Sandia National Laboratories

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DOE Hydrogen, Fuel Cells, and Infrastructure Technologies Program

Systems Analysis Workshop

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Washington, D.C.

Charter

- Sandia's H_2 program objective:
  Provide engineering & science to enable use of H2 as an energy carrier
- SNL's H_2 Program office is in the Combustion Research Facility
  - a user-facility for combustion & energy research
- Program is matrixed to organizations throughout the lab that bring specific expertise:
  - Reacting flows, System engineering, integration and analysis, Materials science, Nuclear and Renewable energy
- Program supported by DOE funding
  - EERE
    - H_2, Fuel Cell, & Infrastructure program
    - FreedomCAR & Vehicle Technologies
    - DER (Distributed Energy Resources)
  - Nuclear Energy (NERI)
  - Fossil Energy (NETL)
- Sandia LDRD funding leveraged to H_2 program

History

- Sandia's H_2 experience spans 40 years driven by Defense Programs
  - Work involves science, engineering, modeling, & systems analysis
  - Gas transfer systems:
    - high-P real-gas eqn-of-state, gas dynamics & heat transfer, solid storage & materials science (70's to date)
- Energy systems programs from 1980 to present
  - Nuclear systems with thermochemical H_2 production
  - Solar central receiver with thermochemical H_2 production
  - Fossil energy to H_2 with sequestration
- Sandia DOE-H_2 program activities began in '94 by Jay Keller
  - Engineering systems analysis (sample projects)
    - Remote Area Power Program: evaluated reformer + FC systems
    - H_2-ICE development & analysis
      - Computer optimized H_2 vehicle/storage system
    - Mine locomotive development
      - Integrated FC control & storage system
  - Safety, codes & standards – experimental/modeling program

Skill Set – People (not all inclusive)

- Analysts currently working on H_2 programs
  - Andy Lutz: Engineering system analysis
  - Tom Drennen, Arnie Baker: Economics
  - Dave Borns: CO_2 sequestration
  - Scott Jones: Renewable systems
  - Greg Kolb, Rich Diver: Solar-to-H_2 via thermochemical cycles
  - Paul Pickard, John Kelly: Nuclear-to-H_2 via thermochemical cycles
  - Lennie Klebanoff: California H_2 Highways, H_2 storage
  - Other analysts with relevant capabilities
    - Steve Thomas, Paul Boggs, Mike Eldrid
      - Optimization software tools for a variety of applications
    - Susanna Gordon, Larry Brandt: team of ~30 analysts & computer scientists
      - System models for Dept Homeland Security & Defense Programs
      - Analysis of radiation, nuclear, chemical, biological security issues

Skill Set – Models that include H2

- **Power parks system model**
  - Developed by Andy Lutz over past 5 yrs
  - Engineering/thermodynamic analysis coupled to economic analysis for components in a local energy station
  - Supported by DOE/EERE/H_2-FC-Infrast Tech-Val program for analysis of demonstration facilities
  - Library of component models:
    - Existing: Reformers (SMR, ATR), electrolyzer, PV collector, compressor, high-P storage, pump, FC stack (efficiency vs power)
    - Developing: ICE gen-set, wind turbine, FC (model I-V curve & parasitics)
  - System models applied to facilities at SunLine, Las Vegas, Hawaii
  - Platform: *Simulink/Matlab*,
    - Uses *Chemkin* (thermodynamics) & *Stanjan* (equilibrium)
  - Limitations:
    - Assembly of a system model requires knowledge of *Simulink*
    - financial assumptions not (yet!) consistent with H2A

Skill Set – Models that include H_2

- *H2Sim*
  - Developed by Tom Drennen & Arnie Baker – Work in Progress
    - Support from Andy Lutz, Dave Borns, Scott Jones, Paul Pickard
  - Economic modeling of H_2 unit cost
    - Production: reforming, gasification, electrolysis, thermochemical (with nuclear & concentrated solar)
      - Electrolysis model gets electricity cost from ***GenSim*** model
    - Transportation: pipeline, truck (gas/liquid), rail, ship
    - Storage: underground, tanks (gas/liquid), metal hydride
    - End-use: vehicle for transportation (cost/mile)
      - Vehicle comparisons: FCV, H_2-ICE, gas-ICE, gas-hybrid, EV
    - GUI makes model easy-to-use!
  - Platform: *Powersim Studio*
  - Limitations:
    - financial assumptions not (yet!) consistent with H2A

Skill Set – Models adaptable to H_2

- Optimization models
  - Software to find parameters that optimize a system given a set of constraints
    - *Dakota*: framework for developing optimization applications
    - *Split*: solves quadratic & general nonlinear optimization problems
    - *MOOCHO*: method for solving large-scale nonlinear optimization problems with nonlinear constraints
  - Platform: C compiler; parallel applications require MPI
  - Limitations:
    - Problem solutions are limited by computer size, time & money,
    - However…
- Computer resources are available for large-scale optimization problems

Skill Set – Capabilities Summary

TYPE OF ANALYSIS	RESIDENT CAPABILITY?	STUDIES SPECIFIC TO H_2?	MODELS SPECIFIC TO H_2?
Resource Analysis	*Yes*	*Yes*	*No*
Technoeconomic Analysis	*Yes*	*Yes*	*Yes*
Environmental Analysis	*Yes*	*Yes*	*Yes*
Delivery Analysis	*Yes*	*Yes*	*Yes*
Infrastructure Development Analysis	*Yes*	*No*	*Yes*
Energy Market Analysis	*Yes*	*No*	*No*

Studies

- Past
  - RAPP: Remote power from H_2 system; Yuma Indian reservation
  - H_2-ICE system optimization
- Current
  - Power Park system analysis: monitor & evaluate H_2 power stations
  - Central-station solar H_2 power plant: analyze solar thermochemical power plant concepts
  - Carbon sequestration in Southwest Regional Partnership
  - Nuclear-to-H_2 via thermochemical
- Planned (funded LDRD projects)
  - California H_2 Highway Blueprint development
  - Optimization of coal/bio gasification for H_2 production
  - H_2 energy system analysis

Future

- Sandia is committed to building a generalized system optimization tool to guide development of the H_2 infrastructure
- How will we make this vision a reality?
  - Draw on expertise in the H2 community
    - Sub-models for evolving state-of-the-art technology solutions
    - Infrastructure analysis expertise (ex: GIS data)
    - Techno-economic analysis procedures (H2A)
    - Codes & standards for implementation options
  - Draw on expertise in the computer science community
    - System assembly algorithms to define a regional/national infrastructure
    - Optimization tools
- Team with university, laboratories, and industry partners
  - Laboratory expertise at NREL & elsewhere
  - University partnerships: Joan Ogden (Davis)

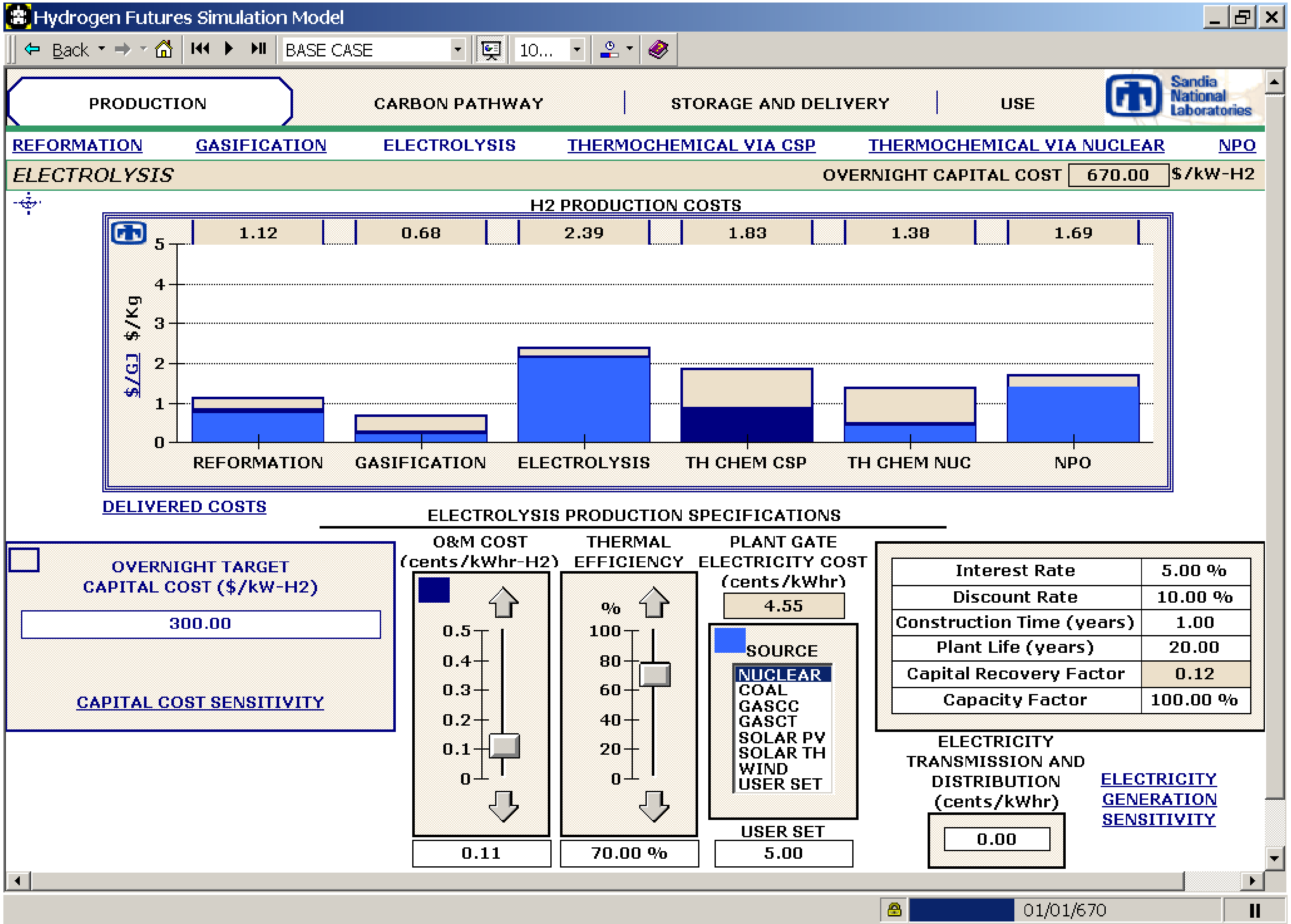
Analysis Issues

Dynamic simulation of integrated H_2 infrastructure should:

- Be ***dynamic***, with respect to an evolving infrastructure
- Be ***regional***, because energy sources & constraints vary throughout US
- Be based on sound ***science*** to provide ***engineering fidelity***
- Include modules for
  - Production alternatives (nuclear, renewable, fossil)
  - Transportation alternatives
  - Distribution/Storage alternatives
  - Utilization alternatives
- Provide ***optimized*** solutions for
  - – Geographic description of a developing H_2 infrastructure
  - – Solution depends on
    - Figures of merit for objectives: cost, emissions, efficiency, …
    - Regional constraints
    - Technology options

Backup Slides

H2Sim Electrolysis analysis page



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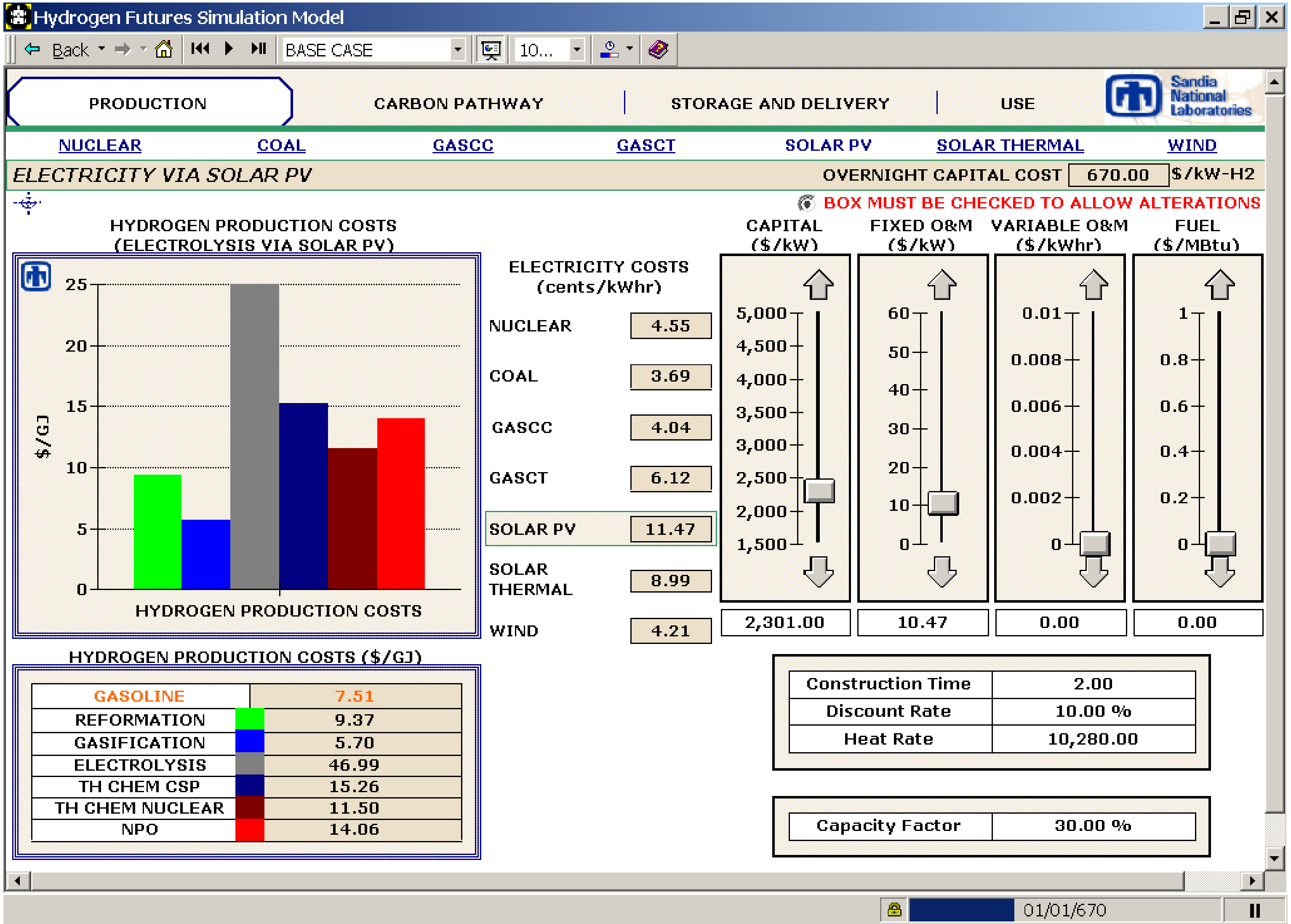
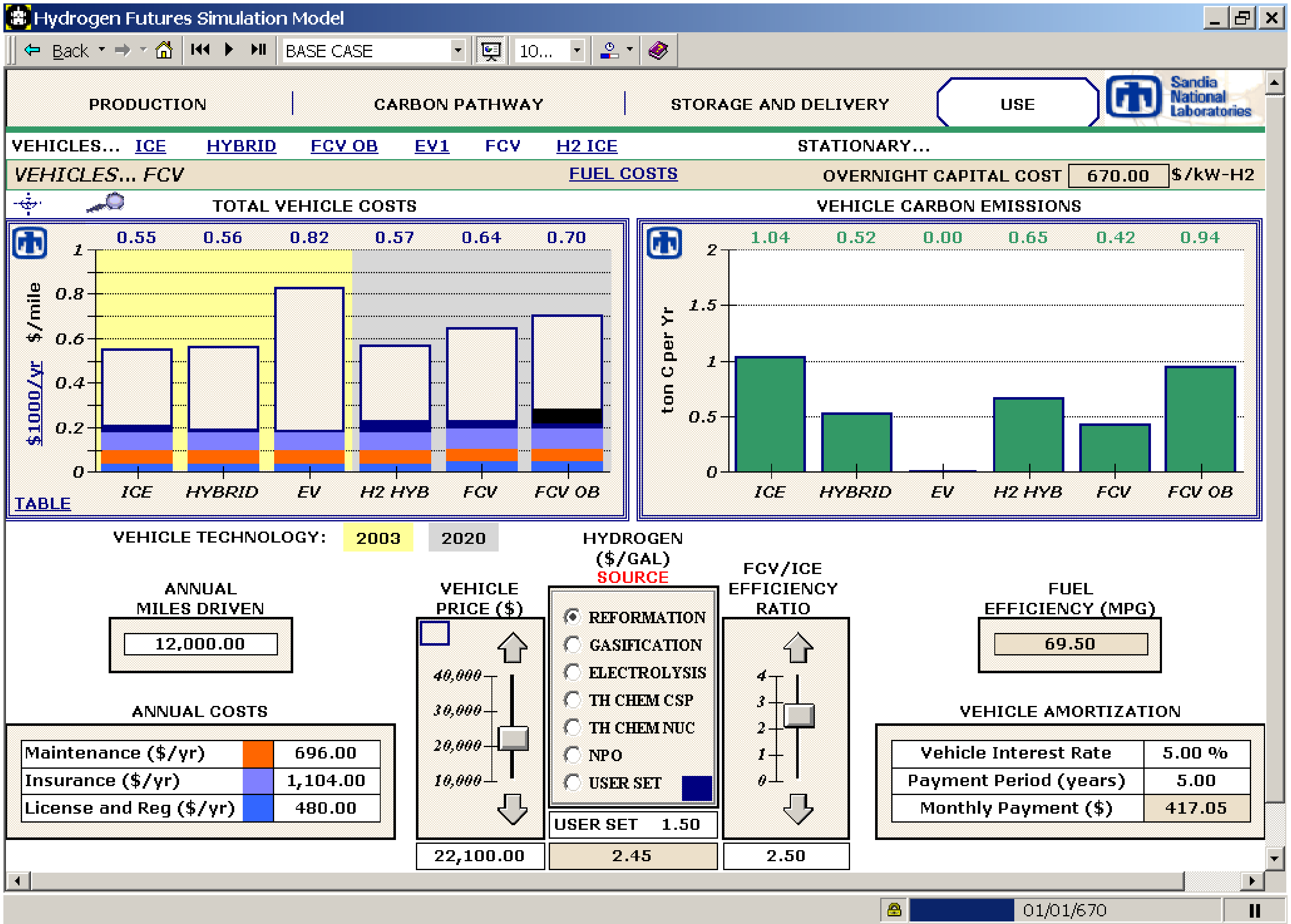
H2Sim Electricity cost analysis from *GenSim*



H2Sim Vehicle Use Page



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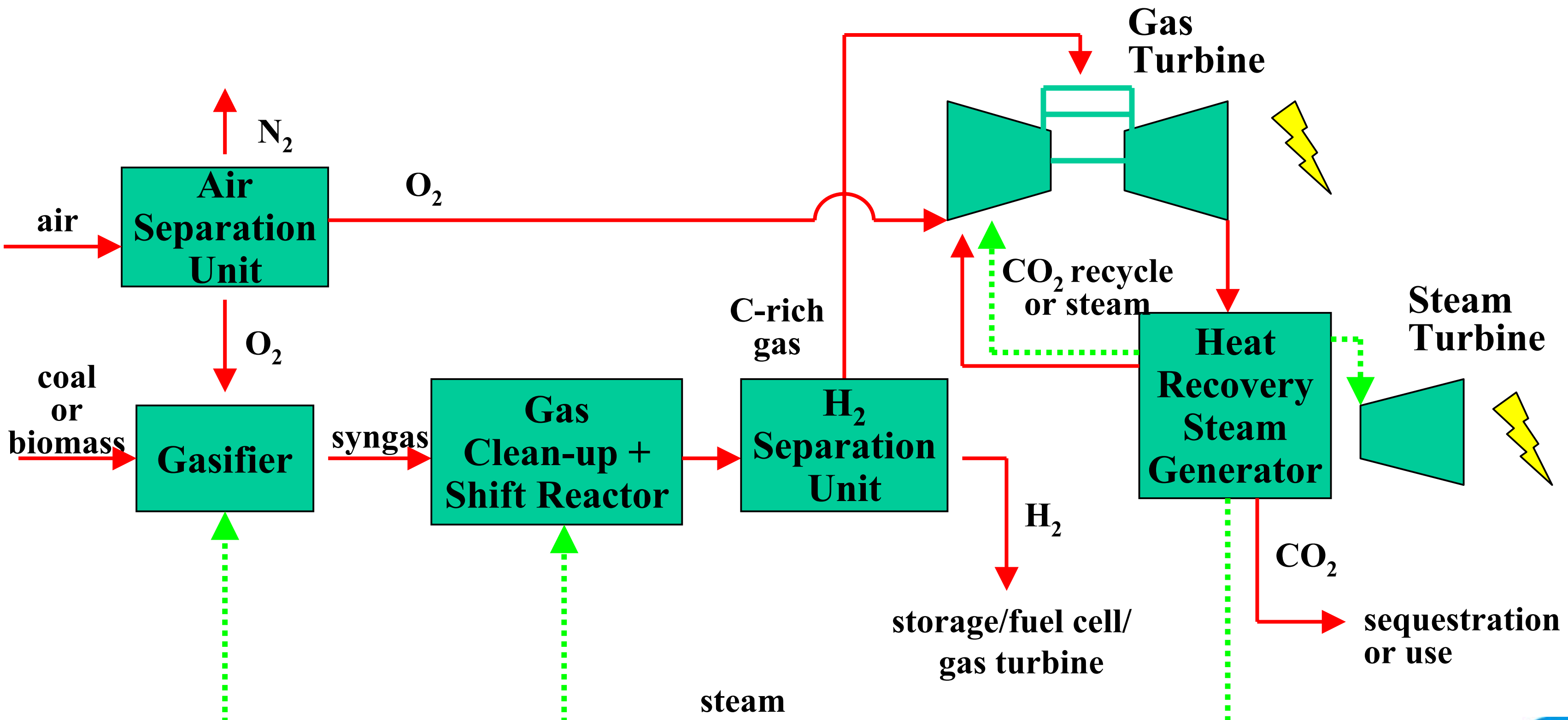
Sandia LDRD Research on Gasification

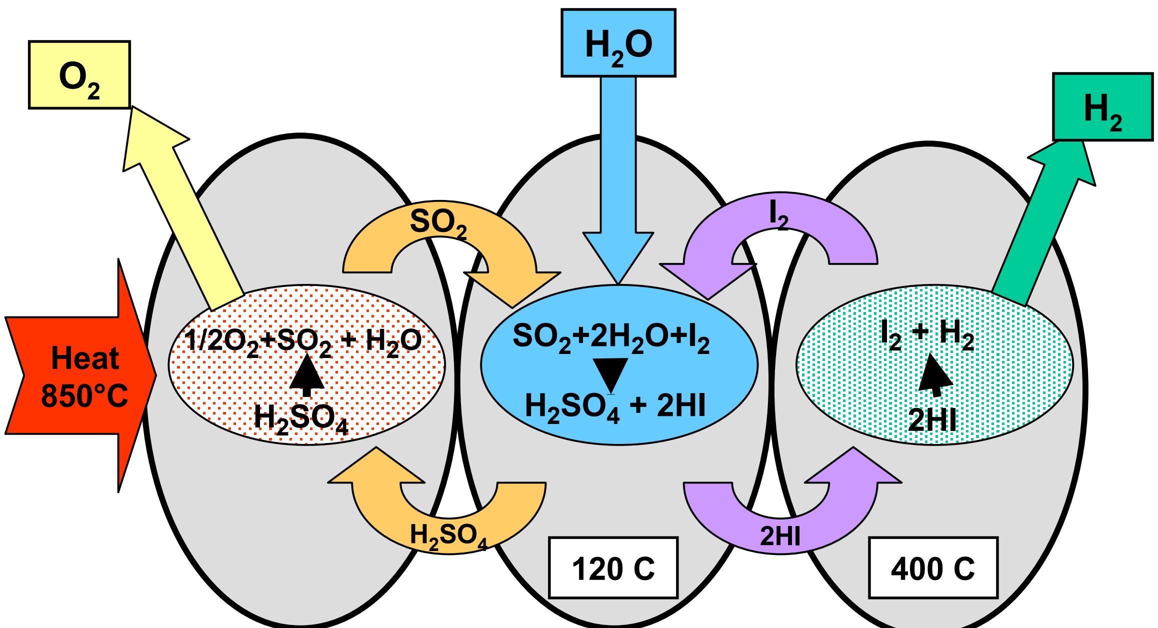
- Optimization of gasification for H_2 production by investigating effects of fuel type, steam/carbon ratio, P, & T on H_2 production using Sandia high-P reactor
- Joint experimental-computational investigation of lean premixed flames for gas turbine burner operation on H_2-depleted syngas with O_2 and CO_2/steam
- Use Simulink model to analyze system performance



Sandia Nuclear-to-H2 Research

DOE - NERI Project (General Atomics, Sandia Labs, U of Kentucky)

- Define nuclear power source options: dedicated H_2 vs hybrid plant options
- Develop performance and cost metrics for technology evaluation
- Examine high efficiency, thermochemical cycles (115 cycles considered)
  - Selected: Sulfur – Iodine & UT-3



Primary Deliverables
- Process step demonstration
- Operational parameters
- Component reaction section design
- Interface requirements
- High T materials data
- Thermodynamic data (VLE)

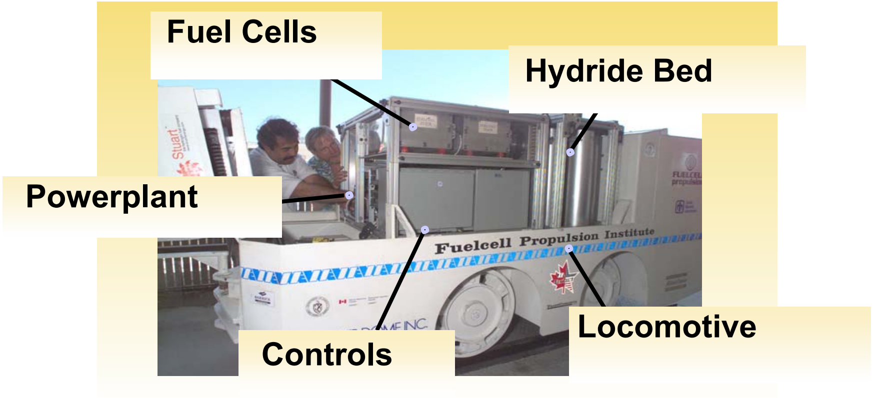
Interface Issues
Species, Concentrations, Recycle Flows, Pressure, Temperature, Control, Configuration

Sandia systems engineering

Challenging new technologies require research, invention, and demonstration. Sandia's systems engineering supports technology development and works with industry to attack the remaining risks.

Sandia integrated enabling technologies:

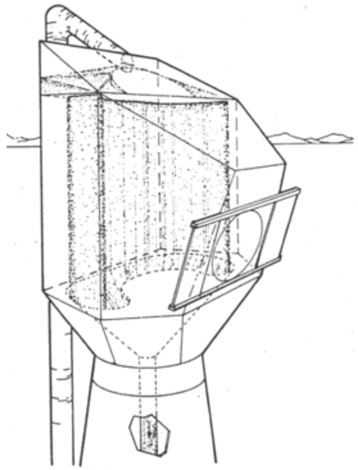
- Commercial components
- The fuel cell balance of plant for fuel cell stacks
- Sandia developed solid storage system
- Complete system including controls



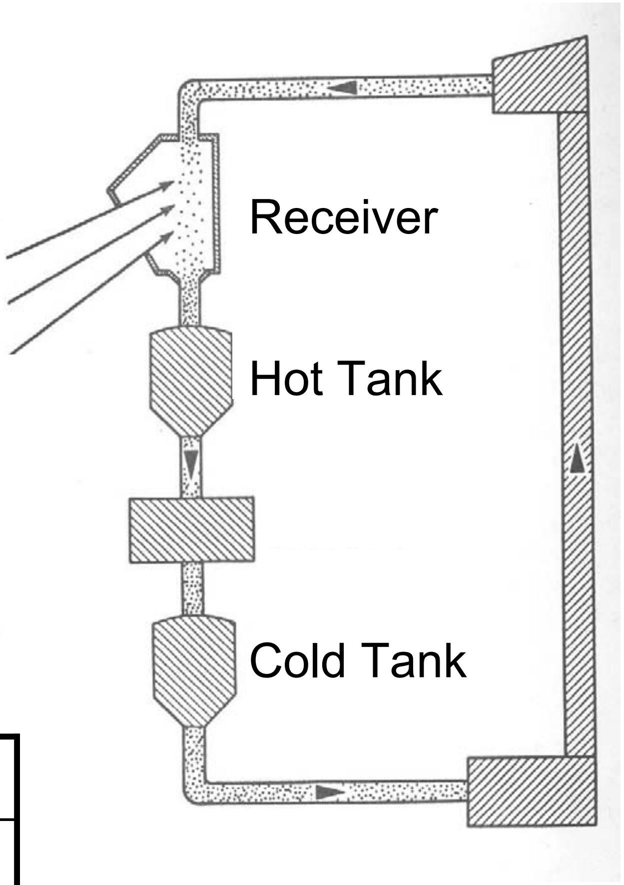
Fuel Cell Powered Mine Locomotive

Central solar-to-H2 system analysis

- Falling particle central receiver



Receiver/Storage Concept



- H2A-like economic analysis
  - Sandia cash-flow model used the major H2A parameters to compute levelized H2 Cost ($/kg)

FCR	PT-electrolyzer	PT-T/C
14%	$4.7	$3.0
10%	$3.5	$2.2

System analysis for Homeland Security

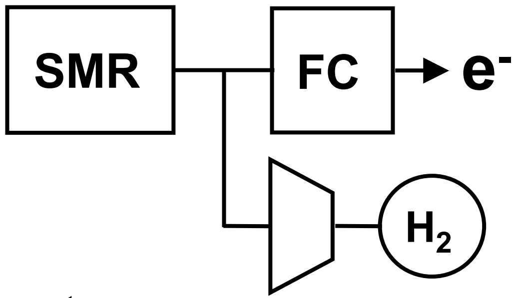
- **PROACT program creates guidance for defense of airports against chem/bio terrorism**
- **Employing a suite of analytical techniques to investigate issues and options**
  - **Vulnerability assessment**
  - **Smoke- and tracer-release tests**
  - **Model-based analyses**
- **Developing broadly applicable guidance**
  - **"Guidelines to Improve Airport Preparedness Against Chemical and Biological Terrorism"**

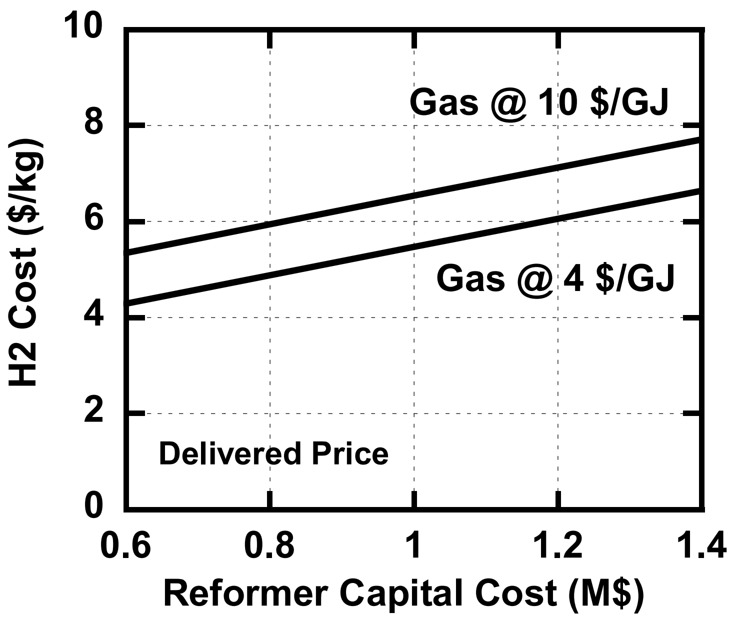
SFO

San Francisco International Airport

Simulink analysis of hybrid power park

- H_2 Generator (SMR) feeds fuel cell and compressed storage
  - Reformer: ~150 kg/day at 68% thermal efficiency (H_2/CH_4 on LHV basis)
  - Compressor: used 82% efficiency from MYPP target
- Hybrid system efficiency = 47%
  - Electricity + Compressed H_2
  - Gas-to-electric efficiency = 29%

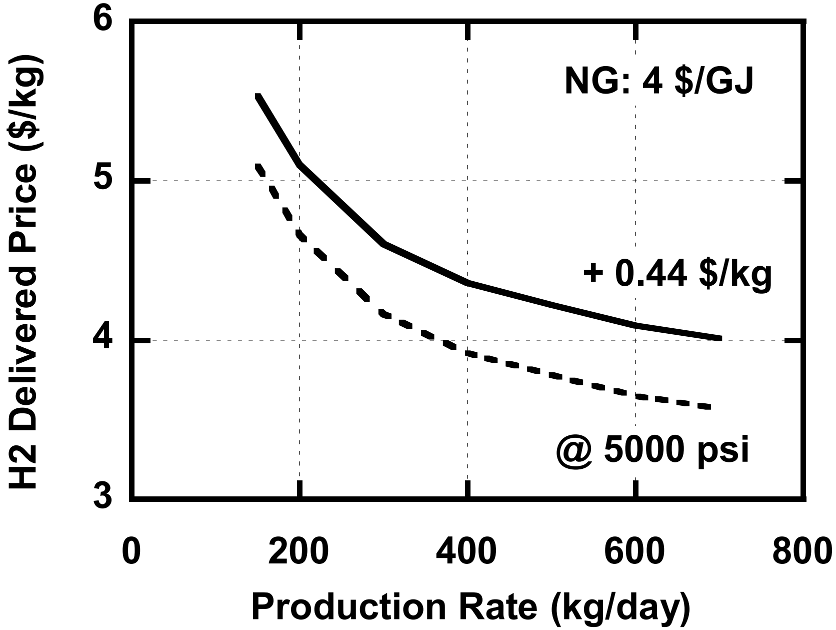


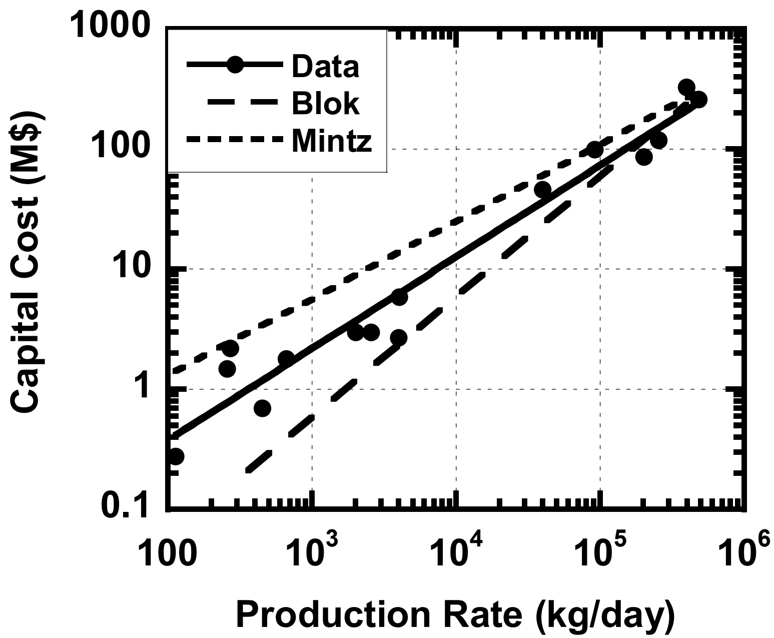


- Economic parameters
  - 10 year life at 10% interest
- Parameter studies:
  - Reformer capital cost
  - Natural gas price
- H_2 cost includes
  - Compressor: capital + power at 8¢/kWh
  - Refueling station: 0.92$/kg (MYPP target)

Cost of H_2 projected for refueling station

- H_2 production rate has non-linear effect on cost
- Use literature correlation to *simultaneously* vary reformer capital cost & production rate
- Add 0.44$/kg for refueling station
  - From DOE 2010 target costing

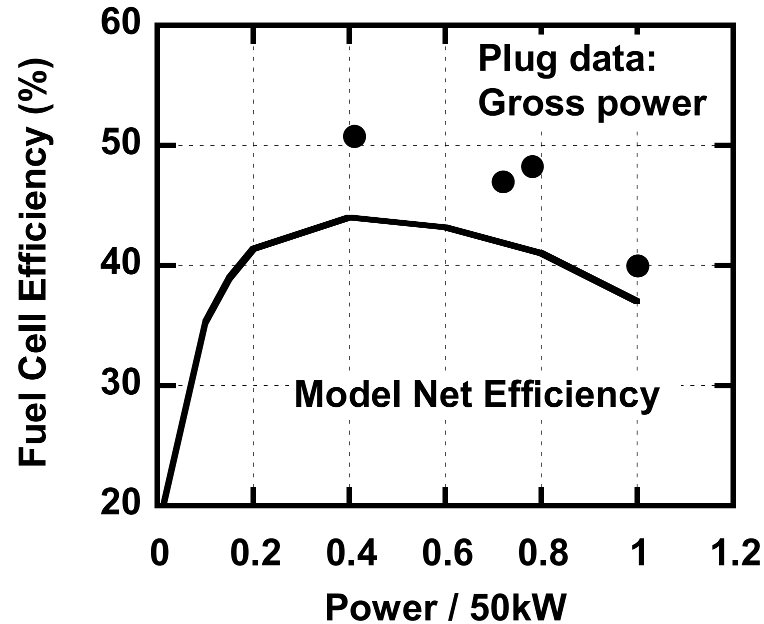




- To meet DOE targets for distributed reforming (4$/GJ gas)
  - **2005: 3$/kg will need 700 kg/day reformer installed for 2.5M$ instead of 3.4M$**
  - **2010: 1.50$/kg requires changing the capital cost vs production rate relation**

Model for fuel cell at hybrid station

- Model uses operation data from Las Vegas station
  - Adjusted efficiency to measurement: 47% for 36kW gross DC power out
  - Assume a 10% reduction to account for parasitics & power conditioning
  - Net efficiency for model = 42%
- Operation data from Plug Power (with permission)
  - Steady-state operation at 36 kW



Cost of electricity for hybrid system

- Economic assumptions
  - Maintenance includes yearly stack replacement
    - Vary O&M cost over range 20-50% of original capital
  - H_2 at 4.81$/kg from reformer at nominal conditions:
    - 150 kg/day production rate
    - 6 $/GJ natural gas