# Off-Board Considerations

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# Off-Board Considerations

Impact of target 60% fuel cycle (well-to-engine) and 90% on-board storage system (tank-to-engine) efficiencies on hydrogen storage material properties

Reference well-to-tank (WTT) efficiencies of physical hydrogen storage

- Compressed hydrogen storage: 700 bar: 54.2%; 350 bar: 56.5%
- Cryo-compressed hydrogen storage: 41.1%
- Cold gas storage: 47.4%

Hydrogen storage in metal hydrides (not discussed in this presentation)

- Relationship between tank-to-engine (TTE) efficiency and thermodynamics of on-board reversible metal hydrides

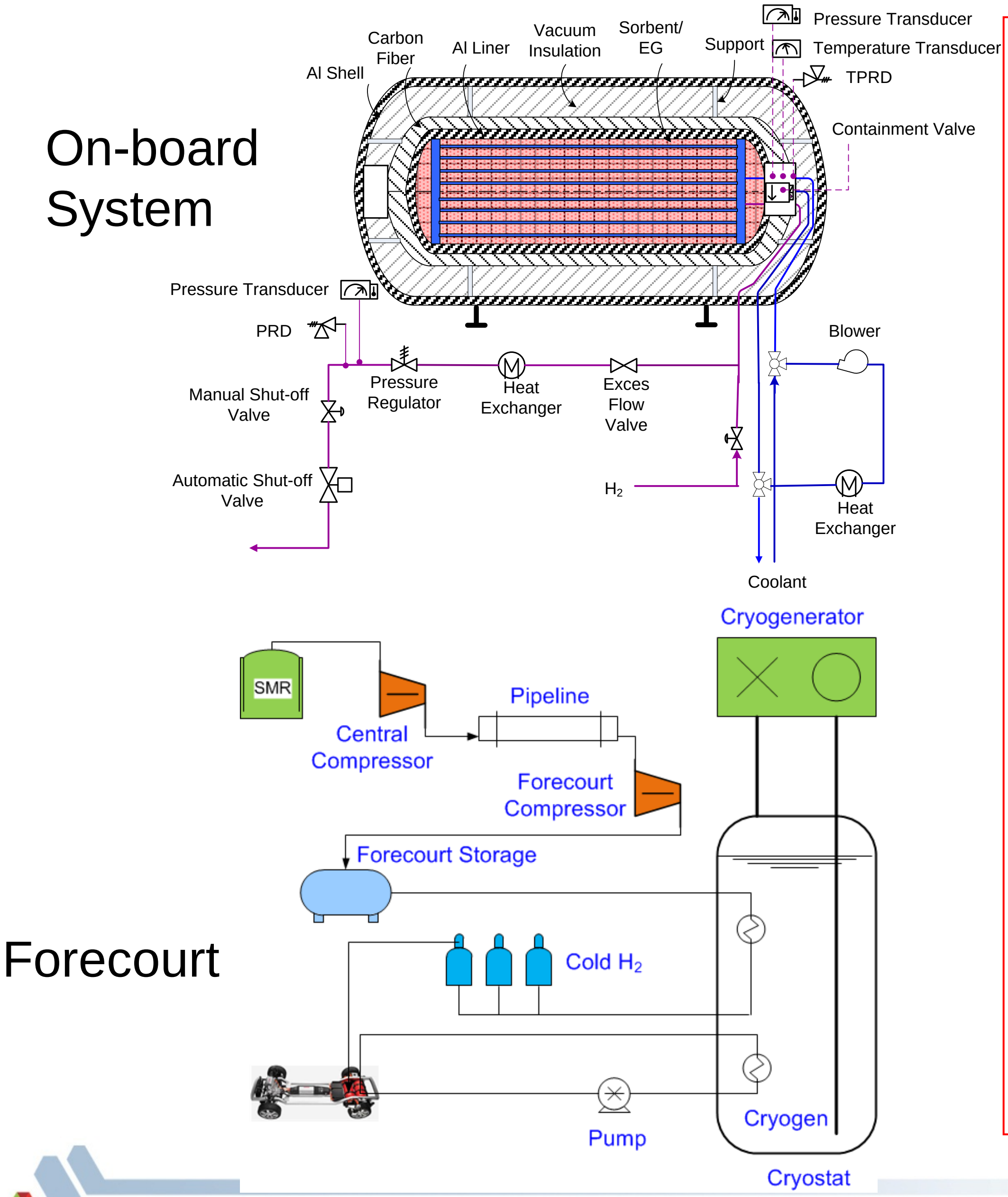
Hydrogen storage in sorbents

- Lower limit on storage temperature imposed by off-board cryogenic cooling
- Acceptable material properties to satisfy on-board and off-board storage targets

Chemical hydrogen storage

- Proposed limits on thermodynamic properties (enthalpy and free energy of decomposition) for acceptable off-board regeneration efficiency
- Acceptable material properties to satisfy on-board and off-board storage targets

# 1. On-Board Sorption Storage System and Refueling Interface



## Key System Requirements

### Storage Medium

- 5.6 kg recoverable $H_2$
- 5-bar minimum delivery P
- Structured Sorbent

### Type-3 Containment Vessel

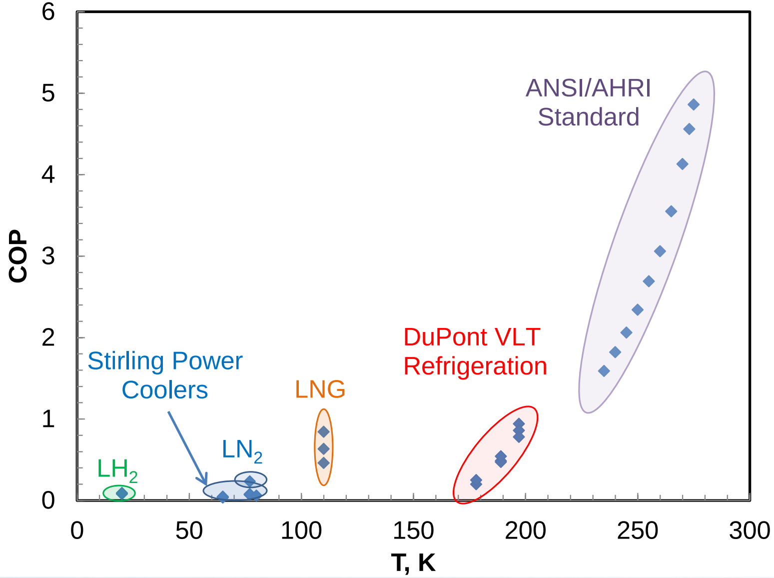
- 2.25 safety factor
- 5,500 P and T cycles
- Toray 2550 MPa CF
- Al 6061-T6 alloy liner

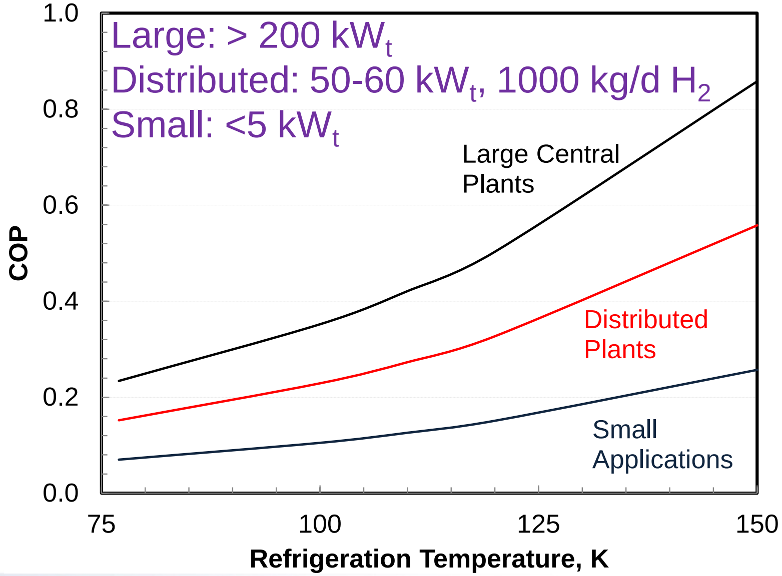
### Heat Transfer System

- 1.5 kg/min $H_2$ refueling rate
- 1.6 g/s $H_2$ min full flow rate
- MLVSI for 5 W heat in-leakage

# Coefficient of Performance (COP) of Cryogenic Systems

| Refrigeration System | T, K | Capacity, $kW_t$ | COP | Comments |
|---|---|---|---|---|
| $LH_2$ | 20 | 200 | 0.081 | Linde Ingolstadt (1992), 13.6 kWh/kg, 4.4 t/d |
|  | 20 | 225 | 0.092 | Linde Leuna (2007), 11.9 kWh/kg, 4.9 t/d |
| $LN_2$ | 65 | 0.5 - 2.5 | 0.037 - 0.046 | Stirling Power Cooler, Stirling Cryogenics |
|  | 77 | 0.8 - 7.3 | 0.070 - 0.077 | Stirling Power Cooler, Stirling Cryogenics |
|  | 77 | 24000 | 0.234 | Large air separation plant, 0.5 kWh/kg, 4860 t/d |
| LNG | 110 | 17000 | 0.46 - 0.632 | Kanfa Aragon $N_2$ expander cycle, 0.4-0.55 kWh/kg, 3000 t/d |
|  | 110 | 17000 | 0.843 | Aragon Dual Cascade mixed refrigerant, 0.3 kWh/kg, 3000 t/d |
| VLT: R-503 | 178 - 197 | 0.2 - 1.9 | 0.2 - 0.94 | VLT refrigeration, DuPont, ozone depleter, higher capacity than R-13 |
| VLT: R-13 | 178 - 197 | 0.1 - 1.2 | 0.25 - 0.78 | DuPont, ozone depleter, to be phased out |
| VLT: HFC-23 | 189 - 197 | 0.1 - 1.6 | 0.86 | Freon 23, CFC free, 10% higher energy consumption than R-503 |
| Commercial Refrigerated Storage | 230 - 245 | 5 | 1.59 - 2.06 | ANSI / AHRI standard refrigerated storage contaniners, cabinets |
|  | 250 - 260 | 5 | 2.34 - 3.06 | ANSI/AHRI Standard 1210 |
|  | 265 - 275 | 5 | 3.55 - 4.86 | Ratings approved by ANSI in Jan 2011 |

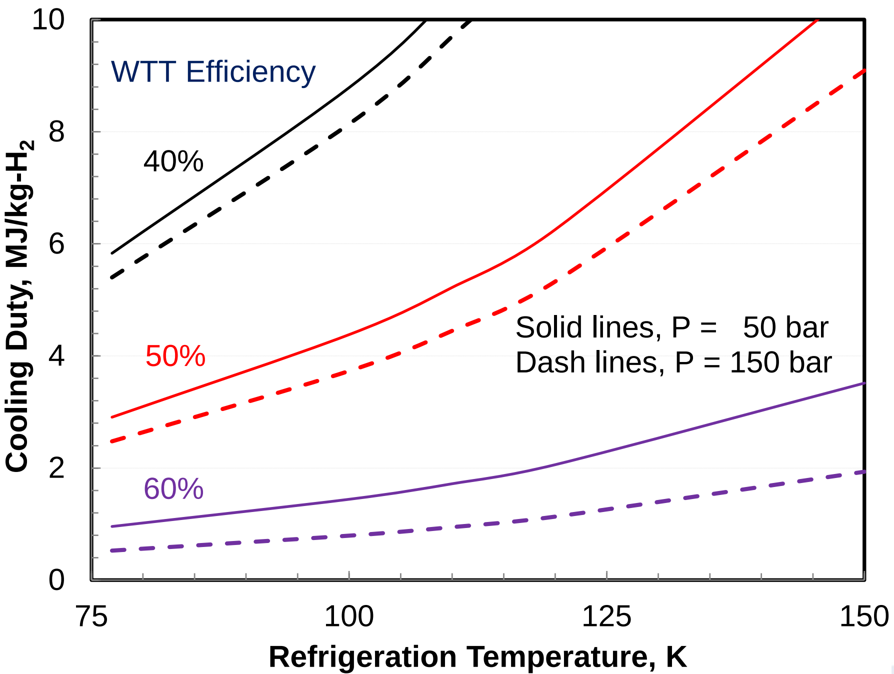




COP (ratio of heat removed to input electrical energy) is a function of refrigeration T and plant size

# Well-to-Tank Efficiency

| Process | Assumptions | Source |
|---|---|---|
| $H_2$ Production at 20 bar | SMR at central plant, 73% efficiency | H2A |
| $H_2$ compression at central plant | Compressor efficiency 88% | FCHtool |
| $H_2$ delivery to forecourt | Pipeline, 50 bar pressure drop | HDSAM |
| $H_2$ compression at forecourt | Compressor efficiency 65% | FCHtool |
| Cooling at forecourt | COP a function of temperature | Various |
| Electricity generation | 35% efficiency | U.S. grid 2015 |
|  | 8% transmission loss | GREET |



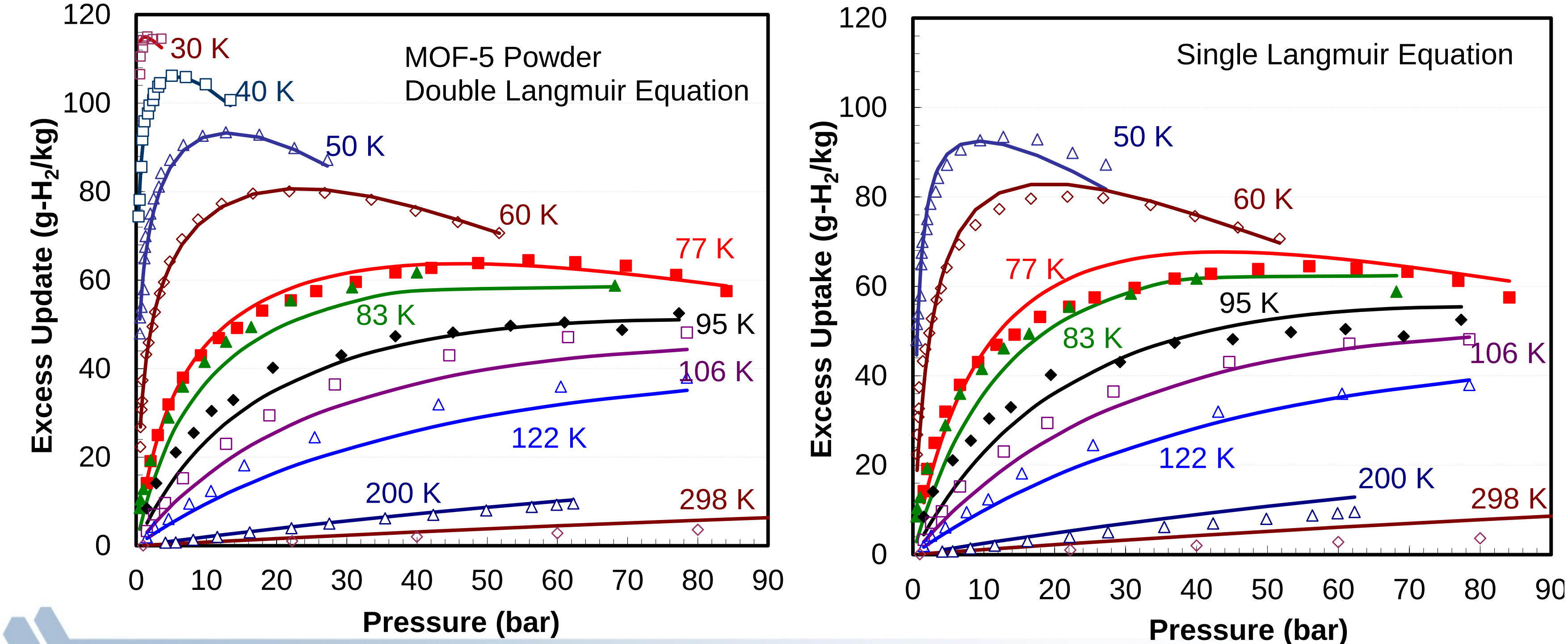
Allowable cooling duty ($Q_c$) determined by coolant temperature ($T_c$) and target WTT efficiency ($\eta_{WTT}$)

- At 77 K, >4-fold reduction in $Q_c$ if $\eta_{WTT}$ raised from 40% to 60%
- For 50% $\eta_{WTT}$, >3-fold increase in $Q_c$ if $T_c$ raised from 77 K to 150 K

# Adsorption Isotherms

Generalized-Langmuir High-Pressure Adsorption Model (Stadie, 2013)

- Available data for $H_2$ adsorption on MOF-5 powder at 60-300 K (W. Zhou, J. Phys. Chem. C 2007, 111, 16131-16137) can be correlated with double-Langmuir equation (two types of invariant adsorption sites of different characteristic energies) with 7 parameters
- Single-Langmuir equation chosen for reverse engineering as it has only 4 parameters and can adequately represent adsorption data: 3 of the 4 parameters can be related to physical material properties

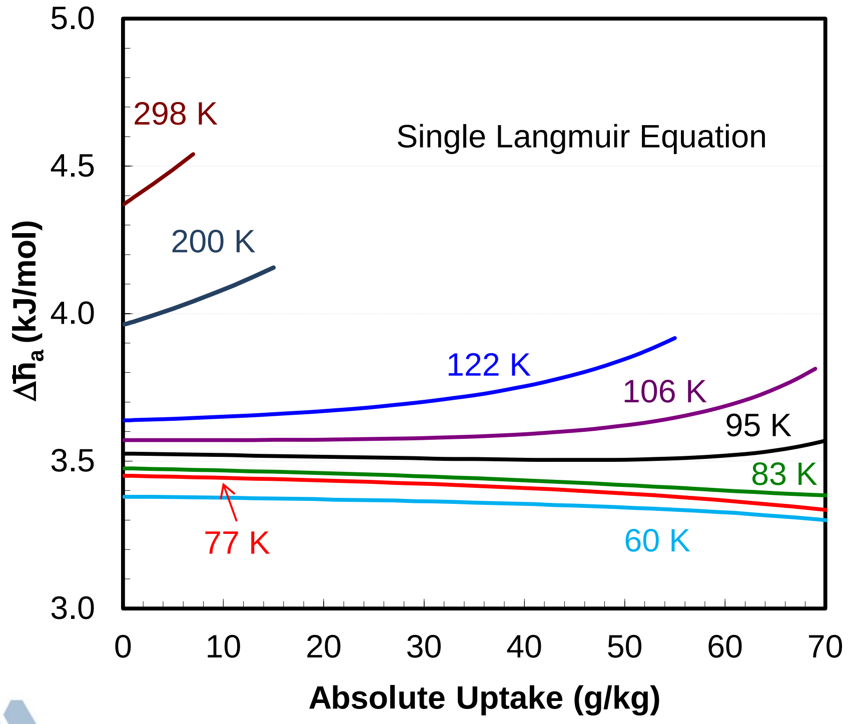


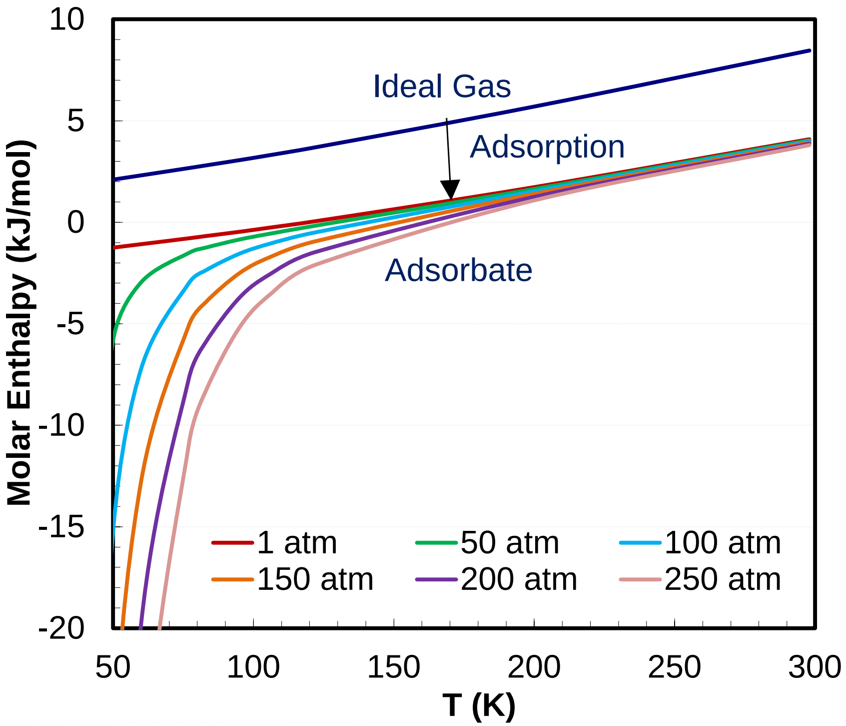
N Stadie, Synthesis and Thermodynamic Properties of Physisorptive Energy Storage Materials, PhD Thesis, Caltech, 2013

# Thermodynamics of Adsorption

Material targets related to single-Langmuir equation for $H_2$ adsorption

- $N_m$: Sorption capacity (g-$H_2$/kg-sorbent), measure of active sites
- $\Delta H^0$: Enthalpy change on adsorption, 3.1 kJ/mol for MOF-5, related to isosteric heat of adsorption
- $\Delta S^o$: Entropy change, 66.5 J/mol/K, varies slightly with temperature
- $V_a$: Adsorption volume, 0.012 $m^3$/kg, a fitted parameter

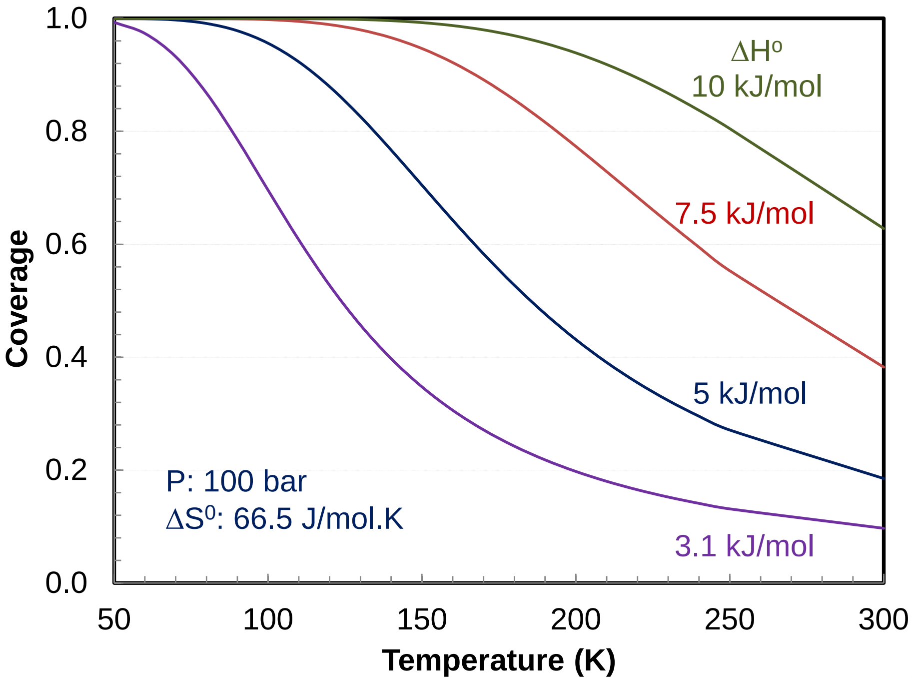


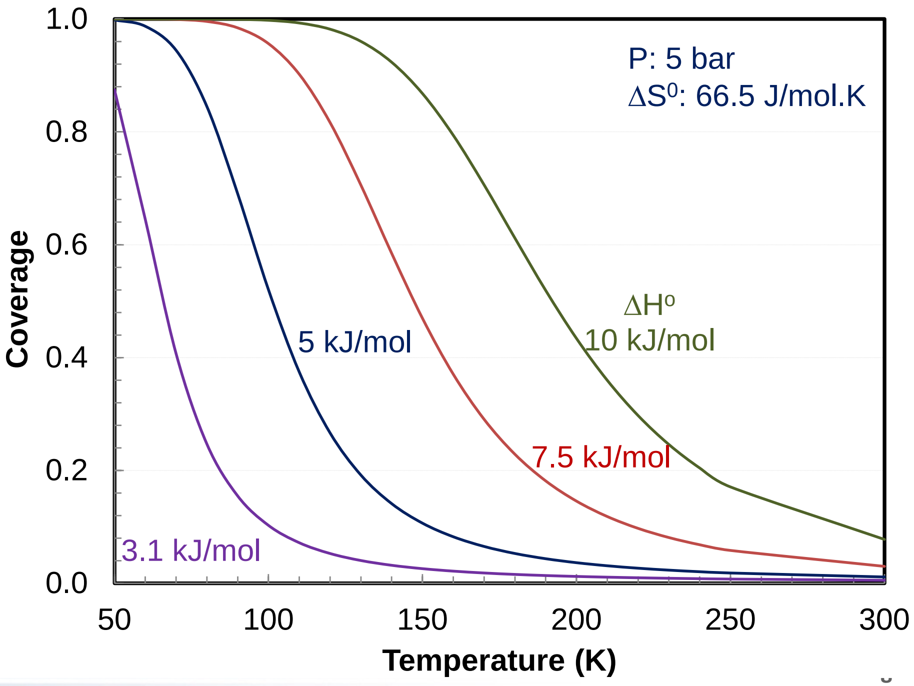


# Advanced Sorbents

Advanced micro-porous adorbents with high specific area (sites) and $\Delta H^o$ > 5 kJ/mol as well as low storage temperatures with sufficient temperature swings are needed.

- Storage temperature depends on $\Delta H^0$. Temperature below 150 K not needed if $\Delta H^0$ > 7.5 kJ/mol.
- Pressure swing alone may not be sufficient for >90% usable $H_2$. Materials with $\Delta H^0$ > 7.5 kJ/mol will require temperature swing.





# Study Parameters

Objective is to determine the peak excess adsorption at the reference $LN_2$ temperature and the bulk density needed to meet the system weight and volume targets at the storage temperature ($T_s$) with constraints on WTT efficiency, refueling time, and minimum full flow rate of $H_2$.

| | | Units | Reference Values | Range of Values | Comments |
|---|---|---|---|---|---|
| Sorbent | Excess Uptake at 77 K | g-$H_2$/kg | 100 | 100-250 | NU-100, ST023 |
| | Enthalpy Change on Adsorption | kJ/mol | 5.0 | 2.5 - 10 | MOF-5, 3.1 kJ/mol, SLI |
| | Adsorption Volume | $m^3$/kg | 0.012 | TBD | MOF-5 |
| | Entropy Change on Adsorption | J/mol/K | 66.5 | TBD | MOF-5, SLI |
| | Bulk Density of Compact | kg/$m^3$ | TBD | 310 - 610 | IJHE 37 (2012) 2723-2727 |
| | Permeability | $m^2$ | TBD | TBD | IJHE 38 (2013) 3268-3274 |
| Operating Temperatures | Off-board Coolant Temperature | K | 77 | 77 - 200 | LN2 - ANSI/ASHRI |
| | Storage Temperature | K | TBD | TBD | |
| | Temperature Swing | K | TBD | TBD | |
| Operating Pressures | Storage Pressure | bar | 100 | 50 - 200 | |
| | Minimum Delivery Pressure | bar | 5 | | DOE target |
| $H_2$ Flow Rates | Refueling Rate | kg/min | 1.5 | | DOE target |
| | Minimum Full Flow Rate | g/s | 1.6 | | DOE target |
| Heat Transfer | ENG/Sorbent Mass Ratio | | 0.2 | 0.1 - 0.3 | |
| | Number of HX Tubes | | TBD | TBD | |

# Reference Sorbent Targets

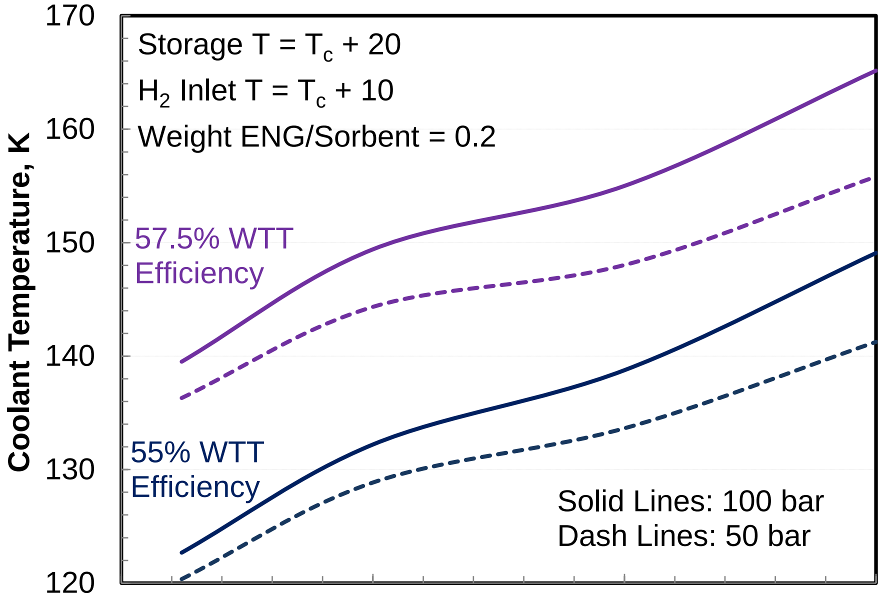
| | Symbols | Levels[4] | Material Targets | Related System Targets | Comments |
|---|---|---|---|---|---|
| **Operating Pressures and Temperatures** | | | | | |
| Storage Pressure | $P_s$ | 1 | 100 bar | | |
| Storage Temperature | $T_s$ | 1 | 155 K | | 20 K above coolant temperature |
| Discharge Pressure | $P_d$ | 1 | 5 bar | 5 bar minimum delivery pressure | In addition to pressure swing, 60-K $\Delta T_s$ allowed for 95% usable $H_2$. |
| Temperature Swing | $\Delta T_s$ | 1 | 60 K | | |
| Off-board Coolant Temperature | $T_c$ | 1 | 135 K | 60% WTT efficiency | COP of distributed cryogenic system depends on $T_c$: 0.45 for $T_c$ = 135 K. |
| **Material Properties[1,2,3,4]** | | | | | |
| Excess Uptake at 77 K | $N_{ex}$(77 K) | 1 | 190 g-$H_2$/kg-sorbent | 5.5 wt% gravimetric capacity | NU-100 showed 100 g-$H_2$/kg-sorbent excess uptake at 77 K |
| Excess Uptake at Storage Pressure and Temperature | $N_{ex}(P_s,T_s)$ | 1 | 120 g-$H_2$/kg-sorbent | | Excess uptake (and kinetics) targets to be met by sorbent mixed in with conductivity enhancement additives and compacted to target bulk density |
| Enthalpy Change on Adsorption | $DH^o$ | 1 | 5-7.5 kJ/mol | | 55% WTT for $\Delta H_o$ = 5 kJ/mol and $T_c$ = 135 K; $\Delta H_o$ = 7.5 kJ/mol needed for 60% WTT efficiency. |
| Usable $H_2$ | | 2 | 95% | | Percent of $H_2$ released with pressure swing from $P_s$ to $P_d$ and temperature swing from $T_s$ to $T_d = T_s + \Delta T_s$ |
| Sorbent Bulk Density | | 1 | 420 kg/$m^3$ | 40 g/L volumetric capacity | Sorption targets are for compacts, not powders |
| Bed Thermal Conductivity | | 1 | 1 W/m.K | 1.5 kg/min refueling rate | High conductivity additives, <20% by weight of sorbent, may be used. |
| Bed Permeability | | 2 | TBD | | |
| Charge Kinetics | | 3 | 30 g-$H_2$/kg-sorbent/min | 1.5 kg/min refueling rate | Refueling from $N_{ex}(P_d,T_d)$ to $N_{ex}(P_s,T_s)$ at 100 bar and 155 K; $T_d$ = 215 K. |
| Discharge Kinetics | | 3 | 2.3 g-$H_2$/kg-sorbent/min | 1.6 g/s minimum full flow rate | Desorption kinetics and minimum usable $N_{ex}$ to be measured at 5 bar and 215 K. |

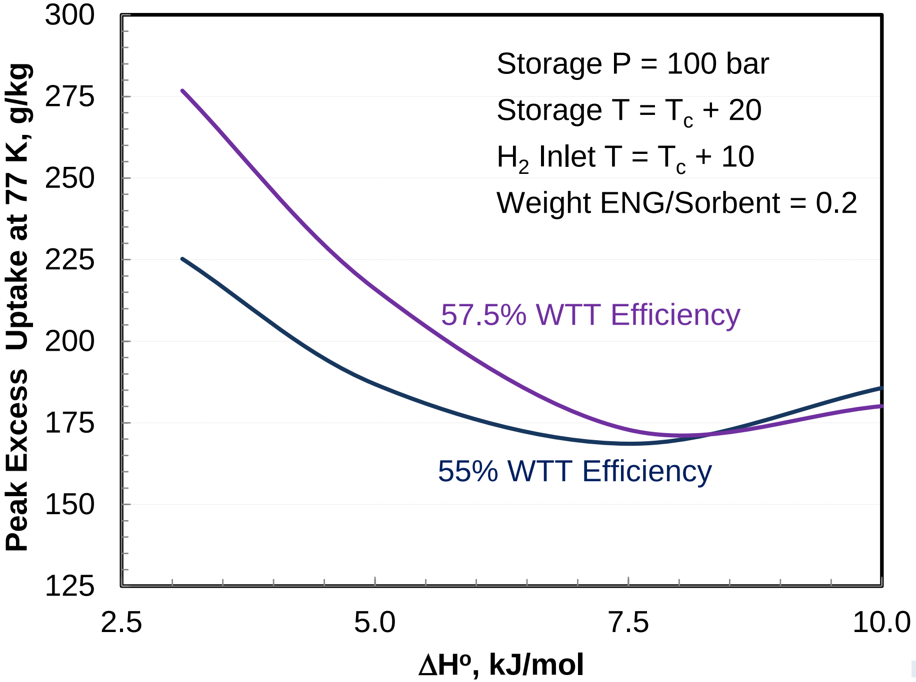
1. The sorbents must satisfy additional requirements for cycle life, purity of hydrogen desorbed, toxicity and safety, as specified in storage system targets.
2. The sorbent must also be tolerant to impurities in fuel hydrogen feed. See the related SAE and ISO specifications for fuel cell quality hydrogen.
3. Allwable cost of sorbents to be determined.
4. Level 1 targets refer to primary requirements. Level 2 targets are also important but may be related to other requirements. Level 3 targets may be less important for sorbents.

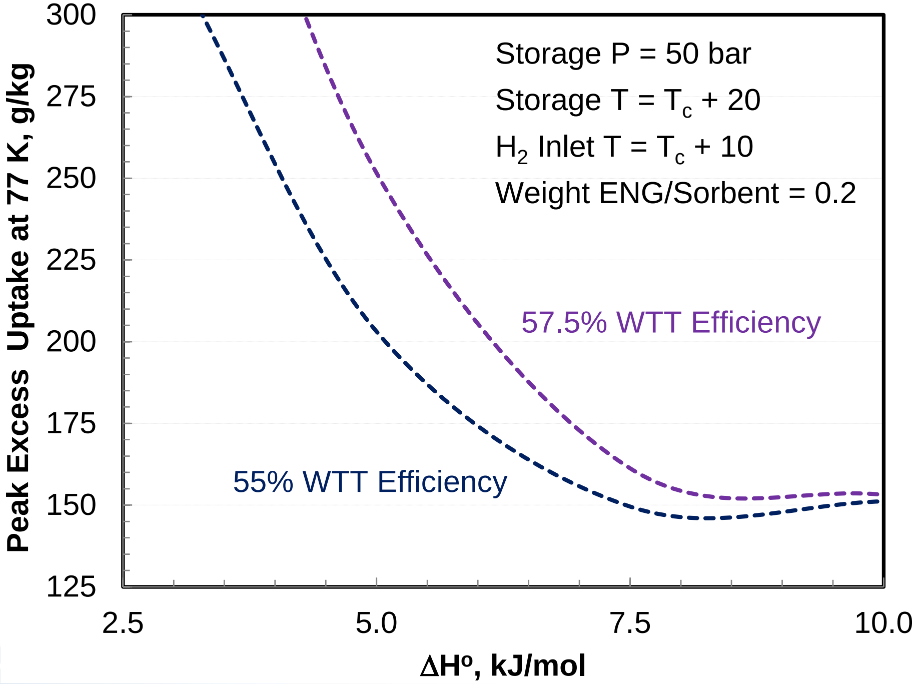
# Sensitivity Study – ΔHº

Adsorbents with ΔHº >7.5 kJ/mol are especially appealing.

- Storage temperatures below 150 K not needed, actually counterproductive
- Advantageous to reduce the storage pressure to 50 bar

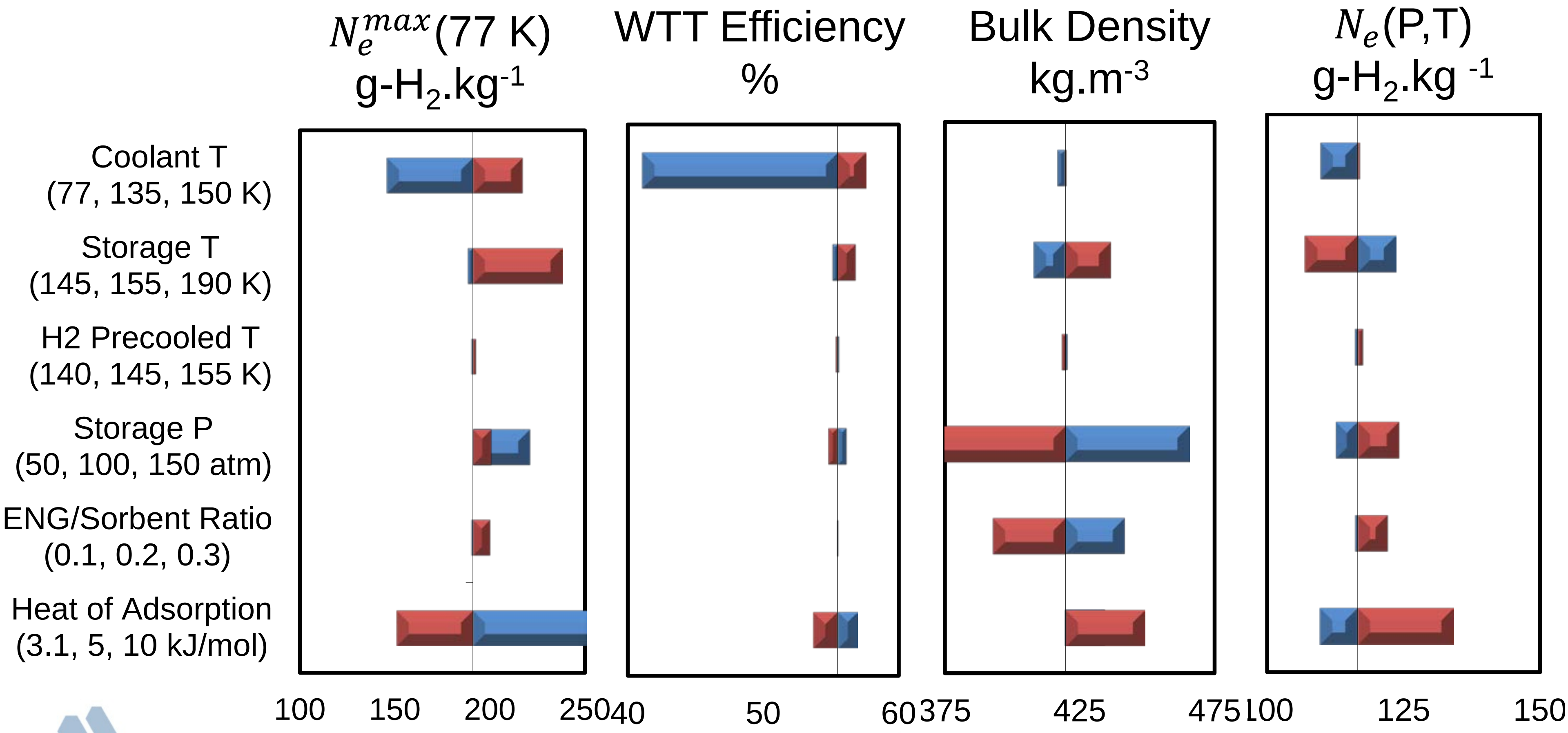






# Summary

The promising sorbent should have >120 g-$H_2$ /kg excess sorption capacity at 150 K or higher temperature and 100 bar pressure, when compacted to 420 kg/$m^3$ bulk density and mixed with 10-20% expanded natural graphite (or other conductivity enhancement materials)



# 2. Chemical Hydrogen Storage Materials

Class of storage materials that release hydrogen through a non-equilibrium process and, therefore, cannot be regenerated by reacting the dehydrogenated product with $H_2$ gas.

- Require off-board regeneration using electrochemical or catalytic processes

1. Negative free energy of decomposition

- Thermodynamically unstable at room temperature and are stabilized by extremely slow kinetics (alane, ammonia borane) or by other chemical means (addition of 3% NaOH to aqueous $NaBH_4$)

2. Positive free energy of decomposition

- Stable at room temperature but can be decomposed at elevated temperatures
- Require a catalyst for adequate kinetics at low temperatures
- APCI patent identifies many cyclic hydrocarbons including perhydrogenated n-ethyl carbazole
- On-board storage system efficiencies may be low since $\Delta H > T\Delta S$, i.e., $\Delta H > 38.8$ kJ/mol for $\Delta S = 130.2$ J/mol.K
- High off-board efficiencies may be possible since the regeneration reaction is exothermic

# Off-Board Regeneration of Chemical Hydrogen Storage Materials

Well-to-tank efficiency ($\eta_{WTT}$)*

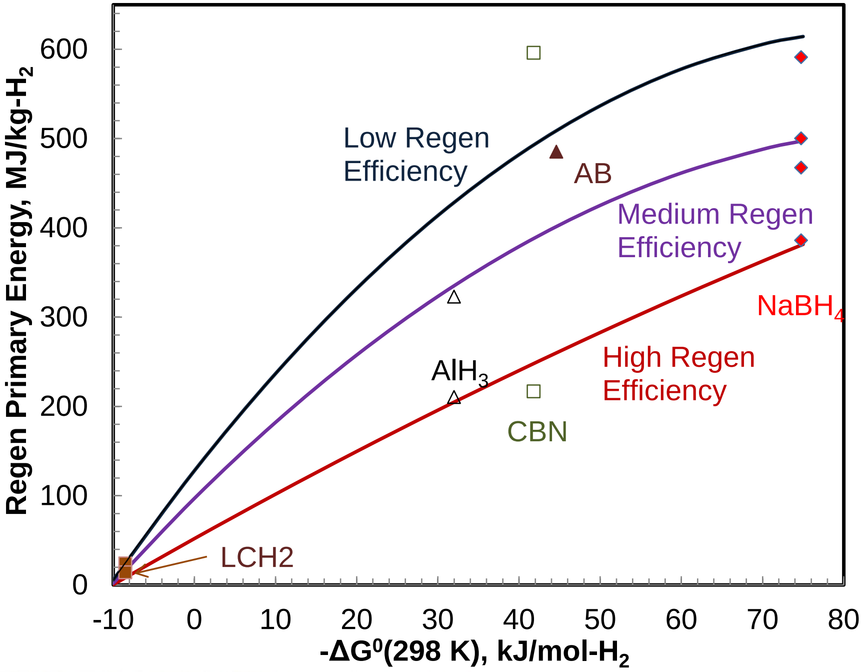
- Ratio of LHV of $H_2$ produced to the primary energy ($Q^f$) consumed in producing (subscript *p*), delivering (subscript *d*) and storing (subscript *s*) $H_2$

$$\eta_{WTT} = \frac{\Delta H_{LHV}}{Q_p^f + Q_d^f + Q_s^f} \qquad Q_r^f = Q_d^f + Q_s^f$$

$\Delta$G determines the off-board regeneration efficiency. Materials with large negative $\Delta$G require elaborate regeneration processes with high demands for primary energy.

- WTT efficiency: 16-21% for $NaBH_4$ (-75 kJ/mol), 8-18% for AB (-45 kJ/mol), 24-31% for $AlH_3$ (-32 kJ/mol), 60-63.2% for n-ethyl carbazole

| | $\Delta G^0$ (298 K) kJ/mol-$H_2$ | $\Delta H^0$ (298 K) kJ/mol-$H_2$ | $\Delta S^0$ (298 K) J/mol.K | Regen Primary Energy MJ/kg-$H_2$ | WTT Efficiency % | Comments |
|---|---|---|---|---|---|---|
| $NaBH_4$ | -74.75 | -57.75 | 57 | 386 | 21.3 | AnH-AqH |
| | Hydrolysis Reaction | | | 467 | 18.6 | AqH-AqH |
| | | | | 500 | 17.7 | An-Aq |
| | | | | 591 | 15.6 | Aq-Aq |
| $AlH_3$ | -32 | 6.6 | 131 | 323 | 24.0 | TMAA no waste heat |
| | Thermolysis Reaction | | | 210 | 31.0 | 50% waste heat |
| AB | -44.6 | -33 | 39 | 485 | 18.1 | Benzophenone |
| | Thermolysis Reaction | | | 1319 | 8.0 | Bayer |
| | | | | 789 | 12.4 | PCUK |
| CBN | -41.8 | -18.97 | 77 | 596 | 15.5 | MeOH/$NaAlH_4$ |
| | Thermolysis Reaction | | | 217 | 30.5 | Formic acid |
| LCH2 | 8.5 | 47.3-53.6 | 130.2 | 24 | 60.0 | Trickle bed reactor |
| | Perhydro N-ethyl Carbazole | | | 14 | 63.2 | Electricity production |



*RK Ahluwalia, TQ Hua and J-K Peng, "Fuel Cycle Efficiencies of Different Automotive On-Board Hydrogen Storage Options," IJHE 32 (2007) 3592-3602

# WTT Efficiency Correlation

Analyzed a $H_2$ production, delivery and regeneration fuel cycle for NA NG and US electric grid: 68% SMR efficiency without credit for steam co-production, 77% with steam export.

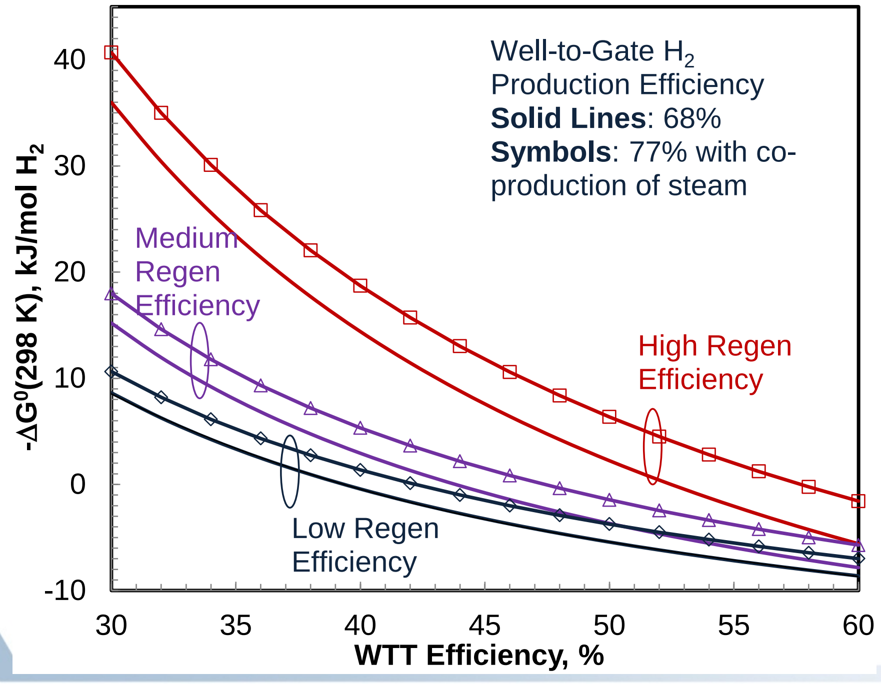
- WTT correlations for high, medium and low regeneration efficiencies

Materials with positive free energy of decomposition

- May meet the 60% WTT efficiency target if $\Delta G^0$(298 K) > 1.6 kJ/mol.

Materials with negative free energy of decomposition

- Even with steam export, 60% WTT efficiency not possible
- With steam export, minimum $\Delta G^0$(298 K) limited to -1.5 kJ/mol for 55% WTT efficiency and -6.4 kJ/mol for 50% WTT efficiency



Definitions of Free Energy and Enthalpy of Decomposition

$AH_m = AH_n + (m-n)/2\ H_2$

$$\Delta G = \left(\frac{2}{m-n}\right)[\Delta G_f(AH_n) - \Delta G_f(AH_m)]$$

$NaBH_4 + 2\ H_2O = NaBO_2 + 4\ H_2$

$$\Delta G = 1/4[\Delta G_f(NaBO_2) - \Delta G_f(NaBH_4) - 2\Delta G_f(H_2O)]$$

***60% efficiency target is for well-to-engine (WTE) efficiency, not WTT efficiency**

# Bounding Thermodynamic and Kinetic Properties

Desired thermodynamic properties of materials for which the WTT efficiencies may be between 50 to 60%

- Over the narrow range of desired $\Delta G^0$(298 K), exothermic materials are unsuitable if $\Delta S$ is between the expected range 80 – 130 J/mol.K
- Materials that decompose above the FCS coolant temperature and require a burner may not be acceptable since the on-board system efficiency is quite low for $\Delta H$ between 20 and 40 kJ/mol-$H_2$

Desired kinetic properties of materials that decompose at 60 – 80$^o$C

- Likely a catalytic process, otherwise the material would have short shelf life and may not meet the 0.05 g-$H_2$/h/kg stability target at room temperature
- Non-equilibrium decomposition kinetics that is independent of back pressure, otherwise the buffer tank would need to be refueled with gaseous $H_2$

| | | **$\Delta S$ = 130 J/mol.K** | | | **$\Delta S$ = 105 J/mol.K** | | | **$\Delta S$ = 80 J/mol.K** | | |
|---|---|---|---|---|---|---|---|---|---|---|
| WTT Efficiency | | 60% | 55% | 50% | 60% | 55% | 50% | 60% | 55% | 50% |
| $\Delta G^0$(298 K) | kJ/mol | 1.6 | -1.5 | -6.4 | 1.6 | -1.5 | -6.4 | 1.6 | -1.5 | -6.4 |
| $\Delta H$ | kJ/mol | 40.3 | 37.2 | 32.3 | 32.9 | 29.8 | 24.9 | 25.4 | 22.3 | 17.4 |
| $P_{H2}(60^oC)$ | atm | 2.9 | 8.9 | 52.1 | 2.1 | 6.5 | 38.0 | 1.5 | 4.7 | 27.7 |
| $P_{H2}(70^oC)$ | atm | 4.4 | 13.2 | 73.3 | 3.0 | 8.9 | 49.4 | 2.0 | 6.0 | 33.3 |
| $P_{H2}(150^oC)$ | atm | 64.3 | 155.3 | 625.2 | 26.5 | 63.9 | 257.2 | 10.9 | 26.3 | 105.8 |

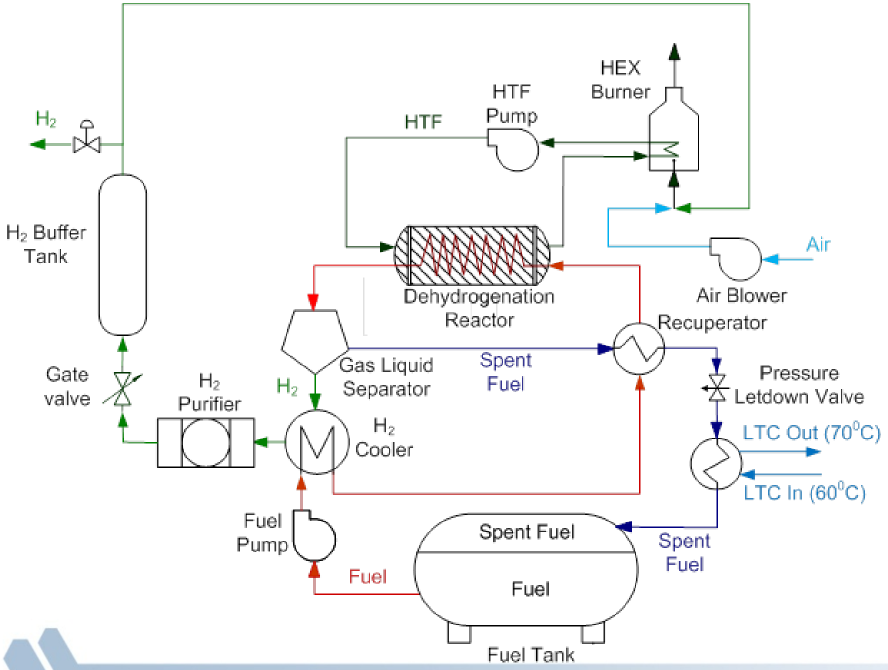
# On-Board Chemical Hydrogen Storage System

Flow system to enable refueling of partially empty tanks

- Volume exchanged tanks for compactness
- Hydrogen buffer for start-up and fast transients
- Reactor operates at elevated pressure, reaction kinetics independent of back pressure, reactor size determined by reaction kinetics and heat transfer
- Fuel may be liquid, slurry or solution

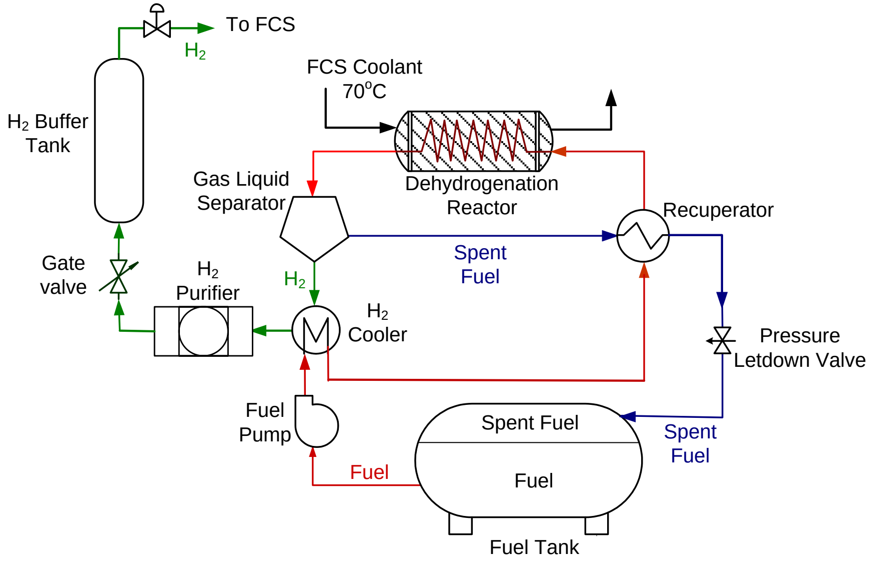
## System with burner*

- 50-kW microchannel HEX burner
- HTF coolant separates burner & reactor



## System without burner

- Thermally integrated with FCS
- Mitigates FCS heat rejection problem

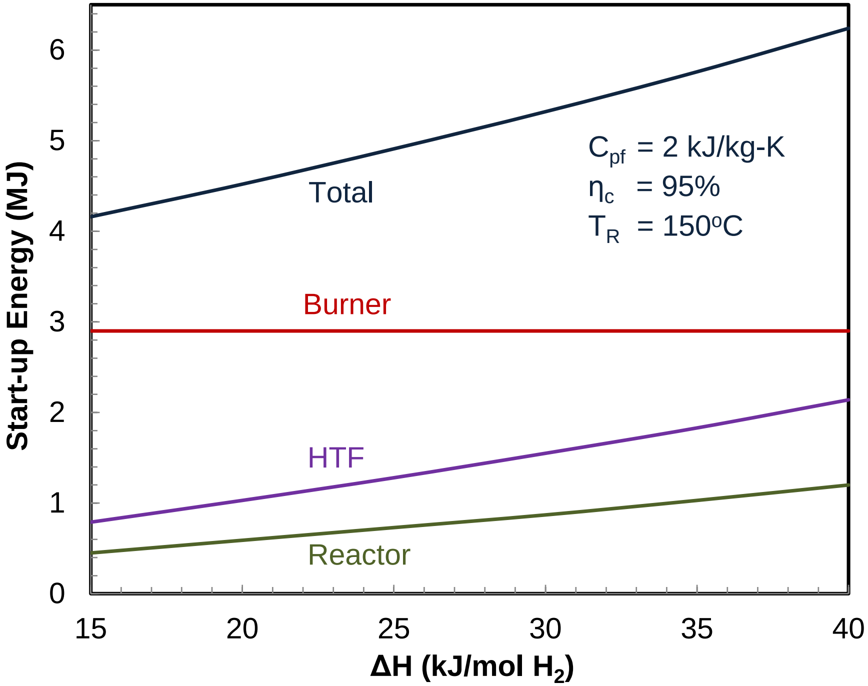


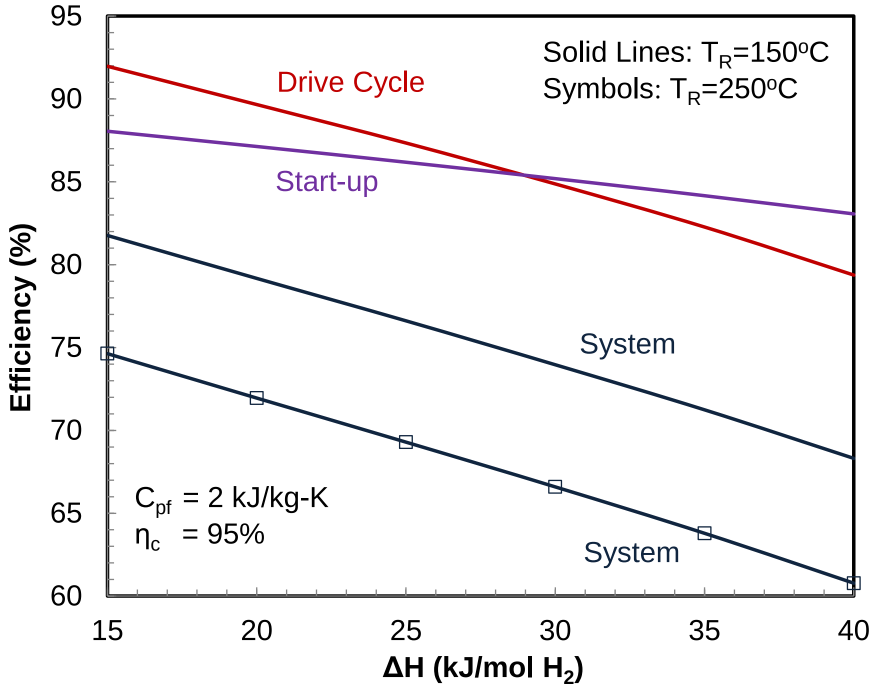
**RK Ahluwalia, TQ Hua and JK Peng, "Automotive Storage of Hydrogen in Alane," IJHE 34 (2009) 7731-7748.**

# Storage System with Burner: System Performance

**Difficult to meet the 90% on-board system efficiency target if a burner is needed to supply the heat of decomposition ($T_R > T_{FC}$)**

- Drive cycle efficiency ($\eta_d$): Ratio of $H_2$ supplied to the fuel cell to the $H_2$ released from the dehydrogenation reactor
- Start-up efficiency ($\eta_{su}$): Related to the fraction of $H_2$ consumed in a trip that is used in bringing the system components to their operating temperatures
- Burner efficiency ($\eta_B$): Burner heat transfer to the HTF as a fraction of the LHV of $H_2$ used in the burner (85% for 60% excess air and $T_R$ = 150°C)



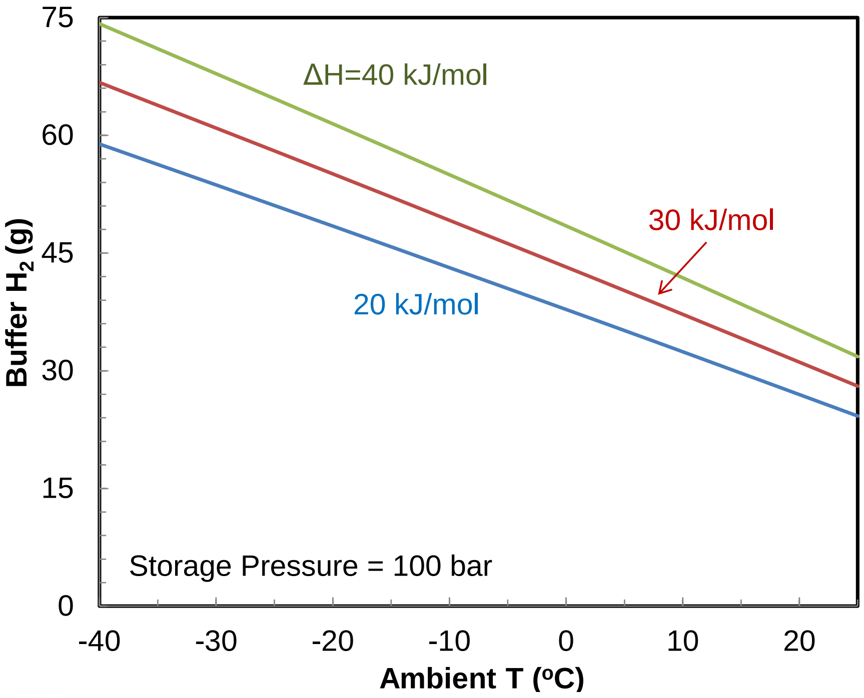


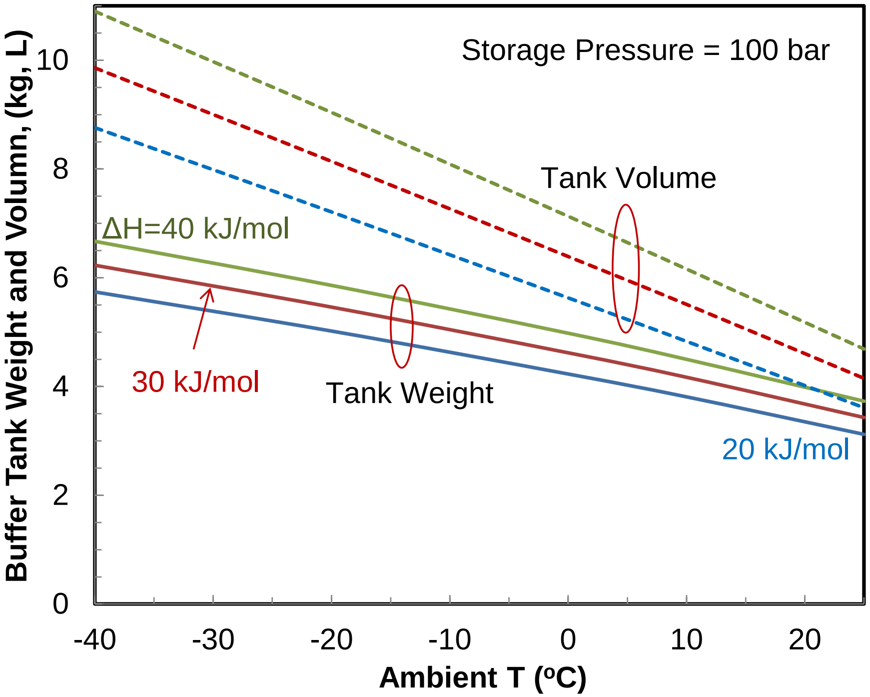
**M Ghazvini and V Narayanan, "A Microscale Combustor Recuperator and Oil Heat Exchanger – Design and Thermofluidic Characterization," IJHMT 64 (2013) 988–1002**

# Storage System without Burner: Buffer $H_2$ Requirements

$H_2$ buffer capacity for FCS startup from -40°C*

- Buffer to supply $H_2$ until the fuel cell and the reactor reach the fuel decomposition temperature (70°C)
- Buffer replenished with excess $H_2$ released from fuel during normal operation when the stack coolant is at its peak temperature (80°C)
- Stack: 2 kW/kg specific weight, 0.5 kJ/kg.K average $C_p$
- Reactor: Thermal mass during startup includes weights of HX tubes, reactor walls, and coolant, 0.5 kJ/kg.K average $C_p$





**RK Ahluwalia, JK Peng and TQ Hua, "Bounding Material Properties for Automotive Storage of Hydrogen in Metal Hydrides for Low-Temperature Fuel Cells," IJHE 39 (2014) 14874-14886.**

# Storage System without Burner: Baseline Material Targets

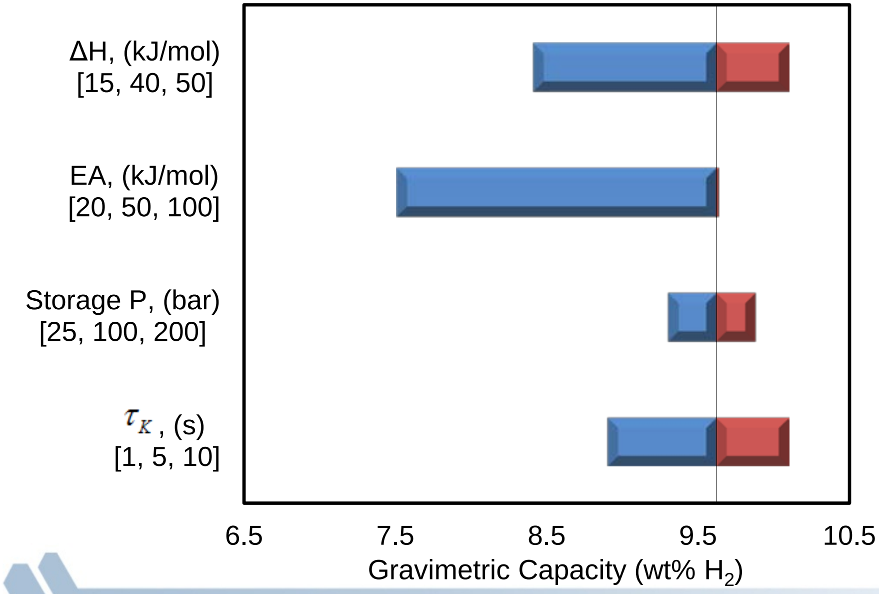
Thermodynamically mildly stable or unstable materials at room temperature that decompose at 70-80°C, 100 bar backpressure

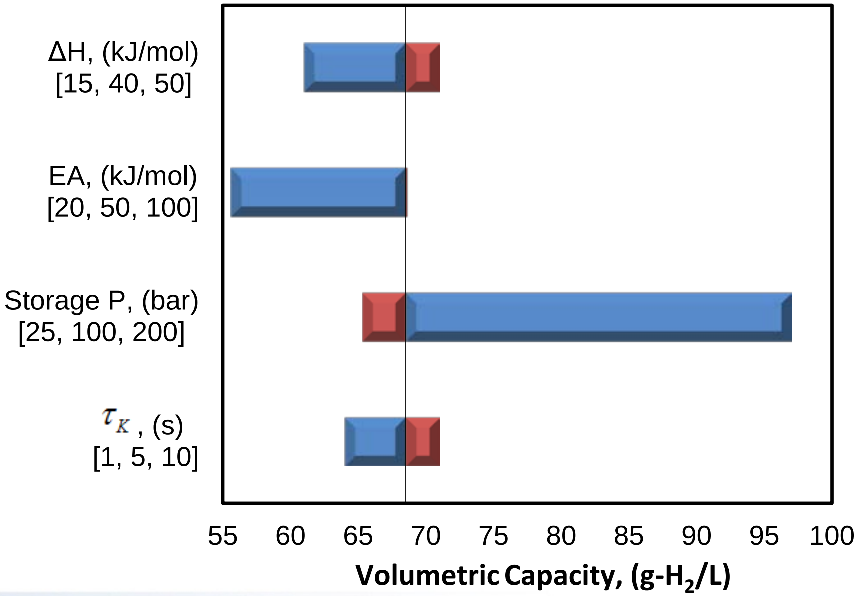
| | | Units | Reference Values | Range of Values | Comments and Relevant Targets |
|---|---|---|---|---|---|
| **Chemical Storage Material** | Free Energy of Decomposition | kJ/mol | 1.6 | -6.4 to 1.6 | 60% WTE efficiency |
| | Enthalpy of Decomposition | kJ/mol | 40.0 | 20 to 40 | 90% on-board system efficiency |
| | Fuel Hydrogen Capacity | wt% $H_2$ | 9.6 | 8.4 - 9.6 | 5.5 wt% system gravimetric capacity |
| | Fuel Volumetric Capacity | g-$H_2$/L | 68.5 | 61 - 71.5 | 40 g/L system volumetric capacity |
| | Decomposition Kinetcs | s | 5 | TBD | Time for 95% conversion at 70°C |
| | Fuel Stability | g/h/kg-$H_2$ | 0.05 | | $H_2$ loss target |
| **Operating Temperatures** | Dehydrogenation Reactor | °C | 70 | TBD | 1.6 g/s minimum full flow of $H_2$ |
| | Heat Transfer Fluid (HTF) | °C | 70 | 70 - 80 | |
| | Spent Fuel Cooler | °C | 50 | 25 - 50 | |
| **Operating Pressures** | Storage Pressure | bar | 100 | 50 - 200 | |
| | Minimum Delivery Pressure | bar | 5 | | DOE target |
| **$H_2$ Flow Rates** | Refueling Rate | kg/min | 1.5 | | Not relevant for liquid fuels |
| | Minimum Full Flow Rate | g/s | 1.6 | | DOE target |
| **Buffer $H_2$ Storage** | Storage Pressure | bar | 100 | 50 - 200 | Start-up from -40°C |
| | Buffer Storage Capacity | g-$H_2$ | 74 | 59 - 74 | |

# Storage System without Burner: Sensitivity Analysis

On-going model testing and validation. As such, results are subject to uncertainties in shell-side heat transfer correlation

- ΔH: Determines reactor heat transfer area and fuel residence time. Reduces heat load on the FCS radiator (advantageous).
- Storage pressure: Determines the volume of the buffer. Volumetric material capacity target increases greatly if material decomposes at 25 bar back pressure.
- Activation energy ($E_A$): Fitting parameter.
- Isothermal conversion time ($\tau_K$): Actual decomposition rate may be controlled by mass transfer (not yet considered in model) and heat transfer as $\tau_K$ is reduced.





# Additional Material Targets

- Fuel should remain liquid and be pumpable over the range of operating temperatures (-40°C to $T_{FC}$).
- No solid phases should form as the fuel is decomposed.
- No gaseous products of decomposition other than $H_2$.

| | Parameter | Reference Value | Comments |
|---|---|---|---|
| **Physical Properties** | Freezing Point | Below -40°C | |
| | Boiling Point | Above 120°C | Vapor pressure should be <1 mPa at 95°C |
| | Viscosity | TBD | Fuel pumpable to 100 bar at -40°C |
| **Stability** | Shelf Life | TBD | |
| | Toxicity and Safety | Non toxic | Compliant with applicable ES&H standrads |
| | $H_2$ Purity | | SAE J2719 and ISO/PDTS 14687-2 specifications |
| **Material Compatibity** | | | Be compatible with materials rotinely used in automtive fuel systems |
| **Off-Board Regenerability** | WTT Efficiency | 60% | Practcal industrial methods for regeneration |
| | Cycle Life | TBD | |
| | Cost | TBD | As per DOE targets |

# Summary and Conclusions

Desired thermodynamic properties of materials for 50 - 60% WTT efficiencies (Based on the experience with $NaBH_4$, $AlH_3$, AB, CBN and n-ethyl carbazole)

- Minimum free energy of decomposition at 298 K: 1.6 kJ/mol for 60% WTT efficiency, and -6.4 kJ/mol for 50% WTT efficiency
- Exothermic materials are unsuitable if $\Delta S$ is between 80 - 130 J/mol.K
- Expected range of $\Delta H$: 20 - 40 kJ/mol-$H_2$

Materials that decompose above the FCS coolant temperature and require a burner may not be acceptable since the on-board system efficiency is <70% for $\Delta H$ = 40 kJ/mol-$H_2$

- Stringent requirement for usable gravimetric capacity if $T_R > T_{FC}$

Desired kinetic properties of materials

- Likely a catalytic decomposition process, otherwise the material would have short shelf life and may not meet the 0.05 g-$H_2$/h/kg stability target at room temperature
- Non-equilibrium decomposition kinetics that is independent of back pressure, otherwise the buffer tank would need to be refueled with gaseous $H_2$
- Preliminary target for decomposition kinetics: 5 s for 95% conversion at 70$^o$C and 100 bar back pressure
- Initial targets for usable gravimetric and volumetric capacities of fuel: 9.6 wt% $H_2$ and 68.5 g-$H_2$/L