Hydrogen and fuel cells

Hydrogen properties

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Hydrogen properties

- hydrogen from – “hydro” + “genes” meaning “water” + “to produce”
- Most abundant element in the universe
- It is richest in energy per unit mass (LHV 120MJ/Kg)
- Hydrogen when burnt in air produces water as the by – product
- Promote the use of diverse, domestic and sustainable energy resources
- Increase the reliability and efficiency of energy systems
- H_2 is widely used in existing chemical industries and refineries
- Long term, large scale storage which can be integrated with renewables

Hydrogen properties

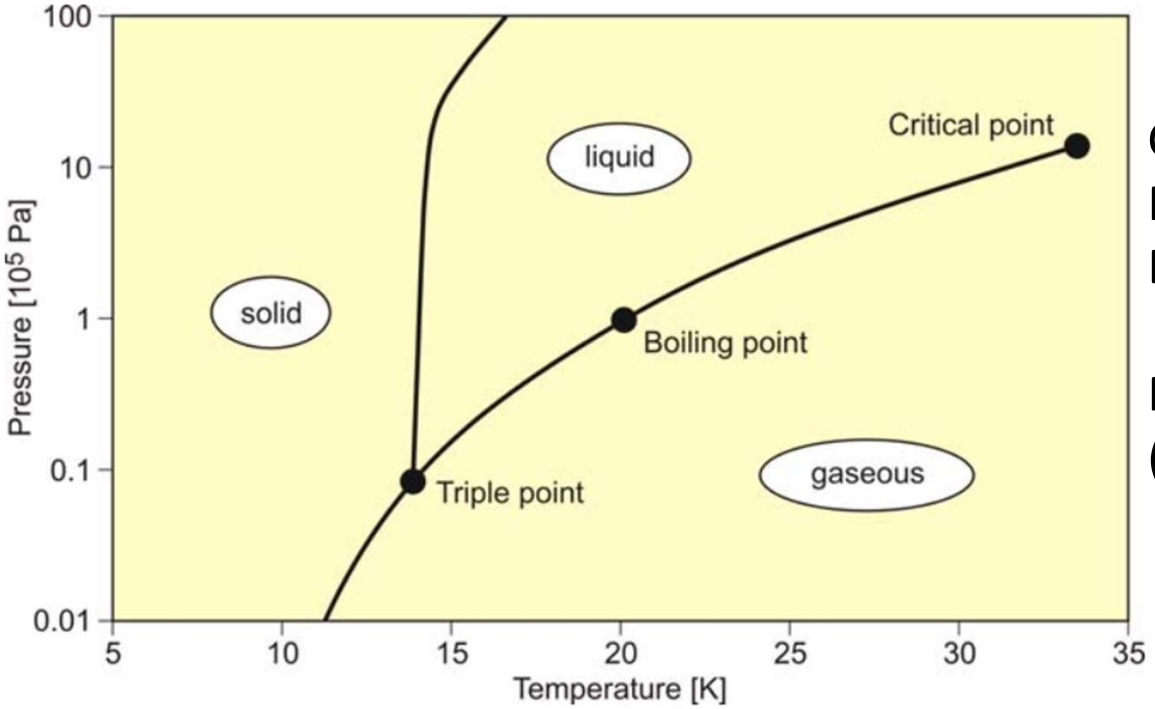
- Found as diatomic molecule, high dissociation energy of 435 kJ/mol
- Colorless, odorless, tasteless, flammable, non-corrosive, non-toxic but can act as asphyxiant
- density of hydrogen is 0.08 kg/m^3
- Diffuses faster
- Buoyancy – rises fast
- Isotopes – (a) Protium- mass 1.008, makes up 99.98%, (b) deuterium – mass 2.014, makes up about 0.02% and(c) Tritium – mass 3.016, occurs extremely small amounts in nature
- Low solubility in solvents, pronounced solubility in metals

Hydrogen properties

Diffusivity

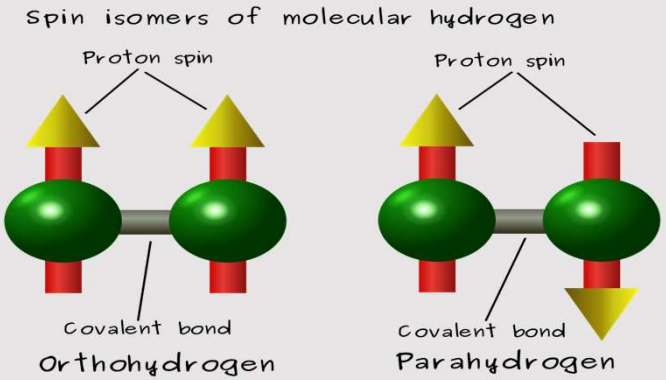
- In the air the
  - diffusivity for hydrogen is: 0.63 cm^2/s
  - diffusivity for methane is: 0.20 cm^2/s
  - diffusivity for vapours: 0.08 is: 0.63cm^2/s

Hydrogen properties



Critical point T= 33.2 K P= 1.3 Mpa
Melting Point 14 K atmospheric pressure
Boiling point 20 K atmospheric pressure

Normal hydrogen is a mixture of ortho (75%) and para (25%) hydrogen



A catalyst is needed to convert hydrogen in para-hydrogen (more stable, slower evaporation rate when stored).

Hydrogen properties

- Hydrogen is a powerful reducing agent

$$(H_2 + CuO \rightarrow Cu + H_2O)$$
$$(3H_2 + N_2 \rightarrow 2NH_3)$$

- Reacts with oxides and chlorides of metals to produce free metals

$$(H_2 + PdCl_2 \rightarrow Pd + 2HCl)$$

- Reacts with salts like nitrates, nitrites and cyanides of Na or K

$$(NaNO_3 + 4H_2 \rightarrow NaOH + NH_3 + 2H_2O)$$
$$(H_2 + 2NaCN \rightarrow 2HCN + 2Na)$$

- Reacts with both metals and non metals to form hydrides

$$(H_2 + Na \rightarrow 2NaH)$$
$$(H_2 + S \rightarrow H_2S)$$
$$(H_2 + Cl_2 \rightarrow 2HCl)$$

- Reacts violently with oxidizers

$$(H_2 + O_2 \rightarrow H_2O)$$

Hydrogen properties

Density –

0.08 kg m^{-3} at NTP (7% of the density of air)

Liquid hydrogen density 70.8 kgm^{-3} (7% of that of water)

Energy Content –

Gasoline 48.6 MJ/kg, diesel 44.8 MJ/kg

Hydrogen 141.8 MJ/kg (HHV), 120 MJ/kg (LHV)

Volume basis –

Gasoline 31,150 MJ/m^3, diesel 31,435.8 MJ/m^3

Liquid Hydrogen 8,491 MJ/m^3

At 15ºC, 1atm 10.05 MJ/m^3

200 bar, 1,825 MJ/m^3

690 bar, 4,500 MJ/m^3

Hydrogen properties

- Flammability range

In air at ambient conditions:

  - Hydrogen 4-75%
  - Gasoline 1-7.6%

- Explosive range 15-59%

  In terms of equivalence ratio:

  - hydrogen: $0.1<f<7.1$
  - gasoline $0.7<f<4$

Hydrogen properties

- Ignition energy of hydrogen is 0.02 mJ Gasoline 0.24 mJ
- Low electrical conductivity
- Prompt ignition even for leaner mixtures.
- Hot spots or hot gases can serve as means of ignition – premature ignition and flashback.

Hydrogen properties

Autoignition Temperature

- Autoignition temperature of hydrogen is 585^{0}C , Gasoline 240 -460 ^{0}C
- Difficult to ignite hydrogen – air mixture on basis of heat alone without some additional ignition source

Hydrogen properties

Flame Speed

- At stoichiometric ratio, hydrogen flame speed is 3.46 m/s
- Gasoline 0.42 m/s

Quenching Distance

- Hydrogen has a quenching distance of 0.64 mm , Gasoline of 2 mm
- Hydrogen flames are difficult to extinguish.
- Tendency of backfire.

Hydrogen properties

Hydrogen Embrittlement

- Factors affecting are hydrogen concentration, purity, pressure, temperature, type of impurity, stress level, stress rate, metal composition, metal tensile strength, grain size, microstructure, heat treatment history etc.

Hydrogen Leakage

- Low density, high diffusivity, dispersion of hydrogen much faster than gasoline.

Hydrogen properties - Summary

Lower heating value: 119.96 MJ/kg

Combustion products: H_2O, NOx

Toxicity: none

Density at NTP: 0.0883 kg/m^3

Flame visibility: Scarce
Colour and/or odour: none

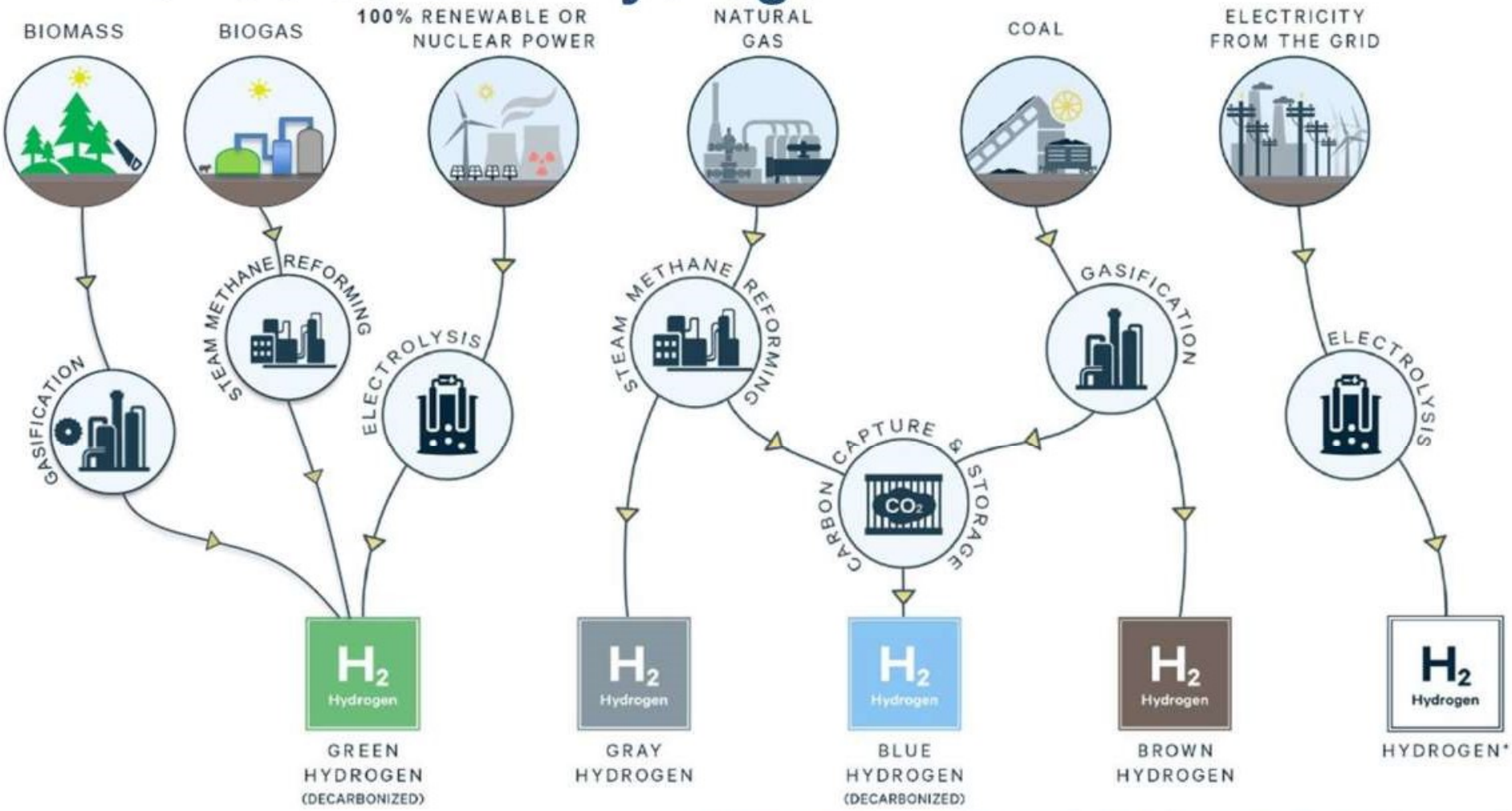
Minimum ignition energy: 0.017 mJ

Flammability range in air: 4 ÷ 75 %vol

Molecule diameter: 120 pm

- Properties of hydrogen makes it different from other conventional fuels
- Studied properties of hydrogen have their own advantages and disadvantages while considering its use as fuel

The “colours” of hydrogen



Adapted from: https://www.rff.org/publications/issue-briefs/investment-tax-credits-hydrogen-storage/

Hydrogen production today is estimated at **70 Mt/yr (million tons):**

- **76% is based on the use of natural gas in steam methane reforming plants.**
- The use of electrolyzers **accounts today 2% of stock.**

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MDPI

Review

An Extensive Review of Liquid Hydrogen in Transportation with Focus on the Maritime Sector

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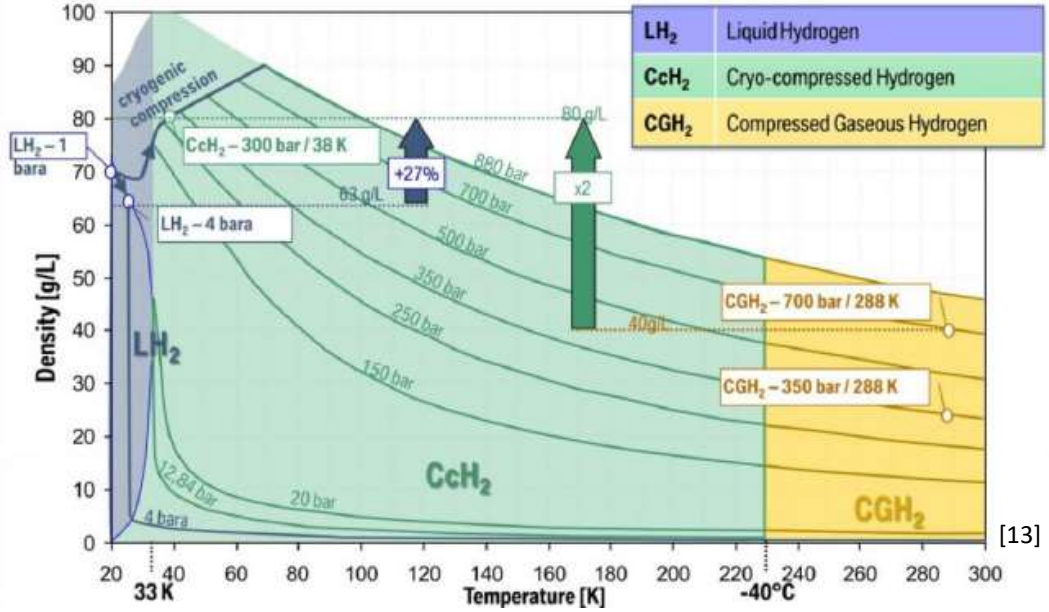
HYDROGEN STORAGE



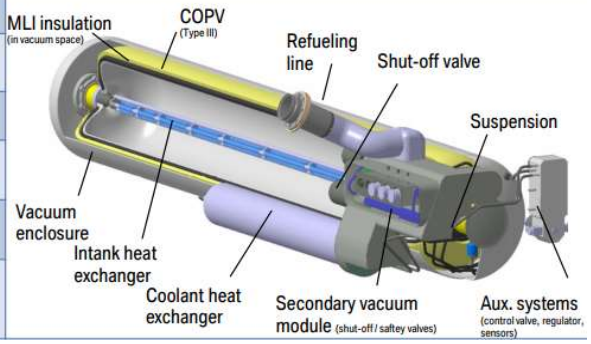
[13]

	Type 1	Type 2	Type 3	Type 4
Market share	93 %	4 %	< 2 %	< 2 %
Structure	Metal	Metal liner reinforced with resin impregnated continuous filament (hoop wrap)	Metal liner reinforced with resin Impregnated continuous filament (fully Wrap)	Resin impregnated continuous filament with a non-metallic liner
Most commonly used	CrMo steel	CrMo steel with glass fiber	aluminium with high performance glass and/or carbon	HDPE liner with carbon fiber
Pressure [bar]	limited to 300	not limited (700 bar)	not limited (700 bar)	not limited (700 bar)
Weight (approx)[kg/L]	0,9 ~ 1,3	0,8 ~ 1,0	0,4 ~ 0,5	0,3 ~ 0,4
Cost (approx.) [US$ / L]	3 to 5	5 to 7	9 to 14	11 to 18

[9], [16]

Max. usable capacity	CcH_2: 7.8 kg (260 kWh) CGH_2: 2.5 kg (83 kWh)
Operating pressure	≤ 350 bar
Vent pressure	≥ 350 bar
Refueling pressure	CcH_2: 300 bar CGH_2: 320 bar
Refueling time	< 5 min
System volume	~ 235 L
System weight (incl. H_2)	~ 145 kg
H_2-Loss (Leakagel max. loss rate I infr. driver)	<< 3 g/day I 3 – 7 g/h (CcH_2) I < 1% / year

+ Active tank pressure control
+ Load carrying vehicle body integration
+ Engine/fuel cell waste heat recovery



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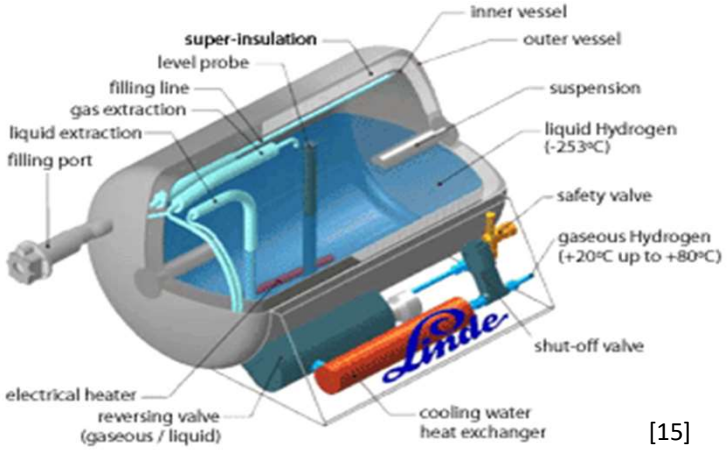


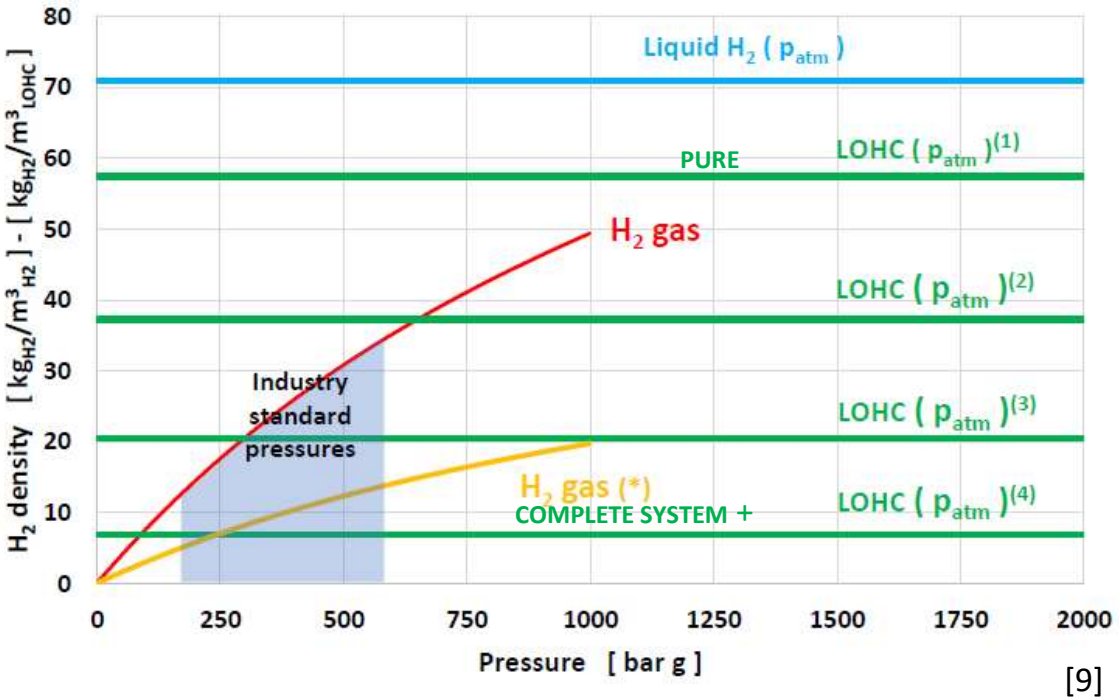
[15]

Example of a tube trailer in a 40-foot container half height [49]

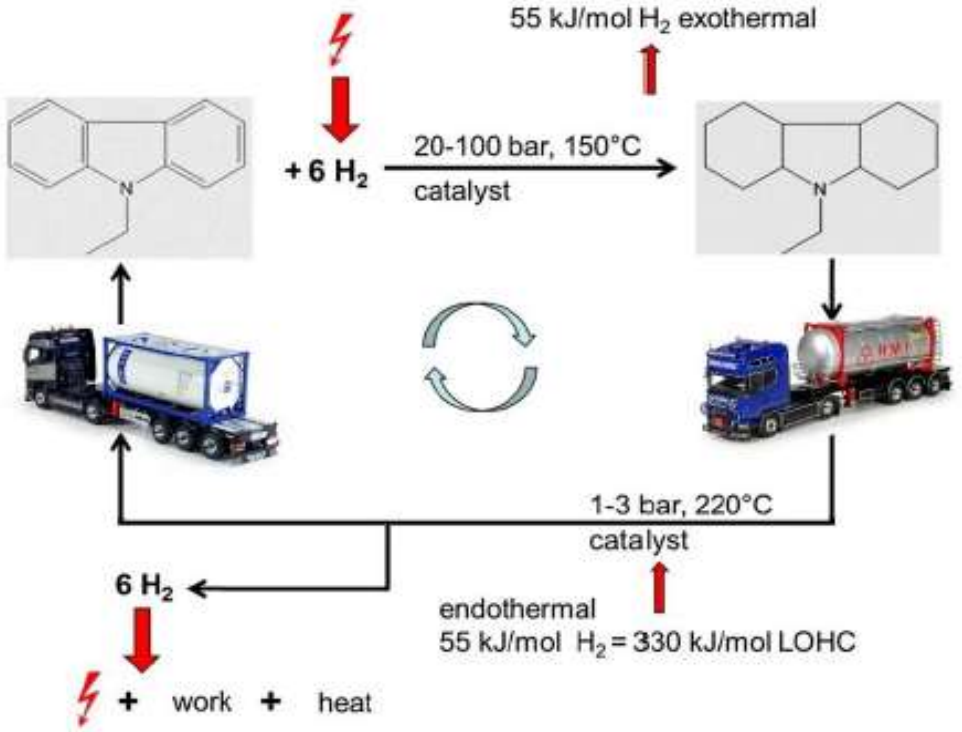
Multiple Element Gas Container (Calvera company)

Series of 16X50 L cylinder packs proposed by the Calvera company

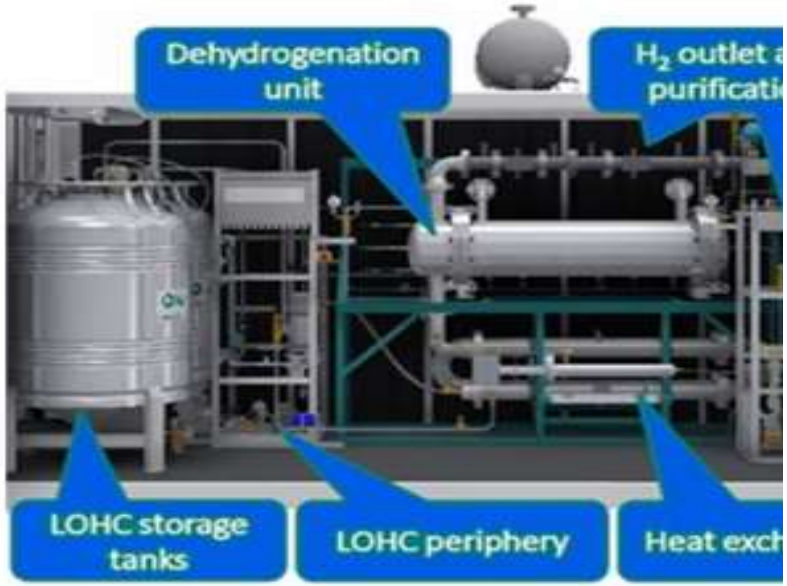
LIQUID ORGANIC HYDROGEN CARRIER



[9]

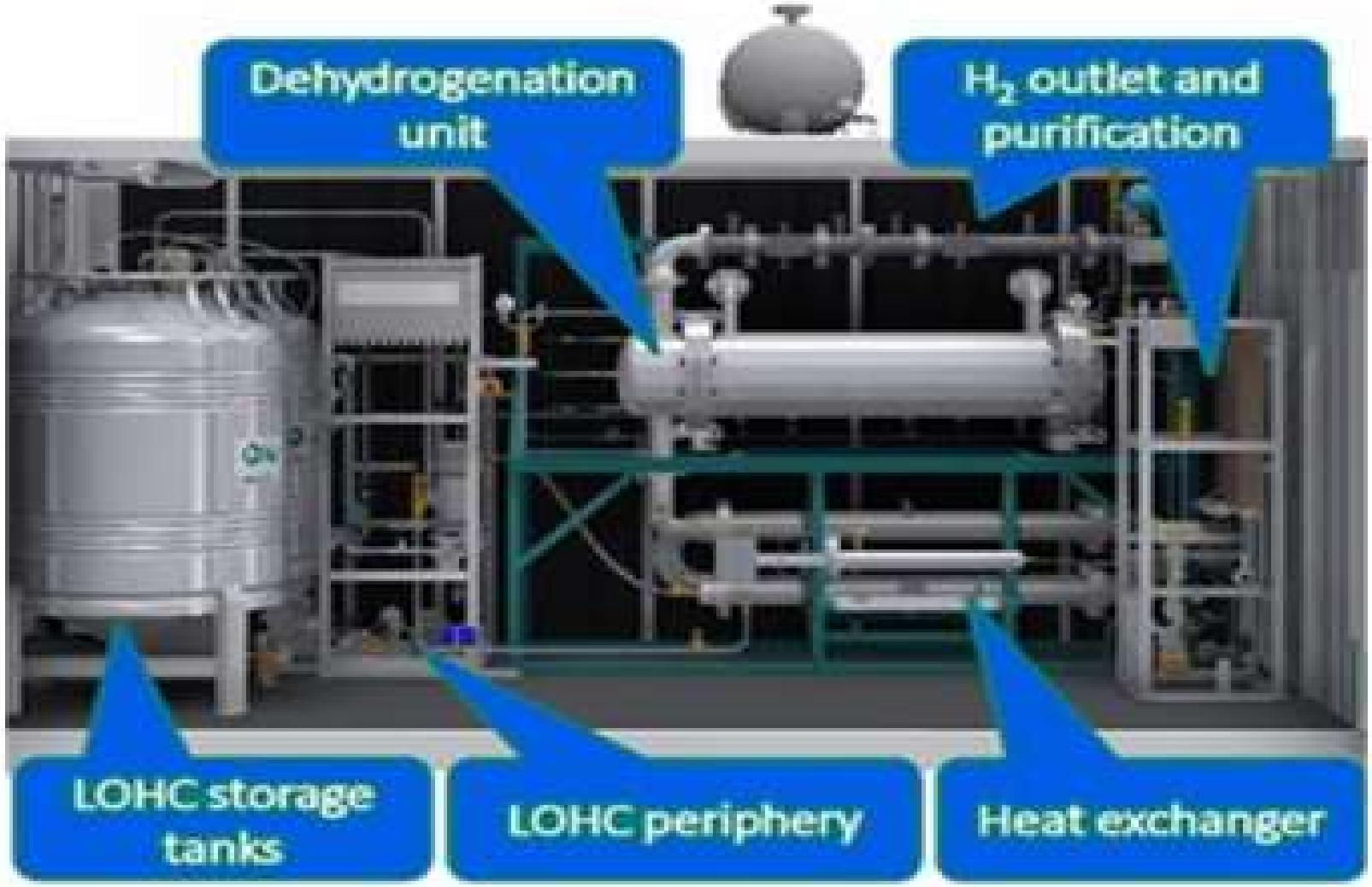


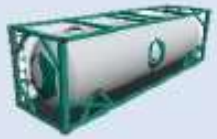
Property	Comment	Mobility	Stationary Storage	Energy Transpo
Storage Capacity	max. 7.2 wt.-% for aromatic systems	!!	!	!
Handling	Melting point, boiling point, viscosity	!	o	!!
Thermodyn. Equilibrium	Hydrogenation and dehydrogenation at moderate conditions	!	!	!
Stability	Thermal and chemical	o	!!	!
Toxicity	Transport restrictions	!!	!	!!
Availability	Price, abundance	o	!!	!!



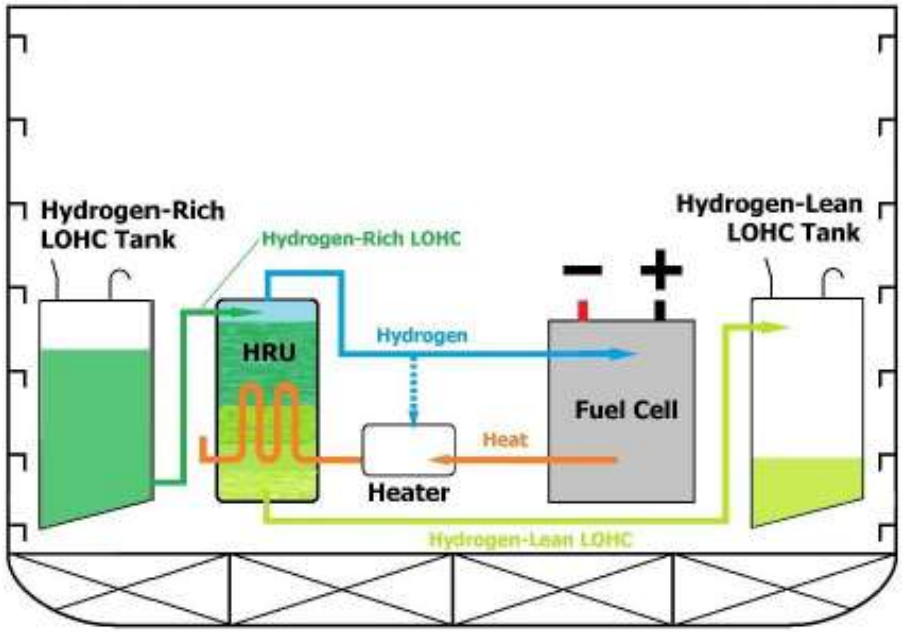
[19]

LOHC plant example

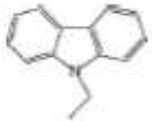
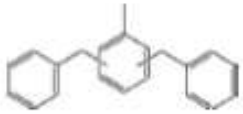
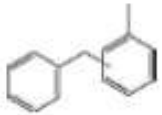
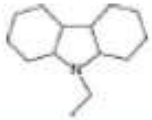
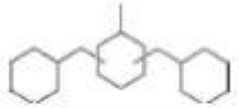
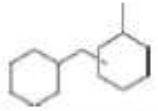


IBC container	1 to 3 m^3	
Swap body container	10 to 24 m^3	
Tank trailer	15 to 30 m^3	

HYDROGENIOUS LOHC STORAGE SOLUTIONS [48]



Schematic representation of a LOHC plant producing hydrogen for the fuel cell [1]

LOHC	TOL/MCH	NEC/H12-NEC	DBT/H18-DBT	BT/H12-BT
H_2 – lean form				
H_2 – rich form				
Chemical formula (H_2 – lean form)	C_7H_8	$C_{14}H_{13}N$	$C_{21}H_{20}$	$C_{14}H_{14}$
Chemical formula (H_2 – rich form)	C_7H_{14}	$C_{14}H_{25}N$	$C_{21}H_{38}$	$C_{14}H_{26}$
Melting point (H_2 – lean form) [°C]	-95	68	-34	-30
Boiling point (H_2 – lean form) [°C]	111	270	390[a]	280
H_2 – capacity [wt. %]	6,1	5,8	6,2	6,2
Energy content [kWh/kg]	2,01	1,91	2,05[b]	2,05
Heat of hydrogenation [kJ/mol_{H2}]	68,3	55	65	65
Cost [€/kg] (1 ton scale)	About 1	About 40	About 4	About 4

a) Diesel: 170-390
b) Li-ion battery: ca. 0,15

CHARACTERISTICS PROPERTIES OF MOST STUDIED LOHC [17]