

October, 1997

MASTER

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

Sentech, Incorporated
Under
Subcontract Number 96DE-GF001-EN1003
Prime Contract Number DE-FC36-96G010170

Prepared for:

Edward G. Skolnik
Energetics, Incorporated

Prepared by:



DOE/GO/10170--76

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

International Energy Agency Annex 11, Subtask B – Interim Report

This document is meant to describe the status of the International Energy Agency (IEA), Annex 11 (Integrated Systems), Subtask B (Analytical Tools) effort being carried out by the Member Nations. This includes Canada, Japan, Italy (inactive at this time), the Netherlands, Spain, Switzerland, and the United States. The Subtask status is taken as of the end of September 1997, following the Fall Experts Meeting. This was held in Toronto, September 23-26.

The goal of this Annex is to identify, compile, and integrate models of hydrogen technology components into system models that will describe overall pathways. Examples would include: PV/electrolysis/pipeline transport/hydride storage/PEM fuel cell utilization or natural gas steam reforming/liquefaction/truck transport/hydrogen refueling station. Component models are developed by the Member Nations and integrated into the desired overall system. Subtask B is concerned with identifying and compiling existing component models from Member Nations, or developing these models from data supplied by the Member Nations via Subtask A.

In a meeting of Annex 11 Subtask Leaders and the Operating Agent in Stuttgart, Germany in the summer of 1996, it was decided to approach the modeling of the various components by assigning a team to each component. The team would consist of a team leader and support members who would provide model development, data, and model validation. This approach was implemented at the Annex 11 Experts' Meeting in Tokyo, Japan in October 1996.

ASPEN Plus[®] was selected as the modeling platform of choice, and this software tool was only available within the group at ECN (Netherlands), and at NREL (USA). It was thus decided that these two organizations would perform the actual model construction after receiving the required input from the Technology Team leaders.

By the time of the last report in July, component models had been completed on the following technologies:

• Coal Gasification	Netherlands (Team Lead)	Netherlands (Model supplier)
• Biomass Gasification	U.S.	U.S.
• Biomass Pyrolysis	U.S.	U.S.
• High Pressure Pipeline	U.S.	U.S.
• Low Pressure Pipeline	U.S.	U.S.
• NG Reforming	U.S.	U.S.
• Chemical Storage	Netherlands	Netherlands
• MeOH Transport	Netherlands	Netherlands
• Liquefaction	Japan	Netherlands

Brief descriptions of these models were given in the April and July reports.

Since that time, we have received four other models. Significantly, we have our first utilization model, proton exchange membrane (PEM) fuel cells, completed. This allows for the first time the

integration of an entire hydrogen pathway from production through utilization to be integrated. The four component models are identified, and then briefly described below:

- PV/Electrolysis Spain/Canada (Team Lead) U.S. (Model supplier)
- High Pressure Storage Canada Netherlands
- Metal Hydride Storage U.S. U.S.
- PEM Fuel Cells Canada U.S.

PV/Electrolysis

As reported earlier, a decision was made to treat electrolysis-based production processes (e.g., PV/electrolysis, wind/electrolysis, grid/electrolysis) as a single component. Thus, this model couples a PV design based on the El Segundo, CA facility with an electrolyzer design from The Electrolyser Corporation. The PV array has a nominal capacity of 40 kW. Solar insolation is the primary factor used in determining the amount of electricity available to the electrolyzer. The model finds the maximum power point, and then determines the corresponding voltage and current. From this, the amount of hydrogen produced by the electrolyzer can be calculated. The electrolyzer converts water to hydrogen and oxygen. Excess water is recycled and the oxygen byproduct is flashed. The hydrogen is purified by converting contaminant oxygen to water in a catalytic reactor. Water is then removed from the hydrogen stream by cooling flashing and recycling. The hydrogen is then dried.

High Pressure Storage

This is a dynamic system. The component model considers an input flow (from a hydrogen production process) that can be valved either through or around a compressor/ high-pressure storage vessel/expansion valve system, and used to meet a demand (or output) flow. The storage system serves to make up differences between the supply and demand flow rates. The model can then determine how much hydrogen is stored and how much is bypassed. It also can calculate the energy consumption associated with storage, all of which is caused by compressor power consumption.

Since ASPEN Plus[®] uses a steady-state simulator, the flows are averaged over a cycle rather than being treated as a function of time.

Metal Hydride Storage

Development of models for metal hydride storage is specific to the particular metal hydride and its properties. It is not practical to attempt to create a single, universal model. The hydrides that were modeled in this exercise were mischmetal-nickel-aluminum, titanium-iron-manganese, and magnesium-nickel. Although each model is unique all (and any other metal hydride that would be modeled) have the same format. In each case, hydrogen, cooling water, fuel, and combustion air are system inputs. The model provides the composition of two hydrogen streams (produced via two desorption steps), flue gas, cooling water return and compressor power demand.

Again, since storage processes are dynamic, the model must run as a pseudo-steady state. Thus, the adsorption processes are decoupled from the desorption processes. In the adsorption portion, the hydrogen is first compressed, and then adsorbed onto the metal, cooling the exothermic process with cooling water if needed. In the desorption process, hydrogen is first released from the hydride in an isothermal depressurization. In the second step, the hydride is heated using natural gas combustion, to remove the remaining hydrogen.

PEM Fuel Cells

The model for the PEM fuel cell is based on a design from the Royal Military College (Canada), and has a maximum output of 3.9 kW. It is based on a hydrogen/oxygen fuel cell, but is assumed to be compatible with a hydrogen/air design with a few modifications.

In the process, hydrogen and air (oxygen) are both humidified and sent to the fuel cell. The amount of each gas is based on the required load, which is a model input. When the power demand is set, the model varies the amount of hydrogen until the demand is satisfied. An assumption is that the user would desire to use the lowest current density possible to meet the demand.

There are still twelve component models out-standing. Some are close to completion. We expect about eight of them to be completed by the end of the calendar year. The goal is to have them all completed, and the final report as well as the model library being constructed by the time of the next experts meeting.

The spring meeting is scheduled for March, 1998, and will probably take place in Switzerland. It is also planned to have what may be the final meeting of this Annex at the World Hydrogen Energy Council Meeting in Buenos Aires in June.

An overall status of the component models as of the end of September 1997, as broken down by technology area, is shown in Tables 1-4.

Table 1. IEA Annex 11 Subtask B -- Status of Source and Production Component Model Development

Technology	TT Lead	TT Support	Date of Receipt or Date Promised	Status
PV/Electrolysis	Spain/Canada	IT,JP,SP,SW,US	9/97	Completed
Wind/Electrolysis	USA/Canada	IT	3 months	Do Not Have
Grid/Electrolysis	USA/Canada	CN,IT,JP,SW,US	3 months	Do Not Have
NG Reforming	USA	CN	3/97	Completed
Biomass Gasification	USA	NE	1/97	Completed
Biomass Pyrolysis	USA		12/96	Completed
Coal Gasification	Netherlands	US	2/97	Completed

Table 2. IEA Annex 11 Subtask B -- Status of Storage Component Model Development

Technology	TT Lead	TT Support	Date of Receipt or Date Promised	Status
High Press CG	Canada	NE, SP	9/97	Completed
Low Press CG	Canada	IT, NE	1-2 months	Do Not Have
Metal Hydrides	USA	IT,SP,JP	9/97	Completed
Liquefaction	Japan	NE,US	6/97	Completed
Chemical Storage (MeOH)	Netherlands	JP	4/97	Completed
Chemical Hydrides	Switzerland	NE	1-2 months	Do Not Have

Table 3. IEA Annex 11 Subtask B -- Status of Transport Component Model Development

Technology	TF Lead	TF Support	Date of Receipt or Date Promised	Status
Transport Tanker	Japan	NE	3 months	Do Not Have
High Press Pipeline	USA	CN	1/97	Completed
Low Press Pipeline	USA	CN	1/97	Completed
Tank Truck	Japan	NE,US	3 months	Do Not Have
MeOH Transport	Netherlands	JP	3/97	Completed

Table 4. IEA Annex 11 Subtask B -- Status of Utilization Component Model Development

Technology	TT Lead	TT Support	Date of Receipt or Date Promised	Status
PEMFC	Canada	IT,NE,SW,US	9/97	Completed
PAFC	Spain	JP,SW,US	1-2 months	Do Not Have
SOFC	USA	CN,NE,SW	?	Do Not Have
MCFC	USA	JP,NE	?	Do Not Have
Gas Turbines/NG Blends	USA	JP, CN (blends)	2 months	Do Not Have
ICE/Gen Sets*	USA		?	Do Not Have
Refueling Stations*	USA	NE	?	Do Not Have

*Components added during Neunburg Meeting