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EG-D05 MSc Dissertation - Electrical Engineering

Investigating feasibility and design of H2ICEs for small scale static applications

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in the

SPEC
College of Engineering

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Declaration of Authorship

I, Edmund Merrow-Smith, declare that this thesis titled, “Investigating feasibility and design of H2ICEs for small scale static applications” and the work presented in it are my own. I confirm that:

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- Where I have consulted the published work of others, this is always clearly attributed.
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Signed:

Date:

"How does that have anything to do with electronics?"

A classmate, when discussing our assigned projects

"It doesn't. I asked for something different."

My reply, which I would regret a few months into the project

PRYFYSGOL ABERTAWE
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Abstract

SPEC
College of Engineering

MSc Electronics and Electrical Engineering

Investigating feasibility and design of H2ICEs for small scale static applications

by Edmund Merrow-Smith

This project explored the feasibility of converting existing petroleum fuelled engines to run on pure gaseous hydrogen for small scale static power generation.

The hydrogen economy is a proposal to deliver energy using hydrogen. Hydrogen could be produced electrically with excess grid capacity, addressing the variable output of renewable energy generation, acting as an alternative to large scale electrical energy storage.

To convert hydrogen back into electricity, fuel cell technologies have been extensively explored. Despite this, fuel cells are still expensive, limiting early adoption of hydrogen economy. The goal of this project is to promote the start of the hydrogen economy by addressing its cost and capital barriers, through assessing the feasibility of adopting small scale combustion engines as alternative to fuel cells. The ultimate goal is to develop inexpensive off-the-shelf conversion kits for targeted applications of varying complexity and needs.

Heat engine theory, existing engine designs and engine design topics are reviewed. A literature review of previous Hydrogen Internal Combustion Engines (H2ICE) attempts and developments is made and a summary given of advantages and disadvantages of H2ICEs and what issues must be tackled when realising one. H2ICE design is discussed and proposals on how best to begin converting existing engine models are made. The fuel systems are included in the discussion. Fuel storage and fuel lines before the fuel pump or restrictor were beyond the scope of the project are only mentioned for the pressure and temperature of the existing fuel. The project concludes that the H2ICE is feasible for the general use, including the target application, and could potentially outperform petroleum engines in efficiency and emissions, and that off-the-shelf conversion kits is a feasible goal, though much development will be needed.

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List of Abbreviations

BMEP	**B**rake (H_2) **M**ean **E**ffective **P**ressure
CN	**C**etane**N**umber
H2ICE	**H**ydrogen (H_2) **I**nternal **C**ombustion **E**ngine
ICE	**I**nternal **C**ombustion **E**ngine
LPG	**L**iquefied **P**etroleum **G**as (propane or butane)
MN	**M**ethane**N**umber
MON	**M**otor **O**ctane **N**umber
NOx	**N**itrogen - **O**xygen compounds
PV	**P**ressure - **V**olume plot
RON	**R**esearch **O**ctane **N**umber
RPM	**R**evolutions (H_2) **P**er **M**inute
TS	**T**emperature - Entropy **S**) plot

Physical Constants

Ideal Gas Constant $R = 8.314\,459\,8\,\mathrm{J\,K^{-1}\,mol^{-1}}$

List of Symbols

F	force	N ($kg\,m\,s^{-2}$)
x	displacement	m
W	work done (typically kinetic energy change)	J
Q	thermal energy or heat	J
U	internal energy or energy stored as state of matter	J
T	temperature	K
P	pressure	Pa ($kg\,m^{-1}\,s^{-2}$)
V	volume	m^3
n	moles	mol
C_V	heat capacity of a gas under constant volume	$J\,mol^{-1}\,K^{-1}$
C_P	heat capacity of a gas under constant pressure	$J\,mol^{-1}\,K^{-1}$
f	degrees of freedom of molecules of a gas	1
γ	ratio of specific heats for gas	1
η	efficiency (ratio of usable to consumed energy)	1

Chapter 1

Introduction

1.1 Motivation

1.1.1 Engines and Hydrocarbons

We will be talking about internal combustion engines (ICE) that use pure hydrogen gas as a fuel (know as the H2ICE). We will be discussing conventional internal combustion engines, how they work, design considerations, and how to modify existing petroleum-powered ICEs to H2ICEs, with a focus on the 4-stroke.

H2ICEs were, perhaps surprisingly, attempted as early as the 19th century. Even then the attraction of cleaner exhaust gases was enough to inspire attempts. Yet up until now, most engines have burnt petroleum fuels (hydrocarbons) and other carbon-based fossil fuels for their power, both for vehicles and electricity generation. This is primarily this is because such fuels can be found underground and extracted, acting as both energy source and fuel. However, there are problems with this.

1.1.2 Problems with petroleum and carbon fuels

Greenhouse gases

Carbon-containing gaseous compounds such as CO_2 and CH_4 contribute to the greenhouse effect that the earth's atmosphere has on its climate. The IPCC fifth report [18] details how increasing concentrations of greenhouse gases in the atmosphere is increasing the greenhouse effect, and the alarming consequences this may, has and will continue to have on the climate.

Local emissions

The emissions from coal furnaces (sulphur compounds, hot ash and partially burnt coal dust, all slightly radioactive), oil furnaces (oil particulates, CO and NOx) and petroleum engines (oil particulates, CO, NOx and often harmful fuel and oil additives) are locally hazardous to the health of people and the environment.

Extraction

When coal, oil and natural gas are extracted from underground or undersea, either the act or the process can be hazardous to workers (particularly coal mines) and the environment (particularly undersea oil and gas fracking).

Limited Supply

The processes that formed these subterranean reserves are extremely slow and as such economic reliance on their extraction is relying on an ever-dwindling natural stockpile.

Concentrated Supply

The concentration of available reserves in some parts of the world cause political issues as political and economic entities compete for rights to the land or extraction, and those that do not have reserves are forced depend on the few countries that have reserves, giving them lots of political power and causing a drain on the balance of trade of countries that must buy from them.

Other Uses

Natural gas and oil are valuable for uses beyond mere fuels, such that Dmitri Mendeleev remarked burning them for fuel "akin to firing up a kitchen stove with bank notes." [26] Such uses include plastics, lubricants, organic chemistry, medicines and countless others that are uniquely possible with complex carbon chemicals and materials that can be made from crude oil.

These problems provide motivation to find alternate sources of energy. Indeed, such sources have already been found, and the real question is harnessing them and addressing the issues these new generation techniques provide.

1.1.3 Renewable Power Generation

Present electric grid power generation output can be varied rapidly thanks to combined gas cycle turbines and hydroelectric dams. Vehicles also require varied power output and local generation, which their engines are designed to provide. The fuel that is not burnt when demand drops stays stored and can be burnt later. The "carbon economy" revolves around this single fact.[1]

Economies that attempt to replace fossil fuels with large scale renewable energy power generation will find that those technologies (wind, wave, tidal, hydro, solar, geothermal, nuclear[2]) feature two important deficiencies that distinguish their realisation from the "carbon economy".

Vehicle transport

These alternatives are wholly unsuitable for powering vehicle transport and must have some form of energy carrier to get the energy from the generation site to the vehicle, either during travel (as in a tram) or stored and delivered at refuelling points (as with battery cars).

Supply variation

The listed alternatives all directly produce electricity, which is not stored by the wires that transport it, at rates that cannot be completely controlled (though hydrogen is an important exception). They are either invariable (such as geothermal), periodic (such as tidal) or functionally random (such as wind), and to not harness all the energy available at any given time is to lose what was let go. Thus an electric grid whose energy comes mostly from these sources suffers from wasting energy when supply out-meets demand, and from brown-outs when demand out-meets supply.

[1] The burning of domestic and commercial waste (such as paper and furniture) in furnaces for power generation is already practised, but will always be limited and varied in weekly output by the nature of the fuel source and like oil, is not so easy to vary in power by reducing fuel input

[2] Nuclear fission is not strictly a renewable energy, but is worth considering here. However, this paper considers the realisation of nuclear fusion in the coming century so unlikely as to be dismissed.

The core problem is that up until now demand has been uncoordinated as supply can be adjusted quickly to match it and the only buffer present in the system is the storage of the fossil fuels. Large scale electrical storage (pumped storage,[3] flywheels, etc) which is potentially infeasible, attaching the energy demand of vehicles to the grid by making them battery powered, and coordinating consumer, commercial and/or industrial demand are examples of proposed solutions to this.

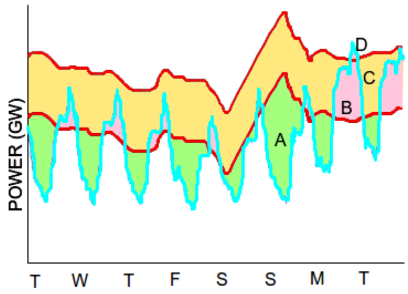


FIGURE 1.1: Typical UK grid demand (blue) with illustrative varying renewable generation (red) for different average production

Figure 1.1 illustrates storage, where attempting to use storage to buffer unmatched supply and demand requires storing a lot of energy if a given week supply consistently outpaces demand (as in this example) or visa versa. A should country such as the UK become dependant on wind power, a plausible week of very little wind might need storage capacities upwards of 1,200 GWh, [24] which may not be feasible. An alternative is to increase average supply , producing large excess, which can then be used

1.1.4 The Hydrogen Economy

The basic premise to the hydrogen economy (and other fuel-energy-vectors such as methanol and methane) is to increase generation above average conventional demand (shown by the higher supply curve in figure 1.1), then use electricity not consumed conventionally (by domestic, commercial and industrial sectors) to produce hydrogen gas, and then use that hydrogen to power off-grid applications such as vehicle transport. The total average demand on the grid now effectively includes vehicles, but the key advantage is hydrogen production can be varied very rapidly so as to very quickly adjust gross immediate grid demand to absorb dips and spikes in demand and supply. Production and electrical storage is now enough to avoid brown-outs without mass demand coordination or mass grid storage, and hydrogen can be stockpiled to continue to supply vehicles during lulls in generation.

Biofuels (which were omitted previously), electric vehicles (using capacitor or battery storage) and hydrogen vehicles are competing existing[4] solutions to vehicle transport. All three are limitedly compatible with each other with the introduction of hybrid vehicles and electric drive-trains. They are heavier, however duel-fuel ICEs that have two tanks with different fuels fuelling the same ICE could make hydrogen and biofuels closely compatible. It must be noted that biofuels compete with food production for fertile land and fertilizer, and soil phosphorous is also limited, to the extent that global biofuel use will likely be limited and impractical in many locations.

[3]Hydro has weekly output limits that vary seasonally, but within those limits, hydro can function as pumped storage by withholding generation until demand rises or supply falls.

[4]Companies in the USA have already brought to market commercially available battery and fuel cell electric vehicles, and engine modifications for diesel and gas biofuels and hydrogen, and some states have seen roadside fuel stations that sell hydrogen gas and biofuels.

1.1.5 Barriers to starting a hydrogen economy

The two primary reasons hydrogen economies are not already common is that petroleum fuels are still available, and that most electric grids and vehicles are equipped rely on them. Agents in countries such as the USA are trying to start hydrogen economies to (among other reasons) reduce local pollution and be less dependant on foreign oil, agents in countries such the UK are attempting to reduce their greenhouse emissions to slow climate change and meet EU goals, while countries such as India who are still developing their infrastructure are attempting to take advantage of their lack of need to integrate with old infrastructure and build to avoid ever having the polluting and import problems of petroleum and coal.

Figure 1.2 illustrates in detail the barriers hydrogen economies presently face. Hydrogen storage can be difficult and dangerous, but cryogenic liquid and pressurized gas are currently available options. Alternatives include atmospheric storage (suitable only for small-scale off-grid applications) and potentially metal hydride-based technology.

It must also be mentioned that alternatives to hydrogen as the fuel exist, such as methanol and methane, which can similarly be made using electricity to produce vehicle fuel, have advantages of being able to re-use some existing carbon-transport infrastructure (in developed countries) but waste more energy in production and as we will see, lack the attractive near-zero undesirable tailpipe emissions.

1.1.6 Promoting the hydrogen economy with the H2ICE

Hydrogen fuel cells are more expensive and wear out faster than petrol and diesel fuelled engines. Improvements are happening, but at a snails pace. Conventional engines are generally less efficient, but currently their low cost outweighs that. Thus, we have motivation to develop hydrogen-fuelled engines, to promote the hydrogen economy, such that when (or if) the (typically) more efficient hydrogen fuel cells improve, uptake will be much easier.

The large number of existing engines also cannot be ignored and a plan that renders these engines obsolete in a short time-frame by quickly replacing all petroleum consumption with renewable generation cannot be considered feasible. Thus we also have motivation to provide conversion at lower cost to their replacement and keep these engines in use.

Other efforts to promote hydrogen economies have included, building roadside fuel stations and subsidizing their supply, making duel-fuel vehicles available that can run off both hydrogen and petrol, encouraging construction of supply points with the promise of existing customers. Figure 1.3 shows the context efforts to promote the university that this project is a part of.

1.2 Goals: conversion kits

Given the large number of existing engines, it would be preferable to convert them to run on hydrogen, rather than replace them with new designs. The prized goal is to develop an inexpensive conversion kit than can be purchased off-the-shelf by customers and be installed follow its instructions either by themselves or by a mechanic to convert any type of engine to run on hydrogen.

There are 6 target applications (and corresponding customer audiences), with increasing difficulty, that should be consecutively developed for.

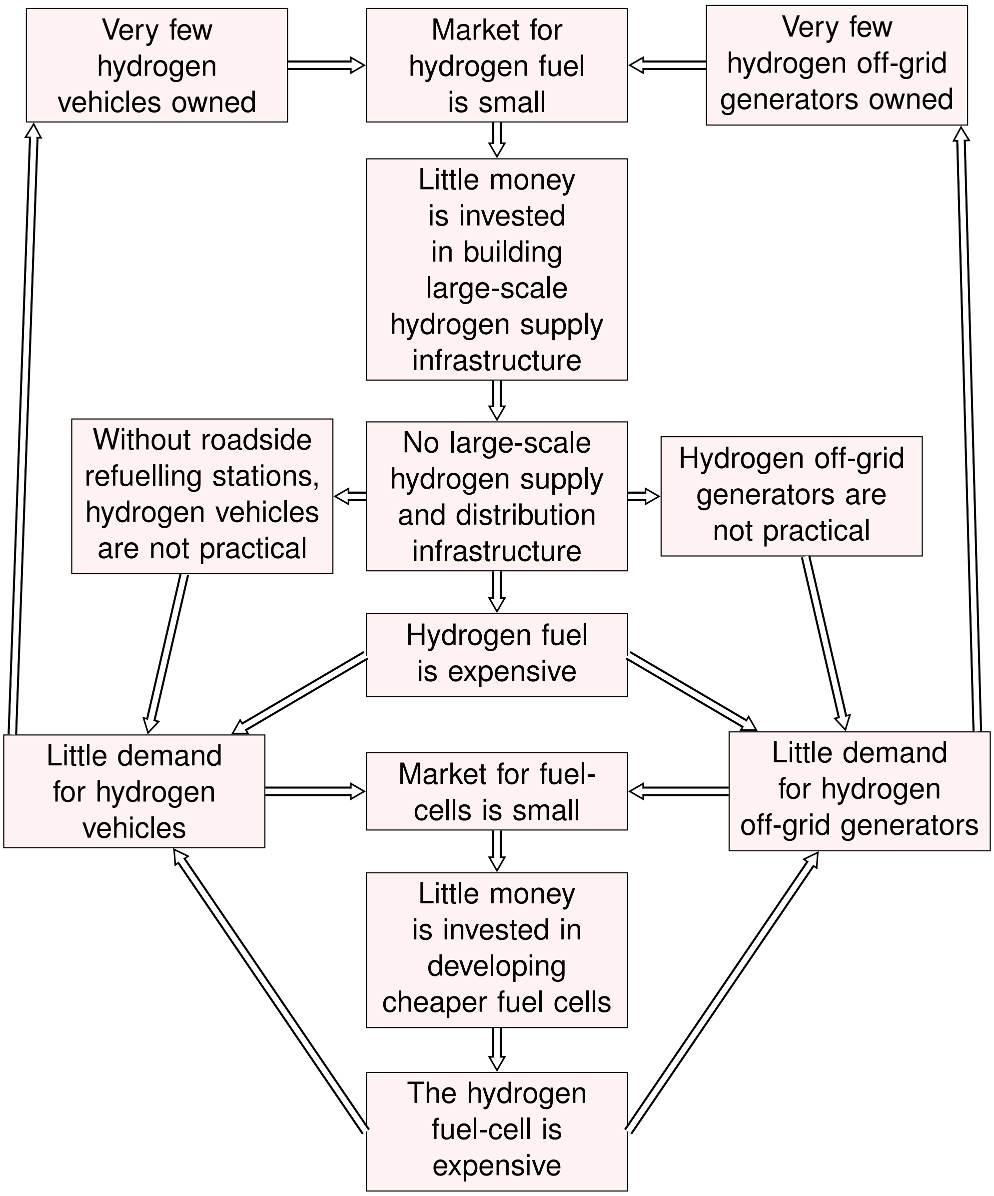


FIGURE 1.2: Economic flowchart of demand and supply for the hydrogen economy, illustrating barriers to its introduction.

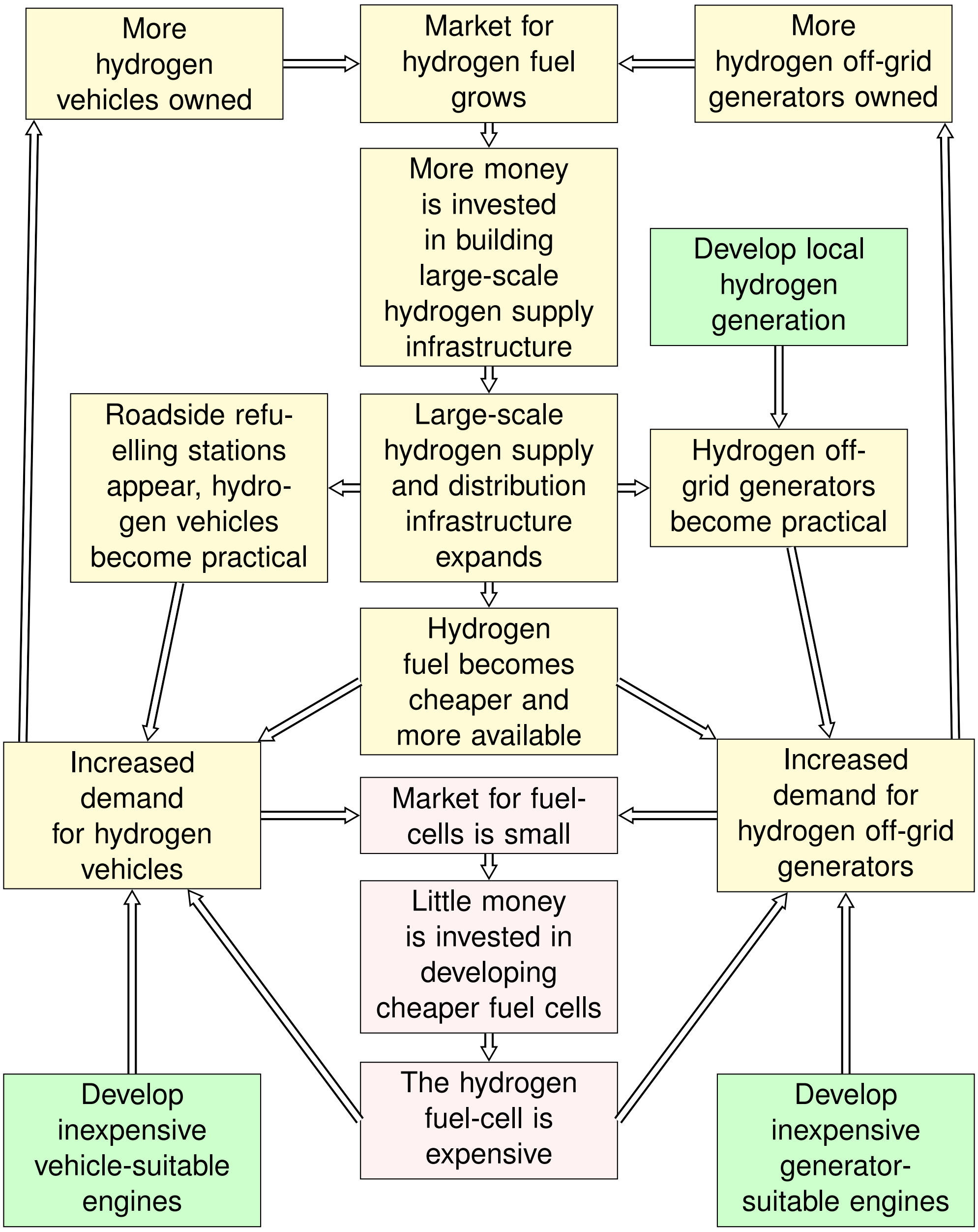


FIGURE 1.3: Economic flowchart of demand and supply for the hydrogen economy, highlighting efforts being made to overcome barriers that this project is a part of.

Prototype The point where this project will begin. It must first be demonstrated that hydrogen as an engine fuel can work. If it does, then in future, in order to familiarize oneself with engines, hydrogen fuel, hydrogen fuelled engines and engine modification, anyone setting out to attempt to provide hydrogen conversion should first familiarize themselves with this step. This is the only step where the safety of the design may be sacrificed somewhat (and made up for by proper procedure to make up for safety to persons and property involved).

Manned off-grid applications Low-power applications (such as for low power, even hand-held equipment on rural farms and forestries) where grid connection is unlikely or troublesome, and where an operator is present to start the generator, run the machinery, to replace or refill and hookup fuel tanks, and to maintain and repair the equipment. Cost is the dominant factor.

Unmanned off-grid sites Medium-power automated applications where inspections are rare (such as remote telecommunications towers) where a local renewable energy generator (such as a solar panel) powers the equipment and produces hydrogen during the day, then at dusk a small battery starts the generator, which powers the equipment at night. Reliability in running and starting are the dominant factors.

General site backup generators Critical, high-power commercial and state applications (such as data storage facilities) that must always be kept online to the extent of requiring large battery or flywheel banks on standby to provide immediate response. A backup generator is used for longer outages, typically a diesel engine in a basement or in a side building, which could be converted to a H2ICE. The site can be expected to handle more complex requirements from advanced fuel storage, starter and control systems and be less concerned about efficiency and cost, but a challenge may come in the engine sizes that come with the high power outputs now required.

Hospital backup generators Similar to general site backups, however hospitals may now be concerned with noise, cost[5] and especially reduced tailpipe emissions.

Public transport and delivery vehicles Buses, plant equipment, tractors, trains and trucks are medium to high power applications where packaging, vibration, reliability, maintenance, cost and expected lifetime begin to become important and conflict with power and weight requirements, but making problematic components larger and more robust (or cheaper and disposable) is still a tolerable approach.

Road vehicles Small to medium power applications where tailpipe emissions, fuel consumption, maintenance, cost, reliability, vibration, and especially packaging become very important, while weight becomes critical. Here every design decision will factor a compromises between improving these conflicting performance factors and removing weight.

[5] A hospital could be expected to have a more thinly stretched budget than a highly profitable data centre with deeper pockets.

Chapter 2

Thermodynamics

We shall first conduct a review of the basic physics underlying engines in order to have it freshly in our minds for analysis of engine design. Theoretical foundations of thermodynamics are widely available in standard thermodynamics textbook, the purpose of this chapter is to clearly highlight the relevant concepts needed to understand the mechanics of how engines produce work from heat and the ultimate limits of how efficient they can be.

2.1 Semantics

2.1.1 Engine

The noun *engine* has an broad etymology that has included *war machine* and *craft [large vehicle]* in the past, and now for software and weather[1] too. So as to clear up understandable semantic confusion, for our purposes, we are referring to *heat engines*; a concept in thermodynamics and a practical human invention that generates work from heat.

2.1.2 Work

$$\text{Work Done} = \text{Force} \times \text{Displacement} \qquad W = \int F\,\delta x$$

Work essentially means useful energy. It takes work to push a car, saw a block of wood or turn an electric generator. A simple definition of work is if a device can lift a weight (say by turning a crank on the end of a pulley), then it has done work. Specifically, a mass of 1.02 kg (a weight (force) of 1 newton on earth) raised by 1 meter produces 1 joule of work. Similarly, if the same weight is lowered by 1 m, then the weight will have done 1 J of work on the crank (and whatever device was connected to it).

2.1.3 Heat and Temperature

$$\text{Heat Capacity} = \text{Mass} \times \text{Material Specific Heat Capacity} \qquad C = mc$$

$$\text{Change in Temperature} = \frac{\text{Heat Added}}{\text{Heat Capacity}} \qquad \Delta T = \frac{Q}{C}$$

Heat and temperature are separate concepts, and this is vital to understand. *Heat* refers, strictly, to the thermal energy of an object (or mass). Temperature is essentially

[1] As we will see, weather systems actually fall under *heat engines* as well.

the average thermal energy of an object. A large object with a low temperature may have the same total thermal energy as a small object with a higher temperature. For this entire work, the collective noun 'heat' refers strictly to thermal energy, and the verb 'to heat' refers to adding thermal energy to an object or gas.

2.1.4 Entropy

Entropy is as a measure of (dis)order, however saying this is not of much help if one is not already familiar with the concept in physics. If a box of dust floating in space has all the dust on one side, then any motion by the dust is more likely to change this situation to one where the dust is more evenly spread throughout the box than it is to leave it unchanged. However, a similar box with evenly spread dust is extremely unlikely to find itself in the first situation. This describes, in brief, the transition of an ordered (in this technical sense), low entropy state, to a more disordered, higher entropy state. Effort may be expended to gather the dust, but the box where this effort came from will grow more disordered (gain more entropy) than the first box will become ordered (lose entropy).

$$\text{Change in Entropy} = \frac{\text{Heat added (or removed)}}{\text{Temperature}} \qquad \Delta Q = \int T\ \delta S$$

Entropy and Temperature are intimately related and both are complex concepts to understand when considering their full definition. Such is beyond this short review, but we will say that entropy is part of an object's state, similar to temperature, and again like temperature has to do with the density of heat, and that every event in the universe increases the total entropy. We mention it only for this chapter, as it is useful in understanding thermodynamic cycles and illustrating their efficiency.

2.2 Assumptions

To discuss thermodynamics, we will use a model universe that is very much simpler than our own, to make the physics clearer. This model universe makes several assumptions:

- Frictionless world (no relation to the second law of thermodynamics)
  - No friction between objects in contact
  - Fluids have no mass, momentum or inertia
  - No effort needed to move through fluids
  - No effort needed to push fluids
- All gases are monatomic ideal gases (such as helium) and that the ideal gas law without high density correction applies
- Perfectly thermally insulating materials are available
- Perfectly air-tight containers and seals are available
- Heat exchange and chemical reactions may take place instantly with no by-products

2.3 Laws of Thermodynamics

These laws describe how heat is able to be converted to work, and what the limits are for it.

0th law All heat is of the same form

1th law Heat and work are two forms of the same energy

2nd law Not all of said heat can be turned into work without the availability of a 0 K heat reservoir

3rd law It is impossible to cool something to 0 K in a finite number of steps.

As we will see later, all heat engines involve a *hot end* and a *cold end* (more formally *heat reservoirs*) and no engine can operate without this temperature difference. This also means that no practical engine can be 100% efficient.

2.4 Adiabatic Process

The term *adiabatic process* in thermodynamics refers to a process where a gas changes state while isolated from its environment. A relevant example is the squeezing of a piston with good insulation, good sealing and no friction.

Combining the ideal gas law with the first law of thermodynamics, we understand what when effort is put into squeezing a gas, the gas heats up, because energy has been introduced into the gas and converted to heat, increasing the total thermal energy of the gas. In reverse, when a squeezed gas is allowed to expand, its temperature drops because that energy has now been converted to work.

The temperature change seen is not due to the original total heat energy of the gas being distributed over a smaller or larger space,[2] or due to heat conduction[3] but because work done on the gas and converted to heat. The ultimate explanation for this conversion involves statistical analysis of the molecular collisions that explain pressure, which can either leave a molecule with more, less or the same kinetic energy it had before the collision. The movement of a container surface changes the distribution of these collisions so as to (on average) add or remove energy from the gas.

For our purposes, an analogy to a spring is preferred (illustrated in figure 2.1). To compress a spring, a force must be applied and maintained over the displacement, meaning work is done on the spring. After compression, this energy is now stored in the spring (ultimately, in the atomic bonds of the spring material).

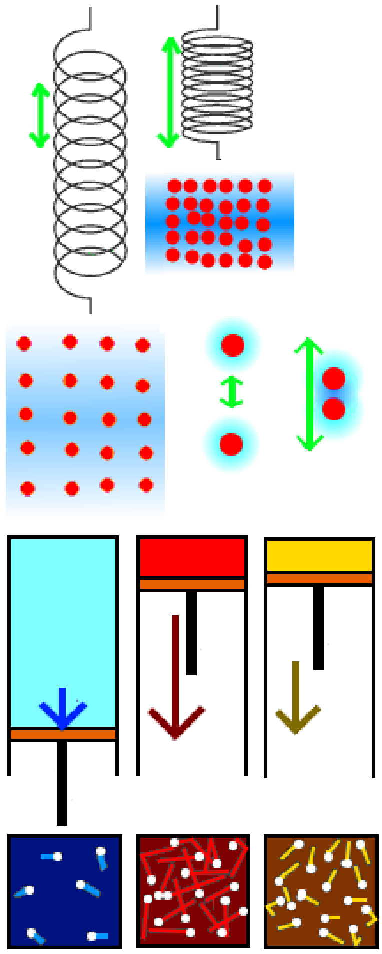


FIGURE 2.1: Energy stored in a compressed gas is somewhat analogous to the energy stored in a spring

[2]It is still distributed over the same mass.

[3]This would decrease, not increase the change seen.

For a piston, the pressure inside increases as it is squeezed, generating a pressure difference across the piston which must be overcome with a force to continue compression. Again, a force is applied over a displacement, so work is done on and the energy stored in the gas. This time, the energy is stored in the added kinetic energy of the gas molecules, resulting in more energetic collisions, so higher temperatures and pressures seen at the container surface.

We can now understand that when a gas is compressed, and then heat is added to it, it can do more work during the expansion than was needed to compress it. The gas can expand to a greater volume then it started at, doing more work total work than was done on it. The pressure is higher during the initial expansion, so more work was also done during the expansion up to the original volume and in fact comparatively little work can be had from the remaining expansion

2.5 P V and T S diagrams

A pressure-volume diagram visually describes how pressure increases during an adiabatic process. We can use a little algebra from the assumptions we've made to calculate how the pressure rises for a gas expanding adiabatically.

The area swept under any curve that describes a given mass of expanding or compressing gas, is the work done on or by the gas, regardless of adiabatic condition. This is clear to see when the volume swept is a prism, so the cross sectional area A and height x can reduce the pressure-volume curve to a force-distance curve. Such a curve would typically start or finish at zero newtons, as in an atmosphere, the force exerted on a cross section is the produce of the area and the difference between the pressure seen inside and outside (p_0) the volume.

Idea Gas Law	$PV = nRT$
First law	$\delta W = \delta Q - \delta U$
No heat exchange	$P\delta V = -\delta U$
Gas specific heat capacity	$c_v = \frac{1}{n}\frac{\delta U}{\delta T}$
Using $R = c_p - c_v$	$n\delta T = \frac{-P}{c_v}\delta V$
	$= \frac{P\delta V + V\delta P}{c_p - c_v}$
Using $\gamma = \frac{c_p}{c_v}$	$0 = \frac{\delta P}{c_v} + \gamma\frac{\delta V}{V}$
Integrating	$k = \ln PV^\gamma$
So for ideal gas nR	$\frac{P_1V_1}{T_1} = \frac{P_2V_2}{T_2}$
for adiabatic condition	$P_1V_1^\gamma = P_2V_2^\gamma$
with no entropy change	$\Delta Q = \Delta S = 0$
In atmosphere with P_0	$F\delta x = (P_1 - P_0)A\delta x$

Figure 2.2 is an example PV diagram of an adiabatic process. The green area W is the work done on the piston. The red area w_0 is the work done by the atmosphere; p_0 is local atmospheric pressure. The work area cannot be plotted for a logarithmic scale as graph area represents exponentially more work the higher the pressure and volume get. It is also known as an isentrope as the equivalent path drawn on a temperature-entropy (TS) diagram would be a vertices line, with no change in the system's entropy.

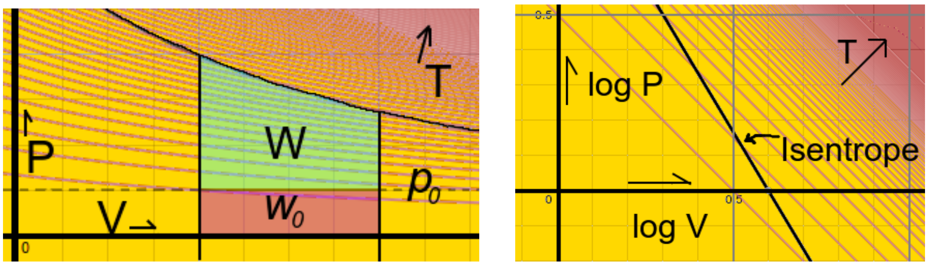


FIGURE 2.2: Linear (left) and logarithmic (right) scaled PV diagrams of an isentropic compression.

2.6 Polytropic Paths

Processes that follow any path other than the curve of an isentrope, exchange heat and change the system entropy. Every curve on the PV diagram translates to the TS diagram and visa versa. Just as the swept area under curves on the PV diagram describes the work done during that curve, the TS diagram describes the heat exchanged. Combining the two, it is now possible to calculate both the heat exchanged and the work done in any thermodynamic process applied to a gas sealed in a piston.

When P, V and T are plotted on logarithmic scales, certain gradients of straight line represent processes where one of these variables is held constant. Figure 2.3 and table 2.1 give the gradient of these lines for both the PV and TS graphs. When these graphs are translated back to linear scales, the areas swept by processes on the PV graph represent the work they do and areas swept on the TS graph represent heat they release. An adiabatic process (the isentropic curve) is special in that, by definition of having no heat exchange, it involves no entropy change, and is reversible and does not require heat reservoirs.

Curve	Constant	$\ln(PV)$	$\ln(T)S$	Work done
Isentropic	Heat	-γ	∞	$C_V(T_1 - T_2)$
Isothermal	Temperature	-1	0	$RT\ln\frac{V_2}{V_1}$
Isochoric	Volume	∞	$1/c_v$	0
Isobaric	Pressure	0	$1/c_p$	$P\Delta V$

TABLE 2.1: Summary of polytropic path gradients

2.7 Thermodynamic cycles

We can now combine these processes to into loops on the PV and TS graphs to form thermodynamic cycles, and analyse the work and heat output of these cycles. The work done and heat absorbed by a given cycle is equal to the area swept within the cycle. These areas will be equal for any given cycle and represent the heat converted to work or visa versa.

Whether the cycle moves clockwise or counter-clockwise defines whether it acts as a heat pump (absorbing work and moving heat from cold to hot) or heat engine (producing work and moving heat from hot to cold). Some cycles may have clockwise and counter-clockwise, in which case clockwise and counter-clockwise areas subtract from one another and the input and output of the cycle is the final area.

The most important cycle is the Carnot cycle, an engine cycle that is special in that for a given maximum and minimum temperature, it produces the most work for the

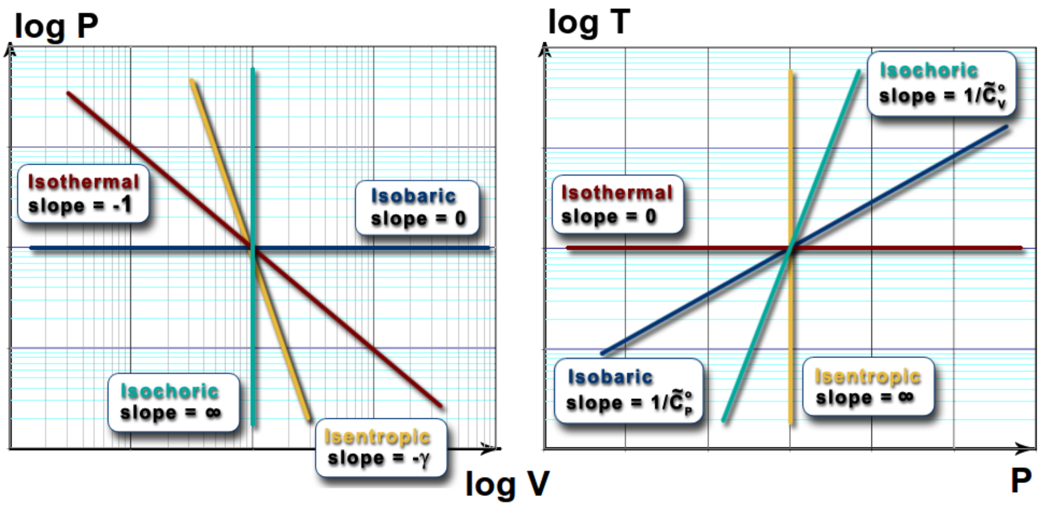


FIGURE 2.3: Summary of polytropic paths [1]
(Note the log-log PV and semi-log TS scales of each diagram.)

least lost heat, so is the ultimate efficiency limit for engine working from a heat difference. This can be demonstrated graphically (see figure), where it is clear that the ratio of input heat to output (wasted) heat is the ratio of areas on the TS diagram within and below the cycle, which is most efficient for the rectangular Carnot cycle, given only a temperature restriction.

In figure 2.4 we see that any deviation from the rectangle reduces Q_{WORK} more than Q_{LOST} or increases Q_{LOST} more than Q_{WORK}, decreasing efficiency. Note that the area below the cycle on the PV graph is the energy needed to start the cycle, but has no component in efficiency.

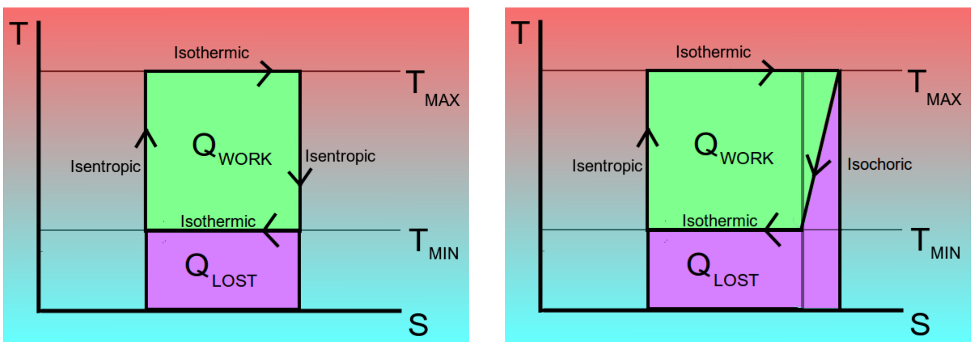


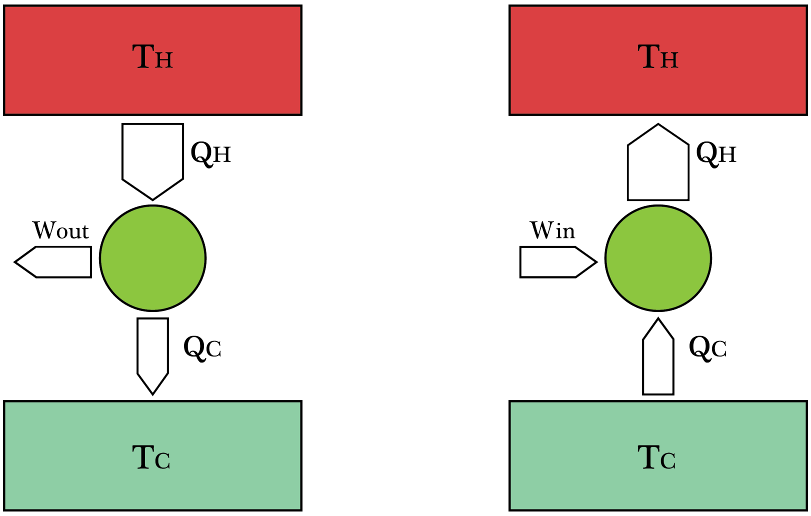
FIGURE 2.4: Perfect Carnot cycle (left) vs example deviation (right)

2.8 Engine cycles

It is useful to know and understand engine cycles other than the Carnot cycle, and pay attention to their efficiency compared to that of a Carnot cycle. For all of these cycles, the bottom-left of the lower two corners is the starting position, where the pressure and temperature of the sealed gas is equal to the local ambient air.

This list is only of a few relevant examples and only include cycles that involve no state change between liquid and gas. The PV and TS graphs of each cycle are laid

FIGURE 2.5: Thermodynamic cycles and their Carnot efficiency



(A) Theoretical Heat Engine (B) Theoretical Heat Pump

heat absorbed from hot reservoir	$Q_H = Q_C + W_{out}$
heat lost to cold reservoir	$Q_C \geq Q_H \frac{T_C}{T_H}$
energy converted to usable work	$W_{out} \leq Q_H(1 - \frac{T_C}{T_H})$
heat engine Carnot efficiency	$\eta = \frac{T_H - T_C}{T_H} \geq \frac{W_{out}}{Q_H}$
heat pump coefficient of performance	$COP = \frac{T_{H/C}}{T_H - T_C} \geq \frac{Q_{H/C}}{W_{in}}$

over the same Carnot cycle graphs in figure 2.6 to act as a reference to make visual comparison between other cycles easer. We should note that practical implementations of these cycles exhausts used air and inhales fresh air, but for analysis we will assume the gas is cooled and re-used to close the cycle.

The ratio of area swept under the top of the TS cycle (the total heat added) to area swept within the TS cycle (the heat converted to work) gives the efficiency. The area swept within the cycle on both the PV and TS graphs represents the heat converted to work, but the area under the lower PV curve represents only the work needed to start and maintain the cycle, and does not factor into efficiency. As a final reminder, these diagrams are on log and semi-log scales, and the value of each unit of area increases along a logarithmic axis, so area on the diagram does not translate linearly to the correct value of work or heat.

2.8.1 Carnot cycle

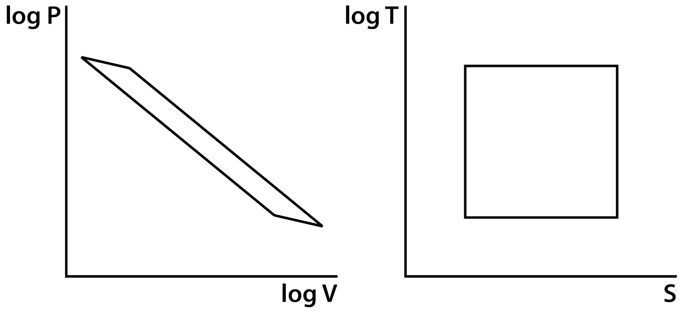


FIGURE 2.6: Carnot cycle

An important feature to note here is that the isentropic expansion expands below the starting pressure and recovers energy during condensation, which unique in this list to the Carnot cycle,

$$\eta = 1 - \frac{T_{COLD}}{T_{HOT}}$$

2.8.2 Brayton cycle

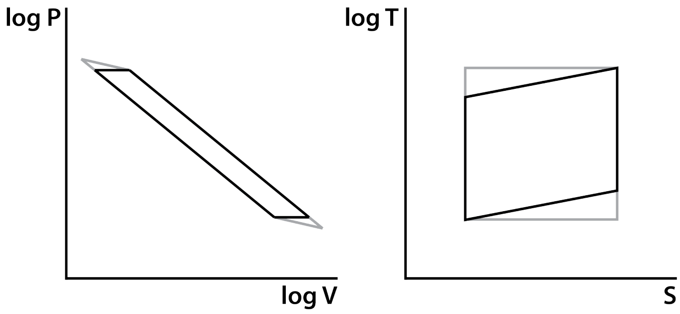


FIGURE 2.7: Brayton cycle

The Brayton cycle is close to the operation of gas turbines and jet engines. It skips the impractical isothermic contraction of the exhaust and adds fuel to maintain an isobaric path, which is more practical than attempting to adjust pressure to maintain an isothermic path.

$$\eta = 1 - \left(\frac{P_{LOW}}{P_{HIGH}}\right)^{1-\frac{1}{\gamma}}$$

2.8.3 Otto cycle

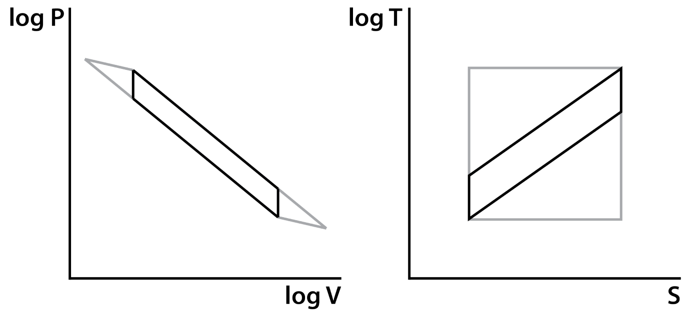


FIGURE 2.8: Otto cycle

The Otto cycle is more practical for many engines than the Carnot or Braydon cycle as the entire cycle stays within a volume difference (forming a compression ratio), where the larger volume limit is the starting point, which is very suitable for a piston engine.

$$\eta = 1 - \left(\frac{V_{MIN}}{V_{MAX}}\right)^{1-\gamma}$$

2.8.4 Diesel cycle

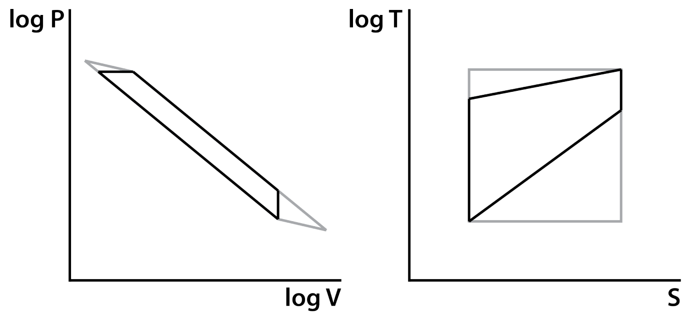


FIGURE 2.9: Diesel cycle

The Diesel cycle is a modification to the Otto cycle replaces the isochoric heat addition path with the more efficient isobaric. For a given compression ratio with the same heat input, an Otto cycle engine is more powerful and more efficient than a Diesel cycle engine, but when the compression ratio is raised to have equal maximum pressure and temperature, the Diesel cycle becomes more efficient, while still maintaining the advantage of the fixed volume difference.

$$\eta = 1 - \frac{1}{\gamma}\left(\frac{\Delta V_{ISOBARIC}}{V_{MAX}}\right)^{\gamma-1}$$

2.8.5 Aktinson cycle

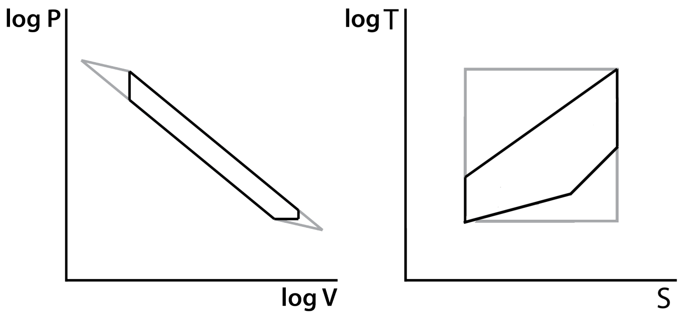


FIGURE 2.10: Aktinson cycle

The Atkinson cycle extracts more energy from the exhaust than the Otto cycle by having the gas expand beyond the starting volume, which may or may not be practical for a given engine.

2.8.6 Lenoir cycle

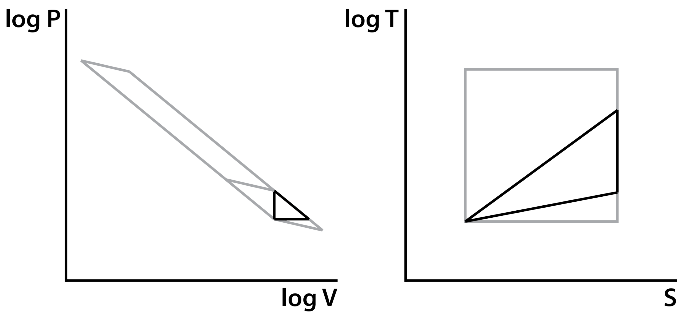


FIGURE 2.11: Lenoir cycle

The Lenoir cycle is the result of an engine that does not compress the gas before adding heat, such as a pulsejet. Efficiency is terrible, whether compared to the original Carnot cycle, or a smaller one for just the temperature difference seen.

2.8.7 Otto cycle with Turbo

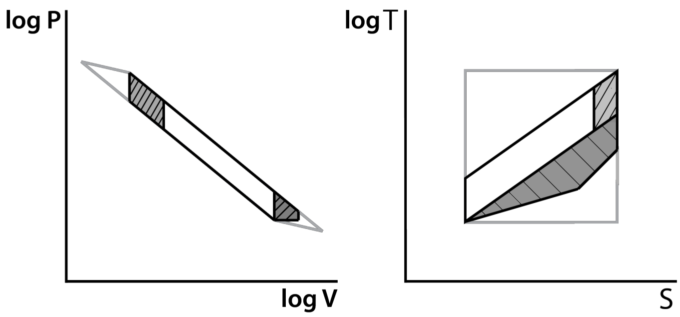


FIGURE 2.12: Otto cycle with Turbo

Otto cycle engines can be fitted with an intake compressor powered by a turbine on the exhaust. This becomes more complicated to analyse as the speed of the turbo

shaft is variable and affects the compression ratio. The turbo can harness the extra shaded work at the exhaust to spool-up (accelerate), but once a maximum speed has been reached, a wastegate opens, losing this shaded region so as not to over-spool the turbo and operate at speeds that would damage it.

2.8.8 Otto cycle with Intercooled and Fully-spooled Turbo

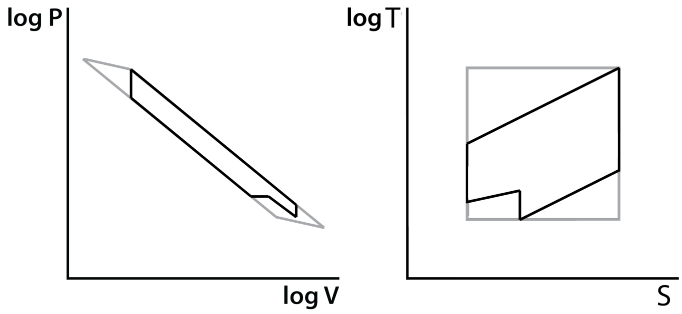


FIGURE 2.13: Otto cycle with intercooled and fully spooled turbo

By adding an intercooler to remove heat from the air between the turbo and the engine intake, a greater initial volume of air can be compressed without needing a larger engine or turbo. This has power-to-weight advantages, but reduces efficiency.

2.8.9 Otto cycle with Intercooled Supercharger

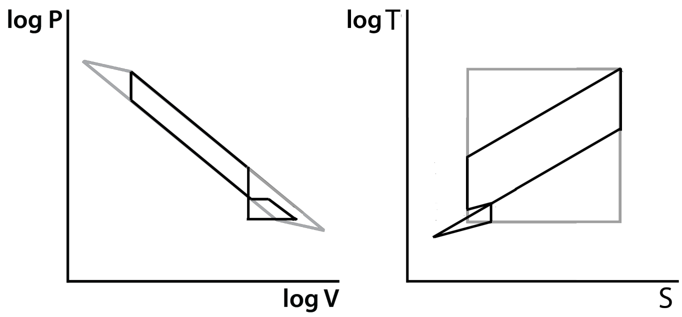


FIGURE 2.14: Otto cycle with intercooled supercharger

A supercharger runs off the engine crank rather than exhaust gas. Combining a supercharger with an intercooler avoids the problems of waiting for the turbo to spool, while increasing power-to-weight, but at such a drastic decrease in efficiency that without sufficient input heat, the work done during expansion is smaller than the work done during compression due to the effective compression ratio being greater than the expansion ratio, which on the PV plot forms a small counter-clockwise loop that takes work out of the engine output.

2.9 Practical Considerations

Internal combustion engines get their input heat from burning fuel, and fuel can burn at any temperature, given the right circumstance. For a quick thought experiment, a methane-oxygen gas mix at 200 K air will burn with a lower flame temperature to the

same mix at 3000 K. Thus for internal combustion engines, the highest temperature reached is not a hard limit.

Without a hard limit on the temperature of the hot heat reservoir, that the Carnot cycle is the most efficient engine cycle possible for a given pair of heat reservoirs loses its relevance. Further, the available temperature limits are unlikely to be the only or even the dominant constraint on efficiency.

Extremely high temperatures are undesirable as they limit the function and lifetime of the engine, but generally pressure is a far more important limit for any real engine design. Additional constants appear when considering engine modification, where some parameters are difficult and undesirable to alter due to packaging, cost or other issues.

For each given constraint, each cycle will perform with different efficiency and maximum power output, as shown in table 2.2.

TABLE 2.2: Best cycles for given metric under dominant constraint

Metric	Constraint	Best cycle
Efficiency	max T	Carnot
Efficiency	max P	Brayton
Power	min V & fix V	Otto
Efficiency	min V	Atkinson
Efficiency	max P & fix V	Diesel
Power	no V	Lenoir

However, all of these cycles are theoretical and without the assumptions made in section 2.2, practical engines have PV plots those in figure 2.15, where the corners are rounded and the plot curves inwards from the theoretical. The cycles we have discussed are useful for analysis by telling us what cycles form from what design choices, and so illustrate the implications to the ultimate efficiency these design choices have, and inform us on how easy it will be to get the real engine cycle to match its design.

We can describe two design choices right now by removing our assumptions and predicting how behaviour changes.

Higher Maximum Temperature

- Increased thermal wear
- Increased chemical reaction speeds
- Increased heat loss through conduction

Higher Maximum Pressure

- Increased mechanical wear
- Greater difficulty sealing gases
- More mechanical strength required

There are also considerations about engine speed and load that make some cycles more practical than others for many applications. We will see later that most Otto or Diesel cycle engine designs are trivially adjusted to recover more exhaust gases such as in the Atkinson cycle rather than isochorically return directly back to the starting point. The reason for this is that it removes the primary advantage that Otto and Diesel cycles provide over Brayton cycles, namely adjustable output with no effect on efficiency. For

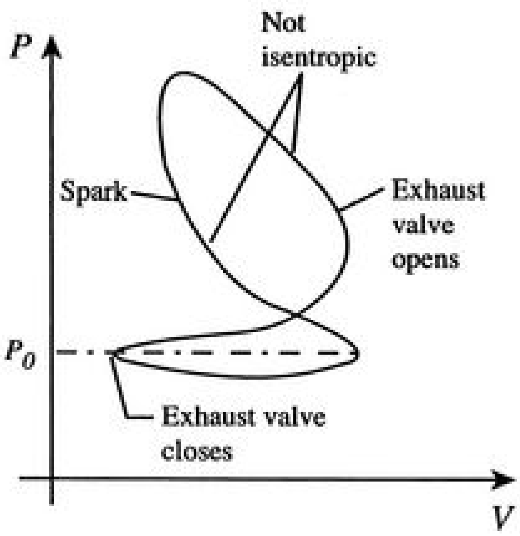


FIGURE 2.15: Typical example of the real PV plot of an Otto cycle engine [2]

a fixed expansion ratio that's above the compression ratio, there will be an input heat rate below which the gas is forced to expand and drop below ambient pressure before being exhausted, requiring work to achieve that is not recovered. Above this heat rate, efficiency drops off as the efficiency gained from the isobaric return becomes negligible compared to the isochoric return, approaching the behaviour of an Otto cycle. Figure 2.16 illustrates this.

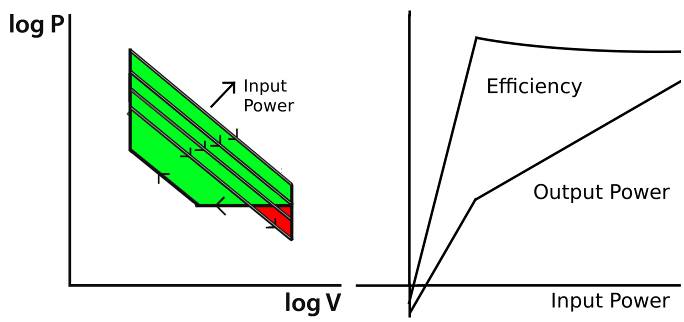


FIGURE 2.16: Efficiency of an Atkinson cycle with input power

Chapter 3

Internal Combustion Engines

3.1 Introducing the ICE

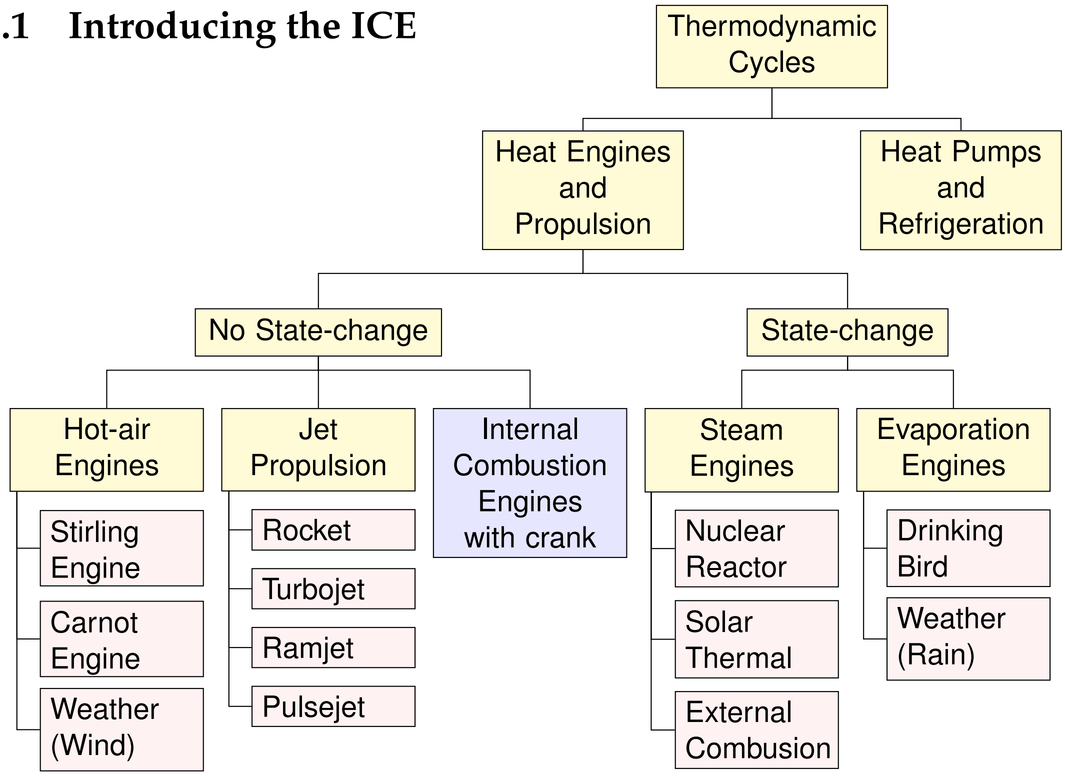


FIGURE 3.1: Categorization of the ICE, with some named examples to compare engine types outside our scope.

With the understanding gained in the previous chapter, it is now possible to think up of any number of ways of extracting work from fuel and air. Inventors and engineers of the past have spent much time inventing countless new engine designs and improvements to old designs, all based on this knowledge. Engines can even be found in nature, where a contained gas is exposed to a temperature difference. Here we find it useful to categorize engines, to contextualize and define our scope, and to illustrate some factors that will and will not arise in the analysis.

We are interested in small-scale (<1 MW), internal combustion engines with crank outputs (currently for off-grid electric generators but with an eye for road and marine vehicle applications). All categorization is arbitrary, and there are too many engine types to be complete, but figure 3.1 satisfies our goal. This illustrates that the engines we will look at will not involve state changes (constant internal energy U), that the number of moles of the work-performing gas may not stay constant (as in hot-air engines), and that any thrust exerted on the engine by the exit momentum of exhaust gases is not beneficial to the engine's performance (as in jet propulsion). Concerning

that last point, however, exhaust gases with momentum will also have energy, and while the thrust may not be relevant, there are 4 other relevant aspects of an engine's exhaust.

- Exhaust gases can produce a lot of noise, which outside of motorsport entertainment, are varyingly undesirable.
- Exhaust gases of a given ICE often have a lot of energy, which can be harnessed.
- Exhaust gases obviously have more oxygen and less carbon dioxide than the intake air, but there are typically other gases or particulates in the exhaust that formed or were picked up during combustion.
- Exhaust gases are often hot, as Carnot cycles that return the exhaust gas to its original intake temperature are typically not practical. This poses a potential burn hazard, and has implications for the chemistry of the exhaust gases.

3.2 Note on assumptions and efficiency

$$\text{efficiency } \eta = \frac{\text{RPM} * \text{BMEP}}{\text{total mean fuel consumption}} = \frac{\text{brake horsepower}}{\text{fuel energy rate}}$$

FIGURE 3.2: Typical description for fuel efficiency of an ICE

The efficiency of and ICE is the ratio of the available power in the crankshaft to the fuel energy of the fuel injection rate, and is typically less than 50% efficient. Besides the inefficiency due to the thermal cycle (called reversibles), there are irreversibilities that arise when we transition a given engine design from a frictionless model to a practical machine. They either directly affect the shape of the P-V and T-S graphs, universally changing them to less efficient shapes, produce a force on the crank that the crank must do work against, or amplify another irreversibility.

Heat Conduction Heat lost to the combustion chamber and piston or rotor must be removed by the cooling system to maintain optimal operating conditions, directly affecting the thermodynamic cycle.

Incomplete Combustion Sometimes some of the fuel goes unburnt (or only partially burnt) and exits the exhaust, and the fuel energy it represented went unused by the thermodynamic cycle.

Variable and Non-zero Combustion Rate The combustion affect the rate of heat release, which affects the thermodynamic cycle.

Combustion By-Products The very high temperatures seen during combustion can cause chemical reactions to occur (such as NOx. These reactions absorb heat energy and store it in their higher energy chemical bonds, directly affecting the thermodynamic cycle.

Mole-count changes The combustion event (and side-reactions) can change the total mole-count of gas, increasing efficiency if the reaction produces more moles (doubly so by reducing temperature and heat loss without directly affecting thermal efficiency), or visa versa.

Leaks Gases in the combustion chamber, before, during and after combustion can leak out, reducing the pressure inside the chamber and affecting the thermodynamic cycle. Gases can gas escape between pistons or rotors and the camber walls (blow-by) and past imperfect sealing on any valves.

Scavenging Despite intake, chamber and exhaust designs that take the aerodynamics into consideration, some of the exhaust gases are not pushed out by the piston and incoming intake gas, and stay in (or reach back into) the combustion chamber, affecting the thermodynamic cycle.

Air Resistance Skin drag of gases moving through their containers, turbulence produced by changing direction, all produce a force against the crank that require work to overcome.

Sliding Friction Despite lubrication, every component that must slide past another produces friction that pulls against the crank.

Vibration Friction Motions inside the engine can lose energy by causing vibrations to occur, which are not recovered, so the crank must work harder to make up for the loss.

Flexing Friction Similar to vibration, materials strain under stress, and not all the work done to flex the material is recovered.

3.3 Designs

3.3.1 Categorizing ICE Designs

Even within just crank-turning ICEs, there are still too many existing and new designs to discuss (and most not worth mentioning), so we find it useful to categorize engines, which will prove useful later for analysis and design of hydrogen fuelled engines.

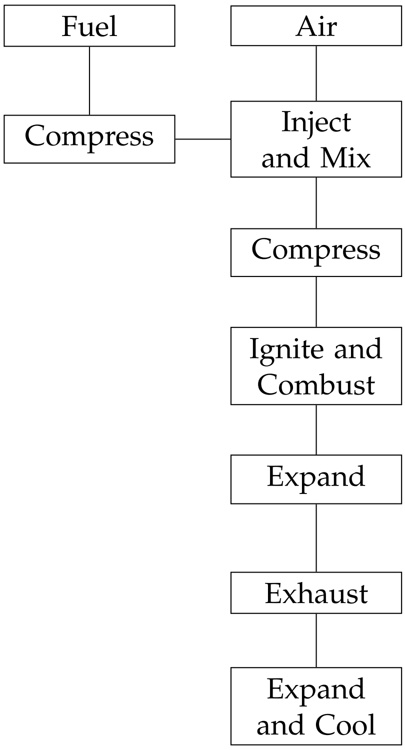
3.3.2 By Fuel

Unlike hot-air and steam engines with external combustion cambers, the physical and chemical properties of the fuel and the character of the flames they produce have a consequences for the design and performance of engines. There are two broad strategies for preparing the combustion chamber and igniting the fuel, shown in figure 3.3, and it is useful to categorize both engines and fuels by how well the properties of the fuel match the strategy of the engine.

Further, an engine may feature a continuous flame and require only an initial ignition at start-up (such as in a gas turbine), or an engine may repeatedly ignite separate flames, requiring a reliable method of ignition for every combustion event (such as a 4-stroke). This further categorizes fuels and engines

Any engine type can, with effort in the design, run on any specific fuel, but most engines are more suited to fuels of one of three fuel types. Specific fuels are rated by how well their properties match the ideal fuel of that type (referred to as the quality of the fuel), and specific engines will be more or less susceptible to problems characteristic of it's type as lower quality fuels are used.

(A) Otto (or Petrol) Engine Operation



(B) Diesel and Turbine Engine Operation

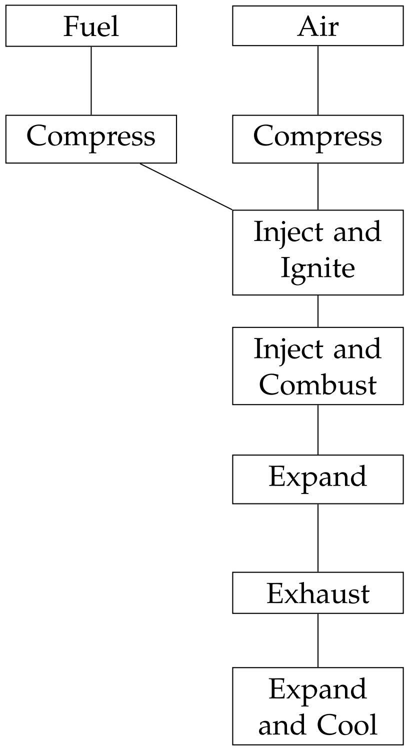


FIGURE 3.3: Charge preparation and ignition strategies

3.3.3 By Operation

Figure 3.4 names and categorizes a few examples of actual engine designs. Most of these can be ran with diesel or otto fuel operation. As will be discussed, only four are worth mentioning in any more detail than name, although rotaries will get a short discussion.

All of these engines perform 4 central tasks (inhale fresh air, expel exhaust gas, compress air or charge, expand under combustion) and 2 side tasks (lubricate components and remove heat).

Reciprocating engines have pistons that continuously move linearly back and forth, shifting the centre of mass of the engine as they do, so have an inherent tendency to produce strong vibration.

Parallel and serial scavenging refers to whether the piston pushes out the exhaust gases before inhaling fresh air or charge (serial), or whether it attempts to perform both tasks at the same time by having the exhaust gases sucked out of the combustion chamber at the same time as fresh air or charge is forced in and displace the exhaust gases.

Rotaries, all invented after most reciprocating engines, both attempt to cure this by having a large rotating body replace the piston and attempt to improve the maximum power output to weight of the engine by having that rotor perform several of the four tasks with each rotation.

[1] In some applications, known as a Turbocrank or simply a Turbo
[2] Know as the Rotary engine at the time, not to be confused with modern usage of the term
[3] Modern usage of the term Rotary engine typically refers to the Wankel engine
[4] Also known as the Rotary-vane, Swing-piston, Swashplate, or "Cat-and-mouse engine"
[5] Sometimes known as the Barrel engine, Z-crank or Swashplate engine

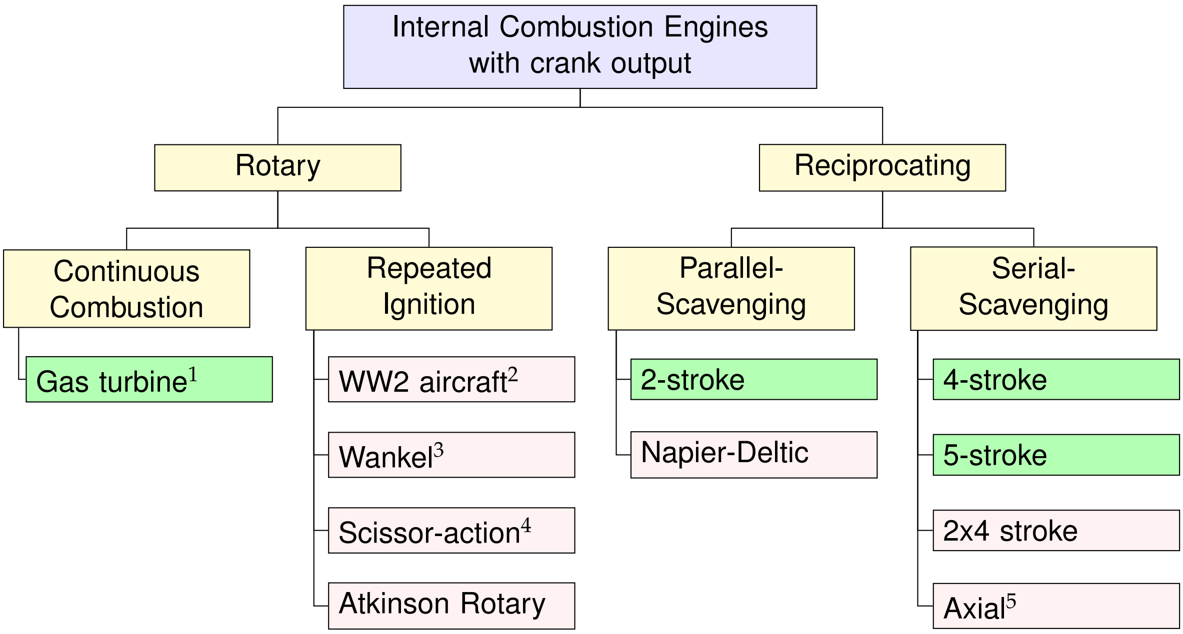


FIGURE 3.4: The ICE in the context of other heat engines

3.4 Fuels

Generally ICEs fall into one of three categories in terms of the fuel they consume, and understanding the ideal and real properties of these fuels is important to understand their operation.

3.4.1 Abstract

FIGURE 3.5: Ideal fuels for each of Otto (repeated ignition), Diesel (repeated-ignition) and Diesel (continuous-ignition)

fuel	autoign. temp.	flame speed	mixing
petrol	high	slow	high
diesel	low	fast	-
burner	low	fast	-

3.4.2 Real

FIGURE 3.6: Properties of common real fuels

fuel	autoign. temp.	flame speed	mixing	ign. energy
petrol	high	slow	volatile	medium
diesel	low	fast	viscous	high
gas fuel	high	-	gas	-
hydrogen	very high	very fast	light gas	low

MON Petrol (or Gasoline) is rated in comparison to the performance of pure octane (C_8H_{18}). Octane Number is usually expressed as Research Octane Number or Motor Octane Number, where a fuel's RON is calculated in the lab from its properties, and MON is derived from engine performance testing. Typical values for commercial fuels are 70 to 100.

MN Methane Number rates gaseous hydrocarbons in comparison to the performance of pure methane (CH_4). Definitionally, methane has the index MN = 100 and hydrogen the index MN = 0.

CN Diesel is rated in comparison to the performance of pure cetane ($C_{16}H_{34}$). Typical values for commercial fuels is around 55.

Generally, MN and MON increase together, while CN and MON are inversely related. See figure 3.8. The CN and MON ratings of hydrogen is contested; see chapter 4.

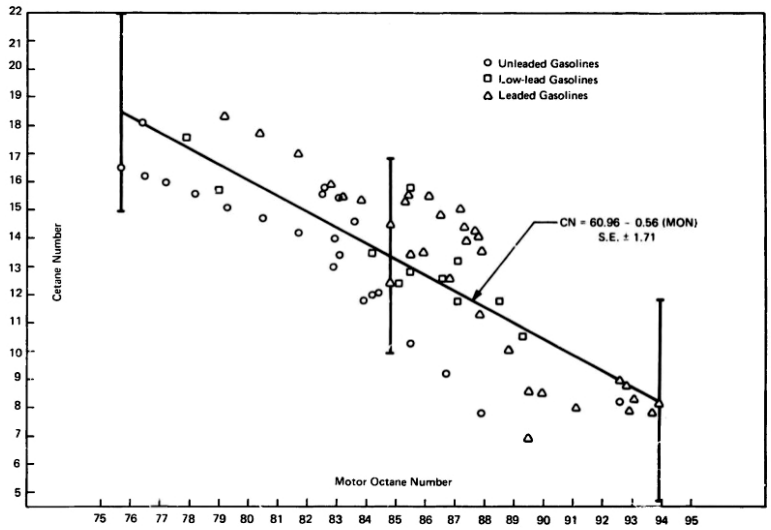


FIGURE 3.7: Empirical data comparing MON and CN of petrol fuels [8]

3.5 Analysis of practical engines

In final preparation for turning attention to hydrogen's potential as their fuel, here we will run though problems faced by the designers of existing production engines. It is with good reason that outside of some niche (generally military) submarine and aerospace applications, the gas turbine, 2-stroke and 4-stroke are by far the most common engine choices (although the 5-stroke, closely related to 4-stroke, stands to offer much).

3.5.1 General

These factors affect all engines.

Friction Lubricating oil is required to prevent excessive wear, seizure of components that slide against one another and reduce frictional loses.

Wear Components wear out and fail after repeated applications of strain. Several factors can accelerate this wearing.

- High combustion chamber pressures flex the chamber walls, inducing wear.
- Corrosion (i.e. rust) accelerates wear.
- Hydrogen embrittlement turns materials brittle, and brittle materials are more susceptible to wear.
- Engine oil degrades with use, losing its lubrication quality, increasing the wear due to sliding friction.
- Erosion from sand and dust affects surfaces that are exposed to intake air, and exhaust gas

Incomplete burn Not all of the fuel burns completely, causing wasted fuel energy to escape through the exhaust.

Emissions The combustion process produces more than just carbon dioxide and water. The elevated temperatures and non-uniform distribution of oxygen and fuel cause some fuel to go partially burnt, forming particulates (often carcinogenic) or carbon monoxide (deadly and odourless), and oxygen and nitrogen to react when heated in absence of fuel, forming nitric oxide and nitrogen dioxide (know together as NOx). Some design choices can reduce emissions at the expense of efficiency.

Temperature Higher temperatures mean greater theoretical thermal efficiency, but result in NOx emissions, increased heat conduction into the combustion chamber surfaces which causes thermal wear and reduced efficiency, and put greater demand on the cooling system, which must keep the materials below a temperature typically not greater than the boiling point of water to maintain the water cooling system and avoid thermal softening of the materials (which increases wear).

Weight Real engines and engine components have weight. Every movement of every component induces vibration, in proportion to the speed and inertia of the component, and requires work done on it (ultimately from the crank) to give it the kinetic energy to move, which is not mostly not recovered due to friction.

3.5.2 2 stroke

While 2 strokes meet their goals of working and having much higher power output per weight, enough to see mass production and application, we can dismiss it for our purposes.

- Lifetime; grinds itself to bits due to having no dedicated lubrication.
- Requires special fuel that is diluted with lubrication oil.
- Lots of exhaust particulates, a problem that gets worse with wear.
- Scavenging issues causing inefficiency as exhaust gas mixes with the incoming air, and intake air escaping down the exhaust, taking unburnt fuel with it (amplifying the particulates problem).

3.5.3 Non-turbine Rotaries

People are quick to cite the Mazda 787B, which won the 1991 24 hours Le Mans endurance race with a wankel engine, as evidence of the wankel engine's viability. However, engines conventionally called "rotaries" suffer badly from their large rotors having poor sealing against the walls of the combustion chamber. Heating and cooling of the rotor on opposite sides means gaps between the rotor and chamber metals must be left to allow for uneven thermal expansion and the sealing between the metals does not last, causing lifetime issues. This also manifests as problems with leaking lubrication oil. We will decide that rotaries need to prove themselves better before they are worth consideration for a fuel where gas leakage is already a greater problem.

3.5.4 Gas turbine

The gas turbines last longer than reciprocating engines, having fewer moving parts and far less sliding friction. However, this only in clean air without much dirt, sand or abrasive dust in it (notably less of an issue for jet planes up in the sky), which erodes the high surface area rotor components of the compressor and turbine, whose performance suffers from rougher surfaces altering the aerodynamic behaviour of the blades.

Gas turbines are more expensive to manufacture and maintain. The mechanical action is simpler with fewer moving parts and less thermal and operational wear, but they run faster so are more important to balance properly and what little mechanical wear there is happens faster. The aerodynamic action is far more complex than intermittently igniting engines, with large, complex parts that are more expensive to design and manufacture, and larger total exposed surface areas leaving them vulnerable to abrasive and corrosive air contaminants.

The lubrication of gas turbines is less about removing friction, as the rotors are all held with ball or roller bearings, so there is no sliding to reduce, but rather the continuous oil application is required to protect from corrosion and carry away heat and contaminants.

3.5.5 4-stroke

The 4-stroke is the most common, most robust engine type and only second in efficiency to some gas turbines. The primary disadvantage of the 4-stroke is the comparatively low power per weight and strong vibrations. Compared to the gas turbine, it is relatively unaffected by abrasive dust and corrosive air (the situation changes for larger particles but air filters typically help there) and less expensive.

The mechanical action is more complex, with more moving parts and many small, complex parts, but runs slower so wear, balance and precision are less important to balance. The aerodynamic action is much simpler, having only to be concerned about tuning the engine speed to the lengths and shapes of the intake and exhaust systems to make use of harmonically assisted scavenging. Most engine components are also isolated from the air, leaving very few surfaces exposed to air contaminants.

Abnormal combustion is a problem in 4-strokes. Modern engines avoid them, but engine modification (or even engine fault) can easily lead flashback (also known as backfire), post- and pre-ignition knock (where a rapid and asymmetric pressure rise develops on the piston head). The quality of the fuel goes hand in hand with these problems.

Lubrication is vital, as there are many moving components, all taking power from the crank and experiencing friction. The engine's oil system typically has a filter in it

to remove contaminants, but engine oil still degrades with time and use and both the oil and filter need periodic replacing.

The seal between the piston and cylinder wall is made complete with a piston ring and engine oil. Valves and ports are designed to fit snugly and can even have rubber or soft metal seals. However, blow by and leaks still occur and during combustion some hot gases force their way out the exhaust, back up the intake, between engine blocks and past the piston into the crankcase.

4-stroke engines produce 4 types of vibration:

Primary Due to the reciprocating motion of the piston. Grows with piston weight and crank length (R)

Secondary Also due to reciprocating motion of the piston, but smaller, and specifically a result of the con-rod (H) not staying vertical.

Rotary Due to rotating components being slightly imperfectly manufactured and always having a heavier end.

Torque Torque is only produced for a quarter of a full cycle, and typically only for half of that cycle again before rapid drop-off. For the rest of the cycle, particularly by the end of compression, each piston absorbs torque. This causes vibration to travel down the crankshaft.

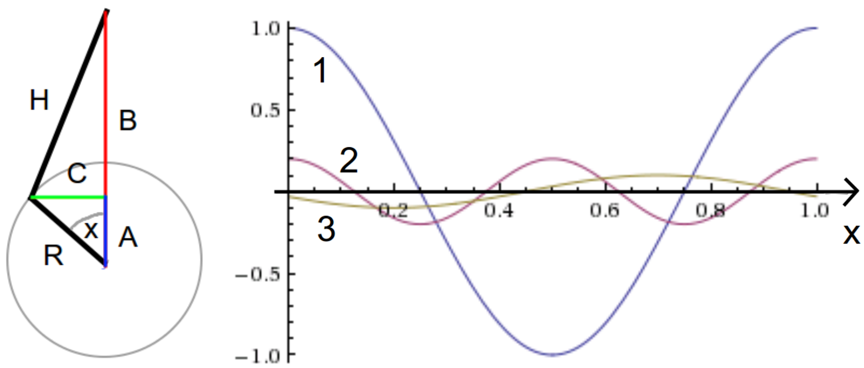


FIGURE 3.8: Primary (1, dependant on 2R) and Secondary (2, dependant on R/H) vibration due to the piston, and derived from the motion of A+B with crank-angel (x). Rotary (3) vibration due other rotating components.

3.6 Major design choices for the 4-stroke

3.6.1 Ignition

Spark Two conductors with an short air gap protrude into the cylinder. A circuit produces a timed high voltage to create a brief ark that ignites the local charge. A flame front then spreads through the charge.

Compression The temperature rise from compression stroke leaves the above the autoignition temperature of the fuel.

Glow ignition A hot object such (as a glow plug, hot spot or hot particulate left over from exhaust gases) heats the local charge until ignition occurs.

3.6.2 Charge Preparation

Homogeneous Fuel is distributed throughout the charge such that a flame front will spread over the whole charge from just one ignition source. Care must be taken to avoid combustion intensity from concentrating, such as any autoignition from combustion raising the pressure inside the cylinder for unburnt charge (detonation knock) or from abnormally high flame travel speed. Typically uses spark ignition, but glow and compression ignition can work in theory.

Stratified Fuel is injected directly into the cylinder at high pressure immediately before ignition and continuing through combustion. The cylinder shape and injector location are chosen to circulate the flame away from the injector and bring fresh air to it. Care must be made to ensure the flame can keep up and stay near the injector, and that unburnt fuel does not build up in the cylinder during combustion, lest it all go off at once (diesel knock). Typically uses compression ignition, with glow ignition for cold starting, though spark ignition is possible.

3.6.3 Injection

Direct or In-cylinder As well as dedicated intake and exhaust ports, the top of the cylinder has one or more dedicated fuel ports so that the fuel is injected into the air as or once it enters the cylinder. Stratified charge strictly implied this injection method.

Port Fuel is injected into the air it enters the cylinder on the intake stroke as close as far down the intake port as possible. Injection stops for other strokes.

Manifold A carburettor, mist injector or some typically low-pressure injection system injects fuel long before the intake valve, before the intake system splits to serve individual cylinders (for engines with more than one cylinder). Typically in or before any plenum or air-box and ubiquitous amongst old petrol cars.

3.6.4 Power reduction

Throttle Part of the air intake system is closable to restrict the total airflow into the engine. The fuel injection is reduced accordingly to maintain a desired fuel-air ratio, and is typically not controlled directly but responds to the actual throttle status (especially for a carburettor). Typical for petrol engines. The throttle creates a negative pressure between it and the engine, which pulls on the crank during intake, reducing efficiency.

Lean burn The air intake is unobstructed and fuel injection is controlled to reduce the total fuel in each burn, regardless of or adjusting for the resulting charge s air-fuel ratio. Typical for diesel engines. Lean ratios are prone to improper combustion.

3.6.5 Intake pressure

Naturally aspirated The pressure at the intake port is at or below local atmospheric (below due to drag inside the intake system). Simpler, lighter, vulnerable to changing conditions.

Boosted A compressor increases the air pressure the cylinder. It adds cost, complexity, wear, drag on the system and another thing to break. More powerful for little added weight, more efficient burn, more reliable intake pressure.

3.6.6 Temperature

Water cooled Coolant flows through the engine block, which is hollow, to keep the bulk of the engine at a constant temperature; this is the "operating temperature" of the engine. However, practically, the operating temperature is actually the temperature setting of the thermostat the coolant enters as or just after after exiting the engine block. This thermostat controls how much water passes through the radiator and how much bypasses it to maintain the desired operating temperature. The choice of this temperature is a factor in the thermal expansion the engine is designed to tolerate (or take advantage of) and the properties of the lubrication oil, which vary with temperature.

Air cooled The engine block is designed with a high surface area on its outside, especially surrounding the cylinder block to radiate heat to the air. Thus there is no control over how effective the cooling system is.

3.6.7 Lubrication

Engines have many moving parts where parts move past one another with little friction. In all these cases, a bearing covered in oil is used. The forces between surfaces continuously push the oil out, so must be constantly forced back in, by direct forced injection between the surfaces. The oil drips down the inside of the engine and gathers at the bottom, where it must be collected, cooled, filtered, stored and pumped in a cycle that continues as long as the engine runs. The oil choice must work with the operating temperature and fuel choice to maintain an acceptable viscosity to perform its tasks. Additives are typically used to promote the desirable properties of an oil.

3.6.8 Sensors

Modern engines use sensors to monitor the state of the engine to stay aware of what part of the engine cycle each cylinder is at, check for faults, and combined with control systems, adjust injection rates and timing, and spark timing or glow plug output. The choice of an engine's sensors is a question between what the sensor adds (functionality, safety, reliability, performance) thanks to monitoring they provide, against the increased complexity, cost, and reliability liability each sensor adds.

Crank and cam position is essential to engines where computers control the spark ignition and/or injection timing, so much so that should crank and cam data be lost, the engine would rapidly lose power and fail,

3.6.9 Scavenging and Tuning

The tubing leading too and from the intake and exhaust port of the cylinder develop standing waves due to how the 4-stroke intermittently opens its valves. With careful design, these waves, the engine speed, the valve timing and the length and shape of the tubes can be *tuned* to as much intake air entering and as much exhaust gas leaving the cylinder. When the standing waves are disadvantageously timed, this effect can instead

prevent proper intake and exhaust. This generally implies that there is an engine speed that is optimal for scavenging, which will typically also be the engine speed at which the engine's highest power output is found.

Additionally, air takes time to accelerate, so the intake valve is typically left open for part of the compression stroke to take advantage of the momentum of the air, and the exhaust is opened early, so as to get the exhaust gases moving by the time the piston starts to push them so the piston sees only a very small increase in pressure for the exhaust stroke. There is also some overlap when both pistons are open, so that the momentum of both gases pushes the last of the exhaust gas out of the cylinder.

3.6.10 Conventional Petrol Engine

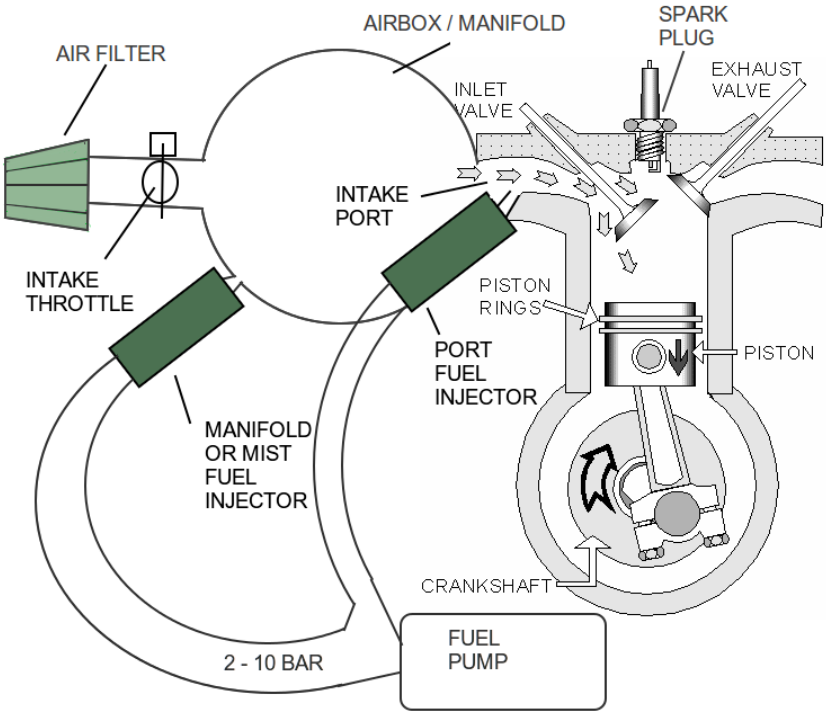


FIGURE 3.9: Conventional petrol engine [3]

Illustrated in figure 3.10; operation described in figure 3.11. Power is moderated by closing the throttle. Fuel injection is adjusted to keep fuel the fuel-air ratio constant. The charge is homogeneous (fuel distributed throughout) at the time of ignition and a spark is used to ignite the charge.

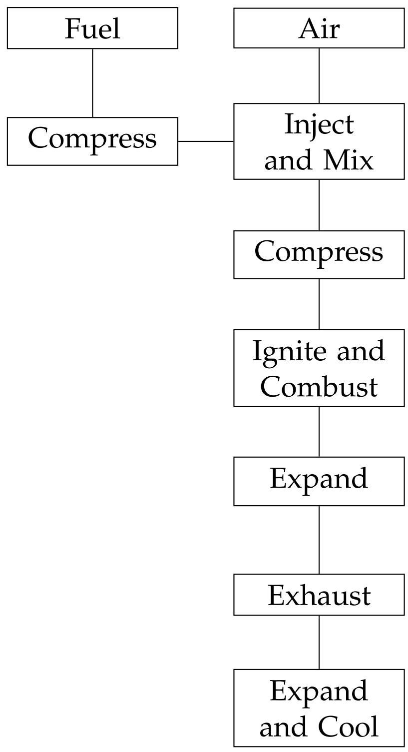


FIGURE 3.10: Petrol Engine Operation

3.6.11 Conventional Diesel Engine

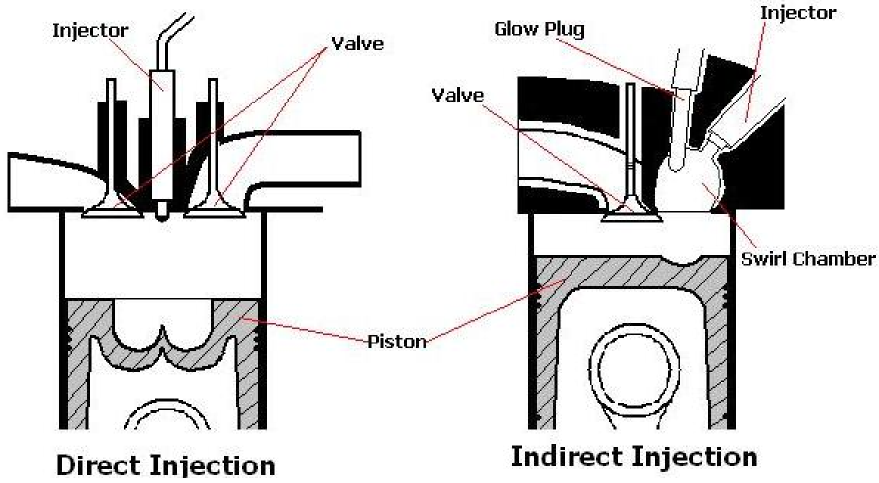


FIGURE 3.11: Conventional diesel engine [4]

Illustrated in figure 3.12; operation described in figure 3.13. Direct injection (left) would expect 100 - 150 bar fuel pressure, indirect injection (right) would expect lower compression ratio and fuel pressure. Power moderated by reducing the fuel rate (lean-burning); the volume of air that is pumped through the system does not change with power output. The charge is stratified (fuel distributed only at the site of injection) at the time of ignition and either a glow plug or the air temperature after compression are used to ignite the charge.

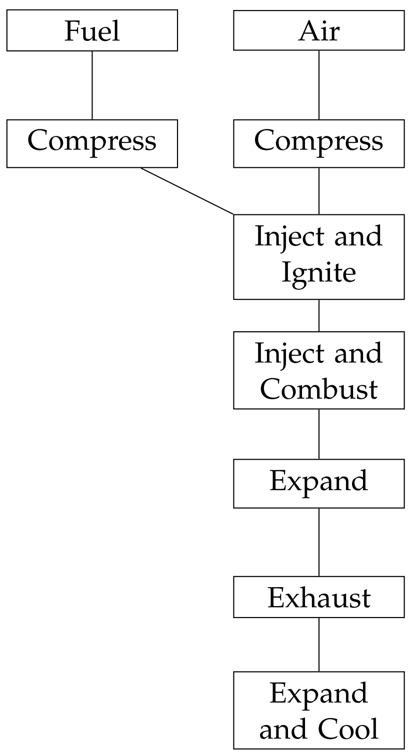


FIGURE 3.12: Diesel Engine Operation

Chapter 4

The H2ICE

4.1 Literature Review

4.1.1 Hydrogen fuel and H2ICE reviews

In 2002, Das[10] wrote a review of all the work on H2ICEs performed at the Indian Institute of Technology (IIT), Delhi. Injection strategies were discussed: carburetion, continuous manifold injection (CMI), timed manifold (or port) injection (TMI), low-pressure direct cylinder injection (LPDI) and high-pressure direct cylinder injection (HPDI, or diesel operation). Obviously both direct injection strategies prevented flashback. LPDI gave lifetime and reliability problems for the injectors, and unburnt fuel in the exhaust from poor mixing. The review found that unassisted diesel operation was not possible, even with compression ratios as high as 29:1, due to hydrogen's 849 K autoignition temperature. Diesel operation was success with duel-fuels, both simple mixtures and using pilot injections of fuels with lower autoignition temperatures to ignite the hydrogen. They found that glow plugs to locally heat and ignite the mixture were required for pure hydrogen fuel under diesel operation, and this was practical without major hardware modification. They also successfully tried hydrogen dilutants to avoid knock.

More reviews in 2002 by White, Steeper and Lutz[36] and in 2009 by Escalante Soberanis and Fernandez[32] made reviews of technical progress of the H2ICE.

Then in 2009, Verhelst and Wallner[35] made a comprehensive review of all issues concerning the H2ICE, both resolved and standing (although they do not mention stratified charge i.e. HPDI). They discuss attempts to apply MON and RON ratings to hydrogen fuel, and conclude the very attempt questionable due to the disparate results attained from different methods.

This review was the only paper found to discuss hydrogen embrittlement of metals. The varying susceptibility to embrittlement between metals is discussed; copper alloys, aluminium alloys and particularly copper-beryllium being resistant, high-nickel alloys and titanium alloys being sensitive, and steel alloys depending highly on the chemical composition, heat and mechanical treatment, microstructure, impurities and strength. They noted that piezo materials (common in fuel injectors) have also been shown to suffer under hydrogen embrittlement. They described how applying a negative voltage to the block and components can slow hydrogen embrittlement for metals known as cathodic protection, but that nothing can be done for piezo materials (although they comment that replacing injectors is cheaper than repair or replacement of other components).

4.1.2 Chemistry

Barron[7] and Dunnill[13] commented on embrittlement and the implications for H2ICEs. Hydrogen embrittlement is a term that refers to a number of materials phenomena. Firstly, most metals are porous to metals, and materials such as polymers that are not, do not suffer hydrogen embrittlement. When metals suffer embrittlement, they stiffen and lose ductility, as the term suggests, affecting the fatigue of the material, but not the strength. It is generally believed that hydrogen radicals, passing through crystal blocks, stop and react with boundary states between crystal blocks, impeding the material's ability to break, re-shape and then re-connect crystal blocks under strain, reducing ductility. It is also know that leaving hydrogen-soaked metal to rest lets the hydrogen porously escape, and this can and often does reduce embrittlement.

Furthermore, Barron[7] commented that transparent ICEs have been demonstrated, (such as the lotus example, made of corundum) which allow for spectroscopy of the gases and combustion event inside the cylinder. It has thus been known since before 1980 that hydrocarbon fuels release significantly large quantities of hydrogen radicals during the combustion event and the materials of the immediate surfaces of the combustion chamber (cylinder head, cylinder block or cylinder liners, piston head and valves), as well as enduring rapid thermal, pressure and mechanical wear, must endure embrittlement. The quantities of hydrogen radicals seen during petrol combustion mean a change from hydrocarbon to hydrogen fuel is unlikely to increase the hydrogen radical quantities by much, especially if diesel operation and lean burning are adopted, is unlikely to increase the hydrogen. This needs confirming, but nonetheless means that the materials found in existing engines is unlikely to be detrimentally susceptible to hydrogen embrittlement.

In 1995, Das[9] reviewed the nature of the $H_2 + O_2$ reaction. They described the explosion limits of the reaction on a PV graph (the mixture is not given but assumed an undiluted stoichiometric hydrogen-oxygen). They describe the mixture's tendency for undesirable combustion events due to the low ignition energy. This implies first that a less energetic spark is required for spark ignition (and so simpler spark plugs possible) and second that pre-ignition is very likely, which combined with the fast flame speed, is potentially very problematic. They assert that many of the pollutants produced by hydrocarbon combustion are not present after hydrogen combustion, save for NOx, which is typically produced less than in hydrocarbon combustion, and indeed with lean operation near-zero NOx emissions is achievable thanks to the wider flammability limits.

In the context of H2ICEs and the hydrogen economy, they note that it is necessary to take into account the ubiquitousness of the petrol and diesel ICE, and plan to convert these to run on hydrogen rather than replace them with new designs. They assert that the comparative merits and drawbacks of hydrogen and specific hydrocarbons as fuels have essentially been identified; hydrogen is a clean burning energy carrier, with an ignition energy that is favourable to spark engines but unfavourable to otto-cycle engines, and wider ignition limits to very lean mixtures which facilitates easily varied engine speed and power output. They emphasise that undesired combustion events are very problematic, to the point of being the main impedance to H2ICE research, citing flashback outcomes (quote) "ranging from a simple misfire to the destruction of the entire fuelling system" and deposits formed by the pyrolysis of lubrication oil being found to be able to ignite cold fuel-air mixtures. Exhaust gas recirculation is mentioned as possibly beneficial to the H2ICE operation.

They discuss the origins of engine knock, where (quote) "according to autoignition theory, knocking takes place due to local pressure imbalances caused by simultaneous autoignition of the last part of the charge. On the other hand, detonation wave theory suggests that there exists a supersonic detonation wave in the end gas which is responsible for the pressure imbalances. It has been observed that knocking conditions are attained because of the acceleration of the primary flame front to speeds of about 400 metres per second. Flame speeds have often been observed to be higher in the entire knocking zone." They also discuss that due to hydrogen's higher flame speed and higher autoignition temperature, knocking is better explained as higher pressure causing faster flame speeds through end gases than detonation by autoignition of end gases in H2ICEs.

4.1.3 H2ICE spark

Most of the papers found concerned attempting to run petrol or LPG engines on hydrogen gas, making only minor modifications outside of the electronics and intake. All of these engines were tested on engine dynamometers, in indoor environments. [15] [38] [11] [33] [39] [20] [14]

After 1990, Lee, Yi, and Kim[21] investigated conversion with a port injection, single cylinder spark engine and improved volumetric efficiency, and produced greater maximum output power. Higher NOx was detected in the exhaust. They also designed and tested a solenoid injection valve for this and concluded that the injection system worked well and was easy to install, flashback was still an issue (though could be handled with injection timing and hot spot removal). They made no mention of intake or operating temperature. They repeated this experiment [37] and placed the injection valve inside the cylinder for direct injection. Jorach, Enderle and Decker[19] also tested direct injection.

After 2000, Verhelst and Sierens[34] found that hydrogen burns cleaner due to wide flammability limits (i.e. lean mixture) and the fast flame speed improved efficiency. They converted a GM crusader v8 spark engine for a city bus, using a sequentially timed multipoint (port) injection system. They pay attention to ignition properties (smaller spark gap), injection pressure (held constant at 3 bar or 6 bar), lubrication oil (finding more blow-by causing hydrogen gas build-up in the crankcase) and the design choice of intake throttle or variably lean mixture. Hydrogen gas was found to be a good insulator, so a shorter spark gap was needed (0.4 mm spark gap, compared to petrol's 0.9 mm), despite low ignition energy, as the original had problems with requiring higher voltages that defeated spark plug insulation. The smaller spark gap functioned acceptably because no fuel-derived deposits built-up and closed the gap.

Alarmingly, after finding significant quantities of hydrogen gas in the crankcase and checking the oil, (quoting [34]) "It appears that the properties of the oil have strongly changed with a serious decrease of the lubricating qualities. The concentration of various additives (both lubricating and wear-resisting, e.g. zincdialkyldithiophosphate) is greatly decreased, esters appearing in the unused oil have almost completely disappeared in the used oil. . . . This is understandable when one knows that hydrogen is used in the industry to harden oils to fats (breaking open the double C-C bonds)." and they confirmed this was not due to engine wear. They suggested forced crank ventilation, catalysts such as copper and the development of special lubrication oils for H2ICEs (that currently are not available) as practical ways of solving this issue.

They found lots of unburnt hydrogen in the exhaust when using ultra-lean mixtures, such as at idle, and solved this by using a throttle on the intake. They proposed

a special throttle that runs wide-open most of the time and only closed for idle conditions. They concluded that a port-injection V8 spark ICE can work with gaseous fuels, including natural gas, hydrogen and hythane (a mixed gas of methane and hydrogen), deliver sufficient power for a city bus without danger of backfire, but needed special features such as the smaller spark plug gap, adjusted injection pressure, oil deterioration countermeasures, and additional calibration of the oxygen sensors for the extremely lean mixtures during engine development.

Heffel[17] outlined the technique of exhaust gas recirculation and described an experiment with a 2 L spark 4-cylinder ford ZETEC conversion to test the concept for the H2ICE. A catalystic converter was also tested and NOx emissions and engine performance measured for both experiments. The intake and exhaust piping were connected via a smaller pipe near the ports, and a fresh-air throttle on the end of the intake was used to provide resistance and suck exhaust gases into the intake, which stayed at 1 atm so throttle resistance was not apparent. For each fuel rate, the percentage of exhaust gases in the intake was increased until the oxygen-hydrogen percentage was at stoichiometric, starting at wide open throttle. They list engine temperature and performance graphs, with impressive results, and found no engine knocking and no pre-ignition (so no flashback). The experiment was performed first at 1500 rpm, and then again at 3000 rpm. [16]

After 2005, Li and Karim[22] investigated engine knock, Mohammadi et al.[25] investigated direct injection and Liu[23] investigated backfire. All were from before 2009 and no other papers investigating spark ignition H2ICEs were found after then.

Finally, prior to this project, Dunnill[12] attempted a low cost, low effort H2ICE by replacing the fuelling system of an electric generator, low-pressure manifold injection, single cylinder, LPG fuelled, air cooled 4-stroke spark engine. It was noted that the engine ran successfully, and smoother at full throttle, but that periodic flashbacks were present, once destroying the fuelling system, and that orange flashes up to a flame arrester were also observed in the soft polymer pipe that connected the fuel system to the 1 atmosphere storage tank. This draws attention to the fact that not only does hydrogen diffuse quickly into air after injection, but that oxygen in the air can diffuse up the injection aperture.

4.1.4 H2ICEs without spark ignition

Most interestingly, in 2008, Antunes, Mikalsen and Roskilly[6] demonstrated a HCCI engine, where no spark was present and instead the temperature rise from compression was the ignition method. They also used hotwire heaters to pre-heat the intake, both to boost the temperature to the required autoignition as compression along was not enough, and was used as a control for keeping sure autoignition was not reached before top dead centre. Using ultra-lean mixtures, the paper claims efficiencies of up to 45%, but it is not stated if this figure includes the energy used to pre-heat the intake, or if it is only the brake horse power against the fuel enthalpy rate.

Two conventional diesel-operation H2ICEs were found. Naber and Siebers in 1998[27] and Gomes Antunes, Mikalsen and Roskilly in 2009.[5]

4.2 Evaluation of the H2ICE

Hydrogen, hydrocarbon gases (meth/eth/propan-e/ol), petrol and diesel, all have their advantages and disadvantages over one another as 4-stroke ICE fuels. Here we

summarize the advantages, disadvantages and teething issues. We can distinguish disadvantages and teething issues in the later being permanent and the former being issues that currently pose problems to H2ICEs, but only because solutions to these problems have not been optimized or implemented, but their optimized forms are within sight.

4.2.1 Pros

Hydrogen Economy H2ICEs function as part of a hydrogen economy, which is a desirable solution to the problem that renewable energy faces in its supply unable to meet domestic and commercial grid demand.

Vs Fuel Cells Within a hydrogen economy, H2 fuel cells outperform H2ICEs in efficiency (although as we have seen, this is not strictly true), but H2ICEs are less expensive to manufacture and maintain and last longer than fuel cells. The 4-stroke ICE also has a much larger background of development than the fuel cell, which is a comparatively immature technology.

Emissions 4-stroke H2ICE exhaust gases contain no CO, no CO_2, no unburnt or partially burnt hydrocarbon fuel, little lubrication oil particulates and less or almost no NO and NO_2.

Deposits Fewer deposits are found on component surfaces due to the absence of hydrocarbon combustion. Deposits from oil degradation are still present, but are less problematic and potentially avoidable with specialized lubrication oils. With fewer deposits, maintenance needed because of them (such as bridged spark plugs and oil filter and oil changing problems) is reduced and design constraints that attempt to minimize them and their problems can be relaxed.

Flame speed The supersonic flame speed means less energy is lost during combustion and that energy can be converted to work.

Low ignition energy This has advantages to needing less energy to ignite the fuel, and simpler devices to perform the task.

Wide flammability limits Ultra-lean fuel-air mixes are possible with hydrogen, which themselves have advantages with reduced emissions, greater total engine efficiency and reduced engine wear.

Very high autoignition temperature This makes H2ICEs almost immune to detonation knocking.

Per oxygen energy release The energy released per mole of oxygen in the cylinder is greater with hydrogen than hydrocarbons, producing more power per cylinder volume. [1]

Fuel-air mixing Hydrogen is gaseous fuel with a very light molecule, so mixes with and diffuses through air much quicker than heavier hydrocarbon gases and vapours, with advantages in more complete combustion.

[1] Mole reduction and higher caloric reaction have opposing effects on pressure (reducing n but increasing T). They may cancel in theory, but in practice resulting increase in temperature means more thermal wear and more heat loss.

Volumetric efficiency Per mole of oxygen burnt, more moles or hydrogen are required than other fuels, and this displaces air when mixed. For direct injection, this has the advantage that greater volumetric efficiency is reached by first inhaling air and then displacing it with hydrogen once the intake valve has closed.

Safety In the absence of hot surfaces, hydrogen-air mixtures are stable. Uncontained hydrogen (like that from fuel leaks) is lighter than air, so in buildings gathers in the ceiling where a flame will do less injury and alone will produce nothing but steam (not withstanding anything else that catches fire, though hydrogen is likely quickly escape any building) and outdoors diffuses into the sky too quickly to form an ignitable mixture near the ground due to any slow leak, unlike hydrocarbons which will pool near the ground and form readily ignitable mixtures. Further, hydrogen has no poisonous properties and, ignition aside, low levels of hydrogen gas inhalation have been shown safe,[31] while exhaust gas contains no "silent killers" such as CO and NOx has a very strong odour.

4.2.2 Cons

Leaks More blow-by between the piston and cylinder occurs, and more gas leaks past the cylinder valve seals due to the physically smaller and faster moving hydrogen and water molecules, which are diluted by larger and slower carbon dioxide molecules in hydrocarbon combustion. This single feature is the central reason why rotaries are likely to be completely unsuitable as H2ICEs.

Mole reduction Two hydrogen and one oxygen molecule will combine to form two molecules of water, decreasing the total moles of gas in the cylinder, and reducing the pressure and therefore the work done during expansion.[1]

Volumetric efficiency (otto) Hydrogen gas displaces air it mixes with, so for manifold injection the intake air is diluted, limiting power due to lower effective oxygen volumetric efficiency.

Storage Although not considered relevant directly to H2ICEs, it must nonetheless be acknowledged that H2ICEs will need a fuel tank to store the hydrogen they burn, and storing hydrogen is more troublesome than storing petroleum liquids and gases, as hydrogen does not condense into a liquid at room temperature and most metals are porous to metals. Insulated cryogenic tanks and high-pressure polymer-lined tanks are currently the only viable methods for high density storage, and are both more trouble than petrol and diesel fuel tanks, whilst atmospheric storage is only suitable for small scale stationary applications.

Safety The health effects of hydrogen gas may be safer, but cryogenic hydrogen poses a safety hazard, and despite hydrogen-air stability, hydrogen gas has a higher flammability rating than petroleum due to the low ignition energy and readily mixing gas, such that sudden release of hydrogen is a much more serious danger. Further, what little NOx that is still produced, the ppm levels found in exhausts[2] are still far above median lethal doses (LD50).[3] NOx is also terribly and surprisingly harmful to the environment.[30]

[2] Although of course this will rapidly reduce as exhaust gas diffuses away from the tailpipe opening.

[3] NO has a recommended exposure limit (REL) and permissible exposure limit (PEL) of 25ppm,[28] while NO_2 has a REL of 1 ppm and a PEL of 5 ppm.[29]

4.2.3 Teething issues

Very high autoignition (diesel) The very high autoignition temperature of hydrogen-air means a dedicated device to assist ignition is required for diesel operation.

Pressurizing More work must be done to pressurize a gas than a liquid, which has implications for efficiency for standard otto and diesel cycle engines only get some of that work back during expansion. This is resolved by using with braydon cycles (i.e. turbo-charging) or atkinson cycles (i.e. non-standard valve timing).

Lubrication oil degradation Lubrication oil degrades in petrol and diesel engines due to deposit contamination, which is reduced in H2ICEs, but is then increased by hydrogenation of oil additives that occurs when hydrogen builds up in the crankcase due to blow-by. This is resolved with one a combination of crank case ventilation (preferably positive to decrease blow-by), H2ICE specific lubrication oils and crank case catalysts to react built up hydrogen.

NOx Hydrogen combustion can produce NOx, and typically does in significant quantities in H2ICEs (but less than with hydrocarbon fuels). This can be resolved with catalytic converters placed along the tailpipe, and by using lean mixtures. Below a given fuel-air ratio, almost zero NOx is produces, above that NOx emission rise sharply to a peak, and then slowly drop-off as the mixture approaches stoichiometric.

Pre-ignition and flashback (manifold and port injection) Due to the ease with which local ignition sources can ignite hydrogen-air mixtures, H2ICEs are vulnerable to pre-ignition under otto-operation, particularly flashback that can destroy the intake and fuelling system (though the damage can be limited with a flame arrestor in the manifold or injection port). This single feature is the central reason why development of the H2ICE has been slow up until now. Meticulous elimination of hot spots, discouragement of hot oil deposits and addressing the mixing of intake and fresh exhaust during valve overlap, for each engine design, is possible but likely impractical without great effort given the sheer variance of existing engine designs. Direct injection is preferred as a solution, though port injection with exhaust gas recirculation deserve development attention.

Supersonic burn There are three issues with the supersonic flame speed of hydrogen combustion.

- Flashbacks are much more energetic and destructive than in petrol engines, resolved as mentioned with direct injection or potentially EGR.
- A rapid pressure climb that reaches higher peak pressure can damage engine components (particularly pistons and their con-rods) and increases mechanical wear. Isobaric burns (i.e. diesel-operation) and ultra lean (so reduced output) mixtures are preferred due to this, although compression ratio reduction (with cylinder-head block sleeves) and component strengthening (reinforced piston heads and con-rods) are also practised with petrol engines when turbo- or super-charging and are applicable.
- A faster temperature climb and higher peak temperatures increases thermal wear and heat loss. The solutions again are isobaric burns and lean mixtures.

Embrittlement Hydrogen embrittlement is an often discussed issue for any handling of hydrogen.

- Firstly, polymer piping and polymer lining address fuel system issues. High pressure static fuel lines need not be concerned with embrittlement as it does not cause them to fail, but high pressure engine fuel lines will suffer vibrations induced by the engine, which may cause reduced lifetime or unexpected failure due to brittle materials wearing quicker under vibration.
- Injector valves can be designed to resist or be immune to embrittlement by avoiding exposure of vulnerable components and surfaces to the fuel.
- The steel and aluminium alloys that typically make the bulk of engine blocks and components are very susceptible to embrittlement, but the alloys that immediately surround the combustion chamber (piston heat, cylinder linings, valve ends, cylinder head) are generally made of special hardier materials. It must be noted that these components suffer from (and are designed to resist) embrittlement as petroleum combustion produces just as many hydrogen radicals as hydrogen gas combustion. So this specific issue with the combustion chamber can be considered already resolved.

Back Diffusion Without the barrier of a liquid's surface tension at the injection aperture, oxygen can dissolve through the hydrogen into the fuel system. There is can build up and ignite, causing damage to the fuel system. This is resolved with maintaining a sufficient difference between the immediate air pressure at the injection site and minimum fuel pressure, as well as a sufficient fluid velocity through the aperture during the time the final valve is open, to ensure as little oxygen diffuses into the fuel system as possible. Additionally, it may be prudent to place secondary valves and flame arrestors further up the fuel system, such as at the point where the fuel leaves the block.

Chapter 5

H2ICE design and conversion

Finally, we understand the theory and design of petroleum ICEs and the H2ICE, and can turn our attention both to designing our own H2ICEs and considering how might be best to modifying a petroleum ICE to run on hydrogen gas with as good a performance we can manage with as little cost and difficulty for the conversion.

5.1 Exploring Ideas

5.1.1 Outstanding Issues

Flashback induced by pre-ignition is clearly too intolerable. Plenty of others have tested H2ICEs operating as otto-engines; all have either found problems with flashback, or made effort to take special measures to prevent it. That it was the single most talked about barrier to further development for most of the literature before 2008, the phenomenon must be considered intolerable and any engine design unacceptable if it has opportunity not have a major design feature that eliminates it. The obvious solution is to keep the fuel and air separate until ignition happens.

This would imply diesel-operation is favourable. However, it is also apparent that hydrogen-air's autoignition temperature not practically achieved reliably with true diesel operation. However, a glow plug or a spark to force ignition would be acceptable and are only not practised by diesel oil-fuelled diesel engines due to the minor added cost and complexity, the redundancy over autoignition and that a spark plug in the path of a jet of diesel oil would quickly build up deposits and short circuit. Given that a diesel-operation H2ICE would rely on such a device for ignition, and that hydrogen-air ignites from hot spots easily, we may think up a way of deliberately inducing a hot spot in or near the path of the fuel injector as a means of ignition that does not require a glow plug powered by the engine's circuit. However, a glow plug will prove easier to install for early designs.

5.1.2 Designs

Pressure release recirculation It is apparent that a gas pump will be required to pressurise the fuel in some situations. For this, it is essential that a pressure release valve that leads from the high pressure side to the low pressure side of the pump be installed and a pressure valve set to the maximum tolerable pressure installed along it. This is also necessary and indeed common practise when forced induction is involved.

Atkinson cycle Otto and diesel cycles lose a lot of energy at high power by releasing exhaust gases before they have expanded as far as they can, thus wasting the energy available. By having cylinder travel further under expansion than it did

under compression, this energy is captured as work. However, how much more the cylinder needs to expand for full capture depends on how much fuel was added, so an application with variable power output requires a variable expansion, or a cut-off is used such that for full power only part of the extra expansion is captured and a minimum power output is implemented below which the exhaust gases reach below-atmospheric pressures and absorb rather than do work, giving rise to idling issues. A simple way of achieving this is by holding the intake valve open for part of the compression stroke, preferably with an adjustable intake cam profile. With the new reduced compression stroke, efficiency is lost, however, when designing an new engine, this can be compensated for by starting with a higher compression ratio, knowing that pressures will not be as high as they were for a standard equal-expansion-compression engine.

5 stroke The 5-stroke achieves the more efficient Atkinson cycle (and for diesel-operation resembles the yet more efficient Brayton cycle), without requiring an external turbine on the exhaust and without needing to sacrifice volumetric efficiency by delaying intake valve open during compression. However, the total hydrogen injected each cycle strongly affects the final expansion of the exhaust, either requiring a variable big-piston valve timing, or toleration of less expansion at high power and pulling against sup-atmospheric pressures at idle. Additionally, low-power single cylinder designs are not possible, so the 5-stroke maybe prove more viable for medium power applications such as vehicles. Note that only the intake and exhaust valve timing of the big piston must be varied, as it is the big piston that performs the final expansion.

Using Turbocharger to power fuel compressor Turbochargers have a turbine on the exhaust to capture discussed extra expansion, then use that work to power a compressor on the intake (effectively forming a small gas turbine where the burner is replaces with a 4-stroke engine). This increases the total compression ratio of the engine, increasing its power and efficiency, but in exchange for greater cost and complexity, and an added poor transient response to engine speed and power output (especially for throttled engines) that comes from the turbo needing to spool up. Given that for direct injection, the work put into displacing air to inject the fuel, and especially for diesel operation where this must be done at high pressure, almost as must work must go to the fuel pump per cycle as is needed for the compression stroke. A turbo could be used to power this fuel pump. The more fuel is added each cycle, the more leftover expansion is left in the exhaust, the more work can be captured by the turbo, the more work the turbo can put into the fuel pump currently needs to do more work to maintain the pressure for the greater flow-rate.

Electronic fuel compressor For such an engine to start, it needs not only work put into the crank to turn it during start up, but work must be done to pressurize the gas ready for injection. Petroleum engine pumps act on liquids, which compress very little, so take very little work to pressurize, thus it is feasibly economical to power the fuel pump from the crank and use a release valve to handle regular pressure overshoots that come when engine speed and power output are such that the fuel pump is doing more work than necessary (though fuel pumps themselves have systems to lock their cranks when no extra work is needed to raise the pressure). For hydrogen fuel, an electronic fuel pump that delivers only enough work from the circuit to pump the gas to the correct pressure may prove beneficial. It would

also go in hand with using a battery-powered starter system to both turn a starter motor and work a fuel pump. It would also work well combined in series with the turbo-powered pump, which cannot be guaranteed to always provide enough work needed to maintain pressure.

Exhaust gas recirculation As has been demonstrated, diluting intake air with recirculated exhaust gas, with the total oxygen-hydrogen kept stoichiometric, is an effective way of reducing knock, NOx, unburnt fuel, peak temperature and efficiency, with only simple modifications to the intake exhaust system and an added throttle (if one is not already installed).

Comprex supercharger An alternative to making use of the extra exhaust expansion is the comprex supercharger, or pressure-wave supercharger. This is similar to the turbocharger, but uses the pressure of the exhaust gas to directly squeeze the intake air in a rotating compartmentalised barrel. When pressures get too high, variable intake valve timing could be used to implement a maximum total compression, which makes the engine more efficient by effectively transferring the duty of compressing the intake air from the crankshaft to the exhaust gases in the supercharger, leaving more power in the crank. Due to the nature of the comprex supercharger, it lends itself to working with exhaust gas recirculation for combined benefits.

Combined-injector-ignition device Concerning the details of direct injection and ignition, an extremely simple solution for spark engines could be to replace the spark plugs (which are typically easy to access without opening the engine due to the need for their regular maintenance) with a fuel line connected to an injector valve, that has either a low voltage spark or small glow plug protruding into the cylinder. It takes advantage of the high engine pressures requiring the access hole to the spark plug to be strong, which could help support the injector in withstanding the high pressure in the fuel line. Such a device (shown in figure 5.1) could make it trivial to convert any engine, given a suitable variety of available device sizes to fit different engines.

Positive crankcase ventilation If the intake is pressurized, then a small branching tube entering the crank, with a hole in the other side of the crankcase, could provide positive crankcase ventilation by forcing fresh intake air through the crankcase. This prevents build up of hydrogen in the crankcase (avoiding rapid oil degradation) and reducing blow-by. However, the effectiveness of the reduction in blow-by needs to be investigated.

Negative crankcase ventilation If the intake is not pressurized, then a small branching tube entering the crank after a slight restrictor, with a hole in the other side of the crankcase, could provide negative crankcase ventilation by sucking fresh air through the crankcase and into the intake. This again prevents build up of hydrogen in the crankcase (avoiding rapid oil degradation) but also recovers that hydrogen for combustion in the cylinder. With reduced pressure in the crankcase, blow-by may increase, the extent of the increase needs to be investigated.

Exhaust-intake heat exchange Using the latent heat of the exhaust to heat the intake tubing, as well as potentially avoiding the need to guard the typically exposed super-hot tailpipe from touch, could pre-heat the intake air and assist in diesel-operation ignition.

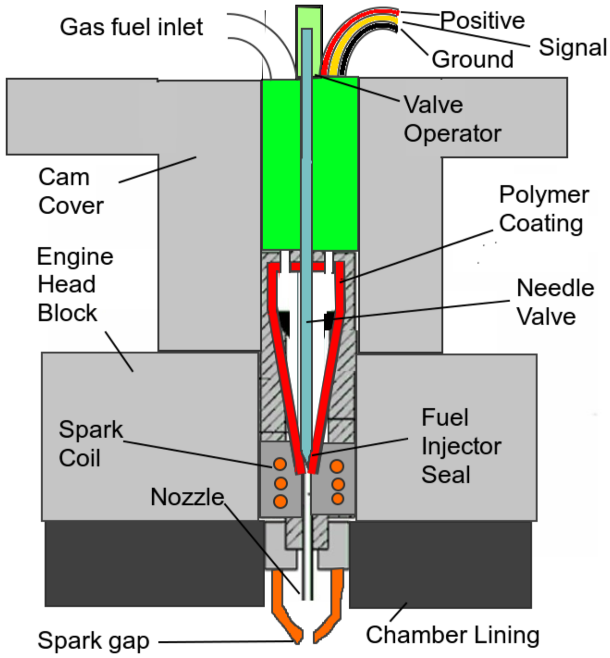


FIGURE 5.1: Combined injector-spark device. Replaces original spark plug, functioning as both direct cylinder fuel injector and spark ignition source. Components exposed to hydrogen are either made of or lined with materials resistant to embrittlement and non-porous to hydrogen.

5.1.3 Ideal design

A quick note to discuss the ideal H2ICE generator, were cost and complexity not an issue. The ideal engine would be a turbocharged 2 cylinder diesel-like engine that has a high compression ratio, a designed hot spot at a point on the surface of the combustion chamber in the path of the injected fuel. A turbo powering the fuel pump is fitted with a motor-generator-unit to prevent over-spooling and power the pump during start up.

Alternatively, a comprex supercharger recovers exhaust gas energy and variable intake valve cam profiling (or direct electronic control of the intake valves) saves the crank work when peak pressure would otherwise exceed maximum pressure. Exhaust gas recirculation is used for its benefits, while the fuel pump is powered electronically.

5.2 Final Recommendation

5.2.1 Engine knowledge

Before any serious practical work is to be done, any investigating team or individual must make an analysis of whichever engine they will be working with, and be aware that:

- The stock intake and exhaust lengths and shapes (as well as the valve timing of cam profiles) are designed (or tuned) with aerodynamics in mind to harmonically produce standing waves that promote intake and exhaust action at certain engine speeds (or hinder, at others) and that adjustment of the intake and exhaust system will have implications for what engine speed, if any, correct harmony is reached.
- Spark timing (otto) and injection timing (diesel) are designed around the ignition delay and flame speed of the engine's fuel, and modifying ignition/injection

timings when making modifications to engines should be expected for best results (hydrogen's supersonic burn means most engines would likely benefit from delaying ignition to closer to top-dead-centre, but beware the next point).

- The strength of the con-rods and piston will be designed for specific pressure curves and consideration for the maximum cylinder pressure these components were designed for is essential to avoiding accidental catastrophic component failure.
- The bolts that hold engine blocks together are under high stress, and the act of unfastening them imposes significant wear on them. For example, the manual of the engine the author worked on with a motor-sport team strongly recommended that bolts holding engine blocks together not be fastened more than three times before being replaced, lest there be a risk of one of them failing totally during operation.
- In general, it cannot be recommended enough to read the manufacturer's manual, paying attention to as much detail as possible, before working on an engine. They are difficult enough to get working at the best of times.

5.2.2 First steps

A diesel-operation engine using the combined-injector-ignition device should be installed, the pump be powered separately from the grid, and the first priority should be to get an engine running that does not suffer knock, leaks, or any form of flashback. In this case, negative crankcase ventilation into the intake is recommended to avoid build-up of hydrogen gas in the testing area, possibly with a dedicated pump also providing positive crankcase ventilation as well until it can be established that the intake really is properly venting the crankcase.

5.2.3 Try After

Once such an engine is operating smoothly, improvements can be tested and efficiency, power, wear and emissions can start to be optimized. Perhaps the easiest first thing to try is intake pre-heating using an intake-exhaust system that exchanges heat to see if it makes ignition more reliable, especially in a cold climate. After that exhaust gas recirculation, possibly with a comprex supercharger, is probably the next simplest thing. However, variable valve timing is a complex feature to attempt, even if the engine came designed with it.

Concluding suggestions for modifications to the first step engine, Atkinson cycle techniques should be explored. Starting with conventional turbochargers with waste-gates to test forced induction and installing a turbine on a H2ICE. A generator on the shaft could be attempted, replacing the function of the waste-gate and capturing more work, although this could prove expensive to develop. Powering the fuel pump with a turbocharger is definitely worth a try, as it effectively achieves an Atkinson cycle that varies its expansion rate (the speed of the turboshaft) with power output.

For a more ambitious step, a 5 stroke with exhaust gas recirculation (should EGR be confirmed to have enough merit to be worth implementing) with variable big-piston valve timing would be worth investigating.

5.3 Conclusion

We conclude here with a quick review and evaluation of target application goals from chapter 1, and a reminder that fuel storage and the fuel system upstream of the fuel pump or restrictor valve, were beyond the scope of this project.

- Prototype
- Manned off-grid applications
- General site backup generators
- Hospital backup generators
- Public transport and delivery vehicles
- Road vehicles

Functioning H2ICEs have been demonstrated in the lab, and we can concluded that they are capable of working well, whether the fuel source be high or low pressure. We have seen that there are many options for optimizing a H2ICE for low NOx emission, high efficiency, and smooth operation. Reliability will need larger scale tests, but there has been no reason found to suggests that H2ICEs will wear faster or be any less reliable than other gas-fuel ICEs. We have seen that H2ICEs can even outperform petrol and diesel engines in efficiency and emissions at the same time.

We have a proposal and an outlined plan to develop H2ICE generators should we now wish to pursue it. We also can already begin exploring simple conversion kits (albeit for simple engines that may sacrifice efficiency and emissions performance). We have also noted that it would be best if any person(s) who pursued practical investigations into H2ICEs have practical experience modifying engines and be very familiar with the engine(s) of choice.

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