestration. This work was performed during the second six months (March 2003- September 2003) of the project under NETL Award No. DE-FC26-02NT41623.

The primary objective of the study is to better understand system design issues and economics for a large-scale fossil energy system co-producing hydrogen (H_2) and electricity with carbon dioxide (CO_2) sequestration. This is accomplished by developing new analytic and simulation tools for studying the entire system in an integrated way. We examine the relationships among the various parts of a fossil hydrogen energy system, and attempt to identify which variables are the most important in determining both the disposal cost of CO_2 and the delivered cost of H_2.

A second objective is to examine possible transition strategies from today's energy system toward one based on fossil-derived H_2 and electricity with CO_2 sequestration. We are carrying out a geographically specific case study of development of a fossil H_2 system with CO_2 sequestration, for the Midwestern United States, where there is presently substantial coal conversion capacity in place, coal resources are plentiful and potential sequestration sites in deep saline aquifers are widespread.

We consider fossil energy complexes producing both H_2 and electricity from either natural gas or coal, with sequestration of CO_2 in geological formations such as deep saline aquifers. The design and economics of the system depend on a number of parameters that determine the cost and performance of the system "components", as a function of scale and geography (components include: the fossil energy complex, H_2 pipelines and refueling stations, CO_2 pipelines, CO_2 sequestration sites, and H_2 energy demand centers). If we know the location, size, cost and performance characteristics of the components, designing the system can be posed as a problem of cost minimization. The goal is to minimize the delivered H_2 cost with CO_2 disposal by co-optimizing the design of the fossil energy conversion facility and the CO_2 disposal and H_2 distribution networks. Research to perform this cost minimization has two parts: 1) implement technical and economic models for each "component" in the system, and 2) develop optimization algorithms to size various the system components and connect them via pipelines into the lowest cost network serving a particular energy demand. Finally, to study transition issues, we use these system models to carry out a case study of developing a large-scale fossil energy system in the Midwestern United States.

Three tasks are ongoing. In our first technical progress report, we described work under Tasks 1 and 2. Most of the work described in this report was performed under Tasks 2 and 3.

Task 1.0 Implement Technical and Economic Models of the System Components

Here we utilize data and component models of fossil energy complexes with H_2 production, and CO_2 sequestration already developed or undergoing development as part of the ongoing Carbon Mitigation Initiative (CMI). (Begun in 2001, the Carbon Mitigation Initiative is a ten-year $15-20 million dollar joint project of Princeton University, BP and Ford Motor Company to find solutions to global warming and climate change.) Additional models for H_2 distribution systems and refueling stations are being adapted from the principal investigator's previous studies of H_2 infrastructure for the US Department of Energy Hydrogen R&D Program (Ogden 1998, Ogden 1999a, Ogden 1999b), and those of other researchers (Mintz et al. 2003, Amos 1998, Thomas et al. 1998).

Task 2.0. Integrated Studies of the Entire System to Find the Lowest Cost Network

As a first step, we developed a simple analytical model linking the components of the system. We consider single fossil energy complex connected to a single CO_2 sequestration site and a single H_2 demand center. We developed "cost functions" for the CO_2 disposal cost and the delivered H_2 cost with explicit dependence on the many input parameters described above (e.g. size of demand, fossil energy complex process design, aquifer physical characteristics, distances, pressures etc.). Analytic sensitivity studies of this "simple system" are used to provide us with insights on which parameters are most important in determining costs.

To study more complex and realistic systems involving multiple energy complexes, H_2 demand centers, and sequestration sites, we are exploring use mathematical programming methods to find the lowest cost system design. From our system modeling, we seek to distill "rules for thumb" for developing H_2 and CO_2 infrastructures.

Task 3.0 Case Study of Transition to a Fossil Energy System with CO_2 Sequestration

In this task, the goal is to explore transition strategies: how H_2 and CO_2 infrastructures might develop in time, in the context of a geographically specific regional case study. We focus on the Midwestern United States, a region where coal is widely used today in coal-fired power plants, and good sites for CO_2 sequestration are available. The goal is to identify attractive transition strategies toward a regional hydrogen/electricity energy system in the Midwest with near zero emissions of CO_2 and air pollutants to the atmosphere.

To better visualize our results, we use a geographic information system (GIS) format to show the location of H_2 demand, fossil energy complexes, coal resources, existing infrastructure (including rights of way), CO_2 sequestration sites and the optimal CO_2 and H_2 pipeline networks. Preliminary results from this task will be described in this report.

INTRODUCTION

In this progress report, we present initial results from an ongoing assessment of fossil H_2 energy systems with CO_2 sequestration. This research was performed during the second six months under NETL Award No. DE-FC26-02NT41623, from March 2003 to September 2003.

Background and Motivation

Production of hydrogen from fossil sources with capture and sequestration of CO_2 offers a route toward near-zero emissions in production and use of fuels. Implementing such an energy system on a large scale would require building two new infrastructures: one for producing and delivering H_2 to users (such as vehicles) and one for transmitting CO_2 to disposal sites and securely sequestering it.

In Figure 1, we show a fossil hydrogen energy system with CO_2 sequestration. A fossil feedstock (natural gas or coal) is input to a fossil energy complex producing hydrogen and electricity. CO_2 is captured, compressed to supercritical pressures for pipeline transport to a sequestration site, and injected into an aquifer or other underground geological formation. Hydrogen is delivered to users via a pipeline distribution system that includes compression and storage at the hydrogen production plant, pipelines (possibly with booster compressors) and hydrogen refueling stations. The design and economics of a fossil H_2 energy system with CO_2 sequestration depend on a host of factors, many of which are regionally specific and change over time. (Variable considered in this study are shown in Figure 1 in italics.) These include:

- The size, type, location, time variation and geographic density of the H_2 demands.
- Cost and performance of component technologies making up the system. Key components are: the fossil energy conversion plant [design variables include the scale, feedstock: (coal vs. natural gas), process design, electricity co-production, separation technology, pressures and purity of H_2 and CO_2 products, sulfur removal options including co-sequestration of sulfur compounds and CO_2, location (distance from demand centers and sequestration sites)], H_2 and CO_2 pipelines and H_2 refueling stations.
- The location and characteristics of the CO_2 sequestration sites (storage capacity, permeability, reservoir thickness),
- Cost, location and availability of primary resources for H_2 production.
- Location of existing energy infrastructure and rights of way (that could be used for siting hydrogen transmission pipelines).

For simplicity, in Figure 1, we have shown a single fossil energy complex, serving a single demand, and one CO2 sequestration site. However, a future fossil hydrogen system could be more complex, linking multiple H_2 demand centers (cities), fossil energy complexes and sites for CO_2 sequestration (Figure 2).

Several detailed technical and economic studies have been carried out for various parts of the system, including CO_2 capture from electric power plants (Hendriks 1994; Foster Wheeler 1998; Simbeck 1999), or H_2 plants (Foster Wheeler 1996; Doctor et al. 1999; Spath and Amos 1999; Kreutz et al. 2002), CO_2 transmission (Skovholt 1993) and storage (Holloway 1996), and H_2 infrastructure (Directed Technologies et al. 1997, Ogden 1999; Thomas et al. 1998, Mintz et al 2002). However, relatively little work has been done assessing complete fossil hydrogen systems with CO2 sequestration in an integrated way. An integrated viewpoint is important for understanding the design and economics of these systems. For example, the scale of the fossil hydrogen plant, can have a large impact on the design and cost of both the hydrogen distribution system, and the system for transporting and sequestering CO_2.

Scope of this Study

The primary objective of this study is to better understand total system design issues and economics for a large-scale fossil energy system co-producing hydrogen (H_2) and electricity with CO_2 sequestration. We consider fossil energy complexes producing both H_2 and electricity from either natural gas or coal, with sequestration of CO_2 in geological formations such as deep saline aquifers. We apply various analytic and simulation methods to study the entire system in an integrated way. We attempt to identify which variables are the most important in determining both the disposal cost of CO_2 and the delivered cost of H_2. We examine the relationships among the system components (e.g. fossil energy complexes, H_2 and CO_2 pipelines, H_2 demand centers, and CO_2 sequestration sites), and apply new simulation tools to studying these systems, and optimizing their design.

A second objective is to examine possible transition strategies from today's energy system toward one based on fossil-derived H_2 and electricity with CO_2 sequestration. We focus on understanding how H_2 and CO_2 infrastructures might evolve over time to meet a growing H_2 demand under different regional conditions. If we know the location, size, cost and performance characteristics of the system components, designing the system can be posed as a problem of cost minimization. The goal is to minimize the delivered H_2 cost with CO_2 disposal by co-optimizing the design of the fossil energy conversion facility and the CO_2 and H_2 pipeline networks. Research to perform this cost minimization has two parts: 1) implement technical and economic models for each component in the system (Task 1), and 2) explore use of optimization algorithms to size various the system components and connect them via pipelines into the lowest cost network serving a particular energy demand (Task 2). Techniques for studying regional H_2 and CO_2 infrastructure development and transition strategies are described, based on use of Geographic Information System (GIS) data and network optimization techniques.

To understand the impact of geographic factors, we are carrying out a case study of development of a large scale fossil H_2 system with CO_2 sequestration, for the Midwestern United States, where there is presently substantial coal conversion capacity in place, coal resources are plentiful and potential sequestration sites in deep saline aquifers are widespread (Task 3).

Three tasks are ongoing. (Results are given for each task in the "Results and Discussion" section below.) Most of the work described in this report was performed under Tasks 2 and 3. (Results from Task 1 were described in an earlier progress report for this contract (Ogden 2003).

Task 1.0 Implement Technical and Economic Models of the System Components

Before developing a total system model, we need to develop technical/economic models for the various parts (or components) of the system. Here performance and cost of each "component" of the system is characterized as a function of scale and other relevant parameters. In this Task, we utilize data and models of fossil energy complexes with H_2 production, and CO_2 sequestration developed as part of the ongoing Carbon Mitigation Initiative (CMI). (Begun in 2001, the Carbon Mitigation Initiative is a ten-year $15-20 million dollar joint project of Princeton University, BP and Ford Motor Company to find solutions to global warming and climate change.) Additional models for H_2 distribution systems and refueling stations are being adapted from the principal investigator's previous studies of H_2 infrastructure for the US Department of Energy Hydrogen R&D Program (Ogden 1998, Ogden 1999a, Ogden 1999b), and those of other researchers (Mintz et al. 2003, Amos 1999, Thomas et al. 1998).

Task 2.0. Integrated Studies of the Entire System to Find the Lowest Cost Network

As a first step, we developed a simple analytical model linking the components of the system. We consider a single fossil energy complex connected to a single CO_2 sequestration site and a single H_2 demand center (see Figure 1). For specificity, we chose a base case hydrogen plant size of 1000 MWth hydrogen output (equivalent to about 600 tonnes H2 per day or 252 million standard cubic feet – see Appendix A for conversion factors). We developed "cost functions" for the CO_2 disposal cost and the delivered H_2 cost with explicit dependence on the many input parameters described above (e.g. size of demand, fossil energy complex process design, aquifer physical characteristics, distances, pressures etc.). Analytic sensitivity studies of this "simple system" are used to provide us with insights on which parameters are most important in determining costs.

To study more complex and realistic systems involving multiple energy complexes, H_2 demand centers, and sequestration sites, we are exploring use mathematical programming methods to find the lowest cost system design. This work is described under Task 2 below. From our system modeling, we seek to distill "rules for thumb" for developing H_2 and CO_2 infrastructures.

Task 3.0 Case Study of Transition to a Fossil Energy System with CO_2 Sequestration

In this task, we explore transition strategies: how H_2 and CO_2 infrastructures might develop in time, in the context of a geographically specific regional case study. We focus on the Midwestern United States, a region where coal is widely used today in coal-fired power plants, and good sites for CO_2 sequestration are available. We consider how fossil energy systems might develop over time to meet an evolving energy demand. The goal is to identify attractive transition strategies toward a regional hydrogen/electricity energy system in the Midwest with near zero emissions of CO_2 and air pollutants to the atmosphere.

To better visualize our results, use a geographic information system (GIS) format to show the location of H_2 demand, fossil energy complexes, coal resources, existing infrastructure (including rights of way), CO_2 sequestration sites and the optimal CO_2 and H_2 pipeline networks. First, a survey of relevant GIS data sets was conducted, and work was begun on building a database. We used this database to answer simple questions about fossil energy systems with CO2 sequestration. Results are given below.

RESULTS AND DISCUSSION

Task 1.0 Implement Technical And Economic Models Of The System Components

In the first progress report for this contract, we described technical/economic models of various parts of a fossil hydrogen system with CO_2 sequestration. These include:

- The fossil energy complex for producing hydrogen and electricity from natural gas or coal
- CO_2 compression and pipeline transport
- CO_2 injection into underground geological formations
- Hydrogen demand for vehicles
- Hydrogen fuel delivery infrastructure (including hydrogen compression, storage, pipeline transmission and refueling stations)

We surveyed estimates for system component costs and performance that are available in public domain literature, and from ongoing work at Princeton University. We synthesized cost and performance estimates for hydrogen production systems with CO_2 capture, hydrogen pipelines, hydrogen refueling stations, CO_2 pipelines, and CO_2 injection sites. In particular, we utilized data and component models of fossil energy complexes with H_2 production, and CO_2 sequestration already developed or undergoing development as part of the ongoing Carbon Mitigation Initiative (CMI) project at Princeton University. Additional models for H_2 distribution systems and refueling stations were adapted from the principal investigator's previous studies of H_2 infrastructure for the US Department of Energy Hydrogen R&D Program (Ogden 1998, Ogden 1999a, Ogden 1999b), and those of other researchers (Mintz et al. 2003, Amos 1999, Thomas et al. 1998).

Details on the models for various parts of the system are given in the first progress report for this contract (Ogden 2003). This work will be updated as better estimates become available. For example, the author is working with the "H2A", a group of hydrogen analysts convened by the USDOE to develop cost and performance estimates for hydrogen technologies. The National Research Council is producing a report on hydrogen that will include models of hydrogen components. The results of these efforts should become available in 2004. Our work will be updated to reflect the new information contained in these studies.

Task 2.0. Integrated Studies of the Entire System to Find the Lowest Cost Options

In Task 2, we combine our "component" models of hydrogen production, CO_2 capture, transmission and sequestration, hydrogen compression, storage, distribution and refueling to describe an integrated system.

Task 2.1. Develop Simple Model for Entire System and Perform Sensitivity Studies

In Task 2.1, we studied total system design and economics, for the special case of a single large fossil energy complex connected to a single geological CO_2 sequestration site and a single H_2 demand center (such as a city with a large concentration of H_2 vehicles). Results for this task were described in the first progress report for this contract. The system is shown in Figure 1. Using the component models from Task 1, we developed a simple analytical model linking the components into a total system. We then estimated the total delivered cost of H_2 with CO_2 sequestration for a number of cases of interest. We conducted sensitivity studies to examine which parameters are most important in determining delivered hydrogen costs. For our base case assumptions (large CO_2 and H_2 flows; a relatively nearby reservoir for CO_2 sequestration with good injection characteristics; a large, geographically dense H_2 demand), H_2 production, distribution and refueling were found to be the major costs contributing to the delivered H_2 cost. CO_2 capture and sequestration added only ~10%. Better methods of H_2 storage would reduce both refueling station and distribution system costs, as well as costs on-board vehicles.

Task 2.2 Explore Use of Mathematical Programming Techniques to Study More Complex Systems.

Although studies of the simple system in Task 2.1 are useful, a mature fossil hydrogen system would potentially involve a number of hydrogen production sites, hydrogen demand centers, and CO2 sequestration sites. To study more complex and realistic systems involving multiple energy complexes, H_2 demand centers, and sequestration sites, we are exploring use of mathematical programming methods to find the lowest cost system design.

Thusfar, we examined the suitability of several mathematical programming methods that could be used to optimize the design of a hydrogen energy system with CO2 sequestration More work on Task 2 remains to be done to understand the best tools for carrying out an optimization of the system.

The basic design problem is shown in Figure 2. We have several hydrogen demand centers (shown in yellow) and primary resources. The question is how to connect these using the lowest cost system (including hydrogen production plants, hydrogen distribution and for fossil hydrogen options, a CO2 disposal system.) The longer-term goal is to compare various possible transition pathways to find the lowest overall cost.

This is a complex nonlinear optimization problem. As a first step, we reviewed the literature to understand how mathematical programming techniques had been applied to modeling pipeline systems. (This is a subset of the overall design problem, as hydrogen production systems are not specifically included in this analysis.)

Several general classes of problems have been studied, relating to optimizing pipeline systems.

Design Optimization: In this category, we consider the design of a new pipeline network. Since the network doesn't exist yet, we must decide how many compressor stations (if any) are needed, where they should be located, where the interconnection of two (or more) pipes should happen, and what size (diameter and length) each pipe segment should be. Constraints may include mass balance at each node, gas flow equation in every pipe segment, the work equation of compressors and limits on the pressure or flow rate. Infinitely many designs can meet the constraints. The design and building cost is used as the objective function to select one design out of the design space.

Steady-State Operation Optimization: In this case, the network already exists, so pipe size, number and location of compressor stations are already known. The objective is to minimize the fuel consumption by compressors, which is determined by the suction and discharge pressure at each compressor station and the flow-rate of gas going through these compressors.

Table 1 summarizes the objective function (e.g. the cost function to be minimized), the constraints, and the optimization variables. Table 2 shows some of the approaches that have been applied to these two classes of pipeline design problems. Dynamic operation has also been treated, but we do not consider this here, because of its complexity.

Literature Review of Mathematical Programming Methods Applied to Pipeline System Design

Linear Programming

In the early years of gas pipeline study, the steady-state operation problem was considered by researchers (Sekirnjak, 1996). They dealt with a very simple network model, consisting of a few sources and sinks. To avoid the nonlinearity caused by the gas flow equation, the network was separated into high, medium and low pressure subsystems, connected by compressors. The pressure drop was neglected within each

	Design Optimization	Steady-state Operation optimization
Objective function	$\mathit{building}\ \cos t = f(\mathit{pipe\ diameter}, \mathit{pipe\ length}, \#\ \mathit{of}\ \mathit{compressor}, \mathit{terrain}, \ldots)$	$\mathit{operation}\ \cos t\ (\mathit{fuel\ comsumed}) = f(\mathit{pressure}, \mathit{flowrate}, \ldots)$

Constraints	1. mass flow balance equation at each node 2. gas flow equation at each pipe segment, i.e. pressure drop equation 3. working equation of each compressor 4. limits imposed on pressure or flow-rate	Same as the left
Optimization variables	pipe diameter and length, location of compressor stations and other interconnection points, etc.	flow-rate, suction and discharge pressure at each compressor station, etc.

Table 1. Objective function, constraints and variables for pipeline cost optimization

Traditional optimization techniques	Pure linear programming
	Nonlinear programming
	    Sequential linear programming (SLP)
	    General reduced gradient method (GRG)
	    Inter-point method
	    Newton-Raphson method
	    Sequential unconstrained minimization technique (SUMT)
	Dynamic programming

Nontraditiona l optimization techniques	Genetic algorithms Simulated annealing Neural network Artificial ants

Table 2. Mathematical programming methods applied to pipeline cost optimization

subsystem, and the only decision variables were the flow-rates through each segment. Thus the network was basically modeled by a set of flow balance equations. This was purely a linear model and then the model could be solved by linear programming techniques. This first optimization application was presented at 12th IGU World Gas Conference in Nice, 1973 (Larcher, et al).

The advantage of LP method is that it has unique optimum, which is the global optimum. The disadvantage is that it can only solve small size network roughly and the pressure difference between sources and sinks here must be relatively small so that three subsystems are enough to make the approximation of constant pressure within one subsystem. Otherwise, two possibilities may appear: one is that the computing error becomes too large to tolerate if we keep the same division of three subsystems. The other is to increase the number of subsystems that is essentially a method of linearizing the nonlinear model, which has its own problems of convergence and tolerance.

Non-Linear Programming

Pipeline system design is an inherently nonlinear problem, so nonlinear programming techniques is a natural tool. Sequential linear programming was used to optimize the steady-state operation of gas pipeline. Edgar (1978) presented a computer algorithm to optimize the design of a gas transmission network. Two solution techniques were used: one was the Generalized Reduced Gradient (GRG) method; the second method was to combine the branch-and-bound scheme with GRG. The techniques were applied to different type of cost functions respectively. Daniel de Wolf (1996) considered the optimal dimensioning of gas transmission network when the net work topology is known. His presented a way to compute the first order derivatives, and used the bundle method (Penalty parameter) for optimization. Siregar (2000) repeated Wolf's work. Djebedjian (2000) applied the sequential unconstrained minimization technique (SUMT) to the operation optimization of hydraulic pipeline system. Benson (2001) took the LOQO nonlinear solver which is based on inner-point method to solve the design problem of small-scale CO_2 pipeline network. Both the network topology and the dimension of pipes are unknown variables in her optimization model.

One prominent problem caused by the nonconvexity is how to judge whether the optimum you get is the global optimum. Since most nonlinear optimization techniques are based on iterative methods and the initial value may determines which optimum is found to some extent, changing the initial value may give another solution. Another approach is to find some upper bound for the objective function at pre-processing and use it as one criterion to discard some local optimums (Wu et al. 2000).

Dynamic Programming

DP has allowed optimization of pressures in steady-state gas pipeline simulations for the past thirty years. This approach allows full used of nonlinear hydraulic models and nonlinear and even discontinuous compressor station models. Any objective function can be used that is a simple sum of costs at each station as a function of flow and inlet/outlet pressures.

The first application on gas pipeline was by Larson and Wong (1968). They applied the method to fuel cost minimization in a single, straight line system and used a recursive formulation, finding the optimal suction and discharge pressures of a fixed number of compressor stations. The length and diameter of the pipeline segments were considered fixed because DP was unable to accommodate a large number of decision variables. The first attempt at optimizing a branching structure in the pipeline industry using DP was by Zimmer in 1975. Recent advances have generated a new DP technique, which is called non-sequential (Carter, 1998) or non-serial DP (Bertelè, 1972). Rather than attempting to formulate DP as a recursive algorithm, in this approach we simply look at a system, grab two or three connected compressor or regular elements, and replace them by a "virtual" composite element that behaves just like its components operating in an optimal manner. These elements can be selected from anywhere in the system, so the idea of "recursion" is really not a good description for this process. The process continues, reducing the number of elements in the problem by one each time, until the system can be reduced no further. Typically, that occurs when there is exactly one virtual element left, which completely characterizes the optimal behavior of the entire pipeline network. The best pipeline operation can then be found by just searching one simple table for the lowest occurring value. Using non-sequential dynamic programming allows one to rapidly and exactly solve these problems even with extensive transmission networks involving extensive branching and looping.

Nontraditional Algorithms

In recent years, a variety of "nontraditional" techniques have been publicized for optimization problems of this sort. Among these methods are Simulated Annealing, Neural Network, Genetic Algorithms and Artificial Ants. The hope is that these methods can give a "more global" optimum. We plan to explore these options further in later work.

Task 2: Future Work

Studies with a simple analytic model linking one hydrogen production center, one hydrogen demand center and one sequestration site were completed, and papers were presented at conferences. Thusfar, we examined the suitability of several nonlinear programming methods for finding the lowest cost hydrogen system. More work on Task 2 remains to be done to understand the best tools for carrying out an optimization of the system.

Task 3.0 Case Study of Transition to a Fossil Energy System with CO_2 Sequestration

In this task, we explore transition strategies: how H_2 and CO_2 infrastructures might develop in time, in the context of a geographically specific regional case study. We focus on the Midwestern United States, a region where coal is widely used today in coal-fired power plants, and good sites for CO_2 sequestration are available. The goal is to identify attractive transition strategies toward a regional hydrogen/electricity energy system in the Midwest with near zero emissions of CO_2 and air pollutants to the atmosphere.

In this task, we hope to derive insights about.

- Time constants and costs. How fast can we implement hydrogen fuel infrastructure? How much will it cost? What are the best strategies? What level of demand is needed for widespread implementation of H_2 energy system?

- Sensitivities to: technology performance and costs, size and density of demand, local availability of primary sources, characteristics of CO_2 sequestration sites, market growth, policies.

- Rules for thumb for optimizing H_2 and CO_2 infrastructure development.

To better visualize our results, we use a geographic information system (GIS) format to show the location of H_2 demand, fossil energy complexes, coal resources, existing infrastructure (including rights of way), CO_2 sequestration sites and the optimal CO_2 and H_2 pipeline networks.

GIS Data for Modeling Fossil Hydrogen Energy Systems with CO2 Sequestration

As an initial step, a survey of relevant GIS data sets was conducted, and initial work was begun on building a database. The preliminary database includes:

- Population density data, which is used to estimate hydrogen demands
- Data on the existing natural gas system
- Information on the electricity system and power plants
- Information on roads, railroads
- Data on the existing gasoline refueling infrastructure
- Information on sites for CO_2 sequestration

We combined this data into a single data base showing features such as hydrogen demand density, location of power plants, etc. This is shown in Figure 8. We use this geographic data as a basis for analyzing alternative configurations for hydrogen supply and CO_2 disposal.

Using GIS Data to Model Hydrogen Demand Spatially and Over Time

Understanding the evolution of a hydrogen fuel delivery infrastructure depends on the spatial and time characteristics of the hydrogen demand. We have developed a simple method to model the magnitude, spatial distribution, and time dependence of hydrogen demand, based on Geographic information system (GIS) data on vehicle populations, and projections for energy use in hydrogen vehicles, and market penetration rates. This method for calculating a hydrogen demand map is described below (see Figure 3).

- First, population density is mapped as a function of location. This information is available in GIS format from US Census data.
- One average in the US there are about three light duty vehicles for every four people (Davis 2000). From this, we can approximate the numbers of light duty vehicles as a function of location (vehicles/km^2). If more detailed information is known about the locations of vehicle fleets, this could be shown as well.
- Next, a market penetration rate for hydrogen is estimated (fraction of new vehicles using hydrogen). This could be done in various ways. For example, one could assume that a "zero emission vehicle mandate" is put in place, so that a fixed fraction of new vehicles sold must use hydrogen. Alternatively, one could devise other criteria for estimating how many new hydrogen vehicles are sold each year, based on projections of when they become competitive with competing technologies like gasoline internal combustion engine technologies. From the market penetration rate, the number of hydrogen vehicles can be found as a function of location and time (H_2 vehicles/km^2 versus time). Table 3 illustrates how the cumulative fraction of hydrogen vehicles in the light duty fleets grows over time, for a very simple model of market penetration. In this simple "ZEV mandate" model, we assume that a constant fraction of all new cars are hydrogen cars (the ZEV mandate level ranges from 10%, 25%, 50%, and 100%). We also assume that new cars sales are 7% of the total fleet each year, and that vehicles are replaced after 14 years. We see that the number of hydrogen vehicles grows linearly in time, reaching saturation at about 14 years. Other market penetration scenarios will be examined in future work.
- The hydrogen use per vehicle (kg H_2/d/vehicle) is estimated from assumptions about hydrogen vehicle fuel economy and miles travelled. A map of hydrogen demand density versus location and time can be calculated (kg/d/km^2). This is shown in Figure 4, for the state of Ohio. The lighter colors are low demand density, the darker colors higher density. The cities of Cleveland, Columbus and Cincinnati are obvious areas of high demand. As time progresses, demand grows, as shown by darkening of the areas around the cities.

Table 3. Fraction of hydrogen vehicles in the light duty fleet as a function of market penetration rate and year, for a simple market penetration model where a constant fraction of new vehicles each year are hydrogen-fueled.

H2 Light Duty Vehicles (fraction of new LDVs)	Year 1	Year 5	Year 10	Year 15
10%	0.7%	3.5%	7%	10%
25%	1.8%	9%	18%	25%
50%	3.5%	18%	35%	50%
100%	7%	35%	70%	100%

Once the hydrogen demand density is known, one has to decide how many refueling stations are required and where they should be sited. The number, location and size of refueling stations have a major effect of the design and cost of infrastructure. This tells us where the hydrogen must be delivered and how much is required. Again, we use GIS data to help guide the process of siting and sizing refueling stations. Let's assume we want future hydrogen stations to be as convenient as today's gasoline stations. In the United States, on average, there is one gasoline refueling station for every 2000 light duty vehicles (Davis 2000), and typical urban stations might serve 3000 light duty vehicles. GIS maps can be used to show where gasoline stations are located. For several cities we examined, stations tend to cluster along major roads in "spoke" or "ring" like patterns. This is shown in Figure 5 for the Columbus, Ohio area. Often, more than one station is found at major intersections or at freeway exits. This suggests that today's convenience level could be preserved, if perhaps 25% of current gasoline stations offered hydrogen. This is similar to results earlier work that estimated the number of alternative fueled stations needed for customer convenience (Kurani and Sperling 1986; IHIG 2003). For typical US urban vehicle densities of 750-1500 cars/km^2, there is one gasoline station per 1.3-4 km^2 (assuming each station serves 2000-3000 cars). Equal convenience might be found with one hydrogen station per 5-16 km^2. If we know the hydrogen demand per km^2, we can find the amount of hydrogen needed at each refueling station as a function of time.

For example, if a fraction fH2 of all light duty vehicles use hydrogen, each vehicle requires on average 0.7 kg H2/day, and there are a total of 1500 LDV/km^2,

the total H2 demand/d/km^2 = fH2 x 1500 LDV/km^2 x 0.7 kg H2/d/LDV
= fH2 x 1050 kg H2/d/km^2

If we want to preserve the same convenience as today's gasoline stations that each serve a total fleet of 3000 cars, and this level of convenience could be achieved with 25% of the current gasoline stations,

minimum number of hydrogen stations per km^2
= (1500 gasoline cars/km^2)/ (3000 cars/gasoline station) x 25%
= 0.125 H2 stations/km^2

The total of H2 cars served per station = fH2 x 3000 cars/gasoline station/25%

Although the economics of hydrogen refueling stations is better at large size, we might wish to limit the size of the refueling stations to better serve markets. If we assume that the maximum size H2 station size serves a total fleet of 3000 cars (similar to stations for today's gasoline cars), the demand at this hydrogen station would be 0.7 kg H2/car/day x 3000 cars = 2100 kg/d/station.)

the total H2 demand per station =

$$\min \begin{cases} fH2 \times (3000 \text{ cars/gaso sta})/25\% \times 0.7 \text{ kg H2/d/LDV} = 8400 \times fH2 \text{ kg/d/station.} \\ (3000 \text{ cars/sta}) \times 0.7 \text{ kg H2/d/LDV} = 2100 \text{ kg/d/station} \end{cases}$$

When fH2 > 25%, more hydrogen stations would be built rather than increasing the size of the stations. This simple hydrogen demand model and refueling station sizing will be improved in future work.

GIS Data for CO2 Sequestration Sites

There are several ongoing projects to model the location, characteristics and capacity of CO2 sequestration sites in the US. A map of possible underground sequestration sites is shown in Figure 6. This database shows the location of saline aquifers and existing brine wells in the US. The MIDCARB project (MIDCARB project**,** http://www.midcarb.org) is particularly relevant to our proposed study of fossil hydrogen infrastructure in the Midwestern US. We are investigating how best to incorporate this work into our study. This will be addressed in future progress reports.

GIS Data on Existing Energy Infrastructure and Rights of Way

We model the availability of resources for hydrogen production and delivery, including the locations of existing infrastructure and rights of way. The location and capacity of existing energy infrastructure and rights of way are an important consideration in developing a hydrogen infrastructure. These include:

- Existing gasoline refueling stations (which give an indication of how transportation fuels are dispensed today, and could be sites for future hydrogen stations).
- Existing hydrogen production plants, storage facilities and pipelines (these might be important for hydrogen supply during the start-up phase of a hydrogen energy system)
- Natural gas transmission and distribution system (hydrogen from natural gas is the lowest cost option in many areas of the US. Hydrogen can be made at a wide range of scales from natural gas.)
- CNG stations (hydrogen stations might be co-located with CNG vehicle fleets)
- Electric power plants (hydrogen might be co-produced at power plants. In many cases, power plants are located near low cost primary resources. These sites might be used for direct production of hydrogen as well.)
- Electric transmission system (electric transmission rights of way might be used by hydrogen pipelines)
- Coal delivery infrastructure (coal might be used to make hydrogen).
- Interstate highways and other limited access roads and railroads. (Rights of way along major roads and railways might be used might be used by hydrogen pipelines.)

GIS databases already exist for many of these systems. As an example, we show the location of electric power transmission lines, coal-fired power plants, CNG stations, the natural gas transmission system, existing industrial hydrogen operations and limited access roads and railroads in Ohio (Figure 7). These data have been combined with population density data in Figure 8 to give a composite picture of demand, potential supply and existing infrastructure.

Designing a Regional Hydrogen Infrastructure Using GIS Data: Preliminary Results

In this section, we present preliminary calculations on designing a regional fossil hydrogen energy system with CO2 sequestration, utilizing data organized in a GIS database. We have used the state of Ohio, as an example, but these techniques could be used anywhere in the US, where similar GIS data are available.

Some characteristics of the energy system in Ohio are given in Table 4. Ohio is heavily reliant on fossil fuels. About 90% of the installed electric capacity is coal-fired.

Table 4. Ohio Energy Statistics

Population	11.1 people
Vehicles	9.7 million light duty vehicles 6.7 million cars 3.0 million light trucks 3.4 million heavy trucks and buses
Light Duty Vehicle Ave. Fuel Economy	20 mpg gasoline
Light Duty Vehicle Ave. Use	10,250 miles/yr
Energy Use	4300 Trillion BTU/y 32% Coal 20% Natural Gas 15% Gasoline 7% Distillate Fuel (other includes fuel oil for heating, nuclear electricity, biomass)
Installed Electric Capacity	27,000 MWe (2.5 kWe/person) 90% coal-fired 65% coal plant capacity factor

Data Base for Designing Regional Hydrogen Infrastructure

In Figure 8, we have created a GIS database that could be used as a basis for designing a fossil hydrogen energy system with CO_2 sequestration for the state of Ohio. Hydrogen demand density (kg/d/km^2) is shown as shading from light colors (low density) to darker colors (high density). Superimposed, we have plotted the location of existing coal-fired power plants (circles proportional to the annual electricity production), limited access roads and railroads, existing CNG stations , and the electricity transmission system. Additional information "layers" that could be added include location and capacity of CO_2 sequestration sites, the existing natural gas transmission system, and existing industrial hydrogen production system.

Matching Hydrogen Demand and Supply

In this section we present some simple calculations on matching regional hydrogen supply and demand. First, we look first at statewide demand at different levels of market penetration, and then at particular cities.

In Table 5, we estimate statewide hydrogen energy use in Ohio for light duty vehicles, and estimate the primary resources needed and CO_2 disposal system required.

First, we summarize projections for future H2 light duty vehicle fuel economy and vehicle miles traveled, and estimate the amount of hydrogen energy that would be needed t produce hydrogen for the entire light duty vehicle fleet. It is assumed that future hydrogen vehicles will be 2-4 times as energy efficient as today's gasoline light duty vehicles (e.g. 40-80 miles per gallon gasoline equivalent on an energy basis). Further, we assume that future cars will travel more, so that the projected miles per year grows from today's average value of 10,250 miles to 15,000 miles per year. The energy required is then about 23-47 GJ (1 GJ=10^9 joules) per year per hydrogen car, depending on the fuel economy.

For a statewide light duty vehicle population of 9.7 million, the energy use is about 0.21-0.42 Quadrillion BTU/y (or 0.22-0.45 x 10^{18} Joules = Exajoules per year). For reference, statewide primary energy use in Ohio today is 4.3 Quadrillion BTU/y, and in the US about 100 Quadrillion BTU/y.

Primary resources needed to make hydrogen are estimated, assuming that all the hydrogen us made from this resource. Producing enough hydrogen for all the light duty vehicles in Ohio would require either:

- 32-64% increase in current statewide natural gas use or
- 27-54% increase in current coal use or
- use of all existing off-peak power (assuming that 50% of the installed capacity could be used off-peak for 12 hours per day), plus an additional 9-44% dedicated power plant capacity to make hydrogen by electrolysis

Of course, not all hydrogen would necessarily come from one source. Still, this highlights that use of hydrogen in mass vehicle markets would entail a significant use of future primary resources.

The statewide CO_2 disposal capacity needed would total about 35,000-70,000 tonnes/day (13-26 million tonnes/year) if hydrogen transportation fuel is made from natural gas, and 75,000-150,000 tonnes/day (27-55 million tonnes/year), if hydrogen is made from coal. Using CO_2 injection wells each capable of handling 2500 tonnes CO_2/day, we would need 14-28 CO_2 injection wells if hydrogen is made from natural gas and 30-60, if hydrogen is made from natural gas. Assuming that the CO_2 sequestration site is operated for 20 years, we would need a CO_2 storage capacity for each well of 18 million tonne CO_2, or statewide a sequestration capacity of 0.26-1.1 billion tonnes CO_2 to dispose of CO_2 from fossil hydrogen transportation fuel production.

Table 5. Projected Statewide Hydrogen Use for Vehicles in Ohio and Required Primary Energy Use and CO_2 Disposal Capacity

Projected characteristics of future light duty vehicles	
Fuel Economy (mpg equivalent) for H2 LDVs	2-4 X current gasoline vehicles = 40-80 mpge
Vehicle use (miles/year) projected for 2050	15,000
Hydrogen use per year (kg H2/d/LDV)	0.52-1.04
Hydrogen energy use per year (GJ/y/LDV)	23-47
Light Duty Vehicle Populations	
Light Duty Vehicles in Ohio (2000)	9.7 million
Hydrogen use statewide	0.22 EJ/y = 211 Trillion BTU
Primary resources required for H2 production if all H2 is produced from single source	
NG (H2 production via 80% efficient steam methane reformer)	277-544 Trillion BTU (32-64% increase in current NG use)
Coal (H2 production via 60% efficient gasifier)	369-739 Trillion BTU (27-54% increase in current coal use)
Electricity (H2 via 80% efficient electrolysis	If all existing off-peak power (assumed to be 50% of 27,000 MWe current installed capacity, available for 12 h/d) is used, additional dedicated power plants for electrolytic H2 production = 9-44% x (the existing electric capacity) would be needed.
CO_2 Disposal capacity needed	
Coal-> H2 plant	75,000 – 150,000 tonnes CO_2/d 30-60 CO_2 wells @ 2500 tonnes/d/well 0.6-1.1 billion tonnes CO_2 over 20 years

NG -> H2 plant	35,000-70,000 tonnes CO_2/d 14-28 CO_2 wells @ 2500 tonnes/d/well 0.3-0.6 billion tonnes CO_2 over 20 years

Matching citywide demand for hydrogen with supply

In Figure 9, we map the hydrogen demand density in the state of Ohio, highlighting the three largest urban areas in Ohio: Cincinnati, Columbus and Cleveland, which are shown in pink. In addition, we have highlighted in blue areas with a vehicle density of more than 200 hydrogen cars per km^2, as likely sites for hydrogen refueling stations, and possibly distribution pipelines.

Using tools in the GIS program ARCGIS, it is easy to select geographic areas for analysis. Regions near each of the three urban areas are highlighted. We then sum up the hydrogen demand over for each city. In Table 6, we calculate hydrogen demand in three cities and statewide, over time, assuming that starting in year 1, 25% of new vehicles sold each year use hydrogen.

Table 6. Daily H2 Demand in Cities (tonnes/day), assuming a market penetration model where 25% of new light duty vehicles sold each year use H2 (the range of values reflects the range of fuel economy projections 40-80 mpg for H2 vehicles).

	Year 1	**Year 5**	**Year 10**	**Year 15**
Fraction of H2 cars in fleet	1.8%	9%	18%	25%
City	**Hydrogen demand (tonnes/ H2/day)**			
Cleveland	6-12	30-60	60-120	84-168
Columbus	4-9	22-44	44-88	62-123
Cincinnati	5-9	23-46	46-92	64-129
Statewide	38-77	192-384	384-768	538-1076

We now contrast the projected hydrogen demand to the size of various hydrogen supply options shown in Table 7. Large coal gasification plants produce 150-600 tonnes of hydrogen per day, while steam methane reformers are more typically in the range 48-480 tonnes hydrogen per day. This suggests that at the levels of hydrogen demand found at year 10 (18% of light duty vehicles use H2), a steam reformer is a better match in size to the city demand than a dedicated coal gasification plant. One large coal to hydrogen plant could provide hydrogen for the entire state, but this would require an extensive long distance hydrogen transmission system (by pipeline or truck).

If higher market penetration of hydrogen cars (for example, if 100% of light duty vehicles used hydrogen), a single city might require enough hydrogen for a dedicated coal plant.

Hydrogen distribution within a city

We can also use the GIS database to look at hydrogen distribution options within a city. In particular, we ask the question "when does local pipeline distribution of hydrogen make sense?" We assume that the hydrogen infrastructure includes a central H2 production plant with small distribution pipelines serving refueling stations, configured in radial spokes (Figure 10). In Figure 11, we plot the cost of hydrogen pipeline distribution versus the

Table 7. Hydrogen Supply and Demand

H_2 Demands	*kg H_2/day*		
1 H_2 FC car (82 mpg, 11,000 mi/y)	0.375		
1 H_2 FC Bus (7 mpge, 50,000 mi/y)	20		
100-1000 H_2 FC car fleet cars (82 mpg, 17,000 mi/y)	58-580		
100 –1000 FC Buses	2000-20,000		
100,000 cars (~1% of cars in LA)	**37,500**		
1 million cars (~10% of cars in LA)	**375,000**		
10 million cars (~100% cars in LA)	**3,750,000**		
H_2 Supplies	*kg H_2/day*	*Size of H_2 FC car fleet supported*	*Size of H_2 FC Bus fleet*
Compressed H_2 gas truck (1/day)	420	1120	21
Liquid H2 truck (1/day)	3600	9600	180
Onsite electrolyzer	2.4-2400	6.4-6400	0.12-120
Onsite steam methane reformer (SMR)	240-4800	640-12,800	12-240
Industrial scale steam methane reformer	**48,000-480,000**	**128,000-1,280,000**	**2400-24,000**
Coal gasifier H_2 plant w/CO_2 seq.	**150,000-600,000**	**400,000-1,600,00**	**7500-30,000**
H_2 from 10% of NG Flow into LA	**1,700,000**	**4,533,333**	**85,000**
H_2 from 1000 MW off-peak power	**240,000**	**640,000**	**12,000**

geographic density of vehicles. We see that pipeline distribution costs rise rapidly at geographic densities of less than about 200 vehicles/km^2. (At these lower vehicle densities, onsite production of hydrogen or truck delivery are less costly than pipelines (Ogden 1999)). In Figure 12, we highlight all the areas in the state where the density of vehicles exceeds 200/km2. In the limit of 100% hydrogen vehicle use, these areas would be possible sites for hydrogen distribution pipelines. We use the GIS database to sum the population in all the highlighted areas. We find that about 70% of people live in areas of high vehicle density that are long term possibilities for pipeline distribution. This suggests that many consumers (30% for this set of assumptions) live in areas where local pipelines will always be a costly mode of bringing hydrogen to refueling stations, even if all the vehicles run on hydrogen.

GIS-aided design of a system for supplying hydrogen to Columbus from coal-based hydrogen plants with CO_2 sequestration

As an example, we consider the design and cost of a system supplying hydrogen to the city of Columbus from a coal to hydrogen plant with CO_2 sequestration. Columbus has a population of about 1 million, with about 700,000 light duty vehicles. Assuming that future hydrogen vehicles have a fuel economy between 2-4X that of today's gasoline cars, and that future vehicles travel more (15,000 miles/year versus 10,250 today) the average hydrogen use per car is 0.5-1.0 kg/d/car. The total hydrogen demand for all light duty vehicles in the city would be 350-700 tonnes H2 per day. (We have not assumed growth in population. If this were included, the hydrogen demand in the future would be greater.)

We now examine possible sites for producing hydrogen for Columbus from coal. From our GIS database (Figure 8), we see several red circles representing coal fired power plants located near Columbus. "Clicking" on various power plant sites, we find that the nearest large coal-fired power plant is the "General Gavin" plant, located along the Ohio river. From the GIS database, the characteristics of this plant are readily available (see Table 8).

From examining the map in Figure 8, we see that there are a number of potential rights of way that might be used to connect the General Gavin plant to the city of Columbus via pipelines. These include electric transmission rights of way (which are ideal, since they run from power plants to cities), railway rights of way and limited access highways. Using an ARCGIS measuring software tool (Figure 13), we find that the distance from the General Gavin plant to downtown Columbus, measured along an electric transmission right of way is 150 km.

Table. 8. Characteristics of General Gavin Electric Power Plant	
Year Built	1974

Type	Pulverized Coal Steam plant with flue gas desulfurization, low NOx burners, SCR
Nameplate capacity (MW)	2600
Electricity production (MWh/y)	17 million
Ave. capacity factor	74%
Coal Consumption (million tonnes/year)	7.2
Coal delivery	100% by barge
Plant Energy Efficiency (kWhe/kWh coal)	30%
CO2 production (tonne/day) (million tonne/y)	50,000 18.6

Assuming that hydrogen could be produced from coal at 65% conversion efficiency, about 18-36% of the current coal consumed at the General Gavin plant would be needed to produce hydrogen for vehicles in Columbus. The General Gavin power plant is operated at only ~ 74% capacity factor today, because it follows electricity load. If this plant is "repowered" with a coal IGCC, with CO_2 capture, and run at a higher efficiency and higher capacity factor, then it might be possible to supply electric needs and make enough H_2 during off-peak electric demand hours for light duty vehicles. (This idea will be analyzed in later work.)

A pipeline bringing hydrogen 150 km from the General Gavin plant to the city would add a relatively small amount to the delivered cost of H_2, < \$1/GJ. H_2 storage at the central plant might add another \$1.5/GJ. Distribution and refueling would add another \$8-10/GJ (Ogden 2003).

A CO_2 disposal system for the fossil energy plant (assuming the same coal consumption as today) would require about 20 injection wells, assuming that each well handled 2500 tonnes CO_2 per day. Most coal consumption would be associated with electricity production. The ratio of electric energy demand to H_2 energy demand for LDVs is about 8:3 (4:3) for H_2 vehicles with 4X (2X) current gasoline fuel economy.

Possible sites for CO_2 sequestration are being evaluated as part of various ongoing studies such as the MIDCARB project. We will be using this data in future work. As an example, we show a map of power plants and existing brine wells in Ohio in Figure 14. If these represented CO_2 sequestration sites, we could estimate the distance from the fossil energy complex using GIS measuring tools, and find pipeline distances and costs. For a CO_2 flow rate of 50,000 tonnes/day, the levelized cost of CO_2 pipeline transmission a 100-200 km and injection should be a small addition to the total hydrogen cost (Ogden, Kaijuka and Wang 2003).

Task 3: Future work

We have developed a GIS data base showing potential demand for hydrogen, location of existing infrastructure, including current coal-fired power plants and major road and railroads (which are potential rights of way for hydrogen or CO2 pipelines) and possible sites for CO2 sequestration. Preliminary results have been presented at two conferences in 2003. We have not yet estimated costs for alternative pathways for developing fossil hydrogen as an energy carrier, or coordinated with other ongoing GIS based studies of CO2 sequestration potential such as the MIDCARB project.

CONCLUSION

During the second six months of research under this contract, we have made significant progress toward understanding the systems aspects of fossil hydrogen systems with CO2 sequestration, and meeting our objectives for the overall project. Below, we summarize by Task the current status of the project and plans for future work.

Task 1.0 Implement Technical and Economic Models of the System Components

Description: Here we utilize data and component models of fossil energy complexes with H_2 production, H_2 distribution systems and refueling stations and CO_2 sequestration being developed as part of earlier work at Princeton and other efforts.

Status: We have surveyed estimates for system component costs and performance that are available in public domain literature, and from ongoing work at Princeton. We have synthesized cost and performance estimates for hydrogen production systems with CO2 capture, hydrogen pipelines, hydrogen refueling stations, CO2 pipelines, and CO2 injection sites. This work was described in the first progress report.

Future Work: Over the next year, we plan to improve these cost and performance estimates. In particular, the principal investigator Joan Ogden has been involved with the H2A group, an ongoing effort at the USDOE, which brings together analysts (funded under various DOE programs) who study hydrogen systems. This group has been reviewing the costs and performance of hydrogen production, delivery and refueling systems. Access to these data will give improved estimates of components costs and performance under Task 1. The National Research Council is producing a report on hydrogen that will include models of hydrogen components. The results of these efforts should become available in 2004. In addition, the PI will check with the latest results from modeling efforts under the CMI project at Princeton. Our work will be updated to reflect the new information contained in these studies.

Task 2.0. Integrated Studies of the Entire System to Find the Lowest Cost Network

Description: As a first step, we developed a simple analytical model linking the components of the system. We considered single fossil energy complex connected to a single CO_2 sequestration site and a single H_2 demand center. To study more complex and realistic systems involving multiple energy complexes, H_2 demand centers, and sequestration sites, we are exploring use mathematical programming methods to find the lowest cost system design.

Status: Studies with a simple analytic model linking one hydrogen production center, one hydrogen demand center and one sequestration site were completed, and papers were presented at conferences. We have looked at several nonlinear programming approaches to modeling CO_2 pipeline disposal systems.

Future Work: More work on Task 2 remains to be done to understand the best tools for carrying out an optimization of the system.

Task 3.0 Case Study of Transition to a Fossil Energy System with CO_2 Sequestration

Description: In this task, we explore transition strategies: how H_2 and CO_2 infrastructures might develop in time, in the context of a geographically specific regional case study. We focus on the Midwestern United States, a region where coal is widely used today in coal-fired power plants, and good sites for CO_2 sequestration are available. To better visualize our results, we use a geographic information system (GIS) format to show the location of H_2 demand, fossil energy complexes, coal resources, existing infrastructure (including rights of way), CO_2 sequestration sites and the optimal CO_2 and H_2 pipeline networks.

Status: We have developed a GIS data base showing potential demand for hydrogen, location of existing infrastructure, including current coal-fired power plants and major road and railroads (which are potential rights of way for hydrogen or CO_2 pipelines) and possible sites for CO_2 sequestration. Preliminary results have been presented at two conferences in 2003. We have not yet estimated costs for alternative pathways for developing fossil hydrogen as an energy carrier, or coordinated with other ongoing GIS based studies of CO_2 sequestration potential such as the MIDCARB project.

Schedule for Completing the Work and Deliverables

Over the year (until August 2004), we plan to complete the three tasks set forth in the original statement of work. In addition, we will use improved understanding from ongoing studies (for example those by the H2A group and the MIDCARB project), to improve our results, especially for Tasks 1 and 3.

REFERENCES

W. Amos, "Costs of Transporting and Storing Hydrogen" NREL report No. NREL/TP 570-25106 November 1998.

Benson, H.Y. and Ogden, J.M.: "Mathematical Programming Techniques for Designing Minimum Cost Pipeline Networks for CO_2 Sequestration", the Proceedings of the Sixth International Conference on Greenhouse Gas Control Technologies, Kyoto, Japan, 2000.

Bertelè, U. and Brioschi, F.: "Nonserial Dynamic Programming", Academic Press, New York, 1972.

Carter, R.: "Pipeline Optimization: Dynamic Programming after 30 Years", Technical Report 9803, PSIG, 1998.

Carter, R., Goodreau, M. and Rachford, H.: "Optimizing Pipeline Operations through Mathematical Advances", Pipeline and Gas Journal, October 2001: 50-51.

Christodoulou, D. "The Technology and Economics of the Transmission of Gaseous Fuels," Master's Thesis, Department of Mechanical and Aerospace Engineering, Princeton University, April 1984.

S. Davis, ORNL Transportation Energy Data Book, Edition 20, October 2000, Table 7.15

Directed Technologies, Inc., Air Products and Chemicals, BOC Gases, The Electrolyser Corp., and Praxair, Inc., 1997: *Hydrogen Infrastructure Report*, prepared for Ford Motor Company Under USDOE Contract No. DE-AC02-94CE50389, July.

Djebedjian, B., Herrick, A. and Rayan, M.A.: "Modeling and Optimization of Potable Water Network", International Pipeline Conference, ASME, Vol. 2, 2000: 1227-1233.

R. Doctor, et al. "Hydrogen Production and CO_2 Recovery, Transport and Use from a KRW Oxygen Blown Gasification Combined Cycle System," Argonne National Laboratory Report , May 1999, Table 7.3

Edgar, T.F.: "Optimal Design of Gas Transmission Networks", Society of Petroleum Engineers Journal, April 1978: 96-104.

Farris, C.B. (1983). "Unusual Design Factors for Supercritical CO_2 Pipelines," *Energy Progress*, 3, 150-158.

Flanigan, O.: "Constrained Derivatives in Natural Gas Pipeline System Optimization", Journal of Petroleum Technology, May 1972:549-556.Foster Wheeler (1998), "Precombustion Decarbonization," Report Number PH2/19, prepared for the IEA Greenhouse Gas R&D Programme.

Foster Wheeler (1996): *Decarbonization of Fossil Fuels*, Report No. PH2/2, prepared for the Executive Committee of the IEA Greenhouse Gas R&D Programme of the International Energy Agency, March.

Goldberg, D.E. and Kuo C.H.: "Genetic Algorithms in Pipeline Optimization", Journal of Computing in Civil Engineering, 1(2), 1987: 128-141.

Hendriks, C.A. (1994). "Carbon Dioxide Removal from Coal-Fired Power Plants", Ph.D. thesis, Department of Science, Technology, and Society, Utrecht University, Utrecht, The Netherlands.

Hoeven, Tom van der and Gasunie, N. V. Nederlandse: "Some Mathematical Aspects of Gas Network Simulation", Technical Report 9206, PSIG, 1992.

Holloway, S. (1996) An overview of the Joule II Project. *Energy Conversion and Management* 37(1-2): 1149-1154.

International Hydrogen Infrastructure Group, private communictions 2003.

Kreutz, T., R. Williams, R. Socolow, P. Chiesa and G. Lozza (2002), "Analysis of Hydrogen and Electricity Production from Fossil Fuels with CO_2 Capture," *Proceedings of the 6th International Conference on Greenhouse gas Control technologies*, 30 Sept-4 October 2002, Kyoto, Japan.

Kreutz, T., Princeton University, Princeton Environmental Institute, private communications, 2002.

Kurani, K, and D. Sperling, 1995.

Larcher, Spitzl, Sekirnjak, Weinberger: "Optimization Problems in the Dispatching of Natural Gas", 12th World Gas Conference of the IGU, Nice 1973.

Larson, R.E. and Wong, P.J.: "Optimization of Natural Gas Systems via Dynamic Programming", Trans. Auto. Cont., IEEE, October 1968, No AC-12: 475-481.

MIDCARB project**,** http://www.midcarb.org

M. Mintz, S. Folga, J. Gillette, and J. Molburg, "Hydrogen: On the Horizon or Just a Mirage?" Society of Automotive Engineers paper No. 02FCC-155, 2002.

Ogden, J., 1998: *Comparison of the Design and Economics of Hydrogen Refueling Station Options*, Report to the U.S. Department of Energy under Contract No. DE-FG36-95GO10061, December.

J. Ogden, 1999a, “Strategies For Developing Hydrogen Energy Systems With CO_2 Sequestration,” *Proceedings of the 10th National Hydrogen Association Meeting*, Vienna, VA, April 7-9, 1999.

J. Ogden, 1999b, “Developing a Refueling Infrastructure for Hydrogen Vehicles: A Southern California Case Study,” International Journal of Hydrogen Energy, vol. 24, pp. 709-730.

Ogden, J. (1999), “Prospects for Building a Hydrogen Energy Infrastructure,” *Annual Review of Energy and the Environment*, 24, 227-279.

Ogden, J. (2003), “Conceptual Design of Optimized Fossil Energy Systems with Capture and Sequestration of Carbon Dioxide,” Semi-Annual Technical Progress Report No. 1, to the National Energy Technology Laboratory, USDOE for DOE Award Number: DE-FC26-02NT41623.

J.M. Ogden, E. Kaijuka and W. Wang, “Modeling Fossil Hydrogen Energy Systems with CO2 Sequestration,” presented at the 2nd National Carbon Sequestration Meeting, Arlington, VA, May 5-8, 2003.

O’Neill, R.P., Williard, M., Wilkins, B. and Pike R.: “A Mathematical Programming Model for Allocation of Natural Gas”, Operations Research, Vol. 27, No. 5, 1978: 857-873.

Sekirnjak, E.: “Practical Experiences with Various Optimization Techniques for Gas Transmission and Distribution Systems”, Technical Report 9603, PSIG, 1996.

Smits, A.J.: “A Physical Introduction to Fluid Mechanics”, John Wiley & Sons, Inc., 1999.

Simbeck, D., 1(999), “A Portfolio Selection Approach for Power Plant CO_2 Capture, Separation, and R&D Options”, *Proceedings of the Fourth International conference on Carbon Dioxide Removal*, Pergamon Press, pp. 119-124.

Skovholt, O. (1993), "CO_2 Transportation System," *Energy Conservation and Management*, 34(9-11):1095-1103.

.

Spath, P.L. and W.A. Amos (1999), “Technoeconomic Analysis of Hydrogen Production from Low BTU Western Coal with CO_2 Sequestration and Coalbed Methane Recovery Including Delivered H_2 Costs,” Milestone Report to the US DOE H2 Program.

J. B. Taylor, J.E.A. Alderson, K.M. Kalyanam, A.B. Lyle, and L.A. Phillips, “Technical and Economic Assessment of Methods for the Storage of Large Quantities of Hydrogen,” International Journal of Hydrogen Energy, vol. 11, p. 5, 1986.

Thomas, C.E., B.D.James, F.D. Lomax, and I.F. Kuhn, (1998). Draft Final Report, *Integrated Analysis of Hydrogen Passenger Vehicle Transportation Pathways*, report to the National Renewable Energy Laboratory, U.S. Department of Energy, Golden, CO, Under Subcontract No. AXE-6-16685-01, March.

U.S. Energy Information Administration (2001). "Energy Outlook 2002, with Projections Through 2020," DOE/EIA0383(2002), U.S. Department of Energy, Washington, DC.

White, Curt, National Energy Technology Laboratory, private communications 2003.

Williams, R.H. (1998). "Fuel Decarbonization for Fuel Cell Applications and Sequestration of the Separated CO_2," in *Eco-restructuring: Implications for Sustainable Development*, Ayres (ed.), United Nations Univ. Press, 180-222.

Wolf, Daniel de and Smeers, Yves: "Optimal Dimensioning of Pipe Networks with Application to Gas Transmission Networks", Operation Research, Vol. 44, No. 4, 1996: 596-608.

Wu, S., Rios-Mercado, R. Z., Boyd, E.a. and Scott, L.R.: "Model Relaxations for the Fuel Cost Minimization of Steady-State Gas Pipeline Networks", Mathematical and Computer Modeling, Vol. 31, 2000: 197-220.

Zimmer: "Dynamic Method Models Gas pipeline", The Oil and Gas Journal, 11(1975)

LIST OF ACRONYMS AND ABBREVIATIONS

CMI	Carbon Mitigation Initiative. Begun in 2001, the Carbon Mitigation Initiative is a ten-year $15-20 million dollar joint project of Princeton University, BP and Ford Motor Company to find solutions to global warming and climate change.
FCV	fuel cell vehicle
GIS	geographic information system
GJ	gigajoule (= 10^9 Joules)
SMR	steam methane reforming.
USDOE	United States Department of Energy Research