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Methodologies for representing the road transport sector in energy system models[☆]

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ABSTRACT

Energy system models are often used to assess the potential role of hydrogen and electric powertrains for reducing transport CO₂ emissions in the future. In this paper, we review how different energy system models have represented both vehicles and fuel infrastructure in the past and we provide guidelines for their representation in the future. In particular, we identify three key modelling decisions: the degree of car market segmentation, the imposition of market share constraints and the use of lumpy investments to represent infrastructure. We examine each of these decisions in a case study using the UK MARKAL model. While disaggregating the car market principally affects only the transition rate to the optimum mix of technologies, market share constraints can greatly change the optimum mix so should be chosen carefully. In contrast, modelling infrastructure using lumpy investments has little impact on the model results. We identify the development of new methodologies to represent the impact of behavioural change on transport demand as a key challenge for improving energy system models in the future.

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1. Introduction

The transport sector is expected to change profoundly over the coming decades as alternative electric and/or hydrogen powertrains are introduced to the market to reduce CO₂ emissions, complementing or replacing the hydrocarbon fuels and internal combustion engine (ICE) designs that have been used since the advent of the passenger car more than 100 years ago [1]. A number of modelling approaches have been used to compare the prospects for, and implications of, various possible future fuels and powertrains. One common approach applies system dynamics modelling to vehicle choice and adoption, and in doing so seeks to explore the

relative importance of different behavioural, technical and economic factors in enabling the adoption of different vehicle technologies [2,3]. Another common approach is to compare different vehicle configurations in a static way, developing detailed depictions of the life-cycle environmental and energy impacts, and the total costs of ownership [4–6].

While these studies have provided valuable insights, they share a common weakness, which is that the wider energy system is assumed to be exogenous to the transport sector. The required level of transport decarbonisation is an exogenous assumption in these models and does not account for the relative costs of decarbonising transport and other sectors. Fuel prices and availability are also provided exogenously

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and are assumed to be insensitive to changes in fuel demand. Moreover, some new transport infrastructure, for example hydrogen pipeline networks, might only be economically-viable if they provide energy services to other sectors as well as to the transport sector.

Energy system models, such as MARKAL/TIMES [7] and MESSAGE [8], do not share this weakness. These bottom-up, dynamic, linear programming optimisation models find the cost-optimal decarbonisation pathway within the context of decarbonising the entire economy. They represent the entire energy system from imports and domestic production of fuel resources, through fuel processing and supply and explicit representation of infrastructures, to secondary energy carriers, end-use technologies and energy service demands of the entire economy. Since energy system models determine whole economy decarbonisation pathways, including the transport sector, they are often employed to provide exogenous boundary conditions for the other model types mentioned above. While no single model methodology is capable of fully evaluating the many options for the transport sector in the future, energy system models provide an important and complementary perspective to the other model types. It is therefore important that the transport sector, including fuel supply infrastructures, is appropriately represented in energy system models.

In this paper, we review how different energy system models have represented vehicles and fuel supply infrastructures in the past. We identify key modelling decisions and examine each of these decisions in a case study using the UK MARKAL model. UK MARKAL is an appropriate model for illustrating the methodological issues that we discuss in this paper because it is a mature model that has been the subject of numerous hydrogen-focused papers [9–13]. We concentrate on private cars in this paper as these dominate transport demand and fuel consumption in most countries, but the infrastructure applies to all forms of road transport and the vehicle methodologies apply equally for other types of road vehicle as for cars (but at a different scale). A full description of how to adapt the methodologies presented in this paper for goods vehicles and buses is given in Ref. [14].

1.1. Difficulties representing the transport sector in energy system models

There are a number of methodological difficulties when representing the transport sector in energy system models that we discuss in this paper.

First, non-cost factors are difficult to represent. Consumers take a variety of factors into account when purchasing a vehicle, including cost, size, colour, safety, features and design, while optimisation models such as energy system models account for only cost so would always invest in the cheapest (i.e. smallest) vehicles if given a choice. It is necessary to make assumptions about the impact of non-cost factors on the vehicle fleet in the future. This is particularly important for new low-carbon technologies whose performance (in terms of range, refuelling time, etc.) is worse than that of existing vehicles.

Second, building the required fuel supply infrastructures for electric and particularly for hydrogen powertrains would

require huge investments, yet such infrastructures are difficult to represent in energy system models because some of the costs (e.g. for pipelines) are sensitive to the geography of the region/country and the energy throughput can be much lower than the maximum, particularly during transitions to new fuels [15,16]. Spatially-disaggregated infrastructure planning models can be used to examine the development of infrastructure and to provide data for energy system models [17].

Third, it is necessary to ensure that the representations of vehicles and fuel infrastructures in the model are internally-consistent. This means that the costs for all vehicle powertrains and refuelling infrastructure should be calculated in a consistent manner using comparable data sources and with clear assumptions. These data should also reflect the scenario being examined, particularly when other models are used to provide input data to the energy system models; for example, demand forecasts for transport (in total distance rather than energy terms) are sometimes taken from external models (e.g. Ref. [18]) and the assumptions used in these models should be consistent with the assumptions used in the energy system model.

More generally, energy system models have very complicated structures as they examine all parts of the energy economy, so it is necessary to avoid overly disaggregating each sector in order to keep the model and particularly the running time manageable; the modeller aims to minimise model complexity without adversely affecting results [19]. From this perspective, the most appropriate methodology is the least complicated one that produces both realistic overall results and the insights required by the study. Modellers might choose to create two versions of the transport sector: a first for general applications and a second more disaggregated version for studies focusing primarily on the transport sector.

1.2. Outline of this paper

In Sections 2 and 3, we examine previous approaches to representing vehicles and infrastructures, respectively, and we identify implicit assumptions and three key modelling decisions that are often not well documented. We also recommend appropriate methodological approaches for representing vehicles and infrastructures in these sections and we illustrate these in a case study in Section 4, in which we develop a full and consistent representation of transport vehicles and fuel infrastructure in the UK MARKAL energy system model. In Section 5, we examine the three key modelling decisions from Sections 2 and 3 using this revised version of the UK MARKAL model. We finish with a discussion some of the drawbacks with energy system models in Section 6.

2. Representing vehicle technologies in UK MARKAL

Energy system models represent the road transport sector as a simple market of vehicle technologies competing to meet demands on the basis of cost. Exogenous forecasts of car transport demand are identified from the literature, in vehicle kilometres, and the various technologies represented in the model compete to meet that demand over all of the years in

order to minimise the total energy system cost over the whole model horizon. Technology capital, operating and fuel costs are considered by the model, with each fuel cost calculated by balancing supply and demand in a dedicated commodity market.

In this section, we summarise the sources of and uncertainties in the cost and fuel efficiency data that underpin energy system models.

2.1. Vehicle market segments

In most bottom-up energy system models, the current and future transport demand is specified exogenously and different technologies compete to meet that demand. Many models [20,21], including UK MARKAL, use a separate demand for each type of vehicle (cars, buses, etc.) but assume that the market for each vehicle type is homogeneous, with no differentiation of size or classes of car and hence little account of non-cost factors. While this is a reasonable assumption for existing powertrain technologies, it is less appropriate for analysing the long-term evolution of the car market and its role in the wider energy system because some technologies are better suited to small, urban cars while others are considered better suited to larger, multi-purpose cars, for both economic and non-economic reasons. The main economic reason is the non-linear relationship between battery capacity and car weight for battery electric vehicles, due to mass compounding,¹ which is necessary to achieve a consistent driving range across market segments [22]. Non-economic reasons include, for example, the limited range of battery electric vehicles, which makes them mostly unsuitable for the larger car markets. For these reasons, transport analysts have increasingly suggested that a portfolio of hydrogen, battery electric and biofuel powertrains will co-exist in future vehicle markets (e.g. Refs. [5,23]).

Disaggregation can offer additional insights about trends in each market segment, for example divergent rates of decarbonisation, which are not available from the homogeneous approach. Some MARKAL/TIMES models do represent the car sector with disaggregated market segments. For example, the US 9-region MARKAL model represents compact cars, full size cars, SUVs, minivans and pickups each as separate categories [24], while the Canadian TIMES model includes a breakdown of small cars, large cars and light trucks [25].

Some models, for example the Canadian [25], French [26], Pan-European [27] and Norwegian [28] TIMES models, and the Belgian MARKAL model [29], disaggregate road transport demand into short- and long-distance journeys. For the TIMES models, this enables vehicle efficiencies (in terms of distance per fuel use) to be higher for long-distance than short-distance journeys if appropriate vehicle efficiency data are available. It also allows modellers to specify the maximum contribution of each powertrain type to each journey distance in each year as an efficient alternative to setting market constraints across

the model (see Section 2.5), although similar exogenous data are required for both methods. However, this approach does not offer any of the advantages of market segment disaggregation discussed above. One solution, adopted by the Canadian TIMES model [25], is to combine journey distance and market segment disaggregation in order to benefit from the advantages of both methodologies.

Although market segment disaggregation enables better representation of variations in the suitability of alternative technologies in different segments, it increases the size of the model and requires assumptions about the future relative market share of each segment. Disaggregating by journey distance similarly increases the model complexity and requires additional data and assumptions. As for any model, such increases in model complexity from disaggregation should be justified by an improvement in the model skill and should be underpinned by data of suitable quality. The modeller should attempt to strike an appropriate balance, which may depend on the research question at hand.

Identifying appropriate levels of vehicle market segmentation is a key decision for energy system modellers. To our knowledge, no studies have reported a comparison of otherwise identical models that have different levels of aggregation in representations of vehicle market. We examine the impact of disaggregating the UK car sector in Section 5.1.

2.2. Vehicles and transport fuels

Vehicle manufacturers are combining low carbon fuels and new powertrain types in a wide array of possible configurations, in order to find the best performing low-carbon vehicles in response to policy drivers. Lower-carbon hydrocarbons (such as Compressed Natural Gas [CNG] and Liquefied Petroleum Gas [LPG]), biofuels, electricity and hydrogen are all contenders. Different conversion devices (engines, fuel cells) and powertrains (parallel and series hybrid, plug-in hybrid) can be combined with these fuels in an array of configurations. In an attempt to reduce model complexity, many previous energy system modellers have chosen to limit the range of options to exclude, for example, the use of plug-in hybrid technology in concert with low-carbon fuels such as hydrogen or biodiesel (e.g. Refs. [25,30,31]).

Table 1 lists a number of vehicle types that could be included in energy system models. In particular, we recommend including hybrid and plug-in versions of hydrogen powertrains and allowing hydrocarbon ICEs the flexibility to use any proportion of biofuels, which is not possible with current vehicles but would require only minor alterations to engine designs in the future. These recommendations exemplify the necessity for imagination on behalf of the modeller to ensure that no prospective vehicle designs are excluded from the analysis.

Hydrogen can be used in modified ICEs as well as fuel cells but on-board storage presents particular difficulties: given the poor efficiency of ICEs compared to fuel cells, hydrogen ICE vehicles have mostly been designed to use liquid hydrogen, despite the high cost of liquefaction, because it has a much higher volumetric density than gaseous hydrogen so can provide sufficient energy for an acceptable vehicle range in a single tank. However, use of liquid hydrogen presents a

¹ Mass compounding means that larger cars require proportionally larger batteries due to the batteries being a substantial proportion of the vehicle weight, which makes electric powertrains relatively cheaper and more efficient relative to other powertrains for smaller vehicles.

Table 1 – Types of vehicle that could be included in energy system models. “ICE” vehicles have internal combustion engines. “FCVs” are fuel cell vehicles.

Vehicle name	Description	Fuels
Petrol ICE NH	Petrol non-hybrid ICE	Petrol and petrol/ethanol blends
Diesel ICE NH	Diesel non-hybrid ICE	Diesel and biodiesel
Petrol HEV	Petrol hybrid ICE	Petrol and petrol/ethanol blends
Diesel HEV	Diesel hybrid ICE	Diesel and biodiesel
Petrol PHEV	Petrol plug-in hybrid ICE	Electricity and petrol and/or petrol/ethanol blends
Diesel PHEV	Diesel plug-in hybrid ICE	Electricity and Diesel and/or biodiesel
Hydrogen FCV NH	FCV – non-hybrid	Compressed hydrogen
Hydrogen FCHV	Hybrid FCV	Compressed hydrogen
Hydrogen FCV PHEV	Plug-in hybrid FCV	Electricity and compressed hydrogen
Methanol FCV NH	FCV – non-hybrid	Methanol
Methanol FCHV	Hybrid FCV	Methanol
Methanol FCV PHEV	Plug-in hybrid FCV	Electricity and methanol
BEV	Battery electric vehicle	Electricity
HICEH	Hydrogen hybrid ICE	Liquid hydrogen
CNG	Compressed natural gas ICE	Compressed natural gas
LPG	LPG ICE	Liquefied Petroleum Gas (also known as autogas)
E85Flexfuel	Flexi-fuel vehicle for E85 ICE	Petrol and high petrol/ethanol blends (up to 85% ethanol)

significant number of practical challenges. The most important is the loss of hydrogen from the car fuel tank through boil-off, which causes both safety concerns and economic losses for the owner. For these reasons, BMW abandoned plans to commercialise a hydrogen ICE vehicle in 2009 and hydrogen ICEs are not currently being pursued by any motor manufacturers. We therefore exclude hydrogen ICEs (both hybrids and conventional) from the runs examined subsequently in the paper, though we recommend that transport sector studies should examine their impact using sensitivity analyses.

2.3. Vehicle costs

Both capital costs and fixed operating and maintenance costs should be represented in models for all vehicles. We have identified several sources of data for estimating vehicle capital costs [32–36], which all provide capital cost estimates for both components and overall vehicles. IEA [37] additionally provides data for fuel cells and fuel cell vehicles. The McKinsey report² [23] draws on proprietary industry data, and can

² Although McKinsey do not claim authorship of this report, it is commonly referred to as the “McKinsey report” and we follow that terminology in this paper.

perhaps therefore be considered to be a more reliable estimate of costs (though possible industry bias in such cases always needs to be considered). Since none of these sources provide capital cost estimates for all the types of vehicle included in this study, we recommend collating and comparing vehicle component costs to estimate vehicle costs using a bottom-up approach, as described for UK MARKAL in Appendix A in the Supporting Information to this paper and in McDowall and Dodds [14].

The costs of new technologies are expected to fall over time. In particular, the costs of electric drive components, fuel cells, automotive batteries and fuel storage technologies are all expected to decrease but the trajectory of cost reductions is highly uncertain. In specifying the future costs of technology for an energy system model, the analyst must adopt one of three possible choices [38]:

1. Assume no technological change.
2. Assume an exogenously-specified trajectory of technological change, with sequential technology ‘vintages’ available in the model. The costs of future vintages are informed by analysis of estimates in the literature, which typically include assumptions about future deployment that may not be internally consistent either with each other or with the resulting output scenarios.
3. Endogenise technological change into the model, such that costs are not specified exogenously but are rather a function of deployment. This has been undertaken by a number of analysts for hydrogen vehicles, including recently by Anandarajah et al. [38], but is not appropriate for a national-scale analysis because technology cost reductions spill over across borders.

For most applications, we recommend following typical energy system modelling practice by adopting the second of these options. The trajectory of cost reductions in the literature varies widely, since the assumed cost reductions are typically either implicitly or explicitly linked to different scenarios of wide scale deployment of the technologies, and with different assumptions about likely learning rates. For most costs in Appendix A, we use the estimates from Ref. [23], since this is based on the expectations of a wide range of automotive industry stakeholders. For each car technology, capital costs are defined for technology vintages, with a new vintage available in each model five-year period. In order to address the significant uncertainty around the future capital costs of technologies, we perform a number of sensitivity runs to examine the importance of plausible variations in future technology costs.

We estimate fixed operating and maintenance costs using estimates of annual running costs, insurance costs and road taxes based on AA [39] and HM Treasury [40]. These are described further in Appendix A.

In energy system models, each type of vehicle is typically assumed to travel the same annual average mileage each year, and both capital costs and operating and maintenance costs are specified in terms of cost per distance (e.g. £m/billion km in UK MARKAL). As a result, assumptions about the average mileage for the average car have a very important effect on the specification of vehicle costs. This introduces a source of

considerable possible error, given significant changes over time in the annual average mileage per vehicle observed in the historical record [41] and given the potential for different usage patterns of vehicles using different powertrains and fuels. For UK MARKAL, we assume that the annual average mileage is fixed over time (at the year 2010 value) and that the mileage is the same for all cars irrespective of the powertrain and fuel. We could exogenously vary this parameter by powertrain or by year to represent heterogeneous consumer behaviour, if there were suitable evidence available or if we wished to examine the impacts of long-term behavioural variations in scenarios, but this would require great care to accurately calibrate the model costs.

2.4. Vehicle energy efficiency

In energy system models, vehicle efficiency data is supplied exogenously for each vehicle and used to calculate fuel consumption. For existing European vehicles, the efficiency of the average vehicle can be estimated from data provided by the UK Society of Motor Manufacturers and Traders on the vehicle stock as a whole [42] and on new vehicle sales. However, these efficiencies are generally optimistically high as the fuel consumption performance of cars on the road is substantially worse than that expected based on standard drive cycle test data, for a whole range of factors including the non-representativeness of standard test drive cycles and the generally poor maintenance habits of many motorists. For the UK, we would therefore recommend using efficiency data from the UK Department for Transport on estimated annual car mileage [41] and total fuel consumption [43] to estimate the efficiency of the average car in the base year. These data are likely to be suitable for most European countries but similar data would have to be obtained in order to check this assertion.

For future vehicle technologies, efficiency data would ideally be drawn from detailed vehicle simulation models that examine the expected efficiency improvement of each component over a drive cycle. This modelled data would then be adjusted to account for the discrepancy between standard test cycles and real-world performance. Unfortunately, relatively few studies report simulation data for the full range of components in a consistent way. An alternative approach is to use data from studies such as Plotkin et al. [33], who simulate the efficiency of a range of different vehicle powertrains and provided forecasts for the years 2030 and 2045. Since this study assesses vehicle efficiencies for the average US vehicle, it is necessary to adjust this data to account for the difference in size and weight between the average US car and the average car in the modelled region. An example of this approach for the UK is in Appendix A.

2.5. Constraints on vehicle market share

The transport sector representation within an energy system model, even when disaggregated into multiple vehicle segments, fails to represent some important features of real-world vehicle markets. Typically in energy system model representations of the transport sector, constraints prevent the model from choosing outcomes that are believed to be implausible in the real world. For example, not every technology type could be expected to be a complete replacement

for the whole passenger car market. In order to represent the limitations on some types of vehicle in particular market segments, constraints can be added to prevent certain vehicle types from exceeding a particular market share.

For models that disaggregate by journey distance, either an upper/fixed limit (TIMES) or only a fixed limit (MARKAL) can be specified to set the extent to which a given vehicle can serve both short and long-distance demand, aiming to reflect the different suitability of vehicle types to different ranges. For models that do not disaggregate by journey distance, such as UK MARKAL, similar model constraints can be achieved by defining market share constraints for each market segment. The constraints in both approaches have similar underlying assumptions based on journey distance data, car industry expertise or information from other sources.

Some suggested constraints for the UK, which are based on studies reporting car industry views and market expectations for technology potential in different sizes of vehicle [44,45], are shown in Table 2. For example, battery electric vehicles are thought unlikely to be widely offered in medium or large sizes because of the problem of mass compounding that is discussed in Section 2.1, so are not expected to be able to capture more than a small portion of the ‘medium-large’ market segment. Given range limitations, it is also expected that battery electric vehicles are unable to capture the full market for small vehicles, though the market potential in this segment is higher. Similarly, car manufacturers are thought unlikely to offer a wide variety of small diesel, small diesel hybrid vehicles or small plug-in hybrids, because the additional costs associated with diesel powertrains and hybridisation come at little additional efficiency gain in this size class [44,45].

The choice of market share constraints is a second key decision for energy system modellers. We examine the impact of using these constraints in Section 5.2.

3. Fuel supply infrastructure

A major barrier to the widespread use of hydrogen or electricity as transport fuels is the lack of infrastructures for delivering these fuels. For electricity, it might be possible to

Table 2 – Constraints on car market share for the UK. The constraints are provided for two market segments (small and medium-large). The market share constraint for the combined market is calculated from the disaggregated market share constraints via a simple average weighted by the relative size of the small and medium-large segments in 2010, assuming that the present composition of the UK car fleet will not change in the future.

	Maximum market share in each market segment		
	Small	Medium-Large	Combined
BEV	60%	10%	24%
Diesel and diesel hybrid	20%	100%	78%
PHEV before 2025	0%	80%	58%
PHEV from 2025	25%	80%	65%

rely principally on home-charging in the short-term while on-street chargers are deployed. For hydrogen, a basic network of production facilities, refuelling stations and delivery mechanisms would need to be created to support the first adopters and this would initially be underutilised during a transition to large-scale hydrogen vehicle deployment. The costs associated with establishing this infrastructure, and bringing it to maturity, are substantial [46].

In addition to the transition costs, a mature electricity or hydrogen delivery infrastructure would be more expensive to construct than the existing hydrocarbon infrastructure. First, the energy density of hydrogen is very low compared to hydrocarbon fuels so a greater storage volume is required per unit of delivered energy, and hydrogen storage is currently very expensive. Second, gaseous hydrogen refuelling is slower than hydrocarbon refuelling and the additional time reduces the number of customers that can be serviced by each refuelling station and hence increases the required number or size of refuelling stations. Third, while home charging of battery vehicles could be low-cost if local electricity distribution network reinforcement was not required, provision of on-street chargers has so far been very expensive.

The delivery costs for hydrocarbon fuels are only a small part of the total cost of the delivered fuel. In contrast, the infrastructural cost of fuel delivery of electricity and hydrogen could be a much greater proportion of the total fuel cost as a result of the factors outlined above. However, these costs are rather uncertain. It is important to assess the extent to which such uncertain assumptions about infrastructure affect the perceived best option for decarbonising road transport using sensitivity studies.

3.1. Representing infrastructure in energy system models

Energy system models represent fuel delivery infrastructures explicitly, in terms of their costs, efficiency losses and lifetimes. The deployment of infrastructures is optimised alongside and evolves with other elements of the energy system and only whole system approaches are able to represent such interactions.

3.1.1. Spatial resolution shortcomings during infrastructure transitions

Energy system models have some shortcomings in the way in which they represent fuel infrastructure (discussed in some detail in Ref. [17]). Investment costs per unit infrastructure are specified in relation to units of capacity (in MW or PJ per annum, for example), with no explicit representation of the spatial structure of demand over which fuel must be distributed. In the real world, the investment costs depend on the capacity of the infrastructure to move fuel over a given distance. A spatially-clustered pattern of demand will require a cheaper infrastructure, per kg of hydrogen delivered, than a spatially diffuse infrastructure (as illustrated by Refs. [47,48]).

In a model without spatial disaggregation, the modeller must make exogenous assumptions (whether explicitly or not) about the spatial pattern of demand. One approach to address the spatial dependence is to build a multi-region energy system model [9,13]. However, this greatly increases

model complexity and a trade-off emerges between spatial detail and model tractability. The main alternative is to assume a spatial pattern of supply and demand off-model, calculate costs accordingly, and implement those costs in the model. This has been the approach used in most previous versions of UK MARKAL, based on assumptions described in Ref. [49] for cities in the USA.

However, the spatial structure of supply and demand (and hence the cost of a given unit of infrastructure per unit of fuel moved) is almost certain to change as a transition to a new fuel unfolds. Several additional factors also drive changing investment costs as demand for the new fuel rises. First, there are scale-economies in infrastructure technologies: a large hydrogen refuelling station is cheaper, per kg of hydrogen dispensed, than a small one [50]. Second, the utilisation rate of infrastructure technologies will vary during a transition, with relatively low utilisation rates in early stages when few consumers have adopted hydrogen vehicles, and higher utilisation rates once adoption has become more widespread. Since infrastructure investment costs are specified in the MARKAL/TIMES framework in units of the actual energy flow, the costs used in the model embody assumptions about utilisation rates. Finally, the cost of capital is much higher for early investors in infrastructure for a new fuel, reflecting high levels of investment risk. As the fuel becomes more widespread, these financing costs fall, and as a result so do the full investment costs. In general, these effects tend to mean that infrastructure investment costs per unit hydrogen delivered fall as a function of the market penetration of the new fuel. This relationship cannot be represented effectively in a linear optimisation model like MARKAL/TIMES.

These problems can be mitigated—though not eliminated—by the use of mixed-integer linear programming approach, rather than linear programming. One such approach is the use of the ‘lumpy investment’ feature of MARKAL to force the model to invest in a minimum level of infrastructure. This enables the modeller to use cost data appropriate for a mature system without allowing the model to gradually build up infrastructure at that cost. Instead, the model must choose to develop a full hydrogen infrastructure or not. Strachan et al. [9] used this feature to examine the creation of a hydrogen pipeline network in the UK MARKAL model, in combination with a GIS model of hydrogen pipeline transmission infrastructure. The strength of the lumpy investment approach is that it improves the internal consistency of the model by ensuring that the capital cost is appropriate for the scale of infrastructure deployment. However, transition costs (those associated with the high specific costs of an immature system) are still excluded from the analysis.

An alternative approach is to use an infrastructure cost curve from a spatially-explicit supply chain model (e.g. Refs. [47,51]) in the energy system model.

3.1.2. Temporal resolution shortcomings

Optimisation models are designed to find the most cost-efficient infrastructure system to supply the required flows of energy but two factors can cause the required amount of energy storage infrastructure to be underestimated. First, energy system models are usually highly temporally

aggregated, with typically only two intra-day time-slices (day and night), so demand peaks for fuel are averaged over the day and storage requirements to meet those peaks are not represented by the model. Second, unexpected interruptions to infrastructure due to accidents, incidents or sub-optimal usage are not considered by models. Energy storage is used in practice to ensure continuity of supply and the required amount of storage is likely to be underestimated in both cases unless the model is forced to construct sufficient storage (for example, by including storage backup costs in the technology costs).

3.2. Previous approaches in MARKAL/TIMES models

Although a number of authors have used MARKAL/TIMES models to examine the possible future of hydrogen in road transport in various countries and regions (e.g. Refs. [21,30,52–59]), few have explicitly reported the detailed assumptions used to model hydrogen infrastructure.

Other than Strachan et al. [9], Gül et al. [56] are the only other authors reporting the use of lumpy investment as an approach to representing hydrogen infrastructure costs. In their treatment of hydrogen infrastructure, Krzyzanowski et al. [57] address the non-linear relationship between hydrogen demand and infrastructure costs by applying ‘endogenous technology learning’ to infrastructure costs. Though not described in their paper, this is presumably applied to represent the relationship between deployment and cost, rather than to represent true ‘learning’. Meanwhile, Rosenberg et al. [60] soft-link MARKAL to a hydrogen infrastructure model and run the models iteratively to converge on a solution.

Most studies that provide any explanation of cost data have developed that data based on assumptions about the spatial pattern of demand and supply (e.g. by specifying average delivery distances), with no changes to the linear scaling of costs with infrastructure and representing the infrastructure investments as continuous rather than as discrete ‘lumpy’ stages. Documentation for the TIAM-ECN model and the US EPA 9-region model both provide detailed discussion and assumptions concerning the specification of hydrogen infrastructure in the models [24,61]. Both describe the assumed spatial structure of the hydrogen infrastructure modelled, and both recommend that a minimum share of production must be derived from distributed sources (at least in early periods) in order to represent the existence of regions in which centralised production and long-distance supply are uneconomic. Shay et al. [24] also provide explicit assumptions concerning assumed level of hydrogen demand (equivalent to a vehicle market penetration of 30%), which is implicit in the specification of costs.

Only two studies [56,57] test the sensitivity of their model results to assumptions about infrastructure costs.

3.3. Guidelines for infrastructure representation

The most important factor is to include all parts of the fuel infrastructure system in the model in a balanced way for all fuels, including additional storage to account for the temporal resolution issues described in Section 3.1.2. We make

recommendations for each part of the system in Section 4.2 and in Appendix B in the Supporting Information for this paper. The assumptions used to derive the infrastructure cost data should be consistent with the assumptions in the energy system model scenarios being modelled.

While this approach should be sufficient to represent the long-term state of the transport sector (e.g. in 2050), it is not likely to accurately represent the timing of any transition to the long-term state because of the spatial resolution and transition issues described in Section 3.1.1.

The third key decision for energy system modellers is whether to use lumpy investments to represent fuel infrastructure. We examine this question in a case study in Section 5.3. For studies examining the transport sector in particular, we recommend that lumpy investment modelling should be considered for pipeline deployment and perhaps for other parts of the system with large capital costs and low utilisation at first, for example the initial deployment of refuelling stations.

4. Transport sector case study for an energy system model

In this case study, we completely revise the transport sector in an energy system model according to the principles laid out in Sections 2 and 3 and we examine the impact on the results of typical model scenarios against the results from the base version of the model. We then use the revised model to examine key modelling decisions in Section 5.

We use the UK MARKAL energy system model for this case study, which is based on the widely used MARKAL/TIMES model paradigm [7]. UK MARKAL [62] portrays all energy flows in the UK energy system and accounts for all energy-related CO₂ emissions. The base model for this study is UK MARKAL v3.26, which was the version used by Ref. [63] for the most recent UK government CO₂ mitigation scenarios.

The model is calibrated to UK energy consumption in the year 2000 and the initial energy service demands to 2050, which are exogenous boundary conditions for the model, are fully described in Usher and Strachan [64]. Transport energy service demands are specified in billion vehicle km per year and are based on the results of a transport demand forecasting model used by the UK Department for Transport [18]. In this case study, we run the model to 2100 under the assumption that demands and technologies do not change after 2050, which allows us to gauge the stability of the post-2050 model solutions. We use the MARKAL elastic demand variant in this study in which welfare (defined as the sum of producer and consumer surplus) is maximised, and hence demand and supply reach equilibrium. Behavioural change in response to increasing energy costs is simulated endogenously by reducing the initial energy service demands.

MARKAL identifies the energy system that meets energy service demands with the lowest discounted capital, operating and resource cost, subject to constraints such as carbon targets, and constraints that force the model to emulate a real-world energy system (such as vehicle market share constraints). Following HM Treasury [65], a social discount rate of 3.5% is used in UK MARKAL. MARKAL allows us to draw

insights about the relative importance of different technologies, costs and policies in the energy system, but the results, as with all models, should be interpreted in light of the limitations of the model framework; MARKAL/TIMES models do not predict the future.

4.1. New implementation of vehicle technologies

We introduce a much wider range of vehicles into our revised version of UK MARKAL than was previously available, including the majority of those listed in Table 1. In contrast to previous model versions, we include a full range of hybrid vehicle types, including hydrogen FC hybrids, and we allow unrestricted use of biodiesel in ICE vehicles. We exclude hydrogen ICEs from our runs in this study for the reasons set out in Section 2.2. We also exclude methanol, despite it having been previously included within UK MARKAL, because there is currently very limited interest from automakers in methanol as a fuel. No previous runs with UK MARKAL have selected methanol as part of the optimal energy mix in any scenarios and it seems unlikely that its exclusion would have an impact on the model results in the future.

The methodology that we use to estimate vehicle costs and efficiencies is summarised in Appendix A in the Supporting Information to this paper. We use the recommended methodology for vehicle efficiency from Section 2.4. Since we do not have detailed vehicle simulation data for future vehicle technologies, we use efficiency data from Plotkin et al. [33] and adjust it using data from Lonza et al. [6] in order to account for the difference in size and weight between the average US and European cars.

In this case study, we examine two approaches to representing vehicle market segments in UK MARKAL. Following the methodology of all previous versions of the model, we first assume that the market for each vehicle type is homogeneous and model only a single size class of ‘average’ cars. We then test a second approach in which we disaggregate the car sector into small and medium-large size classes. In Section 5.1, we compare these two approaches to better understand the potential benefits of vehicle class disaggregation.

In order to disaggregate the representation of cars, it is necessary to identify the characteristics of small and medium-large cars in the existing fleet, in order to calibrate base year technology costs, efficiencies and characteristics. We use data collected by the European Environment Agency [66], which reports the carbon emissions per km and the gross vehicle weight of each car sold in the EU in each year. We specify size classes that correspond to typical industry classifications and identify the average gross vehicle weight and efficiency of each class. We determine the costs and efficiency of each class using a bottom-up assessment of all the component parts, as described in Sections 2.3 and 2.4. Appendix A lists the data that we use. We calculate annual average mileage data for each vehicle class by combining the total distance travelled by small and large cars from the UK National Travel Survey [67] with the number of cars in each class from the SMMT [42].

Finally, we use the market share constraints from Table 2 in both the aggregated and disaggregated versions of the model to represent limitations of electric and hybrid vehicles

for some market segments. We examine the importance of these constraints in Section 5.2.

4.2. New implementation of transport fuel infrastructure

Although a multi-region version of UK MARKAL has been built to examine hydrogen infrastructure [9], most versions of the model, including the base version, assume a spatial pattern of supply and demand for hydrogen from Yang and Ogden [49] and implement the costs from that study in the model. The base version assumes no costs for electric transport infrastructure but does include costs for hydrocarbon fuel infrastructure in the form of a variable operating and maintenance (O&M) cost on the fuel. The source of these variable O&M costs is now unknown but we believe that the treatment of transport infrastructure for different fuels is inconsistent in UK MARKAL, in particular for electric vehicles.

Our revised version of the model takes a consistent approach to representing all fuel delivery infrastructures, including capital and operating costs for pipelines, tankers and refuelling stations. The data for our revised model are summarised in Appendix B in the Supporting Information and are fully described in Dodds and McDowall [16].

We model transmission pipeline infrastructure assuming a configuration similar to that analysed by Strachan et al. [9] in the multi-region version of the model, with a total length of 3500 km and six geographically-separate hydrogen production facilities. The findings of Agnolucci et al. [47], who develop a spatially-explicit model of hydrogen infrastructure for the UK, support this approach. While Agnolucci et al. [47] do not include hydrogen pipelines, their model finds that the optimal spatial configuration of production and supply infrastructure is based on relatively few, large production plants rather than many local small plants. This conclusion would be likely to be strengthened, rather than weakened, if pipelines were included in their model, and we therefore adopt a highly centralised production system in this implementation.

We give the modeller the option of using the ‘lumpy investment’ feature of MARKAL to ensure that the model can only deploy pipeline infrastructure at a scale consistent with the specification of investment costs, which represent a mature and spatially extensive hydrogen refuelling infrastructure. The minimum capacity of transmission infrastructure that the model can deploy delivers 600 PJ of hydrogen per year, which is based on the spatial configuration of the network that is developed in Ref. [9]. The transmission network is linked to high-pressure distribution pipeline networks which supply hydrogen refuelling stations.

We also considered representing the initial deployment of hydrogen refuelling stations using lumpy investments. The H2Mobility consortium has concluded that only 65 small refuelling stations would be required to support the introduction of hydrogen vehicles and that the majority of the UK population could be serviced by 800 medium-sized stations built over 4 years. These two levels of investment are equivalent to a maximum annual hydrogen energy delivery of only 0.3 PJ and 5.9 PJ, respectively. We show in Section 5.3 that such small scale investments can be represented using a linear model with only a negligible impact on model results, so there

is no benefit from using lumpy investments to represent a UK refuelling station network.

4.3. Scenarios examined in this case study

UK MARKAL is most often used to identify strategies to reduce CO₂ emissions to meet government targets. The 80% emissions reduction target in 2050 is represented by a 90% reduction in CO₂ in the model in both [68] and [63] to recognise the uncertainties in the contribution of non-CO₂ greenhouse gases, the emissions from land-use change and emissions from international bunker fuels [68]. In this study, we use an 80% target to be consistent with UK policy and we exclude the UK share of international aviation and shipping energy demands (and hence emissions) in all scenarios. We also examine a second scenario with no constraint on CO₂ emissions.

4.4. Impact of new vehicle technologies and fuel infrastructure

The impacts of introducing new car representations and new fuel infrastructure to the model, with and without the CO₂ emissions constraint, are summarised in Table 3. For the base version of the model, the cost-optimal distribution of vehicles in the post-2050 market is the same for the scenarios with and without the imposition of a CO₂ constraint. In contrast, FCV market penetration reduces from 99% to 44% in the revised version of the model if the CO₂ emission restrictions are removed, as fossil fuels continue to be the cheapest option in the long-term in this scenario.

These trends are expanded upon in Figs. 1 and 2, which show the technology portfolios used to satisfy car demand in the base and revised versions. The impact of introducing new representations of hydrogen FCVs is apparent in Fig. 2, where new hybrid FCVs are preferred to the non-hybrid FCVs in Fig. 1 because the efficiency increase and reduction in fuel consumption outweighs the higher hybrid capital cost. The 11% penetration of fossil fuel powertrains in the base version with a CO₂ emissions constraint is surprising at first sight. It is caused by the imposition of a market share constraint that requires a minimum share of diesel cars in all years. We believe this to be an unreasonable restriction if FCVs can demonstrate similar performance characteristics (speed, range, etc.) to diesel cars in the future so we have removed this constraint in the revised version.

Table 3 – Comparison of car statistics post-2050 for the base and revised versions of UK MARKAL. Results are presented for the scenarios with no CO₂ constraint and with an 80% reduction in CO₂ emissions by 2050.

	No CO ₂ constraint		With CO ₂ constraint	
	Base	Revised	Base	Revised
Hydrogen powertrain	85%	44%	85%	99%
Battery powertrain	4%	0%	4%	0%
Fossil and biofuel powertrain	11%	56%	11%	1%
Well-to-wheel emissions (MtCO ₂)	10	58	3	13
Tail-pipe emissions (MtCO ₂)	6	27	3	0

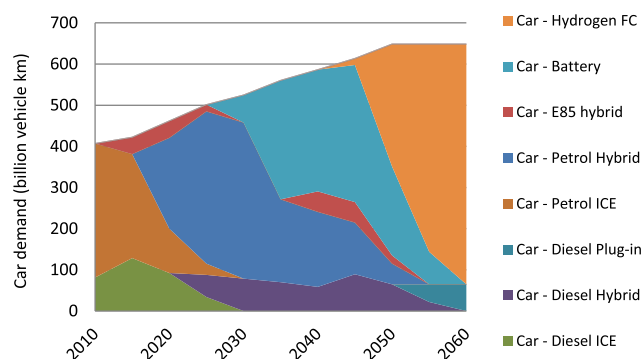


Fig. 1 – Annual car demand fulfilment using UK MARKAL v3.26 (the base version) for an 80% reduction in CO₂ emissions in 2050.

It is notable that the technology portfolios continue to change after 2050 in Figs. 1 and 2, despite all demands and technologies being assumed constant. The two principal contributing factors to this behaviour are the presence of growth constraints on new technologies, which prevent the model from reaching a stable state by 2050 without very early investment in some low-carbon technologies (when they are very expensive), and the presence of cumulative limits on domestic and imported oil, petroleum products and natural gas that are sometimes not reached until after 2050. Running the model beyond 2050 allows us to identify and consider the realism of such trends.

In 2010, well-to-wheel and tail-pipe car emissions are both around 73 MtCO₂ in the model. Table 3 shows that CO₂ emissions from the car fleet after 2050 are always lower than in 2010 but vary substantially between model versions and scenarios. The most important determinant is the presence or absence of an emissions constraint, but the new definition of fuel delivery infrastructure also has an important influence. In the base version, hydrogen is always produced by small-scale electrolyzers at refuelling stations as the model accounts only for the cost of the electrolyser and not for the high cost of on-site storage. The revised version fully accounts for refuelling station costs and hydrogen is instead produced by large centralised production plants (fitted with CCS for the scenario with CO₂ emission restrictions). CCS plants are assumed to

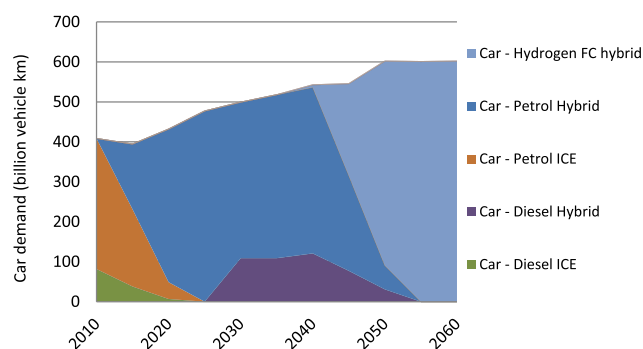


Fig. 2 – Annual car demand fulfilment in the revised version of UK MARKAL for an 80% reduction in CO₂ emissions in 2050.

only sequester around 85% of the produced CO₂ so the well-to-wheel emissions are higher than the tail-pipe emissions in the revised model but are similar in the base model.

Fig. 3 shows the car sector fuel consumption after 2050 for the base and revised models in the scenarios with a CO₂ constraint. Fuel consumption increases by 17% in the revised version, despite the total car mileage demand being lower, as a result of lower FCV efficiencies being assumed in the revised version compared to the base version. The 81 PJ change in fuel consumption could be large enough to have repercussions for model results beyond the transport sector and this demonstrates the importance of choosing technology data carefully.

5. Analysis of the key modelling decisions

In Section 2, we identified the degree of segmentation of the car market and the choice of market share constraints as key decisions for energy system modellers. In Section 3, we identified a third key decision about whether infrastructure should be represented in models using lumpy investments. In this section, we examine each of these decisions using the UK MARKAL model.

5.1. Disaggregating the car market

Disaggregating the car market into small and medium/large segments does not change the cost-optimal car fleet post-2050, with hydrogen hybrid FCV powertrains dominating in both car sizes and with the total CO₂ emissions unchanged. However, the transition to hydrogen powertrains is quite different for the different car sizes as shown in Fig. 4. Larger cars commence the transition to hydrogen after 2035, at a slightly faster rate than the average car, while smaller cars do not commence the transition until 2045 and are not completely converted to hydrogen until 2060. So while disaggregating the car fleet does not change the method of decarbonising the car fleet in this scenario, it does give an insight into the economically-optimal timing for decarbonising different parts of the fleet.

5.2. Market share constraints

The market share constraints listed in Table 2 affect only battery, diesel and plug-in hybrid vehicles so do not change the results of the decarbonisation scenario in Table 3 because

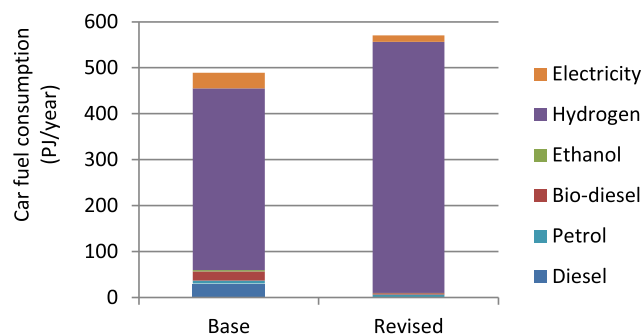


Fig. 3 – Average annual car fuel consumption after 2050 with an 80% reduction in CO₂ emissions.

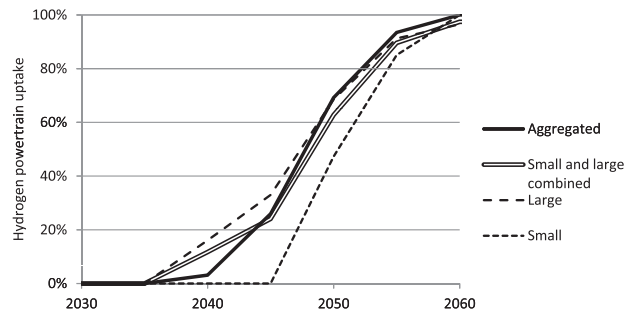


Fig. 4 – Market share of hydrogen cars. The solid line shows the results of the aggregated model in which no differentiation of car markets is made. The dotted lines show small and large cars in the disaggregated model, while the double-line shows the combined market share of small and large cars in the disaggregated model.

hydrogen FCVs dominate by 2050. Although these constraints are effectively redundant in this scenario, they could be important if the scenario assumptions were changed. As an example, we can examine a scenario in which BEVs are assumed to be charged only at home, which removes the requirement to construct costly on-street chargers and makes BEVs cheaper than FCVs in 2050. We use the more disaggregated version of the model for this scenario.

Table 4 shows that removing the market share constraints greatly changes the optimal choice of powertrain in this scenario, both with and without restrictions on CO₂ emissions. BEVs have a much greater market share at the expense of FCVs. Even where FCVs retain some market share, the lower electric infrastructure costs cause the model to choose plug-in hybrid rather than hybrid FCVs. CO₂ emissions also change substantially in the cases with no overall CO₂ constraint. It is clear that the choice of market share constraints can profoundly affect model results.³

5.3. Fuel infrastructure lumpy investments

The revised version of the model is forced to build the hydrogen transmission pipeline network using 600 PJ/year lumpy investments, to avoid the model building only part of a network in the early stages of a transition. We examine the importance of using lumpy investments in this section using a sensitivity study with four scenarios: (i) no lumpy investments; (ii) 600 PJ pipeline lumpy investments; (iii) 1200 PJ pipeline lumpy investments; and, (iii) 600 PJ pipeline and refuelling station lumpy investments.

The uptake of hydrogen powertrains in these scenarios is shown in Fig. 5. Using lumpy investments has no impact on the rate of market uptake and the overall transition to FCVs is unchanged. The three cases with lumpy investments have virtually identical results.

Using lumpy investments improves the internal consistency of the model, by ensuring that infrastructure costs are consistent with the scale of infrastructure deployment.

³ The results also show that the model results are rather sensitive to uncertain assumptions about the costs and form of electric vehicle recharging infrastructure.

Table 4 – Impact of introducing market share constraints in the model for scenarios with and without restrictions on CO₂ emissions. These results are not comparable with Table 3 because the scenarios use the disaggregated car market version of the model (Section 5.2) and because battery vehicle infrastructure costs are much lower as BEVs are assumed to be charged only at home. The results are for the post-2050 period.

	No CO ₂ constraint		With CO ₂ constraint	
	Market share constraints	No constraints	Market share constraints	No constraints
Hydrogen powertrain	17%	0%	71%	23%
Battery powertrain	7%	45%	23%	74%
Fossil and biofuel powertrain	76%	55%	6%	3%
Well-to-wheel emissions (MtCO ₂)	54	73	7	5
Tail-pipe emissions (MtCO ₂)	28	24	1	1

However, technologies tend to be deployed at large scale or not at all in optimisation models, reducing the practical significance of requiring large-scale deployment. Moreover, the use of lumpy investments introduces further complexities, since the model will either over-deploy infrastructure (build lumps of infrastructure with excess capacity) or under-deploy it, with a resulting need to deploy sub-optimal technologies to meet the residual transport demand. This complicates the interpretation of results, as the degree of over- or under-deployment will arise from the modeller's specification of the size of the investment lumps; it will not reflect the real-world phenomenon of under- or over-supply of infrastructure arising from imperfect investor information.

We conclude from this case study that representing hydrogen infrastructure using lumpy investments is unnecessary for a UK-scale energy system model. It might become necessary in a spatially disaggregated model, for example the SHIPMod hydrogen infrastructure model of the UK [47], or if longer pipelines were required to transport hydrogen (around a country with a lower population density than the UK, for example). We do not believe that it is necessary to represent refuelling stations using lumpy investments.

6. Other modelling issues

In this paper, our treatment of the transport sector has concentrated on the representation of transport and fuel supply infrastructure technologies. In this section, we briefly

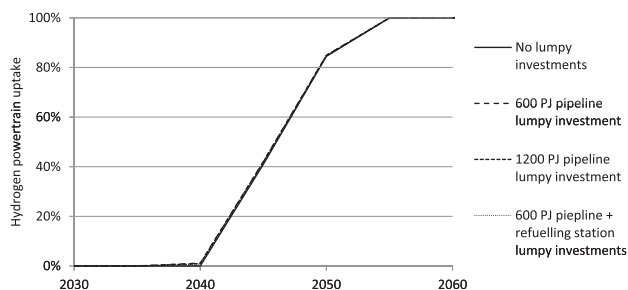


Fig. 5 – Impact of modelling fuel infrastructure as lumpy investments on the transition to hydrogen powertrains. The lumpy investments are applied to the hydrogen transmission pipeline network and the hydrogen refuelling station network (5.9 PJ lumps) as shown in the legend.

discuss a number of wider issues that could affect the representation of the transport sector in models in the future.

6.1. Investor behaviour

Energy system models assume perfect foresight and this assumption is important for infrastructure investments. When the model chooses to invest in infrastructure, it does so with the foresight that the infrastructure will definitely be utilised in the future. In reality, investors in infrastructure are usually faced with almost no foresight about possible future demand levels and there is a substantial risk attached to such investments. One approach to this conundrum is to estimate the minimum level of infrastructure required (e.g. Ref. [46]). Several strategies have been suggested to deal with this conundrum and a number of these are reviewed by Ref. [69]. One approach to investigate the impact of investor uncertainty would be to apply a high hurdle rate to infrastructure technology capital costs to represent the high investment risk. In UK MARKAL, a hurdle rate of 10% is applied to all business-operated technologies to represent the expected return to investors on investment and this could be increased in a “market investment” scenario using information about the perceived risk of hydrogen investments.

6.2. Technological changes

Road vehicles have been operated in the same way since their invention and most models assume that this will continue in the future. Yet technological developments could profoundly change how we use vehicles. For example, driverless cars are being developed that could profoundly affect how we use vehicles [70]. Driverless cars would be available to a much wider proportion of the population who cannot drive (the young and very old, for example) and insurance costs would be lower for young adults; both these trends would increase transport demand. Moreover, ‘Road trains’ could be formed automatically on roads that could increase the aerodynamic performance and hence the fuel efficiency of each car by up to 30%. The impacts of such technologies are difficult to gauge and have not previously been considered by energy system models.

6.3. Behavioural change

The future demand for road transport is a key modelling uncertainty. In some energy system models, the future demand

is forecast endogenously from the base year demand; for example, the ETSAP-TIAM model [71] represents car demand changes as a function of GDP per capita. In other models, such as UK MARKAL, it is supplied exogenously using forecasts from an external model [18]. Yet some external models, such as [18], generate demands based on a small number of economic drivers and have little consideration of wider social or value-driven behaviour change. A good example of a more holistic approach is Eyre et al. [72], who identify the impacts of lifestyle changes then analyse these using UK MARKAL.

People vary their use of cars according to price and these changes are represented in models using elastic demands. In the short-term, demand is primarily affected by fuel price variability. But energy system models operate on long time-scales so use long-run demand elasticities in which demand also depends on the capital and operating costs of the car. There is much uncertainty over the magnitude of these elasticities in the future and the implementation of elasticities is a key issue for energy system modellers.

If consumers do reduce car use in response to changing prices, they are likely to switch transport mode and to use alternatives (walking, cycling or public transport) instead. Mode switching based on limiting overall travel time has been tested in an energy system model experiment [73] but is not normally considered in most mature energy system models. Another option for simulating mode switching would be to add the capability to represent cross-price demand elasticities into energy system models.

We conclude in this paper that the car market is best represented according to market segments because consumers tend to choose cars from particular segments for reasons other than cost and because low-carbon technologies are often better suited to particular segments. Models with segmentation tend to assume that the relative demands in each market segment do not change over time but there is little evidence to support this assumption, particularly looking towards the future.

7. Conclusions

We have reviewed how different energy system models have represented vehicles and fuel infrastructure in the past and have identified three key modelling decisions: the degree of car market segmentation, the imposition of market share constraints and the use of lumpy investments to represent infrastructure. Our case study shows that disaggregating the car market can produce important insights and that market share constraints can greatly affect model results so should be chosen carefully. However, we see little need for lumpy infrastructure investment modelling in most energy system models, as it has little impact on the results but comes at a cost of an increase in model solution time as it uses mixed-integer rather than linear programming. This technique is better suited to infrastructure planning models.

While there is naturally a focus on technology representation in technology-rich energy system models, the impact of behavioural change on future transport demand is another important uncertainty that often receives

comparatively little attention in the energy system modelling literature. The development of new methodologies to represent behavioural change, such as mode switching, is a key area for the improvement of energy system models in the future.

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Appendices A and B. Supplementary data

Supplementary data related to this article can be found at <http://dx.doi.org/10.1016/j.ijhydene.2013.11.021>.

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