# vehicle model

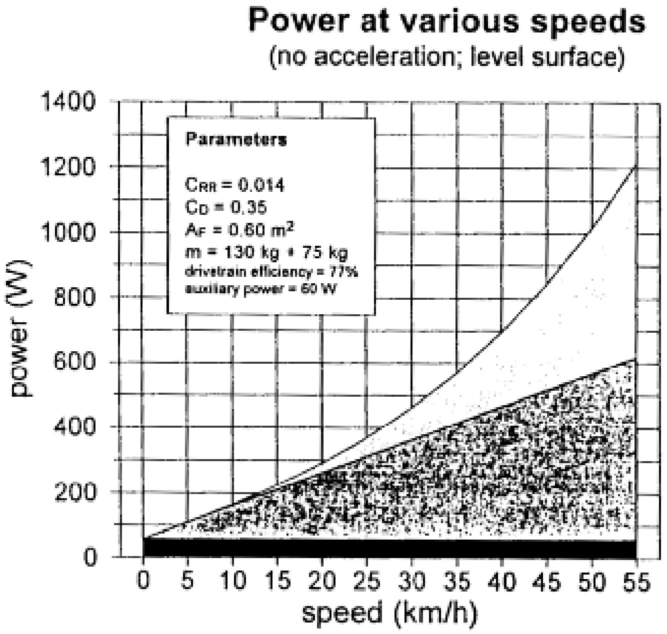
In the computer model used to simulate vehicle performance, the various power demands from acceleration, slope climbing, rolling resistance, and aerodynamic drag are summed to a total power $P_{wheels}$ demanded “at the wheels” by the motion of the vehicle:

$$P_{wheels} = (\, m a v \,) + (\, m g v \sin\theta \,) + (\, m g v C_{RR} \cos\theta \,) + (\, \tfrac{1}{2} \rho_{air} C_D A_F v^3 \,)$$

Future work will integrate the fuel cell power model and an electric motor model with the power required as calculated by the driving model to gain a complete picture of the behaviour of the fuel-cell powered scooter. For now, the motor and controller efficiency $\eta_{drivetrain}$ is modeled as a constant 77% and the auxiliary power $P_{aux}$ (lights, etc.) is added to find the total power required from the fuel cell:

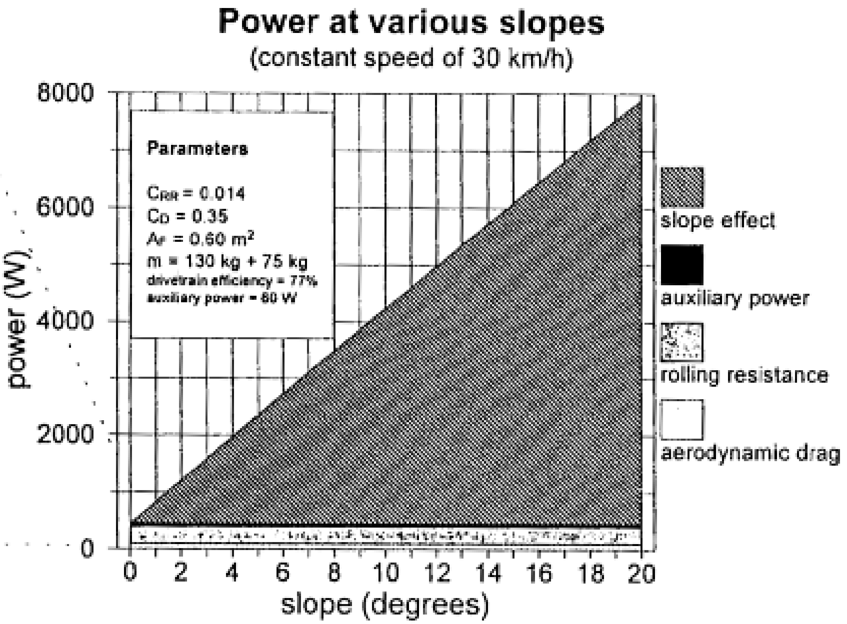
$$P_{output} = (P_{wheels})/\eta_{drivetrain} + P_{aux}$$

The physical parameters were reported from previous scooter studies. Using this equation, the following data were obtained for various theoretical cases:



**Power at various speeds**

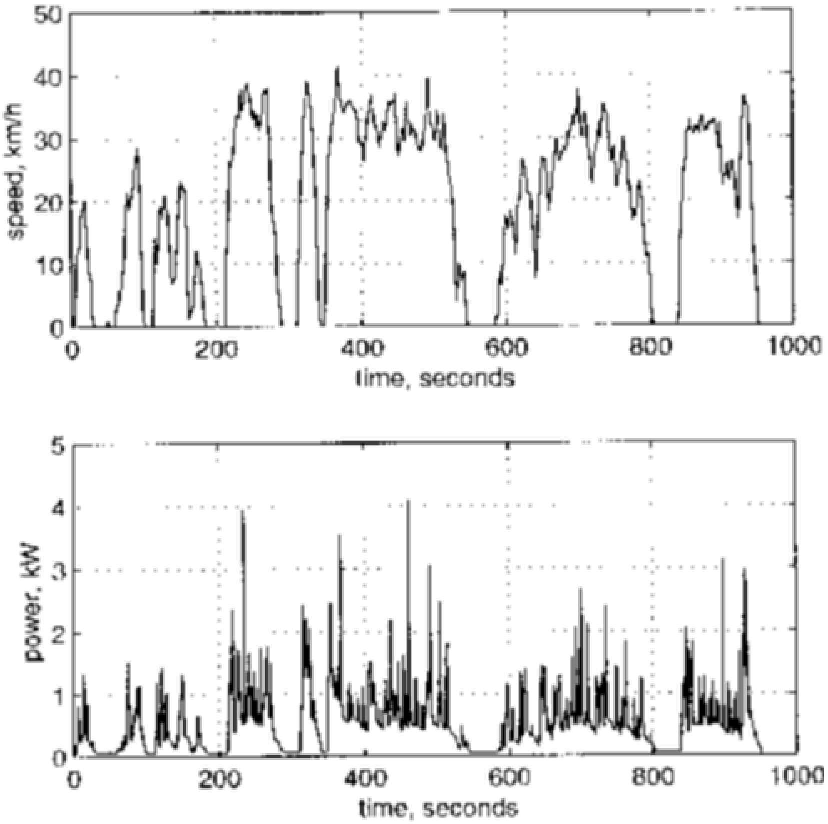
(no acceleration; level surface)



**Power at various slopes**

(constant speed of 30 km/h)

# taipei driving cycle



The Taipei Motorcycle Driving Cycle was obtained from researchers at the Institute of Traffic and Transportation at Taiwan’s National Chiao Tong University. This an actual velocity trace obtained by researchers who followed target scooters on an instrumented “chase vehicle”

Due to inaccuracies in the data caused by, among other things, quantization to the nearest km/h, the data was smoothed using a low-pass filter of the form H(s) = 1/(s+1) with a time constant of 6.3 seconds. Average speed is 19 km/h, total distance 5108 m.

The driving cycle model reveals the following results:

| | |
|---|---|
| Maximum power | 4070 W |
| Average power | 560 W |
| Maximum acceleration | 1.4 km•h$^{-1}$•s$^{-1}$ |
| Maximum deceleration | -2.1 km•h$^{-1}$•s$^{-1}$ |
| Energy usage | 34 km/kWh |
| Equivalent fuel economy | 350 mpge |
| Acceleration energy | 34% |
| Rolling resistance energy | 27% |
| Aerodynamic drag energy | 8% |
| Auxiliary power energy | 17% |

# fuel cell chemistry

The fuel cell is an electrochemical engine that produces electricity from a chemical reaction. Essentially, a fuel cell is the inverse of electrolysis: hydrogen and oxygen are combined to form water, and electricity is released. An electrolyte (in most vehicle applications, a sulfonated fluoropolymer - i.e. PEM, polymer electrolyte membrane) physically separates the two chemicals but allows ions to pass through. At the anode, the hydrogen is oxidized:

$$H_{2\,(g)} \rightarrow 2\,H^+ + 2\,e^-$$

The electrons pass through the load to provide the desired current and end up at the cathode, where the reduction occurs:

$$2\,e^- + \tfrac{1}{2}\,O_{2\,(g)} \rightarrow O^{2-}$$

Electrostatic balance is reached as the hydrogen ions diffuse through the electrolyte to get to the cathode:

$$2\,H^+ + O^{2-} \rightarrow H_2O_{\,(l)}$$

The theoretical energy release of the overall reaction is determined by the free energy change in the overall reaction:

$$H_{2\,(g)} + \tfrac{1}{2}\,O_{2\,(g)} \rightarrow H_2O_{\,(l)} \quad (\Delta G^\circ = 235.4\ \text{kJ/mol})$$

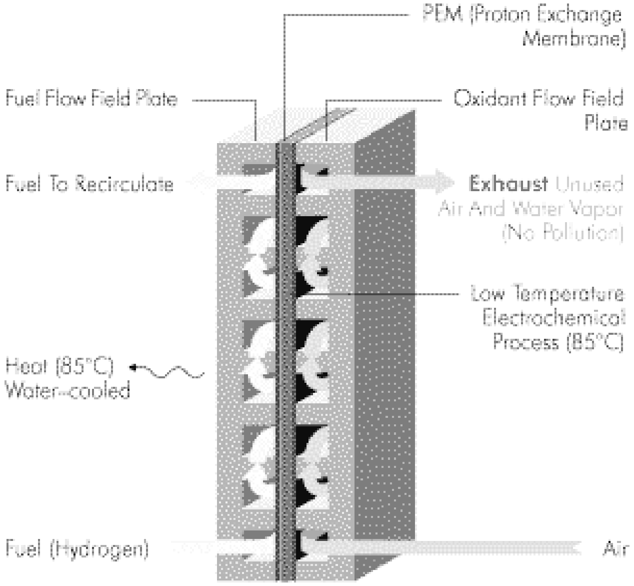
The change in free energy can be used to give the reversible potential of the reaction under standard conditions:

$$\Delta G^\circ = -nFE_r^\circ$$

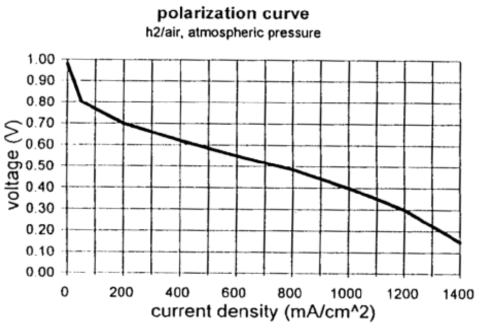
where n is the number of electrons, F is Faraday's constant, and $E_r^\circ$ is the reversible potential. Since n=2 here, $E_r^\circ = 1.229$ V. The reversible potential changes with changing pressure as the Nernst equation:

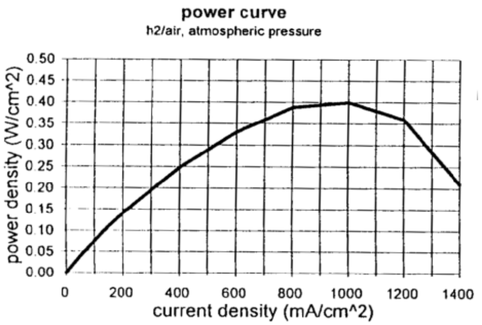
$$E_r = E_r^o + RT\ln\left(\frac{P_{H_2}^* P_{O_2}^{*\,0.5}}{P_{H_2O}^*}\right)$$

Again, n=2. For water in the liquid form, the activity is unity. The partial pressures $P^*$ are measured relative to1 atm.. Essentially, higher pressure means more efficiency.



# polarization curve





source: DTI *Technology Development Goals for Automotive Fuel cell Power Systems* p. 2.3-3

The reversible thermodynamic cell potential, however, is also limited by the kinetics of the reaction. These losses are most often shown in what is known as a Tafel plot or *polarization curve*; cell potential in volts is graphed against versus the cell current density in amperes per square centimeters. The current density basically represents how fast the reaction is taking place (it is the number of electrons per second, divided by the surface area of the fuel cell electrolyte face); voltage as a fraction of the reversible potential ($E_r^\circ$= 1.229 V) is efficiency.

At non-zero current densities, there is what is known as an “activation overpotential”: to drive the dissociation of the oxygen and hydrogen molecules, a certain activation energy must be exceeded. Essentially, the molecules must diffuse in through pores in the metal catalyst, and dissolve into atomic species at the catalyst. The catalyst reduces the height of the activation barrier but a loss of approximately 0.4 V remains due to the still-slow oxygen reaction. Also, competing reactions occur at the oxygen electrode: oxidation of the platinum, corrosion of carbon support, and oxidation of organic impurities.

There a continuous drop in voltage as current increases is due to linear, ohmic losses (i.e. resistance) for ionic conduction through the electrolyte.

Finally, at very high current densities (fast fluid flows), mass transport causes a rapid drop-off in the voltage, because oxygen and hydrogen simply can’t diffuse into the electrode fast enough, and products can’t be moved out quickly enough.

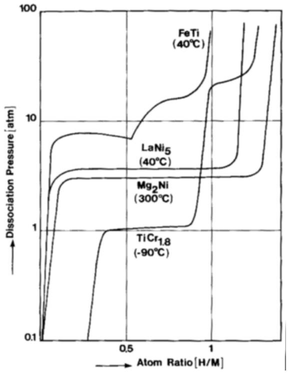
The power curve as a function of current (V•i versus i) shows a characteristic peak beyond which decreasing voltage becomes a stronger negative effect than the increasing current.

# hydrogen storage

At 50% average efficiency, approximately 120 moles of hydrogen are required to travel 120 km. Since reformers are generally too bulky to install in a size-limited vehicle like a scooter, there are two major options for storing the hydrogen: compressed gaseous hydrogen, or adsorbed in metal hydride compounds.

At 250 bar, the 120 moles of hydrogen can be compressed to 14.4 L. This corresponds to an Air Products size “C” cylinder. Made of aluminum, this cylinder would weigh 15 kg without hydrogen, and take up 21.4 L (18 cm diameter cylinder that is 84 cm long). The effective gravimetric density of hydrogen in this case is 1.6%. Current cost is on the order of $300 (Dynetek, 1999)

One disadvantage of compressed hydrogen, that energy is required to compress the hydrogen to storage pressure, can be converted to an advantage if the hydrogen is allowed to expand through a turbine or expander motor as it is released. See discussion under *subsystems*



The pressure-concentration graph at the left shows isothermal filling of the metal lattice with hydrogen. The plateau region represents the actual change in compound structure; at low concentrations hydrogen is simply filling macropores, while at high concentrations the pressure of the vessel is increasing. At higher temperatures the graph shifts upwards.

Example characteristics of a complete TiFe system with heat transfer coils and low-pressure vessel: 1.0 wt% $H_2$ ; 0.024 $g \cdot cm^{-3}$ hydrogen by volume; - 28 $kJ \cdot molH_2^{-1}$ heat of desorption. This corresponds to a mass of 24 kg for the storage system, and a total volume of 10 L. Current prices are about $20/kg TiFe ($480 total), but George Thomas from Sandia estimated a future price of only $5/kg after significant production volumes had been achieved. ($120)

Hydrides offer the inherent safety of endothermic reaction when the hydrogen desorbs; this endothermicity can be used to provide fuel cell cooling.

# subsystems

***Compression and expansion requirements at maximum power (5 kW) for different cycles***

| **type** | **isothermal** | **adiabatic, isentropic** | **adiabatic, 75% efficiency** | **adiabatic, 50% efficiency** |
|---|---|---|---|---|
| Expansion of hydrogen from 250 bar, 300 K to 1.03 bar (0.076 moles/s) | 1044 W<br>(13.7 kJ/mol) | 636 W<br>(8.4 kJ/mol) | 478 W<br>(6.3 kJ/mol) | 318 W<br>(4.2 kJ/mol) |
| Expansion of hydrogen from 250 bar, 300 K to 3 bar (0.076 moles/s) | 841 W<br>(11.0 kJ/mol) | 577 W<br>(7.6 kJ/mol) | 433 W<br>(5.7 kJ/mol) | 286 W<br>(3.8 kJ/mol) |
| Expansion of exhaust gases from 3 bar, 353 K to 1 bar (0.288 moles/s) | 929 W<br>(3.2 kJ/mol) | 818 W<br>(2.8 kJ/mol) | 611 W<br>(2.1 kJ/mol) | 409 W<br>(1.4 kJ/mol) |
| Compression of air from 1 bar, 300 K to 3 bar (0.309 moles/s) | 847 W<br>(2.7 kJ/mol) | 992 W<br>(3.2 kJ/mol) | 1323 kW<br>(4.3 kJ/mol) | 1984 kW<br>(6.4 kJ/mol) |
| Net power required in 3 atm system if tank is full (negative means power available) | -923 W | -403 W | +279 W | +1289 W |

***Total hydrogen expansion energy available (from 14.4 L cylinder, 288 g $H_2$ at 250 bar)***

| **type** | **isothermal** | **adiabatic, isentropic** | **adiabatic, 75%** | **adiabatic, 50%** |
|---|---|---|---|---|
| Total energy available | 1.62 MJ | 0.90 MJ | 0.67 MJ | 0.45 MJ |
| Average specific energy per mole of hydrogen (*) | 11.2 kJ/mol | 6.2 kJ/mol | 4.7 kJ/mol | 3.11 kJ/mol |
| Fraction of electrical power output | 17.1% | 9.5% | 7.1% | 4.7% |
| Average power | 857 W | 474 W | 355 W | 237 W |

The electrical power output and average power are calculated as if the engine were running at maximum output (5 kW), and thus the maximum flow rate and minimum efficiency, for the entire capacity of the cylinder. Note that, as a simplifying assumption, the heat flows required to maintain the systems at a reasonable temperature were not been included.