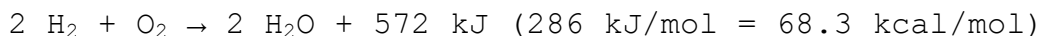## 8. HYDROGEN

General

Hydrogen gas (molecular hydrogen) is highly flammable and will burn in air at a very wide range of concentrations between 4% and 75% by volume. The enthalpy of combustion for hydrogen is –286 kJ/mol (sign minus means the reaction heat is emitted):

$$2\ H_2 + O_2 \rightarrow 2\ H_2O + 572\ kJ\ (286\ kJ/mol = 68.3\ kcal/mol)$$

Under ordinary conditions on Earth, hydrogen exists as the diatomic gas, H_2. However, hydrogen gas is very rare in the Earth's atmosphere (1 ppm by volume) because of its light weight, which enables it to escape from Earth's gravity more easily than heavier gases. However, hydrogen is the third most abundant element on the Earth's surface. Most of the Earth's hydrogen is in the form of chemical compounds such as hydrocarbons and water. Hydrogen gas is produced by some bacteria and algae.

Preparation and Costs

Hydrogen (H_2) can be obtained from different sources:
- fossil fuels (natural gas reforming, coal gasification);
- renewable and nuclear energy: biomass processes, photo-electrolysis, biological production, high temperature water splitting;
- electricity (water electrolysis).

At present, H_2 is produced largely from fossil fuels without CCS (48% from natural gas, 30% from refinery/chemical off-gases, 18% from coal, the rest from electrolysis). Most of today's production (some 65 million tones per year) is for captive use in the chemical and refinery industries. In the future, H2 could be used for power generation and in transport by fueling gas turbines, fuel cells and combustion engines. Used in FCV, H_2 could significantly increase efficiency and emission reduction in transport.

However, using H_2 for energy applications requires more efficient, less costly production processes, ideally with no CO_2 emissions. Decentralized production is the best choice for market uptake as it minimizes the needs for distribution infrastructure. But it is less efficient than large-scale, centralized production, and it makes CCS impractical.

Electrolysis is a well-known electro-chemical process to split water into H_2 and oxygen (O_2) using electricity. Alkaline electrolysis with potassium hydroxide (KOH) electrolyte are

commercially available. Efficiency is a key parameter for electrolysis, as costs are largely determined by electricity costs. Best-practice efficiency could be higher than 85% (Gcal H_2/Gcal electricity), but commercial devices achieve between 55% and 75%. New advanced electrolyzers may approach the upper limit. At high temperatures, heat consumption increases while electricity needs decrease. High-temperature electrolysis (800°C-1,000°C) may therefore offer higher efficiency, in particular using residual heat. Also, high-pressure electrolysis can make H_2 pressurization unnecessary and improve efficiency. New electrolyser concepts are based on fuel cells working in reverse mode. Small-scale polymer electrolyte membrane FC (PEMFC) electrolyzers (60°C-80°C, 15 bar, 50% efficiency) are commercially available. Solid oxide FC (SOFC) electrolyzers functioning at 700°C-1,000°C need more research. Current electrolysis costs are typically above $125/Gcal H_2, but could drop to below $85/Gcal (including pressurization) over coming decades, assuming electricity at $35/MWh and 80% process efficiency. Use of off-peak electricity and large-scale plants may reduce costs, although the cost of CCS is expected to increase the cost of electricity.

Natural gas reforming is a mature technology used in the refinery and chemical industries for large-scale H_2 production. Small-scale reformers are currently used in demonstration H_2 refueling stations (decentralized production). Reforming options include catalytic **steam methane reforming** (SMR), **partial oxidation** (PO) and other variants under development. In SMR, methane reacts with steam at 700°C-850°C to produce syngas, a mixed H_2 and carbon monoxide (CO) gas.

$$CH_4 + H_2O \rightarrow CO + 3\ H_2$$
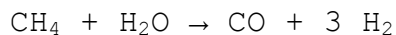
CO is then converted into CO_2, producing additional H_2 by water-gas shift reaction.

$$CO + H_2O \rightarrow CO_2 + H_2$$
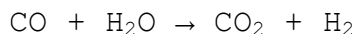
In the PO process, methane reacts initially with pure O_2 to provide syngas.

$$2\ CH_4 + O_2 \rightarrow 2\ CO + 4\ H_2$$
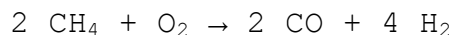
SMR offers efficiencies of up to 80%-85% in large-scale units (excluding H_2 compression). If residual steam is re-used, total efficiency may be higher. Small units have lower efficiency (at least 10-15 percentage points lower) and higher unit costs. Producers have recently much improved the compactness of small scale reformers (10x3x3m) and their capacity (25-30 Gcal/hour), but further R&D is needed to reduce costs and increase efficiency. H_2

compression and CCS (eventually, in large units) may each further reduce net efficiency by some 5-10 percentage points. CCS in small plants is probably not practical. At current natural gas prices, ($25-$40/Gcal), the cost of H_2 from natural gas reforming ranges from between $40 and $60/Gcal H_2 (in large-scale production for captive use) to more than $125/Gcal, with high sensitivity to natural gas prices, processes and economy of scale. Small-scale decentralized production may exceed $200/GJ. Compressed H_2 in tubes may cost $350-$400/Gcal delivered). Projected CCS costs are expected to add $4-$10/Gcal, depending on process and scale.

Coal gasification produces a gas mixture of H_2, CO, carbon dioxide (CO2) and methane (CH_4). The basic reaction is

$$C + H_2O \rightarrow CO + H_2.$$
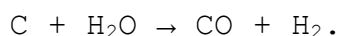
The CO can then be converted into CO_2 and additional H_2 through a water-gas shift reaction. In addition to H_2, the final product offers relatively pure CO_2, ready for pressurization and storage (CCS). Final H_2 purification is needed for most applications.

Although a mature process, coal gasification is currently more expensive than natural gas reforming because of the gasifier and the need for O_2 for the reaction process. Large-scale, integrated gasification combined cycles (IGCC) are considered an attractive option for centralized cogeneration of electricity and H_2, with comparably low CCS costs. Assuming costs of $4-$6/Gcal for coal and $35-$40/MWh for electricity, with 45% electrical efficiency, projected H_2 production cost with CCS would range between $30 and $40/Gcal H_2. IGCC demonstration plants are operating today in several countries to produce electricity (no H_2). They have proved more expensive and less reliable than conventional coal power plants. Cheaper gasifiers and new processes to produce O_2 could make IGCC plants more economically attractive. H_2 is also produced as a by-product from catalytic reforming in refineries, or through off-gas reforming in petrochemical plants, also from ethylene crackers, from chlorine plants and from coke oven gas.

Thermal water-splitting occurs at very high temperatures exceeding 2,500°C, but thermo-chemical processes such as sulphur-iodine (S-I) or bromine-calcium (Br-Ca) cycles may reduce temperatures to below 1,000°C. These processes require low-cost high-temperature heat from nuclear or solar sources, also corrosion-resistant materials. The S-I process is the most promising, with about 43% efficiency and an operating temperature of 950°C. Cost projections suggest a H_2 cost of $40-$80/Gcal using nuclear heat from nuclear high-temperature gas reactors (HTGR), and a cost of $80-$120/Gcal using heat from advanced, megawatt-scale

concentrating solar power (CSP) systems. Both technologies are unlikely to be commercial before 2030.

H_2 from Biomass is the only direct way to produce H_2 from renewable energy without major technology breakthroughs. Biomass can be converted into H_2 via various processes (pyrolysis, gasification, anaerobic digestion etc.). While R&D focuses on gasification, synergies with other fuel production processes (bio-fuels) could open the way to other options and accelerate market uptake. But H_2 production from biomass would compete with bio-fuels and **combined heat and power** (CHP) production. In general, as basic feedstock availability is limited, production from biomass will not benefit from large economies of scale. Costs are expected to be high compared with coal gasification or gas reforming.

Photo-electrolysis produces H_2 using sunlight to illuminate a water-immersed semiconductor that converts the light into chemical energy to split water into H_2 and O_2. This method promises lower capital costs than combined photovoltaic-electrolysis systems and it holds considerable potential for technology breakthroughs. Test-scale devices have shown solar-to- H_2 conversion efficiencies of up to 16%. But cost estimates are premature.

Biological processes derive H_2 from organic matter using micro algal photo-synthesis and cyano-bacteria. These processes require genetic engineering to achieve significant levels of H_2 production. Much research is still needed to demonstrate feasibility.

Projected H2 production costs in Table 1 reflect a range of different technologies, economies of scale and energy prices

Distribution

Pipelines are considered the only option to move large amounts of H_2. They have been used to transport H_2 for more than 70 years. Several thousand km of H_2 pipelines are currently in operation world wide. The energy required to pump H_2 through pipelines is some 4.5 times higher than for natural gas per unit of delivered energy. As a consequence, long distances H_2 transportation for energy use may not be economically competitive. Transportation costs to deliver gaseous H_2 to refueling stations are in the range of \$4-\$8/Gcal, assuming that H_2 compression to refueling pressure is included in the cost of the refueling station.

Liquid H2 transport by truck, rail or ship is more expensive than gas piping. In current plants, the electricity required for H_2 liquefaction at -253°C is about 10-12 kWh/kg H_2, with potential for future reduction to 7 kWh/kg. The cost of liquefaction in large

systems is about $30-$40/Gcal, 75% of which comes from the cost of electricity. Transportation of liquid H_2 by ship over long distances is also more expensive than for *liquefied natural gas* (LNG) since very low-temperature cryogenic technology is needed. Fast ships are required to reduce boil-off losses (0.2%-0.4% of liquid H_2 per day, which could be recovered, however, and used to fuel the ship).

Refueling Stations – Some 140 H_2 refueling stations are in operation world wide (90 under construction) to fuel some 400 FCV and 100 buses used in demonstration projects. Most stations deliver gaseous H_2 at 350 bar. H_2 is either produced on-site from electrolysis or steam reforming, or received from centralized plants. Costs of refueling stations are estimated between $12/Gcal H_2 and $40/Gcal with centralized H_2 production and on-site production, respectively. These costs include investment and H_2 compression. Transportation, distribution and refueling stations may add some $20-$50/Gcal to H_2 production costs.

Storage in FCV

On-board H_2 storage for fuel cell vehicles (FCV) is challenging and may have significant impact on H_2 distribution infrastructure and standards (e.g. operating pressure). The target is to store 4-5 kg of H2 (sufficient for a drive range of 400-500 km) while minimizing volume, weight, storage energy, cost, and refueling time, and providing prompt H_2 release on demand. Storage requires energy-intensive compression at high pressure (350-700 bar) or liquefaction at -253°C. Electrical energy required for compression or liquefaction represents, respectively, some 12% or 30% of the H_2 energy content. Current commercial options do not fully meet requirements for compactness, drive-range, and cost. Liquid or gaseous storage at 700 bar both require more space than gasoline with equivalent energy content. The tank costs more than $3,000-4,000 per vehicle. H_2 storage in solid materials may offer decisive advantages, but this is still under development, with a number of materials under investigation. On-board reforming to produce H_2 from fossil fuels has also proved challenging and expensive.

Infrastructure

Estimates of H_2 infrastructure investment are complicated by significant uncertainty. The cost of H_2 supply infrastructure for road transport is estimated to be in the order of several hundred billion dollars. Assuming large-scale, centralized H_2 production, the cost of worldwide pipeline-based distribution systems for road transport could range from $0.1 to $1.0 trillion. The *incremental*

investment in refueling stations would be somewhere between $0.2 for centralized H_2 production and $0.7 trillion for decentralized production. A full H_2 economy (i.e., widespread use of H_2 in transport and stationary sectors) would require global pipeline investment in the order of $ 2.5 trillion, the bulk of which would be to finance supplying commercial and residential customers. Assuming early retirement or partial replacement of existing natural gas pipelines, a significant part of this cost would be *incremental*. The level of investment needed for H_2 infrastructure is not insurmountable when compared with the $20-trillion investment in energy supply systems that is estimated to be needed if growth in energy demand up till 2030 is to be met.

Potential and barriers

Environmental consequences of the production of hydrogen from fossil energy resources include the emission of greenhouse gases, a consequence that would also result from the on-board reforming of methanol into hydrogen.

Studies comparing the environmental consequences of hydrogen production and use in fuel-cell vehicles to the refining of petroleum and combustion in conventional automobile engines find a net reduction of ozone and greenhouse gases in favor of hydrogen.

Hydrogen production using renewable energy resources would not create such emissions or, in the case of biomass, would create near-zero net emissions assuming new biomass is grown in place of that converted to hydrogen. However the same land could be used to create bio-diesel, usable with (at most) minor alterations to existing well developed and relatively efficient diesel engines.

H_2 is likely to gain significant market share over the coming decades if the cost of H_2 production, distribution and end-use fall significantly, and if effective policies are put in place to increase energy efficiency, mitigate CO_2 emissions and improve energy security.

H_2 production costs should be reduced by a factor of 3 to 10 (depending on technologies and processes) and fuel cell cost by a factor of 10 or more. At the same time, emission reduction incentives of $25-$50/tCO_2 (depending on fossil fuel price) would help to make H_2, fuel cells and other clean energy options more competitive economically.

Under these assumptions, emissions growth over the coming decades could be reduced in proportions that would bring annual emissions in 2050 down to half those projected in a business-as-usual scenario.

Use of H_2 for energy applications would grow during the years starting from 2020 to reach some 12.5 EJ per year (0.3 Gtoe) by 2050, concentrated mostly on the transport sector. Thanks to the high efficiency of FCVs, this relatively limited input of H_2 (2%-3% of projected total primary energy supply) could fuel some 30% of

the global fleet of passenger cars (about 700 million cars). If H_2 for FCV is combined with H_2 used in other applications (refinery and chemicals industries), total H_2 use by 2050 would amount to some 22 EJ (almost four times today's annual use of H_2). Under less optimistic assumptions regarding technology and CO_2 reduction policies, H_2 is unlikely to gain significant market share as alternative fuel and technology options (bio-fuels, Fischer-Tropsch synfuels, hybrids, battery-electric vehicles, etc.) could play a more important role in future.

In addition to costs and competition from other technologies, barriers to H_2 market uptake include the need for dedicated infrastructure. However, no single fuel or technology is likely to meet the expected fast growing demand for clean transport fuels. Various options are therefore expected to play complementary roles in regionally diversified markets.

Table 1 - Typical Data and Figures for H_2 Production & Distribution Technologies

Data Confidence – Industrial H_2 production is based on well known technologies, but new processes with higher efficiency, lower costs and eventually CCS are needed to produce H_2 for energy use. Typical figures for these technologies are more uncertain. H_2 costs are highly sensitive to coal, gas, biomass and electricity prices.
Current H_2 Annual Production: 65 million tonnes per year, equivalent to 8EJ (less than 2% of world total primary energy supply); 48% from natural gas, 30% refinery-gas/chemicals, 18% coal, 4% electrolysis

Efficiency of H_2 production from electrolysis (incl. auxiliaries, no compression

Technology	Alkaline large-scale	Alkaline high-pressure	Advanced Alkaline	PEM	SOFC
Status	Commercial	Commercial	Precommercial	Precommercial	Prototype
T (ºC) P (bar)	70-90 atm. to 25	70-90 up to 690	80-140 up to 120	80-150 up to 400	900-1000 up to 30
kWh/kgH$_2$	48-60	56-60	42-48	40-60	28-39

Efficiency of H_2 production from natural gas reforming (figures in brackets do not include compression)

Technology	Steam reforming, large-scale 50 PJH2/yr, 80 bar		Steam reforming small-scale 0.02 PJH2/yr, 340 bar		Partial Oxidation	Auto-thermal Reforming
Status	Commercial no CCS	Future with CCS	Commercial no CCS	Future no CCS	Commerc. no CCS	Precommerc. no CCS
Effic. %,	72-77 (76-80)	61-70 (62-78)	47 -55 (60-65)	60-65 (70-75)	66-76	66-73

Efficiency of H_2 production from coal gasification without electricity cogeneration (IGCC) - H2 at 75 bar

Technology	Current Gasification		O2-blown Gasification		Adv.CO$_2$ Membrane Separation	Cogeneration		Cogeneration Membrane Separation
Effic. %,	no CCS	CCS	no CCS	CCS	CCS	no CCS	CCS	CCS
	57	51	67	62	64	83	70	77

Note: CCS means Carbon Capture and Storage