# Ford/BASF Activities in Support of the Hydrogen Storage Engineering Center of Excellence

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# Overview

## Timeline

- Start – Feb 2009
- End – Jan 2014
- Percent complete – 0%

## Budget

- Total project funding
  - DOE: $2,051,250
  - Contractor: $430,725
- Funding received in FY08
  - $0
- Funding for FY09
  - $350,000 (planned)

## Barriers

- A. Weight and volume
  - 4.5 wt % and 28 g/L
- B. System cost
  - Target revision in progress
- C. Charging/discharging rates
  - 1.2 kg $H_2$/min (charging)
  - 0.02 (g/s)/KW (min full flow)

## Partners

- Project lead: Ford
- Project partner: BASF
  - Materials synthesis & evaluation
- Center partners: GM, Universite du Quebec a Trois-Rivieres, NREL, UTRC, PNNL, and SRNL

# Relevance - Project Goals

*This project will address three of the key technical obstacles associated with development of viable hydrogen storage systems for automobile applications*

1. Creation of accurate system models that account for realistic interactions between the fuel system and the vehicle power plant

2. Development of robust cost projections for various hydrogen storage system configurations

3. Assessment and optimization of the effective engineering properties of framework-based hydrogen storage media (such as metal organic frameworks, covalent organic frameworks, *etc).*

# Relevance - Project Objectives

Three tasks will be performed to address overall project goals.

**Objectives:**

- **Task 1:** Develop dynamic vehicle parameter model elements for the hydrogen storage system interfaces during realistic operating conditions.
- **Task 2:** Develop a manufacturing cost model for hydrogen fuel systems based on a supply chain assessment.
- **Task 3:** Devise and assess optimized, system-focused strategies for packing and processing of framework-based hydrogen storage media.

# Approach: Project Organization

Ford / BASF activities will contribute to several Technology Areas

**Hydrogen Storage Engineering Center of Excellence**

D. Anton, SRNL
T. Motyka, SRNL

**Materials Operating Requirements**

D. Herling, PNNL

- Materials Centers of Excellence Collaboration – SRNL, LANL, NREL
- Reactivity & Compatibility – UTRC
- Adsorption Properties – UQTR
- Metal Hydride Properties – SRNL
- Chemical Hydride Properties - LANL

Task 3

**Transport Phenomena**

B. Hardy, SRNL

- Bulk Materials Handling – PNNL
- Mass Transport – SRNL
- Thermal Transport – SRNL
- Media Structure - GM

Task 3

**Enabling Technologies**

J. Reiter, JPL

- Thermal Insulation – JPL
- Hydrogen Purity – UTRC
- Sensors – LANL
- Thermal Devices - OSU
- Pressure Vessels - PNNL

**Performance Analysis**

M. Thornton

- Vehicle Requirements– NREL
- Tank-to-Wheels Analysis – NREL
- Forecourt Requirements - UTRC
- Manufacturing & Cost Analysis - PNNL

Task 2

**Integrated Power Plant/ Storage System Modeling**

D. Mosher, UTRC

- Off-Board Rechargeable - UTRC
- On-Board Rechargeable – GM
- Power Plant – Ford

Task 1

**Subscale Prototype Construction, Testing & Evaluation**

T. Semelsberger, LANL

- Risk Assessment & Mitigation – UTRC
- System Design Concepts and Integration - LANL
- Design Optimization & Subscale Systems – LANL, SRNL, UQTR
- Fabricate Subscale Systems Components – SRNL, LANL
- Assemble & Evaluate subscale Systems – LANL, JPL, UQTR

**Technology Area**

Technology Area Lead

- Technology Team – TT Lead
- Technology Team – TT Lead
- Technology Team – TT Lead

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# Approach: Task 1 related Quad Chart

**Technology Area:** Integrated System Modeling

**Technology Team Lead:** M. Veenstra

**Technology Team:** Framework & Power Plant

**Team members:** Ford, UTRC, GM

**Date:** March 17, 2009

## Objectives:

- Develop the common aspects of the modeling framework which will be used by all partners in the integrated power plant / storage system studies.
- Construct models for the power plants, FC and ICE, which will be used in both the on-board rechargeable and off-board rechargeable system modeling.
- Establish operation conditions focused on drive cycles and examining refueling.
- Determine the modeling elements that will be supplied to the vehicle level simulations.

## Accomplishments:

- Agreed to best common platform is Matlab / Simulink

## Key Milestones:

1. Identify common modeling framework and provide partners with interaction assumptions. *(6/09, Ford/UTRC)*
2. Determine boundary conditions for the key vehicle to H2 storage system operating parameters. *(6/09, All)*
3. Construct baseline FC model. *(9/09, Ford/UTRC)*
4. Characterize the boundary operating conditions through initial profile modeling and data analysis. *(12/09, Ford/GM)*
5. Establish generic operating profiles and conduct interaction evaluation of models. *(6/10, Ford/GM)*

## Issues:

- Need to link tasks and modeling efforts between partners in order for foundational assumptions to be established.
- Need a common understanding of existing model structures.
- Identify the method and approach in handling proprietary data and modeling algorithms.
- Obtain necessary boundary data to validate the models.

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# Approach: Task 2 related Quad Chart

**Technology Area:** Performance, Cost & Energy Analysis
**Technology Team:** Manufacturing and Cost Analysis
**Date:** March 17, 2009

**Technology Team Lead**: D. Herling
**Team members:** PNNL, NREL, UTRC, Ford, GM

## Objectives:

Near Term:
- Determine figures of merit
  - Net Present Value, Internal Rates of Return
  - Potential Costs/Benefits
  - Probability component requirements
  - Determine variables for alternatives analysis
- Determine Scope of Analysis Model Requirements
- Determine which Model(s) could potentially meet objectives with least adaptation requirements.

## Accomplishments:

## Key Milestones:

1. Develop model(s) *(5/09)*
2. Obtain key data *(5/09)*
3. Link model(s) as necessary *(8/09)*
4. Obtain preliminary results *(09/09)*

## Issues:

Near Term:
- Adapt existing models for this analysis
- Need Key Data:
  - component listings
  - available cost data
  - potential manufacturers
  - manufacturing processes

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# Approach: Task 3 related Quad Chart

**Technology Area:** Materials Requirements

**Technology Team Lead:** R. Chahine

**Technology Team:** Materials Properties: Adsorbents

**Team members:** BASF, Ford, GM NREL, UQTR

March 2009 v1

## Objectives:

- Develop selection criteria and down select base adsorbent
- Develop initial base line model
- Establish materials properties database for use in modeling and system engineering by HSECoE partners
  - Perform initial screening tests (calorimetry, kinetics, composition) for storage system materials
  - Produce material characterization and generate engineering property data base
- Model H2 uptake (serves also for metering)
- Derive Heat of adsorption

## Accomplishments:

## Key Milestones:

1. Develop adsorbent selection criteria *(4/09)*
2. Indentify materials properties needed for center modeling and engineering activities *(4/09)*
3. Establish who, what, when for property characterization measurements *(4/09)*
4. Model base line adsorption *(5/09)*
5. Survey available adsorbents *(5/09)*
6. Down select candidate *(6/09)*

## Issues:

- Need to establish proper distribution of measurement tasks
- Availability of analytical resource (equipment, etc)
- Material availability for evaluation, or information to synthesize materials

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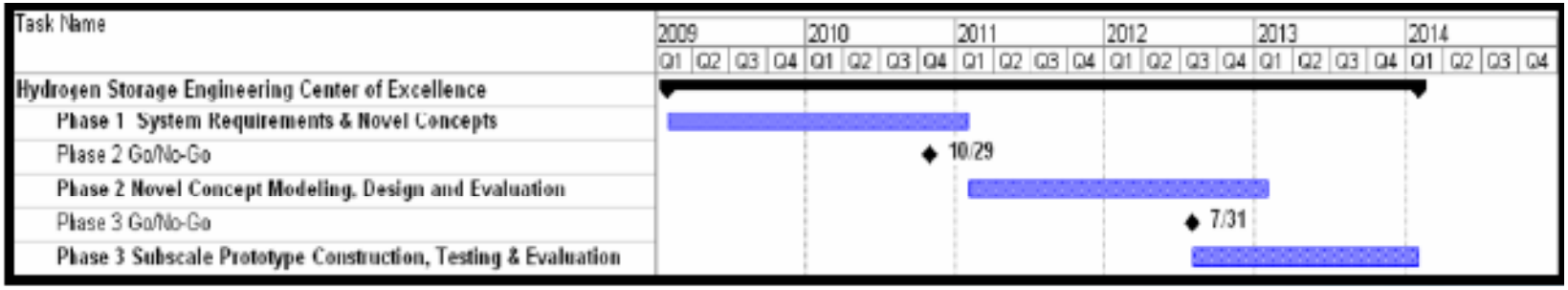
# Accomplishments & Progress

- Kick-Off meeting held Dec. 2008, Washington, D.C.
- **Project Start: Feb. 1, 2009**
- Team and Center Milestone Go/No-Go negotiated, Feb. 28, 2009
- Face to Face Meeting held Feb. 23-25, 2009, Golden, CO
- Draft Safety Plan Formulated

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# Collaborations

- **BASF** (industrial subcontractor): framework materials synthesis, processing, and characterization
- **GM** (industrial collaborator): team member for sorbent materials operating parameters, system/vehicle-level modeling, and structured materials
- **Universite du Quebec a Trois-Rivieres** (university collaborator, R. Chahine): team leader for sorbent materials
- **NREL** (federal lab collaborator): team leader for vehicle level modeling
- **UTRC** (industrial collaborator): team member for structured materials and on-board system modeling
- **PNNL** (federal lab collaborator): team lead for cost modeling
- **SRNL** (federal lab collaborator): team lead for transport phenomena

# Proposed Future Work: Task 1

## *Task 1: Dynamic Operating Parameter Model*

***Phase I:***

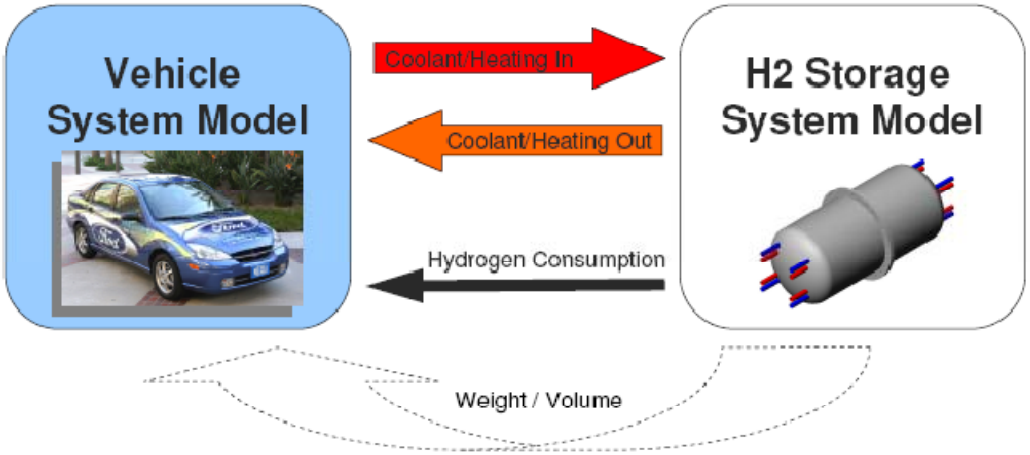
- Perform system engineering for boundary operating parameters
- Analyze experimental operating data and noise characterizations
- Establish model structure and parameter profiles

***Phase II:***

- Complete model structure and validate parameter interactions
- Expand model for design variations and trade-offs

***Phase III:***

- Translate dynamic operating parameters into test profiles
- Develop design recommendations based on operating parameters



# Proposed Future Work: Task 1

## *Task 1: Dynamic Operating Parameter Model*

Illustrative Example of a modeling interface evaluation of operating conditions

**Vehicle Available Heat Input**

$$\text{heat flow (kJ/hr)} = C_p \cdot \Delta T \cdot \text{coolant flow}$$

$C_p$ = coolant heat capacity

$\Delta T$ = allowable temperature drop in coolant

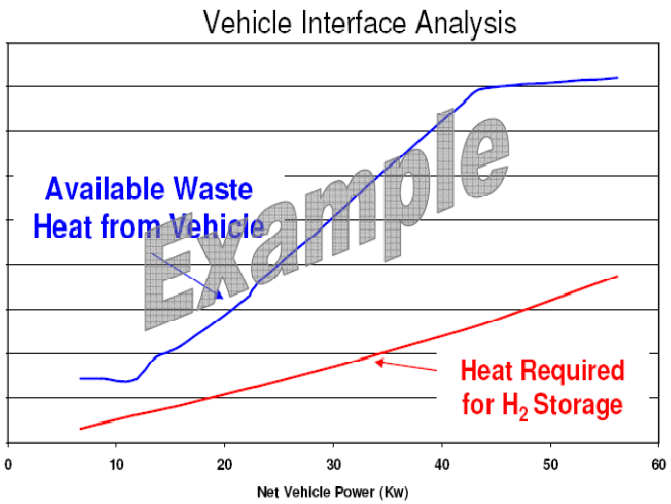
Coolant flow obtained from vehicle data

**H2 Storage System Required input**

$$\text{heat flow (kJ/hr)} = \Delta H \cdot H_2 \text{ consumption rate}$$

$\Delta H$ calculated with Van't Hoff equation

H2 consumption rate obtained from vehicle data



# Proposed Future Work: Task 1

*Task 1: Go/No-go Milestones*

**Phase 1 Go/No-Go (10/31/2010)**

- Pursue development of unified system simulation tool that couples the dynamic powerplant subsystem module with various hydrogen storage system and BoP modules. The development decision will be based on weighing the potential benefits of a unified model vs the complexity involved in constructing it.

**Phase 2 Go/No-Go (7/31/2012)**

- Based on validation against available sub-system components and potential to provide predictive data, further evolve model to enable development of design recommendations for hydrogen storage system prototypes planned for Phase 3.

# Proposed Future Work: Task 2

*Task 2: Manufacturing Cost Analysis*

***Phase I:***

- Conduct hydrogen storage system and component decomposition
- Develop predictive material usage and analysis assumptions
- Assess initial manufacturing elements for the cost model

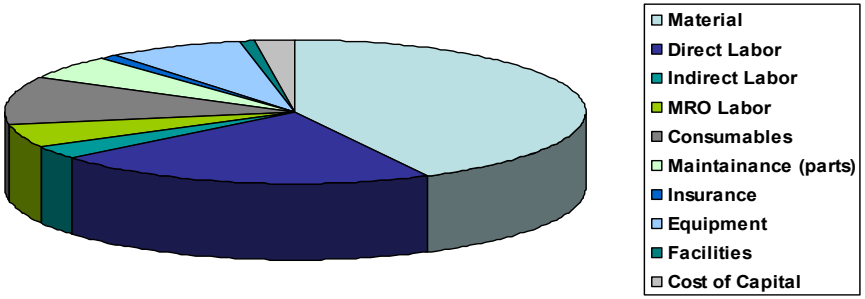
***Phase II:***

- Confirm manufacturing assumptions and validate initial results
- Conduct sensitivity and trade-off analysis of model approach

***Phase III:***

- Recommend hydrogen storage system solutions based on cost
- Evaluate potential commercialization paths for hydrogen storage

Illustrative Example

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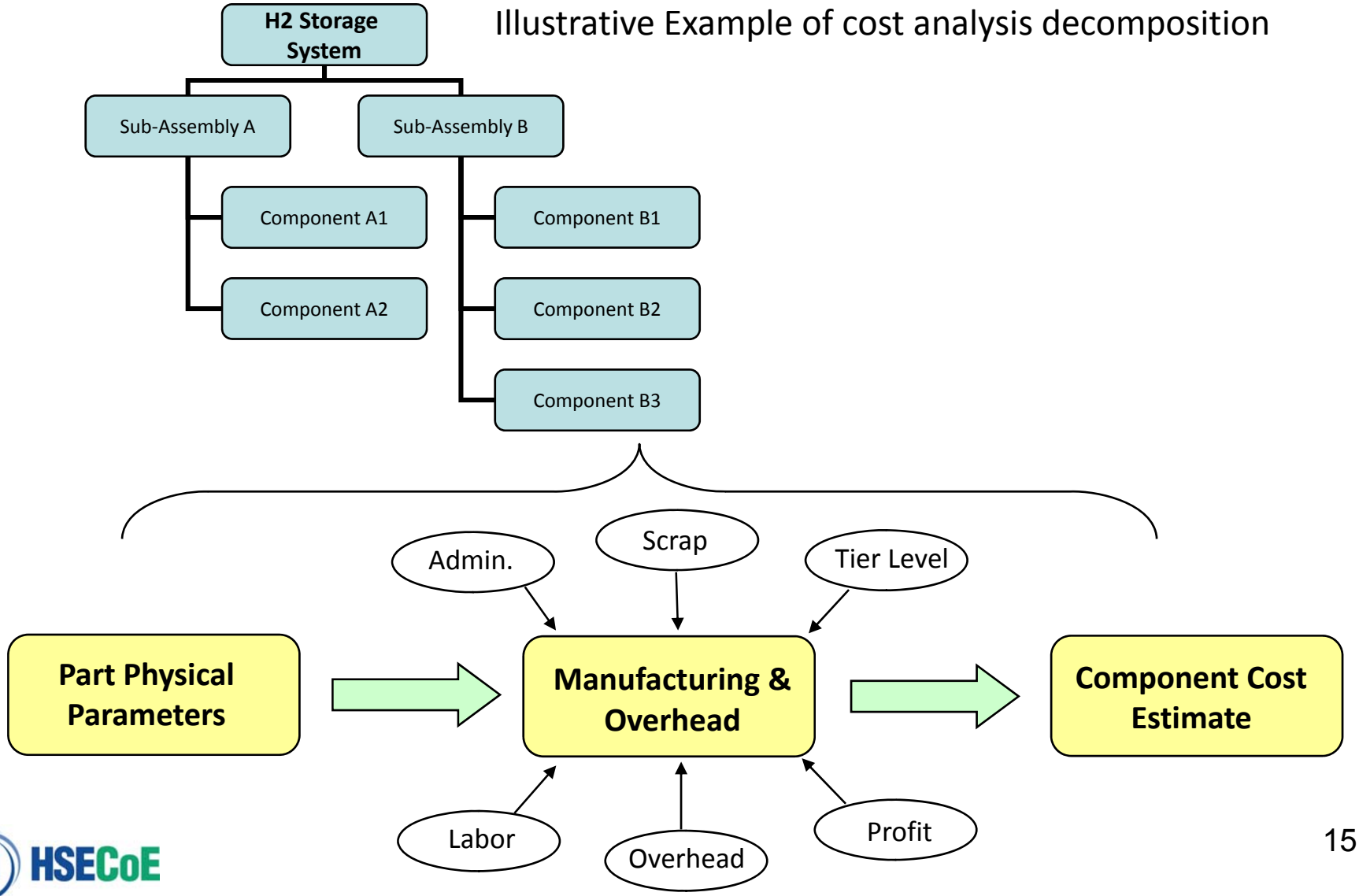
# Proposed Future Work: Task 2

## *Task 2: Manufacturing Cost Analysis*

Illustrative Example of cost analysis decomposition



# Proposed Future Work: Task 2

*Task 2 Milestones*

**Phase 1 (10/31/2010):**

- Based on the ability of the model to predict manufacturing cost of existing or previously analyzed hydrogen storage systems and/or components within an acceptable error band, pursue extending cost analysis models to new storage system concepts.

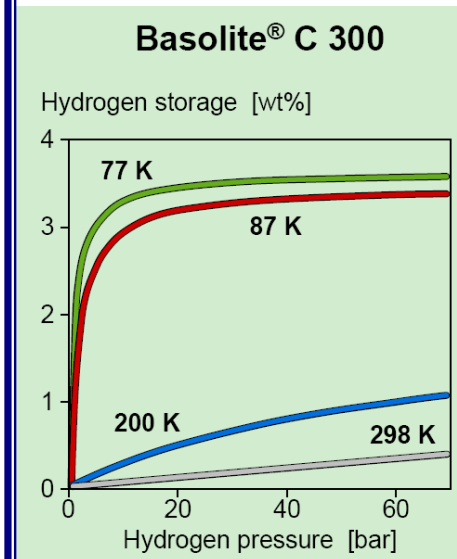
**Phase 2 (7/31/2012):**

- Based on the ability of the model to predict cost for new hydrogen storage system designs and production processes, and a demonstrated capability to perform sensitivity analyses in support of that ability, pursue extending the model to cost optimization studies in Phase 3.

# Proposed Future Work: Task 3

*Task 3: Optimized Adsorbent Media*

Example FM




***Phase I***

Establish preliminary Processing-Structure Properties (PSP) relationships for framework materials (FM)

- Literature review & down-selection of FM (coordinated w/ Sorption CoE)
- Establish baseline materials properties of select *powder FM*
  - Physical properties: thermal conductivity, powder density, stability, etc.
  - Storage properties: capacity, kinetics, $H_2$ purity, T-P excursions, etc.

Generation 1 structured media synthesis & evaluation

- Systematically explore binder agents, thermal conductivity aids, & various densification strategies (compaction, shaping)



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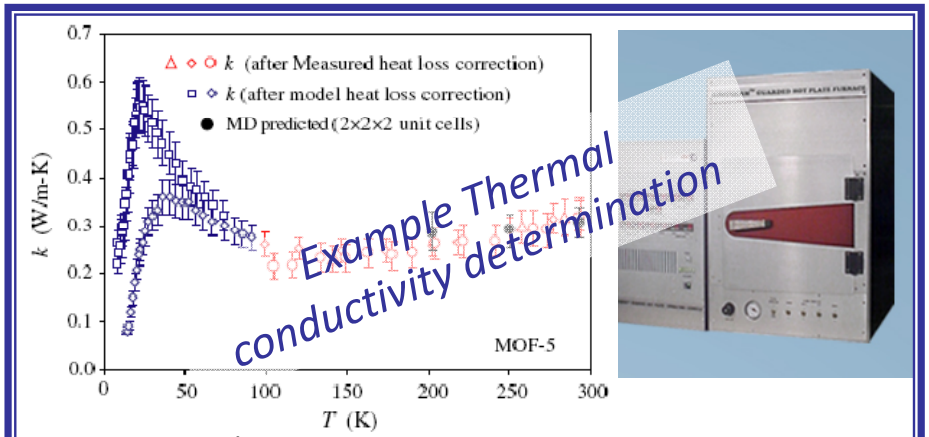
# Proposed Future Work: Task 3

*Task 3: Optimized Adsorbent Media*

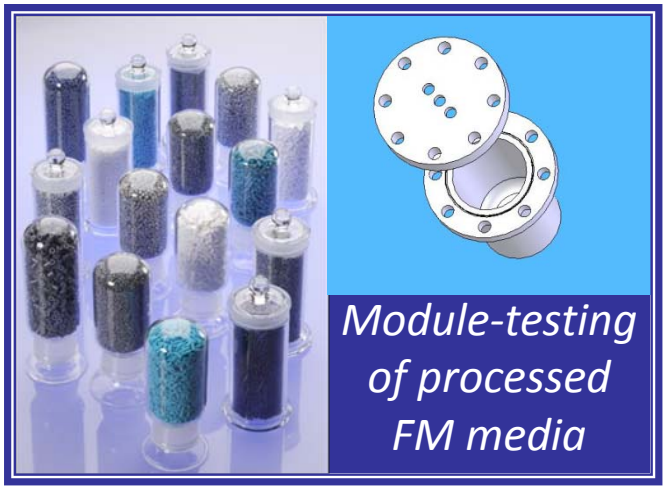
***Phase II***

Optimize packing schemes for *processed FM* and performance evaluation via instrumented testing module(s)

- Down-select promising processing approaches from Phase I (Gen. 1 media) for additional optimization (Gen. 2 media)
- Measure impact of processing routes on physical and storage properties via testing-module evaluation




B. L.. Huang *et al*, *Int. J. Heat & Mass Trans.*, **2007**, *50*, 405



# Proposed Future Work: Task 3

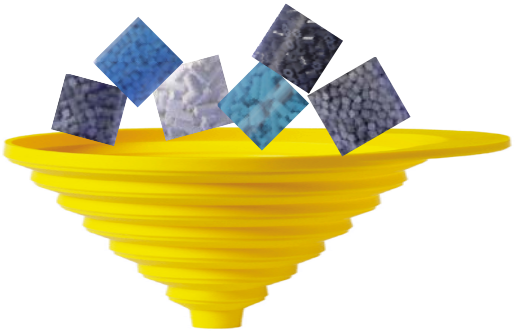
## *Task 3: Optimized Adsorbent Media*

***Phase III***

Prototype construction, testing, and evaluation

- Synthesize and pack (optimal) down-selected FM media into prototype vessel
- Conduct "vehicle simulation" evaluation of prototype properties

*Down-selection of processed FM concept*



*Sorbent Prototype*

*(*assuming 'Go' decision*)*

*Storage-system FC vehicle simulator*

# Coordination between Ford and BASF: Task 3

- Perform literature review to identify gaps in measured properties of FM; cross-check with BASF & S-CoE databases
- Conduct round-robin materials evaluation in conjunction with BASF
- Collaborate with BASF on novel concepts for media structuring
- Measure "engineering properties" of structured media and jointly devise optimal processing strategies
- Participate in Center down-selects
- Design & build instrumented evaluation module using BASF-supplied FM

- Synthesize and supply FM to Ford (phase 1-3) and other CoE partners (phase 3, as appropriate)
- Share existing materials data
- Conduct round-robin materials evaluation in conjunction with Ford
- Lend expertise in development of structured FM (shaping, binders, *etc*)
- Participate in Center down-select decisions, and in discussions with Sorption CoE.
- Provide input to Center efforts on manufacturability and cost modeling

# Proposed Future Work: Task 3

*Task 3 Milestones*

**Phase 1 (10/31/2010):**

- Based on the potential for processed (i.e., pelletized, extruded, etc) sorbent media to achieve 70% of the system-level DOE targets for capacity and kinetics on a materials-only basis, pursue optimized (Gen 2) processing schemes to further improve properties.

**Phase 2 (7/31/2012):**

- Based on the potential for Gen 2 media to achieve 100% of the system-level DOE targets for capacity and kinetics on a materials-only basis, and demonstration of sufficient thermal conductivity to enable low-cost system design, pursue Phase 3 activities focusing on loading of media into sub-scale prototype.

# Summary

As partners within the newly-launched HSECoE, Ford and BASF will contribute to three areas critical to engineering commercially-viable hydrogen storage systems

1. Creation of accurate system models that account for realistic interactions between the $H_2$ storage system and the vehicle power plant
2. Development of robust cost projections for various hydrogen storage system configurations
3. Assessment and optimization of the effective engineering properties of framework-based hydrogen storage media (such as metal organic frameworks, covalent organic frameworks, etc).