# Development of an Advanced Chemical Hydrogen Storage and Generation System

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Project ID #: STP 12
Contract #: DE-FC36-05GO15056

# Overview

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The Hydrogen Battery Technology Company

## Timeline

- Project start date: February 2005
- Project end date: February 2010
- Percent complete: 40%

## Barriers

- Weight and Volume
- Efficiency
- Heat removal

## Budget

Total project funding (5 Year)

- DOE share: $2.4 million (80%)
- MCEL share: $0.6 million (20%)

Funding received for FY06:

- $250 K

Funding for FY07:

- $180 K requested
- $200 K obligated

## Project Targets

| | 2005 | 2006 | 2007 |
|---|---|---|---|
| System volumetric capacity (kWh/L) | **1.0** | **1.1** | **1.2 (Est'd)** |
| System wt% | **3.9** | **4.2** | **4.5 (Est'd)** |

## Partners

Center of Excellence – Chemical $H_2$ Storage.
PNNL – System modeling and engineering.

# Objectives

## Overall:

- Improve capability to store and release $H_2$ from chemical hydride
- Meet DOE 2007 target and beyond:
  - 1.2 kWh/L (36 g $H_2$/L) and 1.5 kWh/kg (45 g $H_2$/kg).
- Leverage MCEL engineering expertise and guide Center research

## Last Year:

- Developing modeling tool for hydrogen release reactor.
- Collecting data for fuel compositions.

## This Year:

- Validation of modeling results with experimental data (on-going.)
- Conceptual system design based on modeling.
- Submitted preliminary draft to TIAX & ANL
- Preparing materials for DOE "go/no-go" decision on SBH for Q4FY2007.

# $NaBH_4$ System Development

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| Catalyst Modeling | Reactor Modeling | Conceptual Design | System Design |
|---|---|---|---|
| Oct. – Dec. 05 | Jan.- Aug. 06 | Sept. 06 - Sept 07 | Oct. 07 –Sept. 08 |

**PNNL Collaboration**

- Develop modeling tools
- Lattice Boltzmann calculations
- Macroscopic modeling
- Validate model
- Optimize Conversion
- Optimize reactor dimensions
- Increase throughput
- Fluid dynamics

09/30/07

- Reactor features
- BOP designs
- Safety evaluation

Go/No-Go

- Sub-system testing
- System testing
- Prototype Demo:

  > 45 g $H_2$/kg

  > 36 g $H_2$/L

# Current Status

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| Target | MCEL Results (previous experience) | MCEL Results (current design estimates) | Go/NoGo Decision (2007) |
|---|---|---|---|
| System Gravimetric Capacity | 1.3 kWh/kg (87% to target) | 1.5 kWh/kg (meets target) | 1.5 kWh/kg |
| System Volumetric Capacity | 1.1 kWh/L (30% SBH system) (92% to target) | 1.22 kWh/L (30% SBH system) (meets target) | 1.2 kWh/L |
| Storage System Cost | 6.7 $/kWh net | (pending) | 6.0 $/kWh net |

# Accomplishments for FY2006

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- **Reactor modeling activity making progress.**
  - Developed reactor packing sub-module.
  - Completed microscopic modeling of reactant flow in the reactor.
  - Established macroscopic reactor model that matches the experimentally observed parameters.
- **Generated experimental data to validate modeling results.**
- **Started to use the model to predict performance parameters.**
- **Begin to build model in Star-CD.**

# Improve System Level Storage Capacity

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## Reduce Fuel Volume

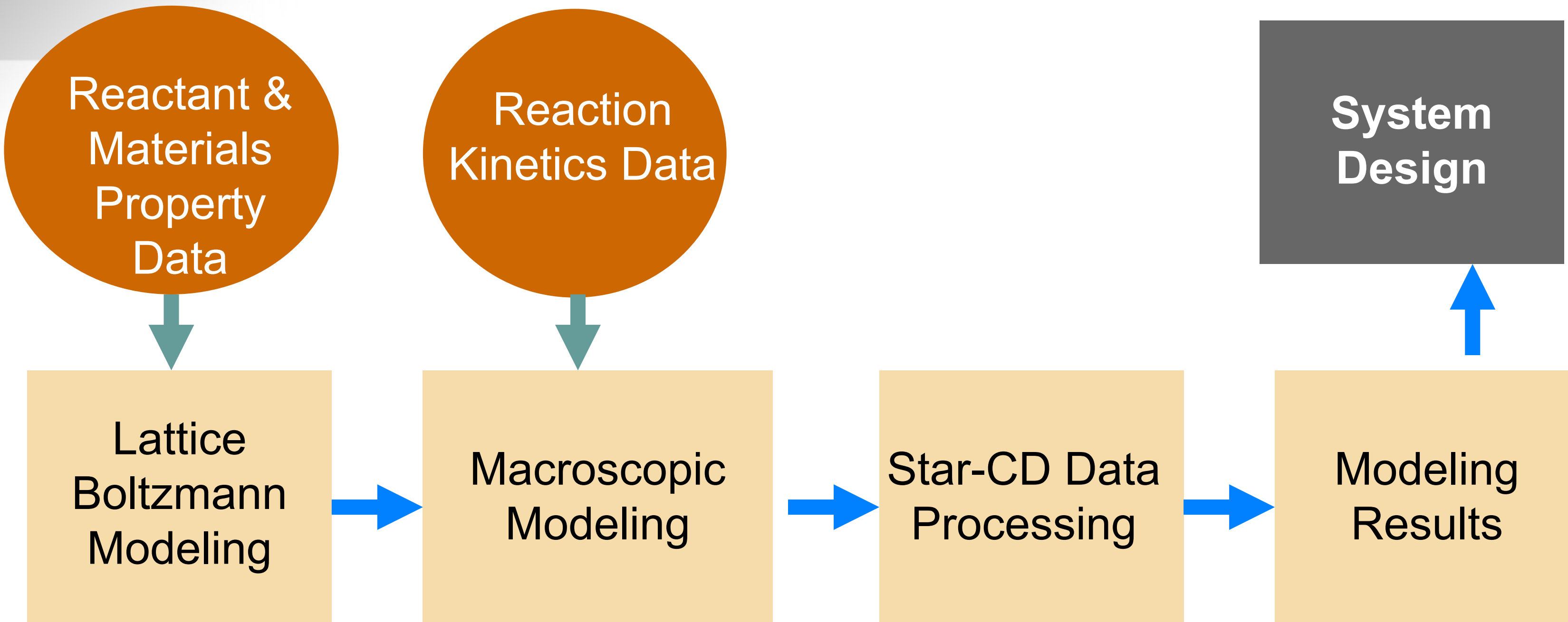
- Increased fuel concentration (30% weight/weight).
- Improved catalyst's ability to process concentrated fuel.
- Volume exchange tank design - increase volume usage.

## Reduce Volume of Balance of Plant (BOP)

- Relationship between reactor liquid hold-up and size of ballast.
- Manage heat exchange – size of exchanger.
- Improve gas-liquid separation – size of separator.

# System Development

## Modeling Approach Overview




**Develop "Tool Box" applicable to other chemical hydrogen storage systems**

- Means to handle microscopic reaction basics
- Means to handle multi-phase reactions
- Means to incorporate thermodynamic and kinetic data
- Means to apply to other chemical hydride systems

# Reactor for $H_2$ Release

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## Preliminary Modeling

- 10x100 segmentation of reactor – simplifies heterogeneous microscopic properties into multiple homogeneous sections.
- Solves the flow, energy and species transport equations for multiphase flow through a catalyst bed reactor.

- Two-dimensional (axial and radial) finite-volume formulation.
- Transient solution to reach a steady state.

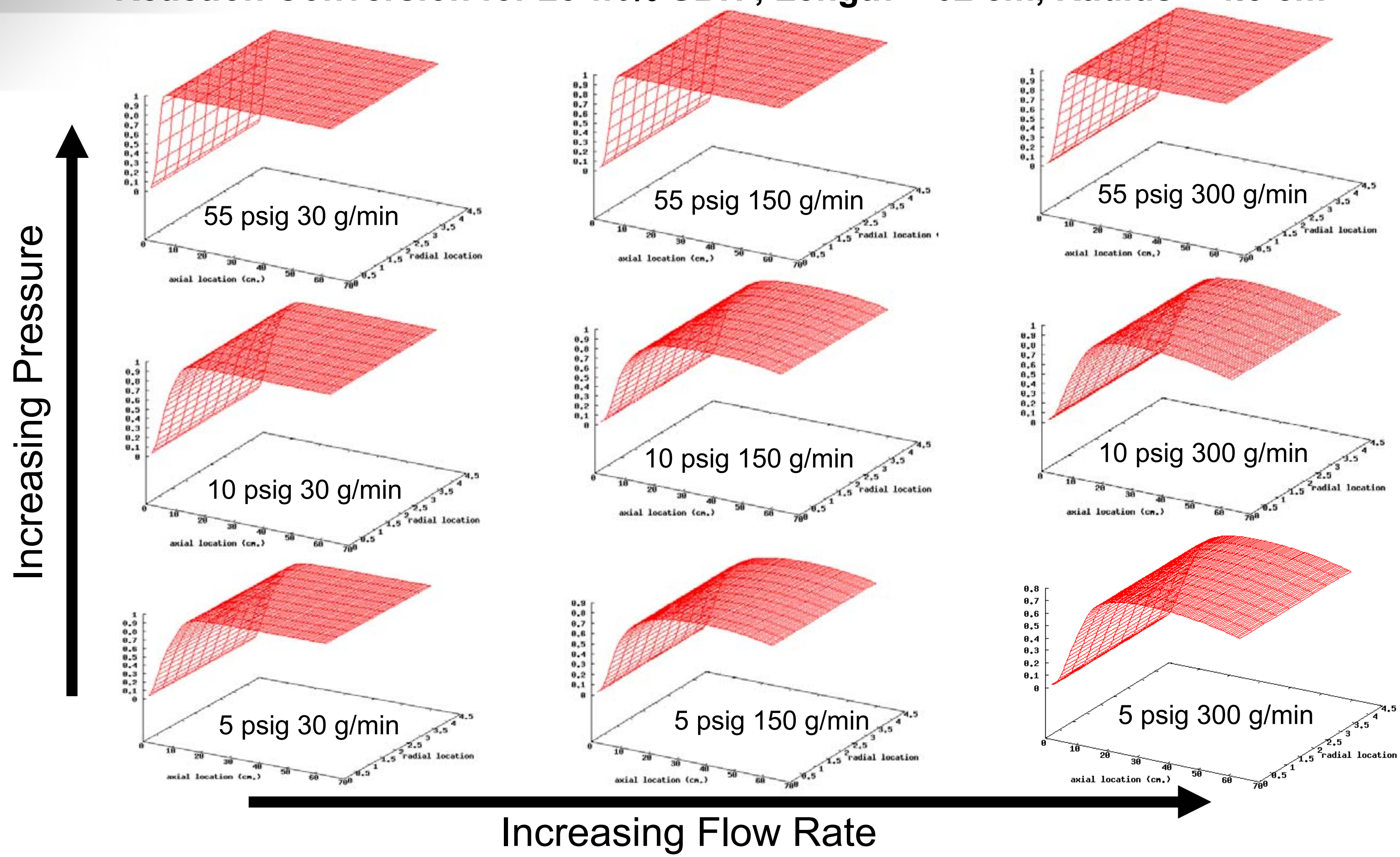
**Reactor Schematic**

# Technical Accomplishments

## Lattice-Boltzmann Modeling (PNNL)

- **Reactor model was used to predict outcome of various operation conditions**

**Reaction Conversion for 25 wt% SBH , Length = 62 cm, Radius = 4.5 cm**



# Key Findings for FY 2006

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1. **Modeling Method** has been validated as a tool to simulate and predict the experimental results.
2. **Reaction Kinetics** is critically important to establishing the validity of the model.
3. **Validation**: Steady state profiles of temperature, $NaBH_4$ concentration, pressure drop, and $H_2$ flow rate correspond to experimental data.
4. **Simulation:** Effects of fuel flow rate, fuel concentration, and system pressure were determined.
5. **Design Optimization**: reactor geometry, catalyst porosity, active control of pressure and temperature will have strong influence on the simulation results.
6. **Benefits:** Initial simulation results already generated additional insights to be used to optimize system design and operation.

# On-Board System Design (2007 version)

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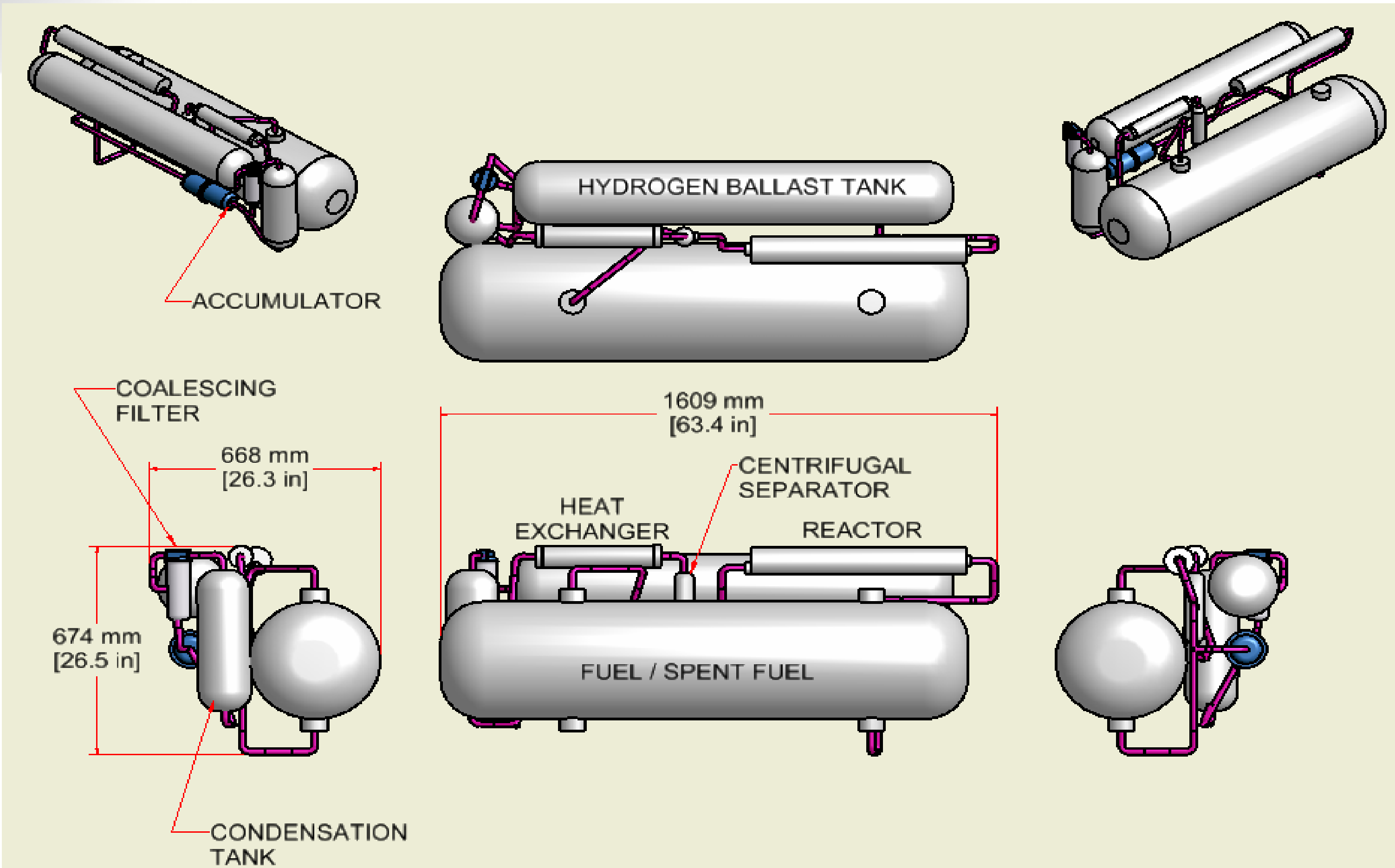
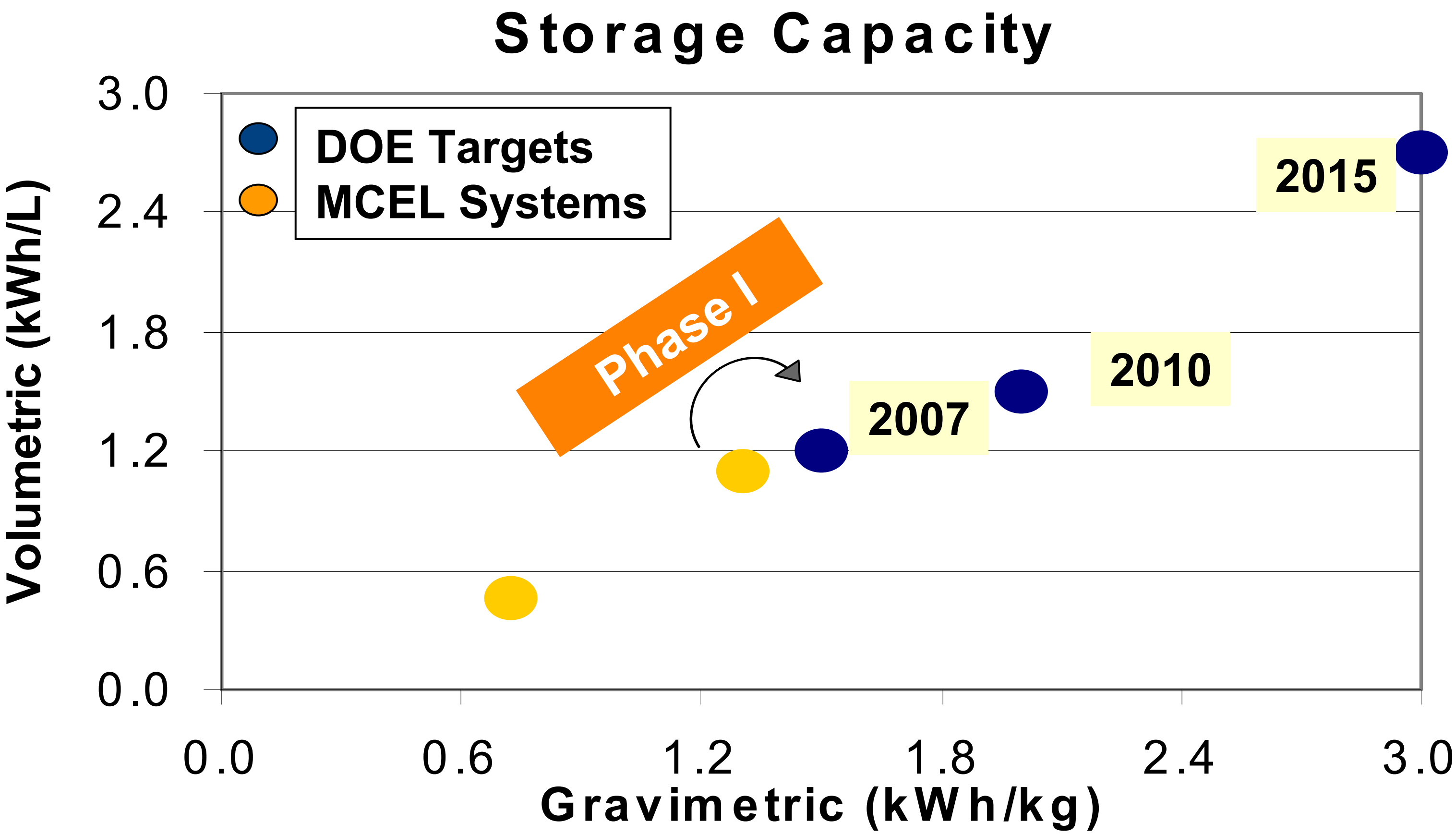



Components to be fabricated in a “mass” production method.

# Storage Capacity Progress
## Towards DOE Targets




**Note:** MCEL Gen-I & Gen-II Prototypes were developed prior to the current DOE sponsored project. Experience from those prototypes has been used as benchmark and guidance to assist this Center of Excellence Research.

# Future Work (till end of 09/2007)

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- Pending Go/No Go Decision, work from June to September 2007 will focus on:
  - Improving cost estimates,
  - Refining estimates for equipment sizing,

  and

  - Compiling a “final” report that summarizes all data and tools developed under this project.

# Summary

- Center Collaboration
  - Collaboration with PNNL has been very productive
- System Development
  - Developed tools and methods to optimize and improve on-board hydrogen generator
  - Heat and water management can be accomplished by better understanding of operating conditions
  - Borate precipitation can be managed by balancing fuel concentration and reactor pressure and temperature