Hydrogen Storage Systems Analysis Meeting

955 L'Enfant Plaza North, SW, Suite 6000
Washington, DC 20024-2168

March 29, 2005

SUMMARY REPORT

Compiled by
Romesh Kumar
Argonne National Laboratory

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Meeting Objectives

The objective of this meeting was to familiarize the DOE research community involved in hydrogen storage materials and process development with the systems analysis work being carried out within the DOE program. In particular, Argonne National Laboratory (ANL) has been tasked to develop models of on-board and off-board hydrogen storage systems based on the various materials and technologies being developed at the DOE Centers of Excellence and elsewhere. An important aspect of ANL's work is to develop models that can be used to "reverse engineer" hydrogen storage systems, i.e., determine the viable matrix of material, thermodynamic, and kinetic properties that would be needed for a given system to achieve the desired performance and cost targets.

DOE has requested that a "Storage Systems Analysis Working Group" be formed to leverage expertise, avoid duplication, and facilitate communication of storage related analysis activities. This meeting was used as a basis for starting such a group. The working group will meet formally twice a year (at DOE Annual Program Review in May and at a major conference such as Fuel Cell Seminar or MRS Meeting in November/December).

Summary of Presentations

The meeting agenda is shown in Appendix A. The meeting participants (some, by calling in) are shown in Appendix B.

After introductory and overview remarks by DOE and ANL, D. Anton of United Technologies Research Center (UTRC) described a 1-kg H_2 prototype sodium alanate system. This was followed by a presentation by S. Lasher of TIAX on how the UTRC prototype data can be used to evaluate the manufacturing cost of such a hydrogen storage device. Following up on the sodium alanate case study, R. Ahluwalia of Argonne then discussed how the various thermodynamic and kinetic factors determine the performance of such a system, and how one may assess what improvements in material properties would be needed to meet one or more of the performance and cost targets for such systems. The Argonne presentation also discussed a preliminary analysis of a hybrid (elevated pressure, lowered temperature) activated carbon hydrogen storage system.

Representatives from the three Centers of Excellence then provided overviews of their future analysis plans and what they see as the significant materials and process characteristics in complex metal hydrides (W. Luo, SNL), chemical hydrogen storage (C. Aardahl, PNNL), and carbon-based materials and sorbents (M. Ringer, NREL) approaches for hydrogen storage.

These discussions and presentations at the meeting are summarized below.

DOE Introductory Remarks (S. Satyapal)

The main objectives of the meeting are to introduce analysis-related activities that are underway within the various hydrogen storage projects and will form part of the work of the Centers of Excellence as their research gets underway. Meetings like this that involve participation by the different groups will help to identify and reduce areas of overlap and duplication, as well as to identify opportunities for complementary research. A Storage Systems Analysis Working Group could be a forum to promote cross-communication on an ongoing basis.

The types of analyses envisaged for this activity include: systems analysis for performance and cost; design, analysis, engineering, and optimization of reactors, including consideration of hybrid approaches, materials properties, and thermal management; and life-cycle analyses, including energy balances, life-cycle costs, environmental impact/cradle-to-grave and emissions analyses. Such analyses are needed for various on-board vehicular hydrogen storage options, such as metal hydrides, chemical hydrogen storage, carbon-based/adsorbent systems, as well as physical storage (tanks) and hybrid concepts.

ANL Overview (R. Kumar)

Various approaches are being considered or pursued for on-board and off-board hydrogen storage. Each approach has different characteristics, such as operating conditions, thermodynamics, energetics, and kinetics. System-level models can help to identify component and performance issues, as well issues of effectively interfacing the hydrogen storage system with the fuel user, i.e., a fuel cell or an internal combustion engine.

Argonne's role in hydrogen storage system development will be to work with the DOE contractors and the researchers at the three DOE Centers of Excellence to: model and analyze various developmental hydrogen storage systems; conceptualize and analyze hybrid approaches that combine features of different systems; develop modeling tools to "reverse engineer" particular technologies; identify interface issues and opportunities for material and/or energy integration; and identify data needs and research directions for the development of effective, efficient hydrogen storage systems.

Sodium Alanate Case Study, UTRC (D. Anton)

United Technologies Research Center designed, fabricated, and tested a "first generation" 1-kg prototype hydrogen storage system based on catalyzed $NaAlH_4$ for use in automotive polymer electrolyte fuel cell systems. Models for the reaction kinetics of the two-step hydrogen charge-discharge processes were developed to track the in-tank composition (weight fractions) of the different sodium-aluminum hydrides (i.e., NaH, Na_3AlH_6, and $NaAlH_4$). The thermal effects were analyzed to determine the number and size of heat transfer tubes (24 tubes of 3/8-in diameter, with 4% dense aluminum foam support). It was determined that a composite tank, rated for 1500 psi at 250ºC, rather than a stainless steel tank, was needed to approach the gravimetric goals. Media densification is a major factor in improving volumetric density; however, the densification method needs to be scalable and applicable to the storage vessel as a whole, including means to load the media into the vessel.

The presentation discussed the design of the first prototype, various components, assembly, powder loading on the foam support, and loading of the supported media into the vessel. As fabricated, this prototype had 19 kg of the hydride at an average density of 0.44 g/cc (with a peak hydride density on the foam disks of 0.60 g/cc) in the vessel designed for 100 atm pressure. The hydride represented 39% of the total mass of the vessel.

The system was tested for hydrogen charging and discharging. Charging was carried out at 70 bar and 100 bar at 80, 100, and 120ºC for 24 h; for the discharging tests, the standardized charging conditions were 100ºC, 100 bar, 24 h. Discharging was measured at 80, 90, 100, and 110ºC down to 2 bar over 24 h. The data were consistent with those obtained with 1 g samples of the media. Integrated system modeling using these data showed that, for the current system, the volume of the system is slightly lower than that of a 5000-psi tank of comparable H_2 capacity, while the mass is 50% higher. Using 2015 projections of 7.5 wt% media, 70 wt% media loading, and an optimized system configuration, the sodium alanate system is projected to offer a 20% lower mass and a 50% lower volume than the current 5000-psi tank.

Manufacturing Cost Analysis of Prototype Sodium Alanate Systems, TIAX (S. Lasher)

TIAX has conducted a manufacturing cost analysis of the sodium alanate system as part of its project to assess the performance and costs of different hydrogen storage options. The cost model is based on process models and performance and technical assessments. It includes materials costs and processing and manufacturing equipment costs, and it can be used for sensitivity analyses to determine the relative influence of the different cost contributors. For the sodium alanate system, TIAX evaluated the material and processing costs of the media, the tank, and the heat exchange system. The purchased cost of other components (pump, blower, valves, pressure regulator, etc.) was included in the model.

The system design used for the cost model was based on data in the literature and from developers. The system was designed for 5.6 kg of available H_2 (based on ANL drive-cycle modeling of a mid-size SUV hybrid fuel cell vehicle). Several key assumptions were: media H_2 capacity of 4 wt%; powder packing density of 0.6 g/cc; minimum and maximum temperatures of 100 and 186ºC; and maximum pressure of 100 bar. The tank design incorporated the heat exchanger tubes to provide cooling during charging and heating during discharging. The balance-of-plant needed for thermal management and flow control was included in the assessment (see the presentation for details).

The TIAX analysis showed that a media H_2 storage capacity greater than 7 wt% would be needed to meet the near-term gravimetric targets, and that such a sodium alanate system would have a volume comparable to that of a 5000 psi compressed gas tank. The manufactured cost of the sodium alanate system, approximately \$13/kWh, is projected to be comparable to that of a

10,000 psi compressed gas tank. Although media cost and capacity are major parameters affecting total system cost, the tank hardware and the balance-of-plant contribute about 60% of the total cost and about 50% of the total system weight. Further, if part of the stored hydrogen is used to provide the thermal energy for the discharge step, the amount of stored hydrogen would need to be increased by about 25%.

Performance Analysis of Sodium Alanate Systems, ANL (R. Ahluwalia)

This study examined a sodium alanate hydrogen storage system for use with a high-temperature (120ºC) polymer electrolyte fuel cell system, where the fuel cell waste heat could be used to provide the thermal energy of the dehydriding reaction. If the stack waste heat is not used, there will be an 18–25% penalty in net system efficiency. A preliminary model of the sodium alanate tank system was developed using GCtool, a systems analysis software package developed at Argonne. The model included $NaAlH_4$-Na_3AlH_6 thermodynamics, first order charge and discharge kinetics (derived from Sandia data), transient thermal model for the heat transfer fluid, heat exchanger tubes, support foam, the metal hydride powder, and the liner, carbon- and glass-fiber wraps, and the insulation. The stack coolant temperature of 115ºC and the required minimum hydrogen discharge pressure of 3 to 8 atm limit the metal hydride capacity to 3.7 wt%. During charging, for a 10-min refueling time for 5.6 kg of H_2, the average cooling duty is 173 kW, with a peak cooling duty of nearly 1 MW.

With the assumption that the stack waste heat at 115ºC is used for hydrogen desorption, and that a hydrogen evolution rate of 1.6 g/s (0.02 g/s-kW for an 80-kW fuel cell system) must be achievable at all times, it was determined that the maximum depth of discharge of the metal hydride may not exceed 59.6% due to the first order kinetics of hydrogen adsorption/desorption for sodium aluminate. With a maximum state of charge of 95% (limited by kinetics of hydrogen refueling), the recoverable hydrogen is 1.4 wt% in the hydride media. With the set of design parameters used (see the presentation for details), the recoverable hydrogen storage capacity corresponds to 0.7 wt% of the hydride storage tank. Sensitivity analyses showed that this value can be increased to 1.7 wt% if the desorption kinetics can be increased 10-fold, the heat transfer tubes can be made of aluminum alloy, and the contact resistance between the tubes and the aluminum foam can be reduced by an order of magnitude.

Preliminary Analysis of Medium-P, Low-T Activated Carbon Systems, ANL (R. Ahluwalia)

Argonne has also conducted a preliminary analysis of activated carbon hydrogen storage systems that may use a “hybrid” approach of combining elevated pressures and reduced temperatures to achieve storage capacity targets. Analyses were conducted using published adsorption data for commercially available activated carbon AX-21, pressures to 100 bar absolute (bara), and temperatures of 150 K (hydrocarbon refrigerant) and 77 K (liquid nitrogen refrigerant). It was determined that just the carbon medium, i.e., without the containment and other tank internals, can achieve the near-term volumetric target of 1.2 kWh/L (36 kg/m^3) at 77 K and storage pressures in excess of 65 bara. However, if the minimum hydrogen delivery pressure is 8 bara, even the carbon by itself cannot meet the recoverable hydrogen target capacity at storage pressures of 100 bara or less. The carbon can meet the target if it can be warmed up by 50 K, i.e., for 77 K to 127 K, as the pressure is reduced from 100 bara to 2 bara.

For the system as a whole, i.e., including the tank but not incorporating any internal heat exchange hardware, the AX-21-based system can meet the near-term 4.5 wt% gravimetric target at 77 K, but it would not meet the volumetric target of 1.2 kWh/L. Neither target can be met with AX-21 at 150 K. Sensitivity analyses have identified the improvements in activated carbon characteristics needed for such systems to meet the targets.

Systems Analysis Considerations for Complex Metal Hydrides, SNL (W. Luo)

The materials issues and characteristics identified as being important for system performance include:

1. Enthalpy of the charging and discharging reactions;
2. Heat transfer rates, material volume change, material packing, heat exchanger design;
3. Gas transport, media packing, hydrogen quality;
4. Sorption/desorption kinetics, heat and mass transfer, cycling effects;
5. Mechanical stresses, pressure and temperature cycling, molar volume change;
6. Material safety, reactivity; and
7. Life-cycle analyses.

In the first phase, work at this Center will investigate engineering properties, material safety, effects of contaminants in hydrogen, and material synthesis and processing. Subsequently, engineering issues of scale-up will be addressed.

Systems Analysis Considerations for Chemical Hydrogen Storage, PNNL (C. Aardahl)

Chemical-based hydrogen storage can achieve high volumetric and gravimetric energy storage densities. Two significant challenges are chemical reversibility (on-board or off-board) and kinetic control. This Center will investigate chemical hydrogen storage based on hydrolysis, dehydrogenation, and dehydrocoupling, as well as processes yet to be developed. Studies will include thermodynamics, catalysis, kinetics, and analyses.

For this type of storage, regeneration of the "fuel" is likely to be conducted off-board. Engineering and analysis activities will, therefore, be carried out separately for the hydrogen generation and the fuel regeneration components of these hydrogen storage systems.

Systems-Level Considerations for Carbon-Based Hydrogen Storage, NREL (M. Ringer)

The major analysis activity conducted by this Center to-date is the H2A hydrogen delivery system analysis. This analysis examines movement of hydrogen by a compressed gas truck, liquid hydrogen truck, or pipeline, which require compressors and liquefiers. The Excel-based model calculates the portion of the delivered hydrogen cost that is attributable to the different delivery components. Thus, for example, the cost of hydrogen delivery as a compressed gas can be evaluated as a function of the storage pressure, delivery distance, and the delivered amount of hydrogen. At 3000 psi storage pressure, delivering 100 kg/day over a distance of 100 km will have an estimated cost of $1.40/kg of H_2 (see presentation for details).

Future work will include similar analyses of metal hydride, chemical, and carbon-based storage and shipping approaches.

Action Items and Next Steps

The Storage Systems Analysis Working Group is tentatively scheduled to meet biannually, typically in conjunction with the Fuel Cell Seminar in November and the DOE Hydrogen Program Review in May. Other topical meetings or workshops may be convened as needed. It is anticipated that smaller teams will have monthly conference calls on specific storage analysis efforts. Final reports of the Working Group will be made available on the public DOE website.

APPENDIX A

AGENDA

Hydrogen Storage Systems Analysis Meeting

March 29, 2005, Washington, DC

01:00 PM	Welcome	S. Satyapal / DOE/EE
01:05 PM	Objectives of Meeting / ANL overview	R. Kumar / ANL
01:15 PM	$NaAlH_4$ prototype system	D. Anton / UTRC
02:00 PM	Cost analyses of H_2 storage systems	S. Lasher / TIAX
02:45 PM	Break	
03:00 PM	H_2 storage system-level considerations	R. Ahluwalia / ANL
03:45 PM	Systems considerations and plans: Metal Hydride Center	W. Luo
4:00 PM	Systems considerations and plans: Chemical Hydrogen Storage Center	C. Aardahl, / PNNL
4:15 PM	Systems considerations and plans: Center for Carbon-based Materials	M. Ringer / NREL
4:30 PM	Discussion	All
4:55 PM	Wrap-up and Next Steps	R. Kumar / S. Satyapal
5:00 PM	Adjourn	

APPENDIX B

MEETING PARTICIPANTS

Hydrogen Storage Systems Analysis Meeting

March 29, 2005, Washington, DC

Last	First	Org	E-mail	Phone
Aardahl	Christopher	PNNL	Christopher.Aardahl@pnl.gov	509-376-7022
Aceves	Salvador	LLNL	saceves@llnl.gov	925-422-0864
Ahluwalia	Rajesh	ANL	Walia@anl.gov	630-252-5979
Anton	Don	UTRC	AntonDL@utrc.utc.com	860-610-7174
Blair	Larry	DOE/Consultant	larry.blair@ee.doe.gov	505-896-6686
Bowman	Robert	SNL	robert.c.bowman-jr@jpl.nasa.gov	
Cleary	Bill	ANL	bill.cleary@ee.doe.gov	202-586-1570
Duffy	Michael	NREL	Michael_Duffy%exchange@ee.doe.gov	303-275-3022
Gronich	Sigmund	DOE/EE	Sigmund.Gronich@EE.DOE.GOV	202-586-1623
Heben	Michael	NREL	michael_heben@nrel.gov	303-384-6641
Joseck	Fred	DOE/EE	Fred.Joseck@ee.doe.gov	202-586-7932
Keller	Joe	SNL	jokelle@sandia.gov	925-294-3316
Kelly	Michael	Mcell	Kelly@millenniumcell.com	
Ko	Jui	Quantum	JKo@qtww.com	949-399-4500
Kumar	Romesh	ANL	kumar@cmt.anl.gov	630-252-4342
Lasher	Stephen	TIAX	lasher.stephen@TIAXLLC.com	617-498-6108
Luo	Weifang	SNL	wluo@sandia.gov	925-294-3729
Motyka	Theodore	SRNL	ted.motyka@srnl.doe.gov	803-725-0772
Ordaz	Grace	DOE/EE	Grace.Ordaz@ee.doe.gov	202-586-8350
Read	Carole	DOE/EE	Carole.Read@ee.doe.gov	202-586-3152
Ringer	Matthew	NREL	Matthew_Ringer%exchange@ee.doe.gov	
Satyapal	Sunita	DOE/EE	Sunita.Satyapal@ee.doe.gov	202-586-2336
Sheahen	Tom	NREL	tom_sheahen@nrel.gov	202-646-5216
Sirosh	Neel	Quantum	NSirosh@qtww.com	
Thomas	George	DOE/SNL	george.thomas@sbcglobal.net	775-771-3324

Note: Names shaded in yellow participated in person, those shaded in blue called-in, while names without shading are additional people involved in the storage analysis activity.