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Introduction

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1.1 Study motivation

Future transportation systems face a broad range of requirements. They must be economic, clean, low-carbon, efficient, and reliable (to name just a few). These characteristics must be based not only on the vehicles, but also upon their fuel supply chains. Using hydrogen as a fuel offers a possible solution to satisfying global mobility needs, including sustainability of supply and the potential for significant reduction of greenhouse gas (GHG) emissions.

Because hydrogen is an energy carrier that must be produced from primary energy resources, sustainability also implies that the hydrogen must be cleanly and economically produced, whether this involves carbon capture and storage (CCS), renewable energy resources, or long-term nuclear solutions.

This does not mean that a sustainable future must be static, and the evolving vision of sustainability is increasingly coming to incorporate concepts of flexibility and resilience.

This book is about research issues that are at the intersection of hydrogen and transportation, because the study of vehicles and energy carriers is inseparable. This book presents analysis of light-duty vehicles (LDVs; i.e. cars and light trucks, not heavy trucks), set in the context of other competing technologies, the broader energy sector and the overall economy.

1.1.1 Size and complexity of the problem

The size and complexity of the transportation system are undeniable. Transportation represented 29% of US energy use in 2009 (EIA, 2010b), and the share is similar globally (EIA, 2010a). The historic availability, affordable (though volatile) price, and excellent physical and chemical properties of oil have long made it the

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dominant transport fuel, with 95% of US transportation energy demand, including ship, rail, and air use, being satisfied by petroleum (EIA, 2010c). The size of the transportation infrastructure is vast and permeates the very fabric of our human environment on both the physical and social levels. On the supply side, this includes oil production, transport, refining, and distribution; on the demand side, it includes not only the stock of vehicles and roads produced, but also demographic patterns and a society built on division of labour and cheap transportation. Both the scale and complexity of this infrastructure mean that changes must be gradual.

The analytic and policy complexities of the transport sector are significant. Both the costs and benefits of our current system are great, and they affect a large number of stakeholders in different ways. Some of these costs and benefits are unremarkable; for example, the costs of traffic accidents and the benefits of personal freedom are largely uncontroversial, if difficult to quantify. The dominant problems of dependence upon oil are the increasing cost and decreasing reliability of future supplies, and the environmental consequences of our ever-increasing demand, due primarily to the costs associated with predicted future climate change. Both of these problems have costs and benefits that are unevenly distributed around the globe, with implications for social equity, global development, and international security.

The role of carbon dioxide (CO₂) as a GHG deserves, perhaps, special mention in this discussion of problem complexity. While the relative contribution of ever-increasing CO₂ levels compared to other factors affecting climate change (e.g. solar wind, oceanic oscillations, and cloud/water vapour feedback) is still a subject of some debate, the consensus of the scientific community is that further increases in CO₂ levels are likely to lead to long-term costs due to climate change, increased storm intensity, changes in rainfall patterns, and rising sea levels. There are also arguments about the economic priorities of avoiding CO₂ emissions versus adapting to climate change while addressing other global problems (Lomborg, 2009). But it is clear that reducing CO₂ emissions is a very significant global concern.

1.1.2 Energy security

Predictions of future gaps between dwindling oil supplies and growing demand will not be fulfilled as long as market prices can function to incentivise new production and allocate production to the most valuable uses. But that does not mean that the production of cheap crude will not decline, or that those people unable to afford future prices will not suffer. The expectation is not the ‘end of oil’ but the end of cheap, easy, and reliable oil. Not ‘peak oil’, but a transition to resources that are ever more difficult to find, extract, and afford. This is a present continuation of the historical shifts from wood to coal to oil, and ongoing shifts to gas and presumably nuclear (interrupted, but now possibly resuming). The depletion of current reserves,
and the increasing marginal cost of extracting oil from new reserves or existing reserves of lower quality is the driving force behind the development of competing energy resources. As Sheik Ahmed Zaki Yamani said, ‘The Stone Age didn’t end for lack of stone, and the oil age will end long before the world runs out of oil’ (Maass, 2005). We will leave oil behind when it is too expensive to compete.

For the present though, it is not just cost and global availability that are a concern for energy security. Geopolitical concentration in supply and the international competition for supply as global demand patterns shift are not new in the history of oil. The fungibility and easy transport of oil mean that the market is global, but prices are still volatile. This volatility leads to economic disturbances that are painful in and of themselves; and also serves to deter the development of competing energy resources.

1.1.3 Climate change mitigation

The current transportation sector is a major source of CO₂, contributing 23% of total emissions worldwide in 2006 (IEA, 2008b), and the difficulty of reducing emissions is out of proportion even to its contribution. Vehicle emissions are the hardest source of CO₂ to eliminate because they are numerous, small, mobile, and distributed. In contrast, fixed site emitters like power plants are larger and much more amenable to efficiency gains, fuel switching, or CCS (a technology that is still in the demonstration phase). Even small, fixed site emissions, such as from residential heating, are much more amenable to fixes like better insulation or replacement by biomass (wood) or heat pumps. One of the advantages of using hydrogen as a transportation fuel is that emissions are moved from the tailpipe back up the supply chain to where the hydrogen is produced. Depending upon the source of the hydrogen, the CO₂ emissions per vehicle kilometre can be increased (e.g. hydrogen from coal), reduced (from natural gas), or virtually eliminated (renewable energy or nuclear).

These major problems of energy security and climate change provide great impetus to transition beyond oil to a different future energy and transportation system, but this does not guarantee that future transportation systems will be based on hydrogen. Hydrogen has a long history of being called the ultimate fuel, and the latest wave of enthusiasm and inevitability has only recently begun to ebb again. There is significant need for objective, unbiased analysis of the potential that hydrogen holds in transportation, and where its use can most benefit the economy in general.

The dominant expectation is that hydrogen in vehicles will be used by fuel cells rather than internal combustion engines, due to the high efficiency that exceeds the thermodynamic limits of combustion. This is compatible with and benefits from the current trend to increased electrification in vehicle drivetrains found in hybrids and electric vehicles. The chief disadvantages of hydrogen vehicles are the still high costs of fuel cells and the relative balance that must be struck between tank size
and limited driving range (currently as much as 400–600 km), due to the low volumetric energy density of current hydrogen storage methods. These problems have meant that commercial demonstration of hydrogen-fuelled vehicles is still lacking. Battery-powered vehicles currently have a more limited range (100–200 km), but with the additional advantage that it is much easier to transport and deliver electrons (electric power) than protons (hydrogen), as the distribution infrastructure for electricity is already in place. In contrast, a hydrogen vehicle fleet will likely involve building a new distribution infrastructure of pipelines and tankers that will not only prove more expensive, but also form a barrier to market penetration.

1.1.4 No guarantees

The potential benefits of hydrogen are very great, but its competition is far from standing still in both the areas of drivetrains and energy carriers. Improvements to the internal combustion engine (ICE) continue through electromechanical controls (e.g. variable valve timing and compression, and mixed multi-fuel metering), multi-fuel engines, and many other schemes. Hybrids and electrical vehicles are at or near the cusp of commercialisation, and battery energy densities are continuing to climb. On the fuel side, there are many alternatives to produce alternative fuels with volumetric energy densities that are higher than hydrogen, including natural gas, syngas, a range of synthesised liquid fuels like alcohols, bio-ols, Fischer-Tropsch, etc. These gases and liquids can stem from a wide range of primary energy resources, including coal, biomass, algae, and direct microbiological sources. Thus, the advantage that hydrogen may be produced from many different energy resources is in fact shared by other fuels, each with their own unique advantages. Hydrogen is therefore by no means guaranteed to be the fuel of the future, and only a careful and detailed analysis of its costs and benefits in comparison with other drivetrains and energy carriers will reveal its strengths and weaknesses. It is indeed likely that no one energy carrier will continue to dominate all economic, environmental, and social (or consumer) criteria, so individual choices in the marketplace will have a key role in determining the vehicle of the future.

1.2 Primary objectives

The primary objectives of the research reported in this book were to perform a comprehensive and holistic analysis of the impacts of implementing hydrogen as a fuel into future LDV fleets while considering the effects on other energy sectors. Important issues have included centralised versus decentralised production, competing distribution methods, suitable vehicle drivetrains and onboard storage, full energy chain cost, environmental and safety concerns, the feasibility of transition
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to a hydrogen infrastructure, and the effect of different policy options on implementing such a transition.

1.2.1 Fuel use and emissions identities

As a background to discussing the structure of the research programme that forms the basis for this book, it is worthwhile to recall the basic identity equations that form the basis for total vehicle fuel use and emissions, namely:

\[
\text{Fuel use} = (\text{population}) \times (\text{cars/person}) \times (\text{km/car}) \times (\text{fuel use/km}) \quad (1.1)
\]

and adding an additional factor for emissions:

\[
\text{Emissions} = (\text{fuel use}) \times (\text{emissions/fuel use}) \quad (1.2)
\]

This chain of factors illustrates that, if the goal is to reduce the total amount of fuel used or emissions, it is not sufficient to look only at the individual vehicle. The equations must be summed over the entire vehicle fleet to understand total fuel use and emissions, and it must be understood how the fleet is projected to change over time in order to forecast total fuel use and emissions into the future.

1.2.2 Trends in fuel and emissions factors

Based on the factors in Equations (1.1) and (1.2), it is worth mentioning how trends in the relatively recent past have influenced each factor in the chain.

Population growth

Population growth, and policy options to control it, is beyond the scope of this book, but it is worth noting that differential, national population growth rates form a key driver for transportation demand, and resource demand in general.

Fleet growth

The per capita ownership of light vehicles is dependent upon per capita income, and hence economic growth over time. This factor includes shifts between vehicle types (e.g. from scooters to cars to SUVs), and thus fleet composition. Fleet penetration depends on competing vehicle characteristics (price, mileage, safety, etc.). Factors relevant to fleet penetration studies include vehicle fuel type and availability, various policy options (e.g. taxes, subsidies, feebates, etc.) and social acceptance.

Annual vehicle use

Travel per vehicle is primarily determined by demographic patterns (e.g. commute distances) and per capita income. Increasing income can also shift mileage between vehicle types.
Fuel use

Engine efficiency gains over the last decades have been significant, while the vehicle fuel use per kilometre has stagnated. The reason for this has primarily been the consumer choosing vehicle performance over economy, particularly in vehicle classes exempt from mileage standards (Bandivadekar et al., 2008a). Reallocating engine efficiency gains to fuel economy is important for reducing total fuel use and carbon dioxide emissions. Other key ways to reduce fuel use and emissions include vehicle downsizing and lightweighting.

Emissions

The emissions per unit of fuel used can be divided between local emissions (NOx, VOC, particulates, etc.) that are determined by engine and exhaust treatment technology, and global emissions (i.e. CO₂) that cannot practically be scrubbed from vehicle emissions and depend upon the carbon content of the fuel.

1.3 Scope of work and approach taken

Based on the factors and trends discussed above, the scope of the research and the approach taken followed the basic steps below, that is, to:

• Analyse individual technology impacts (for both energy carriers and drivetrain technologies)
• Analyse vehicle trade-offs for a large number of vehicle designs
• Analyse changes in fleet composition, and the resulting changes in total fleet burdens over time
• Analyse technology choice strategies using least-cost optimisation

More concretely, this scope of work was translated to the following separate research tasks that are shown in Figure 1.1 below, which shows the structure of the research programme that generated the results described in this book.

• Well-to-tank analysis of hydrogen production from multiple primary energy resources (including renewables), in addition to competing fuels (Chapter 2).
• Heuristic, rule-based generation of vehicle designs, including drivetrain simulation to produce multi-attribute characterisation on a vehicle and kilometre basis (Chapter 3).
• Assessment of atmospheric hydrogen concentrations related to fossil-fuelled vehicles and estimates of the effects of the introduction of hydrogen vehicles (Chapter 4).
1.4 Organisation of book

The book is organised by chapters corresponding to each of the individual research tasks shown above. A brief description of each task and chapter is given below.

1.4.1 Life cycle assessment

Energy technologies generally involve a related chain of steps including resource extraction, transportation, refining or conversion, distribution, use, and disposal. A life cycle assessment (LCA) is necessary in order to integrate the potential environmental impacts of each step in the chain. For transportation systems, this is usually called a well-to-tank analysis if the chain ends with the fuel and a well-to-wheel analysis if
the chain includes final use in the vehicle. Use of LCA guarantees that all the relevant material, resource, and energy flows throughout the complete chain are considered, which is a strict prerequisite for comparative environmental assessment of energy systems. LCA is particularly important for hydrogen because as an energy carrier most of its burdens are associated with the production step rather than final end use.

Chapter 2 presents an overview of the environmental performance of various current and future routes to hydrogen production, including fossil, renewable, and nuclear energy as the primary sources. Production using fossil energy is based on chemical conversion from coal and natural gas, as well as production of electricity for electrolysis. The direct production of hydrogen from renewable energy focuses on innovative solar processes, and production via electrolysis is based on a range of renewable generation technologies. The assessment considers centralised production with transport and distribution to the point of sale, as well as smaller, distributed, and on-site (fuelling station) production methods.

The chapter compares the various production pathways for producing 1 kg of H₂ with the combustion of energy-equivalent quantities of conventional fossil vehicle fuels in a EURO3 standard passenger car engine.

The LCA performed was based on the ecoinvent database (ecoinvent, 2009), which is the world’s most comprehensive and transparent LCA database. The impact assessment was conducted using a range of indicators: cumulative primary energy demand (fossil and nuclear) and the cumulative emissions of GHGs, suspended particulate matter (PM), volatile organic compounds, nitrogen oxides, and sulphur dioxide.

1.4.2 Heuristic vehicle modelling

Well-to-wheel analyses have in the past typically been performed based on a rather limited number of generic or typical vehicle types. In Chapter 3 the approach that was used instead was to automate the generation of vehicle designs based on a set of rules to ensure consistency between component weights, power, etc. The design variables (or options) that were combined to form different designs included vehicle class and weight, type of drivetrain and fuel, degree of electrification (from zero for conventional designs to one for electrical vehicles, with hybrids in between). In addition to these exogenous variables, a range of dependent variables endogenous to the vehicle design were also determined. By automating the design process and integrating it with a drivetrain simulation of each vehicle, it was possible to perform repetitive modelling of a very large number of designs composing a ‘virtual fleet’.

A range of characteristics (multi-attribute analysis) was calculated for each vehicle design, including not just drivetrain attributes (e.g. energy use and emissions), but
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also characteristics including vehicle performance, utility, range, safety, materials use, and cost. These attributes were then used to perform trade-off analyses and multi-attribute analysis for different preference profiles.

Areas of analytic emphasis included study of the synergistic and competitive relationship between hybrid and fuel cell vehicles (FCVs), impacts of variations in the degree of electrification, lightweighting, and correlating vehicle weight to energy use.

1.4.3 Hydrogen emissions

Molecular hydrogen (H\textsubscript{2}) present in the atmosphere is not a direct GHG, but it is removed from the atmosphere through a chemical process that competes with the process that removes methane, a potent GHG. H\textsubscript{2} is therefore effectively an indirect GHG. Present internal combustion engine vehicles (ICEVs) are the dominant source of anthropogenic hydrogen to the atmosphere. Large-scale use of hydrogen as a vehicle fuel, in parallel with increasing H\textsubscript{2} production for non-transport-based end uses, could lead to an increase in atmospheric hydrogen.

Chapter 4 first provides an overview of atmospheric hydrogen, including the major sinks and sources, with particular emphasis on the anthropogenic contribution from technological processes (i.e. motor vehicles and H\textsubscript{2} production, distribution, storage, and non-transportation-based end uses). It then relates the influence of vehicle technology and driving patterns to hydrogen emitted in vehicle exhaust, and qualitatively and quantitatively compares emissions from current and future vehicle technologies. These emissions are scaled using various scenarios for time periods throughout the twenty-first century to quantify global H\textsubscript{2} emissions from road-based transportation. H\textsubscript{2} emissions from non-transportation sources are also scaled up based on various leakage and loss rates, using these same scenarios. The scaled results from transportation are then combined with results from the non-transportation-based sources to find overall global, anthropogenic H\textsubscript{2} emissions from technological processes, based on various vehicle fleet composition scenarios and H\textsubscript{2} production strategies for industrial and direct energy-based end uses.

1.4.4 Fleet modelling

People purchase cars based on a wide range of factors, including cost, mileage, fuel availability (infrastructure), and the behaviour of other people around them. The aggregate choices of people that are reflected in vehicle fleet composition dynamics are therefore non-linear and exhibit a range of feedbacks. This makes the use of systems dynamics particularly interesting for the purposes of modelling market penetration of different fuels and technologies, and the impact that different
policy options can have upon the rates and ultimate levels of market penetration into the vehicle fleet.

Chapter 5 focuses on understanding the market dynamics of technology penetration into the vehicle fleet, and, in particular, on the interplay between technology introduction and the availability of fuel (or energy carrier) infrastructure. These dynamics reveal a range of behaviours, such as hybrid vehicles prolonging dependence on fossil fuels, technology lock-in that can delay bridging to ultimately cleaner vehicles, and rebound effects (increased driving) due to improved fuel economy. This modelling includes current technologies (gas and diesel vehicles), as well as competing future technologies (natural gas and hydrogen vehicles). It also shows that, in addition to zero-emissions vehicles, reductions in fleet size and vehicle travel are important in reducing total fleet emissions. The effects of different policy options on fleet penetration have also been examined, as well as the levels at which they can tip technology adoption into alternate system states.

### 1.4.5 Energy–economic modelling

The energy–economic analysis in Chapter 6 expands the consideration of vehicle energy carriers and technologies by setting them in the wider context of the whole energy sector. It uses a least cost optimisation model (MARKAL) to determine constrained capital investment in all stages of the competing energy chains. These chains include primary resource extraction (e.g. oil), conversion to energy carriers (e.g. hydrogen, electricity, or synfuels), transportation (e.g. hydrogen pipelines versus pressurised tank trucks versus local production) to the final demand technology that converts energy into consumer services (e.g. vehicles that provide transport). By making investments in all steps of the many competing energy chains to minimise net present costs, the global, multi-region model can incorporate energy system interactions, technical change, and economic and demographic driving forces. Such a model assumes perfect foresight (i.e. certain forecasts), so it serves as a complementary comparison to the system dynamics modelling of the previous chapter that models without foresight.

The model can include policy scenarios by imposing emissions caps, or modifying costs by adding taxes or subsidies. The results of this chapter show hydrogen can be an important option for achieving stringent GHG targets over the long term, but strict emissions caps or other strong incentives are necessary to achieve vehicle and infrastructure deployment. Hydrogen transport is identified as a potential bottleneck that could reduce hydrogen’s attractiveness, and the mid-term investment that is required to keep the long-term option for hydrogen open is found to be moderate compared to other power sector investments.