



Representation of Hydrogen in the UK, US and Netherlands MARKAL Energy Systems Models

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1 Introduction

Various modelling approaches have been used to analyse the development of a hydrogen economy in the UK. This include the MARKAL energy system model. This paper details the modelling of potential UK hydrogen development in the UK MARKAL model and compares this approach to the MARKAL models in the Netherlands and the United States. A review of other models of hydrogen development are explored in depth in UKSHEC Working Paper 29 (Joffe and Strachan 2007). These include models specific to the UK namely the Hydrogen Infrastructure Techno-Economic Spatial (HITES) model (Joffe et al, 2004), and the THESIS model (Dutton 2005).

1.1 Background to the UK MARKAL energy systems model

MARKAL (acronym for MARKET ALlocation) is a widely applied bottom-up, dynamic, linear programming (LP) optimisation model. It was developed in the late 1970s at Brookhaven National Laboratory and has been continually supported by the International Energy Agency (IEA) via the Energy Technology and Systems Analysis Program (ETSAP).

MARKAL portrays the entire energy system from imports and domestic production of fuel resources, through fuel processing and supply, explicit representation of infrastructures, conversion to secondary energy carriers (including electricity, heat and hydrogen), end-use technologies and energy service demands in the industrial, commercial, residential, transport and agricultural sectors. A highly simplified reference energy system – focusing on the electricity component of the full model – illustrates how these components are linked to each other as in Figure 1 below.

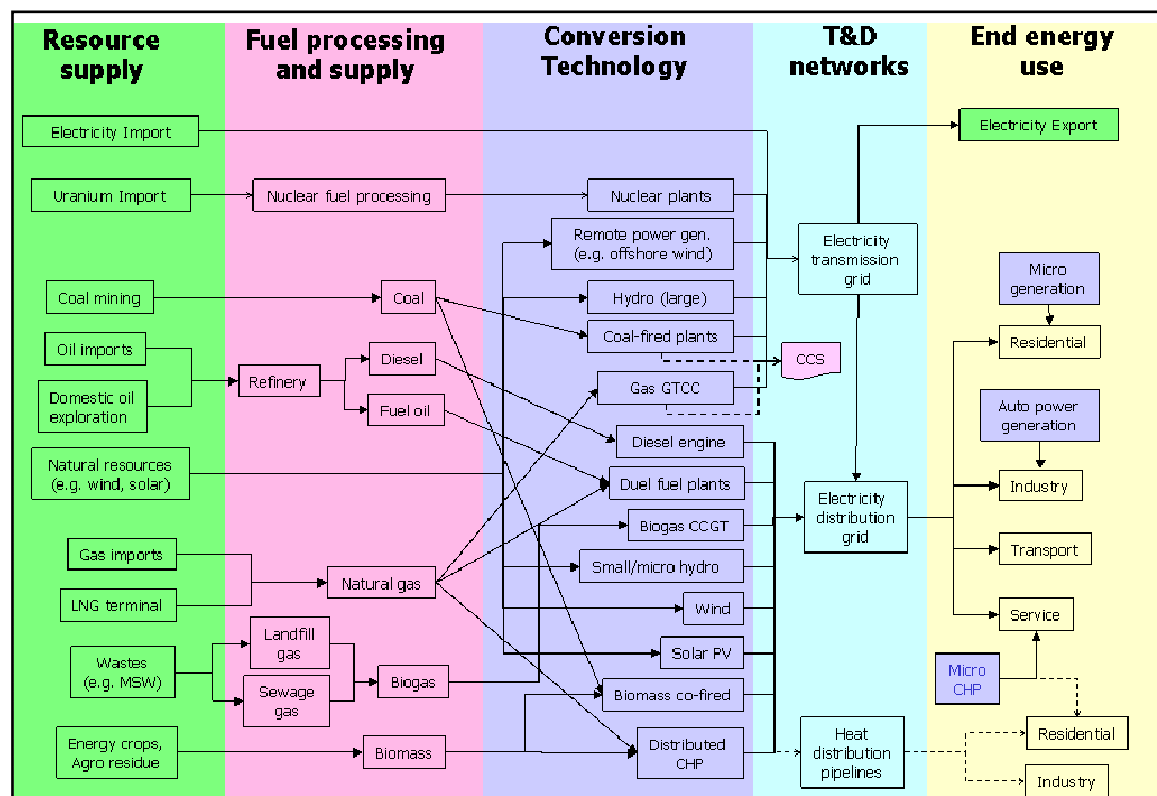


Figure 1: Highly aggregated example of a MARKAL reference energy system (RES)

As a perfect foresight optimization model, MARKAL minimizes the total system cost by choosing the investment and operation levels of all the interconnected system elements. The participants of this system are assumed to have perfect inter-temporal knowledge of future policy and economic developments. Hence, under a range of input assumptions, which are

key to the model outputs, MARKAL delivers an economy-wide solution of cost-optimal energy market development.

The construction of the UK model entails definition of the specific characteristics of the UK energy system, including resource supplies, energy conversion technologies, end-use demands, and the technologies used to satisfy these demands. In particular, the current model is developed based on a previous model (FES, 2003), and supplemented by stakeholder workshops and a wide range of peer reviewed data sources¹. Inputs into the model include base levels for global energy price curves (DTI, 2006), and detailed energy service demands in units of useful energy. These energy services demands were calibrated to final energy consumption projections that were published by the government (DTI 2006). A full description of the UK MARKAL model is given in Strachan et al (2006).

In order to replicate the physical, regulatory and policy aspects of the whole UK energy system in MARKAL, some hundreds of constraints are introduced to the model. These are designed such that the optimization of the model database of technological pathways occurs under a realistic engineering and economic framework of the deployment of new infrastructures, fuels and technologies.

The model is calibrated in its base year (2000) to within 1% of actual resources supplies, energy consumption, electricity output and installed technology capacity. The principal calibration source is DUKES (2006). In addition, considerable attention is given to near-term (2005-2010) convergence of sectoral energy demands and carbon emissions with the econometric outputs of the government energy model (DTI 2006). The model solves in 5-year time steps for an optimal evolution of energy pathways and technology deployment and use.

Further detailed information on the MARKAL modelling system, including the economic rationale of this partial equilibrium model, an explanation of the linearization process for energy supply and demand as well as explicit representations of the mathematical equations used in the solution algorithm is given in Loulou et al (2004).

1.2 MARKAL strengths and limitations

MARKAL is widely used, proven and continually evolving model for assessing a wide range of energy and environmental planning and policy issues. Its well understood analytic framework (least-cost equilibrium computation in efficient or regulated markets) is ideally suited for assessing the role of technology in achieving environmental and policy goals. One of the major strengths of MARKAL is that it represents the entire energy system and the entire energy chains from primary energy resource to energy service demand. This allows the model to choose *combinations* of primary energy resources and technologies in minimising the cost of meeting energy service demands within the specified constraints. Hence it can identify synergies between measures on the demand and supply sides, as well as the infrastructure that connects them.

This, in turn, allows competition in areas of the energy system not captured by more specific models that focus only one part of the system. For instance, competition could be for finite primary energy resources between different energy carriers, e.g. electricity and hydrogen, which might be used for differing end uses, such as domestic energy vs. transport. Imposition of a CO₂ emissions constraint adds an extra dimension to this competition, as it enables the optimisation of the energy system for cost-effective emissions reduction. The use of resources is then driven not only by cost, but also by the efficiency of whole energy chain and consequent emissions per unit of energy service. This enables the best use to be identified for

¹ Three stakeholder workshops on road transportation technologies, electricity generation technologies and hydrogen were held. For further details on model calibration and validation, please see Strachan et al (2006).

low-carbon energy sources in reducing CO₂ emissions, e.g. renewable electricity being used directly as electricity or natural gas used in for combined heat and power (CHP). Additionally, MARKAL allows for analysis of various other constraints on either demand or supply side of energy system making it a powerful tool in investigating various environmental policies, such as imposing the share of renewable resources in electricity generation.

One of difficulties of representing infrastructure in linear programming (LP) models such as MARKAL has been that discrete, large investments can be difficult to represent properly. This is because the model will try to build a fraction of such investments, e.g. half a nuclear plant or 10% of a large-diameter hydrogen pipeline. This has been addressed within MARKAL by the introduction of a ‘lumpy investment’ option which only allows whole numbers of certain large scale investments to occur. The use of this feature turns MARKAL into a mixed-integer linear program.

Last, MARKAL it is a coherent, open-source and transparent framework, where the data assumptions are open and each model output may be traced to its technological cause.

MARKAL’s weaknesses includes its data intensiveness, including characterization of technologies and the UK reference energy system. Like all models, results are driven by the quality of input technology and other parameter data, and can be sensitive to small changes in data assumptions. However, stepped supply curves, and market share algorithms can partially remedy this. In practice when running the model, extensive sensitivity analysis is used to explore thresholds and tipping points between alternate energy technology pathways.

MARKAL has a limited ability to model behaviour, such as hidden costs of technology switching. However, growth constraints, damping costs, and “hurdle” rates, demand elasticities partially remedy this. Also, MARKAL has a limited representation of economic impact of energy policy, although an extended version, (MARKAL Macro), links the energy system to a simple neoclassical Macro module (see section 2.5). This linkage facilitates a demand feedback (in addition to technological change) in response to price signals.

MARKAL as a non-geographical model, is limited in directly representing the spatial aspects of the system, such as the locations of resources and demands, as well as the infrastructure required to link the two. For incumbent energy supply infrastructures, such as those for electricity and natural gas supply, changes are generally small and incremental additions to an already established system. As such, these limitations do not present an insurmountable barrier to approximating the costs and trade-offs involved in any further infrastructure development. However for hydrogen, infrastructure is likely to develop in areas of resource availability and where potential demand is sufficiently dense to justify these investments. One approximation to remedy this problem might be introduction of these resource-infrastructure-demand options explicitly as competing technologies. There is ongoing work to link it to a geographical information systems (GIS) framework (See Section 2.5 and Strachan et al, 2007).

A further limitation of the MARKAL framework is its representation of energy storage technologies, of which hydrogen may be one. The ability to store energy is essential in any energy system, whether this is in the form of primary energy (coal, natural gas, biomass, hydro); indirect storage of electricity (batteries, pumped hydro, supercapacitors); or as hydrogen. In particular, storage of electricity to buffer variations in both supply and demand is essential, especially in a context of an increasing proportion of inflexible power generation (nuclear and renewables, except hydro). A more flexible and detailed seasonal and diurnal structure is being enabled through a project between the MARKAL model developers and the US MARKAL team at the U.S. Environmental Protection Agency (MARKAL/ANSWER, 2006)., and is discussed in section 2.5

1.3 Background to key hydrogen technologies

Production

There are generally considered to be four major hydrogen production pathways for the UK: steam methane reforming, coal gasification, biomass gasification / pyrolysis and electrolysis. These production technologies are reviewed in detail in UKSHEC Working Paper 25 (Hawkins and Joffe, 2006)

Large scale fossil routes to hydrogen currently provide the cheapest option for production, although their large-scale implies a substantial requirement for H₂ distribution. Small scale SMR currently appears more expensive, but with room for significant reductions if it becomes widespread.

Fossil fuel pathways contribute to CO₂ emissions, coal more so than gas. Adding CO₂ capture to fossil plants may increase the cost of hydrogen by 10-20%, excluding the costs of CO₂ transport and sequestration. The cost of CO₂ transport and sequestration are difficult to predict, since the technologies are uncertain, costs are likely to be very site-specific, and depend on economic factors such as enhanced oil and gas recovery revenues.

Estimates for cost of hydrogen from biomass vary widely; a major uncertainty is the cost of biomass, and the size of the resource potential. Waste biomass may be available much cheaper than dedicated fuel crops, though not in as large or predictable volumes.

Electrolysis is currently the most expensive option; the major component is electricity price, and unless stranded electricity resources are used it is difficult to see electrolysis being competitive in many situations.

Storage & Distribution

Hydrogen storage and distribution technologies have been reviewed in detail in UKSHEC Working Paper 21 (Hawkins, 2006). The characteristics of hydrogen transmission technologies are summarised in Table 1. The main point to note is that costs are very sensitive to distance and capacity (flow rate). Previous research has illustrated the trade-offs between the least cost option, depending on distance and capacity, as shown in Figure 1.

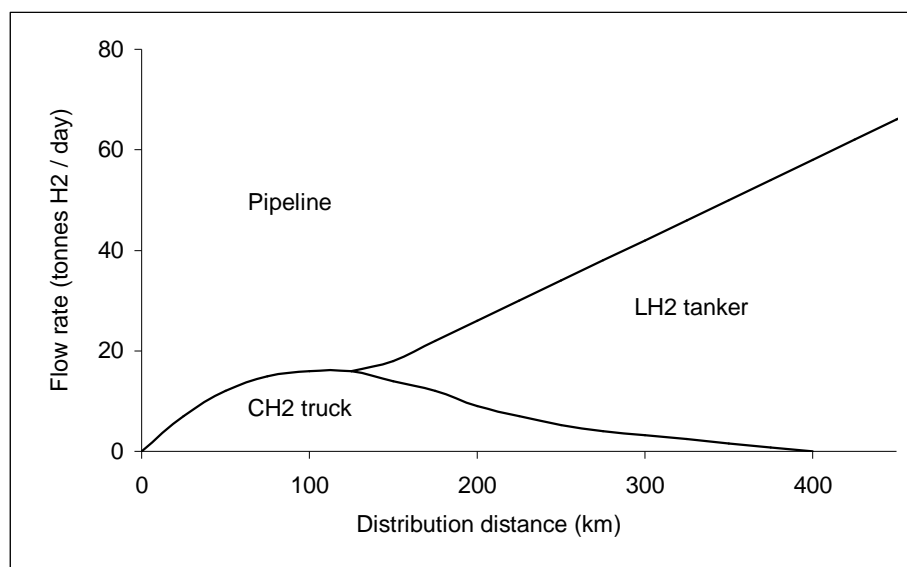


Figure 2: Least-cost H₂ distribution method as a function of distribution distance and flow rate

However, Figure 1 is based only cost, not practical considerations. For example, delivering 500 kg/h by tube trailer would require more than one truck delivery per hour. Simbeck and Chang (2002) suggest tube trailer delivery is suitable up to capacities of up to about 13 kg/h, and LH₂ trucks are suitable up to 1000kg/h, while pipelines can deliver up to 100 000kg/h.

Also pipelines offer a storage and buffering capacity, and their useful lifetime is likely to be longer than their investment lifetime, so companies might see investments in pipelines as strategic. However, the high capital cost of pipelines makes investment less likely if the market for hydrogen is uncertain. Decisions on the mode of transport are linked to the mode of storage, for example if both the producer and consumer are using liquid storage, then it makes sense to transport hydrogen as a liquid.

Comparing transportation costs with the cost of production is difficult since both vary depending on the pathway and technology. The cheapest options for producing hydrogen (large scale fossil fuel routes) might cost around \$1/kg. The cheapest option of transporting hydrogen is by high capacity pipeline, which can cost less the \$0.1/kg over 100km. However, if hydrogen is liquefied and transported by road, the cost is likely to be over \$1/kg – possibly more than the cost of production. Hence the costs of hydrogen transport are a significant factor when analysing the cost of hydrogen.

² The exact trade-offs between the different distribution modes will depend on energy prices, changes in technology costs and other things such as policy interventions. However, while the ‘switching points’ may shift, the underlying relationships remain the same and the shapes on the graphs would be largely unchanged.

Table 1: Characteristics of major hydrogen transportation options

	Pipeline	Liquid (road)	Liquid (ship)	Tube trailer
Advantages	Large volumes High efficiency Also provides storage and buffering Low variable cost	Higher volumes than compressed gas High efficiency	Could allow international transport Very high volumes	Can be deployed at small scales
Disadvantages	Capital intensive Needs large volumes of hydrogen to justify pipeline costs Required volume increases with distance	Expense and inefficiency of the liquefaction process Boil off losses Increases road traffic	No experience of LH2 shipment Not feasible until large supply and demand exists Boil off losses are more significant than road	Small deliveries per truck Energy inefficient Can't handle large capacities Increases traffic
Suitable for	Large and very large quantities of gas Where pipeline storage is used	Large quantities of gas Where liquid storage is used	Very large quantities of gas International transport	Small quantities of gas Small distances
Capacity	Up to 100 000 kg/h (3.9GW)	Up to 4000kg per truck	Potentially 10 million kg per shipment	Up to 400kg (delivered) per truck
Capital costs	\$200,000 - \$1,000,000 /km \$0.1 - \$2.0 per kg H2 or more depending on distance and capacity	\$300,000 - \$400,000 per truck \$0.3 / kg H2 (excluding liquefaction plant)	\$155 million for LNG barge could be 3-4 times higher for LH ₂ barge	~\$300,000 per truck \$0.10 - \$0.40/ kg
O&M costs	Energy costs of pipeline compressors ~\$0.03 /kg	Driver labour @ ~ \$18 /h \$0.02 - \$0.20 /kg	Crew labour and fuel Uncertain	Driver labour \$0.5 - \$2.0 / kg
Total cost				
\$/kg/100km	\$0.10 - \$1.00	\$0.3 – \$0.5	\$1.8 - \$2.0	\$0.5 - \$2.0 / kg
Energy required	Pipeline compressors	Transport fuel	Transport fuel	Transport fuel
Efficiency	99.2% per 100km	99% per 100km for transport 75% efficiency of liquefaction.	fuel use unknown boil-off 0.3% per day	94% per 100km

Source: Hawkins (2006)

Fuel cell vehicles

Hydrogen vehicle technologies have been reviewed in detail in UKSHEC Working Paper 22 (Hawkins and Hughes, 2006). Fuel cell vehicles (FCVs) are estimated to be about 2-3 times more efficient than conventional gasoline vehicles and 1.5-2 times more efficient than the diesel electric hybrids. Well-to-wheels analysis suggests greenhouse gas reductions of 30-60% compared with conventional gasoline vehicles, if hydrogen is produced by SMR and transported by pipeline. Comparable savings - 25-50% compared with conventional gasoline - appear to be achievable with advanced diesel hybrids. GHG gas savings will be far greater if carbon capture technologies, renewables, or nuclear energy is used to produce hydrogen.

Long-term costs of FCVs are somewhat uncertain, although comparison with baseline vehicles suggests FCVs will cost anywhere between 15-50% more than conventional vehicles, once in mass production.

Performance of fuel cell vehicles does not match conventional vehicles, but is close given the early stage of development, and likely to improve. The performance of FCVs is well matched for urban driving. The most significant challenge is improving the storage capacity to give an adequate range between refuelling; this may be addressed by the use of lightweight materials for vehicle body, substantially reducing the vehicle's energy demand.

Hydrogen internal combustion engine (ICE) vehicles, particularly in a hybrid configuration with a battery, offer a lower cost option for H₂ vehicles in the early stages of a hydrogen economy. It is likely that these will gradually be displaced by fuel cell vehicles as the costs converge and the higher efficiency of FCVs comes to the fore.

Power generation

Hydrogen power generation technologies have been reviewed in detail in UKSHEC Working Paper 24 (Hawkins, Joffe and Hughes, 2006). In the near term, it seems unlikely that fuel cells running on pure hydrogen will find widespread market applications for stationary power production. However, opportunities for hydrogen fuel cells look more encouraging for certain niche applications, in particular for back up or off grid power, or as an energy carrier for scenarios where the primary resource is remotely located, or the availability of the resource does not coincide with demand, e.g. for intermittent renewable electricity.

The market prospects for hydrogen fuel cells in distributed CHP applications are currently limited by the high capital costs of the units. This is evidenced in part by the fact that manufacturers are currently concentrating their efforts on niche applications such as uninterruptible power supplies, where a premium can be demanded. The quick start up capability of PEM fuel cells would be useful for load following in small scale domestic applications, and this technology looks likely to benefit from future cost reductions as a result of the research being devoted to it for automotive applications. However, the requirement of PEM cells for pure hydrogen means that domestic applications would be heavily dependent on a hydrogen infrastructure.

1.4 Background to E4 modelling of hydrogen

1.4.1 Representing the potential roles of hydrogen

One of the main challenges in modelling hydrogen is to represent the ways in which it might actually be used. Like electricity, hydrogen is an energy carrier that produces

zero emissions at the point of use. However, unlike hydrogen, electricity technologies are widespread and there is an already-established infrastructure for its production and distribution. It therefore becomes important to identify the situations in which electricity, natural gas and petroleum, the current dominant energy carriers, are not cost-optimal to meet the demands of the energy system and where hydrogen might be able to do so.

Environmental issues, notably CO₂ emissions and resulting concerns over global climate change, and local air emissions and health concerns could be significant drivers of hydrogen diffusion. This would require low-carbon sources of hydrogen and/or low polluting end-use applications. Security of supply is another potential driver with the option of restructuring an energy system to utilize more domestic fossil or renewable resources. In addition, joint production process where hydrogen is a co-product of industrial production may offer a cost effective supply of hydrogen.

Additional opportunities relate to the storage of hydrogen. While storage of hydrogen is not trivial, it is easier to store significant quantities of energy as hydrogen than by storing electricity in batteries. Hydrogen could therefore potentially have a role where energy storage is important:

- fuel storage onboard vehicles;
- portable power;
- back-up power; and
- energy storage to buffer the electricity system.

The main role of hydrogen in end-use sectors is likely to be in the transport system, with possible niches in the portable power and back-up power markets. However, the latter point on 'electricity storage' is potentially very important in an energy system such as the UK's which could potentially incorporate substantial proportions of intermittent renewables, and/or other inflexible electricity generation such as nuclear.

Its potential role as a buffer for the electricity system needn't necessarily mean that all of the hydrogen produced at times of excess electricity supply would be used to regenerate stationary power. Much, or indeed all, of this hydrogen could be diverted to the transport sector.

Major uncertainties in the development of hydrogen as a significant proportion of the UK's energy supply, include the funding and timing of fuel infrastructure provision, the requirement and opportunities of hydrogen storage, the total productive capacity from alternate feed-stocks at various cost levels, and the safety (and public perceptions of safety) of hydrogen supply and use, as well as development and diffusion of cost-competitive hydrogen end use technologies.

1.4.2 Key modelling issue - resource competition

In general terms, the primary energy resources that might be used for hydrogen production have other potential uses in generation of electricity or heat. As such, there is competition for these resources for meeting different energy service demands. For each type of resources, the available technologies have differing costs and efficiencies for conversion of primary resources to secondary energy such as electricity, hydrogen, heat, biofuels etc.

Modelling of a developing hydrogen energy system requires that this resource competition be taken into account, so that the result is hydrogen supply in the context of the overall energy system. One approach to this would be to project forward the prices of energy supplies, so that a model can decide the least-cost hydrogen pathway

given these energy prices, as well as technology costs. However, energy prices are, in most cases, the *result* of the competition for the resources.

An alternative approach is to model the energy system as a whole, together with a full representation of available energy resources and allow competition for these resources to determine both their prices and how they are used.

1.4.3 Key modelling issue - hydrogen infrastructure development

Except in a very few industrial areas, there is no pre-existing infrastructure for hydrogen supply; as such, hydrogen infrastructure would develop from scratch. Furthermore, a number of different approaches to hydrogen infrastructure development exist, using different scales of production and requiring different types of distribution links:

- Large-scale centralised H₂ production, requiring extensive H₂ distribution links to points of demand (e.g. refuelling stations), either by road in liquid form, or via an extensive pipeline system;
- Small-scale onsite production, requiring no distribution infrastructure;
- ‘Medium’-scale production within urban ‘distributed networks’, distributing hydrogen via short pipelines.

In selecting pathways for hydrogen infrastructure development, a model must effectively trade-off between centralised production and minimisation of distribution infrastructure, i.e. between the economies of scale available in H₂ production and the costs of H₂ distribution. Economies of scale for production are known, or can be estimated. However, as discussed by Martinus, Smekens & Rösler (2005), costs of H₂ distribution – particularly for pipelines – are strongly dependent on the distribution distance and flow rate.

The least-cost method of distributing pure hydrogen depends both on the flow rate and the distance of distribution, as illustrated in Figure 1. In particular, pipelines are favoured at short distance and high flow rates, while liquid hydrogen is the favoured distribution method over long distances.

2 Overview of UK MARKAL depiction of hydrogen

The UK MARKAL model has a representation of hydrogen that covers production, distribution and end-use in transport and power generation. The structure of the hydrogen module is illustrated in Figure 2. Implicit in the model (although not shown in Figure 2) is the dynamic nature of the hydrogen chains with costs reflecting new vintages of technologies or global learning rates.

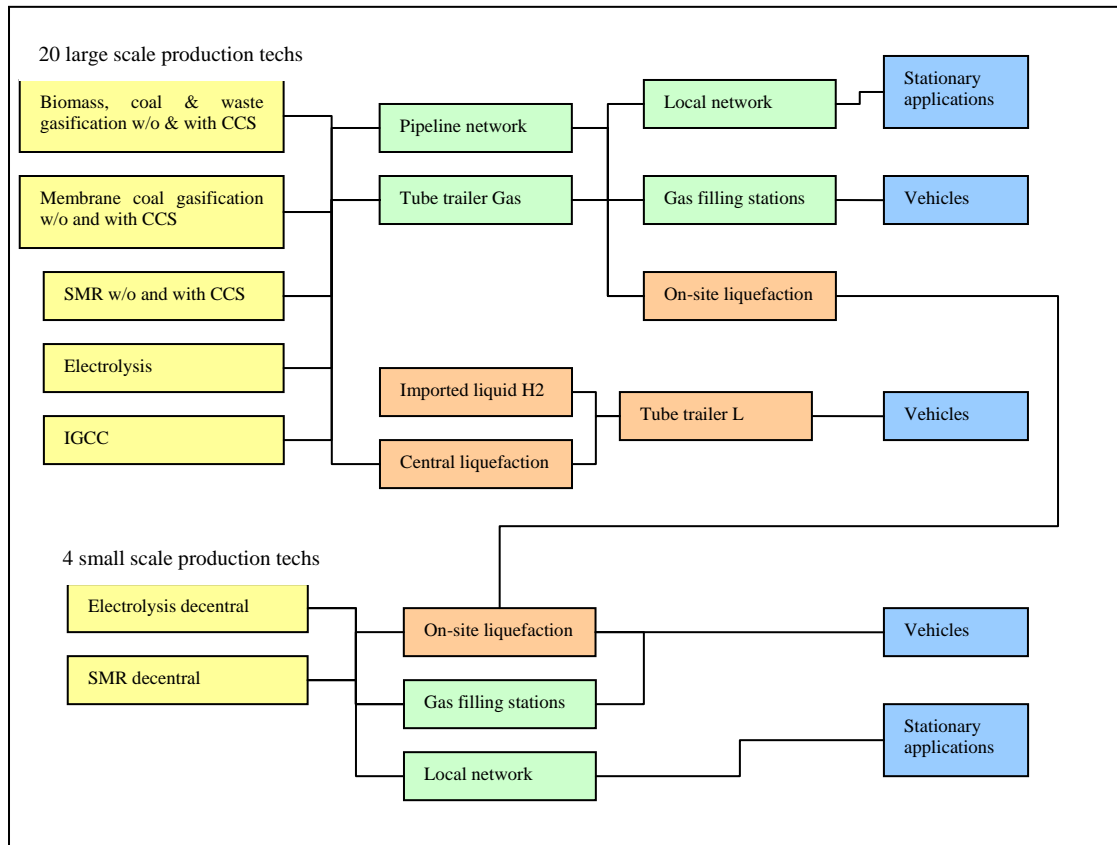


Figure 3: Structure of the hydrogen module in the UK MARKAL model

2.1 Hydrogen production

As presented in Figure 2, the UK MARKAL model includes a very detailed presentation of H_2 production technologies. These are electrolysis, steam methane reforming, gasification of coal and biomass, as well as municipal waste and import of hydrogen from outside the UK. CCS is included as an option for the reformation and gasification processes.

These production options are represented at two scales with the corresponding technologies as follows:

- **Large-scale production** from reforming of natural gas, electrolysis of water or gasification of coal, biomass or municipal waste;
- **Small-scale production** from natural gas reforming or water electrolysis.

The option to import from outside the UK is also included for liquid hydrogen.

2.2 Hydrogen infrastructure

Where hydrogen is imported or produced at a large scale, it is assumed first it arrives at a transmission point, and then it is distributed for supply to potential end uses. All three main hydrogen distribution technologies have been included: via pipelines or distribution by road in either liquid or compressed form. As pipelines deliver H_2 to the point of use, there are distribution technologies specific to the end use sectors.

However, as mentioned earlier, the flow rate and distribution distance have a key role on the distribution costs of H_2 . Additionally, on the demand side, each type of transport would require a filling station at different capacities at different spatial

proximity. For example, while air and rail transport would require few large fuelling hubs – which might be close to resource or import sites – due to their large scales, while cars would need filling stations throughout the country with lower flow demands to each station. On the other hand, buses would use relatively small depots when travelling in short distances as they are mostly based in urban areas. Heavy good vehicles, though, would need few truck services located on major road networks with high flow demands.

Hence, the UK MARKAL model has been updated to develop a H₂ distribution system that takes into account distance and flow rate relationship as well as characteristics of the end use options. Following Yang and Ogden (2006), four H₂ distribution systems are assumed to take place based on distance and flow rate. Yang and Ogden (2007) argue that a distribution distance of 50km versus 300km, and a flow rate of 15t/day versus 100t/day significantly affect the costs. Hence, in the UK model, each transport mode is assigned to a quadrant in a 2x2 grid, formed by these two axes for all three distribution networks. Table 2 below presents each transport mode in one of these quadrants.

Table 2: UK hydrogen distribution network by transport mode

		Distribution Distance	
		Short (50 km)	Long (300 km)
Flow rate	High (100t/day)	Air, rail, ship	Heavy goods vehicles (HGV)
	Low (15t/day)	Bus, 2 wheeler	Car, LGV (LGV)

However, these different types of transport also require H₂ in different forms. While air transport requires only liquid H₂, the other transport types may take H₂ in liquid or compressed form with the exception of 2-wheelers and rail transport. Hence, for several types of road transport – namely, buses, cars, HGVs and LGVs – and air transport on-site H₂ liquefaction technologies are introduced, in addition to the centrally produced and distributed liquid H₂ chain. These on-site liquefaction technologies can take gaseous H₂ either centrally produced and distributed via pipelines or tube trailers, or locally produced gaseous H₂.

For the distribution of H₂ to the power generation sector, it is assumed that they are low flows and will be travelling in long distances.

As the small scale H₂ production is assumed to take place at a site close to demand points, there are no distribution or transmission costs associated with them. Instead the distribution is via the electricity or natural gas infrastructures.

2.3 Hydrogen end-use technologies

Technologies to use hydrogen in the transport sector are available for air transport, rail and several types of road transport: buses, cars, light goods vehicles (LGVs), heavy goods vehicles (HGVs), and 2-wheelers. In road transport fuel cell vehicles use gaseous H₂, whereas vehicles with internal combustion engine require liquid H₂, and these both are enabled in the model. Vehicle technologies are vintaged to represent the development over time of the characteristics of new vehicles.

In the stationary power generation sector, storage technologies, large poly-generation H₂ production plants, and micro-generation options utilizing hydrogen (both CHP and electric-only) have been introduced. From these, H₂ generated electricity can flow to the dedicated service and residential sector electricity and heat carriers or to the generic ELC and LTH carriers (which also flow to industry, and transport).

2.4 Technologies and data sources

Within the UK MARKAL model, the hydrogen module is one part of the larger model of the energy system. The hydrogen-specific technology data that is included in the model is presented in the Appendix, within various tables. Consolidated data is given for transport technologies due to the sheer number of vintaged technology in this module. Further explanation for this data is given in Strachan et al (2006). Not included in the Appendix are additional technologies that serve multiple purposes in the model (including servicing hydrogen chains)³

An important aspect of the technological representation within MARKAL is how costs and performance of technologies change with time, especially those that are immature, such as hydrogen and fuel cell technologies. In order to represent the changes in the technology over time, the model has used technologies vintages. This means that the technology is represented by several database entries, each applying to installation of that technology in a particular year. Use of this approach enables representation of the gradual turnover of the technology stock as the technology improves.

While the best data and projections from literature have been used, clearly the future development of immature technologies is, to some extent, uncertain. It is therefore very important to undertake sensitivity analyses for these parameters, in order to ascertain the degree to which this affects the overall results.

2.5 Extensions

While UK MARKAL has considerable strengths in its integrated approach to the energy system, and specifically captures important distribution aspect of flow and distance in its hydrogen module, it is important to identify areas where it can be improved.

An innovative modelling project sponsored by the UK Department for Transport will address two major limitations of current energy system modelling of hydrogen infrastructure development. Firstly, MARKAL is a non-geographical optimisation model, which therefore does not consider directly the locations of demand or resources in its representation of the future energy system. H₂ has no existing transmission infrastructure and would be expected to develop different in areas with concentrated demands and/or access to primary resources for H₂ production. Secondly, the current model has only limited depiction of seasonal and daily demand changes and the resultant need to balance supply and demand. Understanding temporal aspects is especially critical considering the potential requirement to store significant amounts of H₂, especially if it were required to provide a balancing mechanism in electricity provision.

This project will develop a Geographical Information Systems (GIS) based spatial model for the optimisation of H₂ infrastructure for the UK, to allow the explicit consideration of H₂ distribution⁴. This spatial model will have an integrated two-way linkage and interaction with the UK MARKAL model. Secondly, this work will extensively improve the temporal representation of demands in the MARKAL model, to 5 diurnal and 12 seasonal slices. This will allow explicit consideration of daily load

³ e.g., natural gas pipeline can deliver gas to power plants or distributed H₂ production sites

⁴ i.e., improving the current approximation of hydrogen distribution flow rates and distances as in the current MARKAL model

duration curves as well as peak seasonal supply and demand periods, thereby enabling the explicit consideration of the role of H₂ in energy storage.

To our knowledge this is the first time that an integrated E4 energy model has been linked to detailed spatial and temporal components. However, this research topic has been discussed within energy modelling forum and conferences for some time, including the publication of proposals and methodologies on linking energy models and GIS frameworks (e.g., Biberacher, 2006).

One additional extension that has been implemented is the MARKAL-Macro model, which link UK MARKAL to a simple neoclassical growth model. This has the twin advantages of allowing energy service demands to be endogenous and to explicitly calculate GDP, investment and consumption effects in the overall economy from various energy and environmental policies changes in the energy sector. In the lexicon of energy modelling, this links the ‘bottom-up’ technology focused approach to the ‘top-down’ macro economic approach. MARKAL-Macro hence combines very rich technological characterization of energy system with a dynamic inter-temporal general equilibrium model.

2.6 Summary

The current hydrogen module of the UK MARKAL model includes all of the main technologies that are expected to feature in a future ‘hydrogen economy’.

It also encompasses a very detailed H₂ infrastructure system by taking into account the two key determinants of this system cost, namely flow rate and distribution distance. Hence the model allows for analysis of the trade-offs between the central production of H₂ and its distribution via pipelines or road transport for each transport type. This is done by representing all resource-distribution-end use options explicitly as competing technology.

While this representation allows for analysis of trade-offs between different uses as well different distribution systems in any transition to a hydrogen economy, there are other MARKAL approaches to address these issues. Two of these (for the Netherlands and the USA) are discussed in Section 3. Additionally future extension in the UK model are being pursued to improves it spatial and temporal resolution

3 Comparison with other MARKAL models

3.1 ECN Netherlands

The ECN MARKAL model is being used as part of the EC HyWays project to develop a roadmap for hydrogen and fuel cells in the European Union, as well as another project called Cascade Mints. The modelling of hydrogen using MARKAL is an extension of ECN’s existing MARKAL model for Western Europe, incorporating a greater level of detail and sophistication than the previous characterisation. The description here of ECN’s modelling of hydrogen in MARKAL is based on Martinus et al (2005), and is summarized in Figure 3.

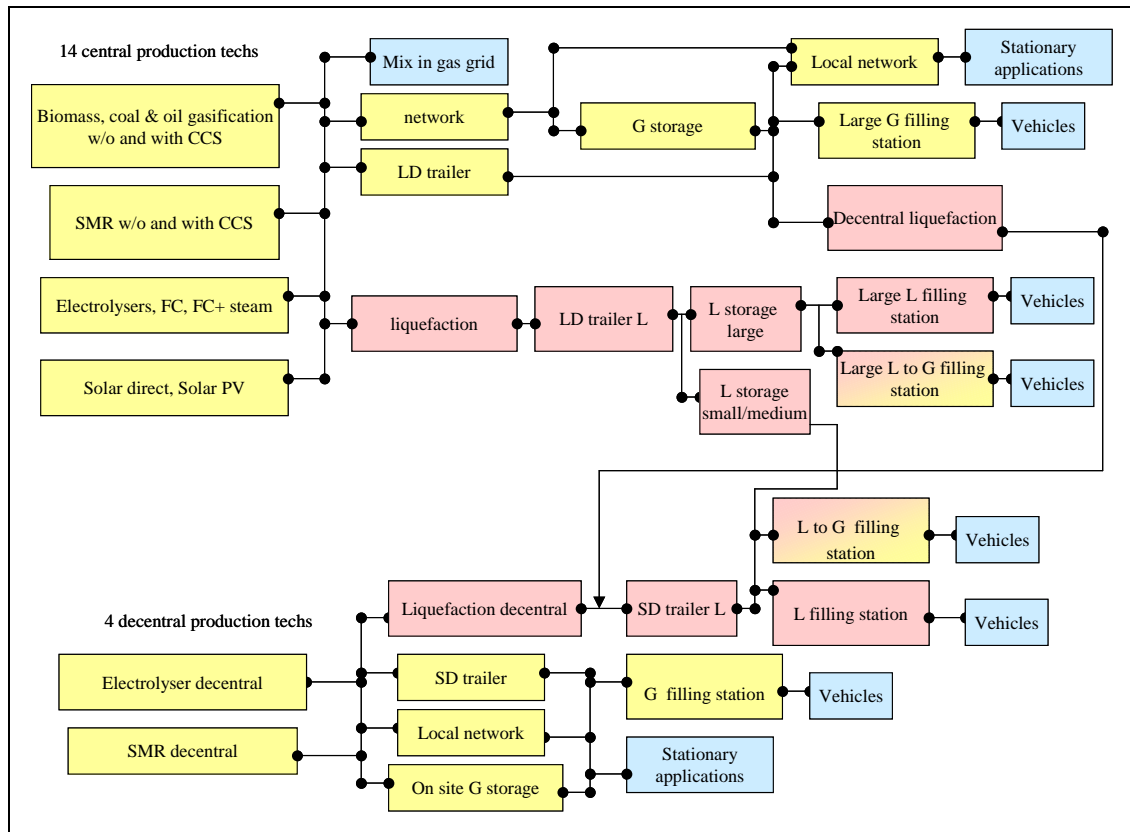


Figure 4: Structure of the hydrogen module in the Netherlands MARKAL model

3.1.1 Hydrogen production

Potential sources of hydrogen included in the ECN MARKAL model are production via electrolysis, steam methane reforming, direct solar production and gasification of coal and biomass, as well as by-product hydrogen supplied from industrial processes and import of hydrogen from outside the region modelled. However, by-product hydrogen offers limited penetration, due to a high assumed cost compared with dedicated production. CCS is included as an option for the reformation and gasification processes.

The model categorises production into at two scales: centralised and decentralised. Decentralised production can either by via electrolysis or SMR. All of the above production options are available at the centralised scale, including the option of CCS for the thermal routes (SMR and gasification).

Speculative H₂ technologies, such as biological production, have been excluded due to insufficient detail available to represent the technology fully.

3.1.2 Hydrogen infrastructure

Infrastructure for transportation and distribution of hydrogen covers each of the main options:

- distribution by road in compressed or liquid form;
- development of a dedicated H₂ pipeline distribution network; or
- mixing H₂ with natural gas in the existing pipeline system.

However, the latter option of mixing H₂ and natural gas requires the development of separation technologies, e.g. membranes which allow only H₂ molecules to pass

though them. These have not been assumed in the ECN model and the mixture would therefore only be used in natural gas applications, as a way of reducing the carbon content.

As discussed in section 1.4.3, the least-cost method of distributing pure hydrogen depends both on the flow rate and the distribution distance. In particular, as acknowledged by Martinus et al (2005), representation of pipeline distribution is difficult, due to the number of independent parameters that characterise pipeline development. The issue of distances is handled by drawing a distinction between the local hydrogen ‘distribution’ pipeline systems and longer distance ‘transmission’ pipelines, in a similar way to the treatment of natural gas pipeline infrastructure.

Handling of flow rates is a particularly important issue for H₂ pipelines, as the incremental unit cost of energy transmission capacity falls substantially with increasing diameter, and therefore capacity (Yang & Ogden, 2004). The ECN model addresses this using the ‘lumpy investment’ feature, which is a relatively recent development in MARKAL, allowing different capacities of pipeline to be specified and only of each built. This representation of hydrogen pipelines is being investigated as part of ECN’s Cascade Mints project.

For distribution by road, hydrogen will tend to be transported in liquid form over long distances, while tube trailers carrying compressed hydrogen are more favoured by shorter distances. The ECN work has therefore assumed a different distribution distance for each method. The flow rate is a less important factor for distribution by road, as this would only affect the *frequency* of delivery, which makes the cost of distribution approximately proportional to the quantity distributed.

The ECN model explicitly represents refuelling stations in its infrastructure representation, with the option to dispense H₂ either in liquid or compressed with two different sizes available. The inclusion of different sizes of refuelling stations again requires the use of the ‘lumpy investment’ feature and is seen as important in looking at the initial build-up phase of infrastructure, where low utilisation of refuelling facilities could adversely affect the economics of H₂.

3.1.3 Hydrogen end-use technologies

In the ECN MARKAL model, end-use technologies that use hydrogen appear in the transport and industrial sectors as well as in buildings within the residential, commercial and service sectors.

Hydrogen in the transport sector

Demand for transport services is quite disaggregated in the ECN model, with fixed splits between different modes, e.g. public and private transport. Furthermore, for private vehicles, demand is split between city, regional and inter-regional drive cycles. Hydrogen vehicles using both fuel cells and internal combustion engines (ICEs) are included, with liquid hydrogen an option for larger vehicle types.

Hydrogen in buildings

The hydrogen technologies in buildings are fuel cells that would provide distributed combined heat and power (CHP) generation. The characterisation of these fuel cells is not very detailed, due to the current immaturity of CHP fuel cells. The possibility to mix hydrogen with natural gas, supplied via the existing pipeline network, is not treated as a hydrogen end-use, as it is assumed that this mixture is used in the same technologies that use natural gas.

Hydrogen in industry

Inclusion of technologies in the industrial sector that use hydrogen as an energy input are limited to the generation of heat and power. Boiler technologies have been included, which could use surplus hydrogen produced in other industrial processes. In addition, CHP technologies similar to those in the buildings are included for distributed production of heat and electricity.

3.1.4 Data sources

Technology data in the ECN model has been continually updated including implementation in the framework of two projects partially funded by the European Commission: Cascade Mints and HyWays. Key data sources include Amos (1998); and Krewitt and Schmid (2005). In addition the use of technological clusters for endogenous technological change is implemented sectorally (e.g. in hydrogen production, and this approach is discussed in Febers et al (2003)

3.1.5 Summary

The ECN MARKAL model represents a hydrogen 'system' in a similar way to that usually used for electricity systems, separating production, distribution and end-use. Hydrogen can be used for applications in the transport sector, distributed heat and power generation and in industry. It can also be mixed with natural gas in the existing pipeline system, although no separation technologies have been assumed, so this mixture would be used directly in existing natural gas technologies.

The ECN model allows the model the flexibility to choose appropriate combinations of H₂ production and distribution technologies. However, while this flexibility allows a large number of plausible solutions for H₂ infrastructure development, it also allows some implausible solutions as well.

3.2 US EPA model

The US MARKAL model is run by the Environmental Protection Agency (EPA), with a focus on regulated pollutant emissions from energy use in the US. While CO₂ is tracked, the focus of the modelling is on more local pollutants such as NO_x and SO₂. A full documentation is given in Shay et al (2005), and the hydrogen module is summarized in Figure 4.

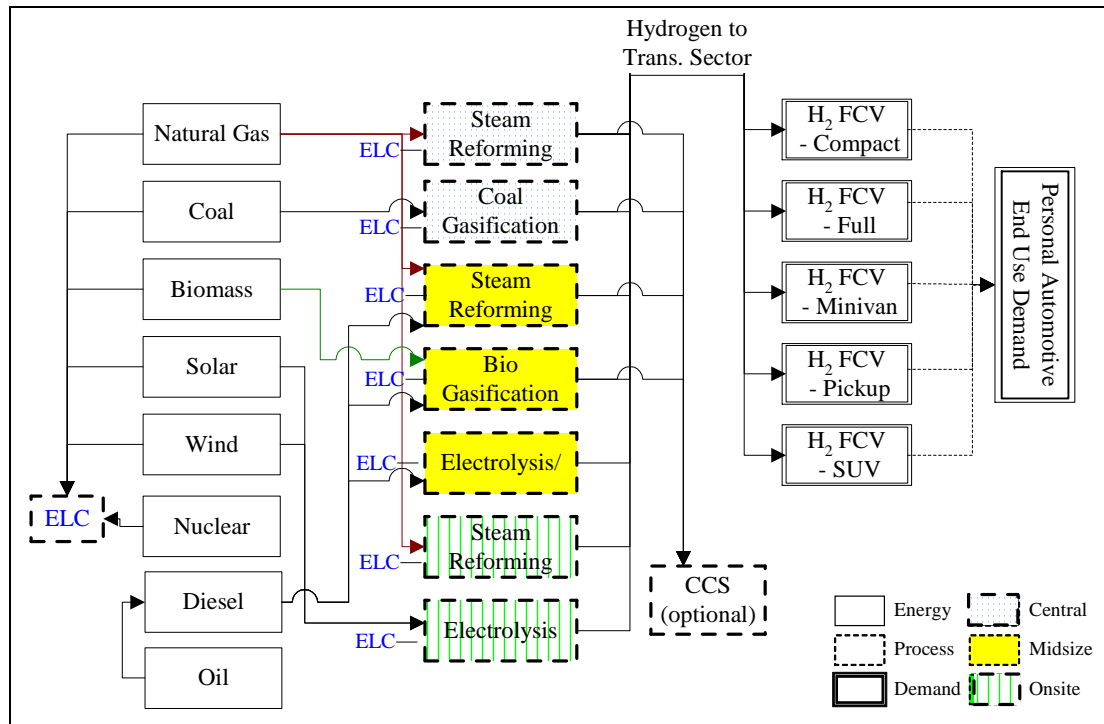


Figure 5: Structure of the hydrogen module in the US MARKAL model

3.2.1 Hydrogen production

The hydrogen production technologies considered are at three scales:

- Central (large) scale production, 1200 tonnes H₂ /day capacity, via coal gasification or steam methane reforming (SMR);
- ‘Mid-size’ production, 24 tonnes H₂ / day capacity, via SMR, grid electrolysis or biomass gasification;
- Decentralised (small-scale) production, 480 kg H₂ /day capacity, via SMR or electrolysis using electricity from the grid or non-grid solar or wind power.

All of the thermal (i.e. non-electrolysis) production routes are represented as options both with and without carbon capture and storage (CCS), with the exception of decentralised SMR.

3.2.2 Hydrogen infrastructure

The hydrogen component of the US EPA model is based on analysis of infrastructure development in a report by the National Academy of Engineering (NAE)⁵. This report analyses the different types of H₂ infrastructure that would be appropriate to supply hydrogen based on different situations and using different production scales.

The options in the model have been constructed to form complete ‘production plus delivery’ infrastructures, each of which would supply hydrogen all the way to the end user. For the large-scale production facilities, pipeline distribution is assumed, while the mid-size production is combined with H₂ liquefaction and distribution by road. The decentralised production option requires no distribution infrastructure.

⁵ National Academy of Engineering - The Hydrogen Economy: Opportunities, Costs, Barriers, and R&D Needs (2004). <http://www.nap.edu/books/0309091632/html/>

As such, each of the options is equivalent from the end users perspective and the option selected by the model is therefore simply a function of the size and growth rate of demand. The model uses the lumpy investment option to ensure that only whole numbers of each option can be selected.

3.2.3 Hydrogen end-use technologies

In the US EPA MARKAL model, hydrogen is only considered as an option in the transport sector. Within the extensive representation of the transport sector within the model, hydrogen can be used in a subset of vehicles, grouped as ‘personal automotive services’: cars, minivans, pickups, large vans and sports utility vehicles (SUVs). Hydrogen is not considered as a fuel for buses, aircraft, trains, heavy trucks, marine transport or ‘transportation off-highway’.

The model has quite extensive aggregation of transport service demands. Within the personal automotive services demand, cars, van and light trucks compete on cost to fulfil the demand for vehicle-miles. In this subsector, hydrogen options for each of these vehicles compete with those fuelled by gasoline, diesel, ethanol, methanol, liquefied petroleum gas (LPG), compressed natural gas (CNG) and electricity. Bounds are used to constrain some options in certain years and extensive vintaging is used, to represent the changing performance of vehicles purchased in different years.

3.2.4 Data sources

The data on infrastructure costs was drawn from the NAE report, based on the scale of production and required infrastructure for delivery to refuelling stations. In addition, endogenous technological learning was assumed for H₂ production technologies, using a progress ratio of 92% for production technologies with CCS, and 90% for those without⁶. The cumulative deployment of H₂ technologies to date was taken from Suresh, B., R. Gubler, et al. (2001).

As the focus of the EPA modelling has a particular focus on the emission of local and regional pollutants, their model also includes substantial amounts of data on the emissions for each technology. This data was obtained from three reports: Contadini & Diniz, et al (2000), S&T Consultants Inc. (2003) and Mann & Spath (1997).

3.2.5 Summary

The US EPA model uses a very ‘aggregated’ representation of H₂ infrastructure to circumvent the limitations of MARKAL in its optimisation. Instead of allowing the model to choose potentially implausible combinations of H₂ production and distribution, the model instead incorporates distribution infrastructure into its representation of H₂ production technologies. This means that all H₂ production technologies represent options for ‘delivered’ hydrogen and allows centralised and decentralised options to compete on a level playing field.

However, this approach removes the flexibility of the MARKAL to a wider variety of combinations of H₂ production and distribution pathways, potentially limiting the results to a subset of the possible or plausible solutions for H₂ infrastructure development.

⁶ The use of endogenous technological learning in MARKAL links the costs of technologies to their cumulative uptake, on the basis that learning takes place as a product matures, resulting in cost reductions. A progress ratio is applied to the technology cost, reducing the cost by a certain fraction for each doubling of cumulative uptake. Thus a progress ratio of 90% means that each time that the uptake of that technology double, the cost decreases by 10%.

4 Conclusions

The MARKAL framework provides a way of modelling the development of a hydrogen economy within the context of the overall energy system. However, it also presents a number of challenges in representing hydrogen as part of a future energy system. It has strengths in analysing the energy system as a whole, enabling analysis of issues such as resource competition, selection of entire energy chains and synergies between choices in different parts of the system. Nevertheless, key challenges exist in relation to its representation of infrastructure development, particularly in the case of hydrogen.

The current UK MARKAL model includes all of the main hydrogen technologies and provides a framework to analyze the development of hydrogen within the overall context of the energy system. All possible options of hydrogen infrastructure are represented by taking into account the impacts of distribution distance and flow rates on the cost of distribution technologies, hence on the network cost. Further, it encompasses a framework to analyze the impact of these parameters on distribution network for each transport type explicitly. Hence, it allows the analysis of trade-offs inherent in determining the degree of centralisation of H₂ infrastructure and selecting distribution options.

The Dutch MARKAL model has used a similar approach to this, although attempts have been made to address specific issues for H₂ infrastructure such as pipelines and refuelling stations. The US model takes a different approach, bundling the distribution infrastructure together with H₂ production, so that all of the supply options are for 'delivered' hydrogen. In doing so, this takes plausible descriptions of H₂ infrastructure produced 'off-line' and includes them in the model wholesale.

Work on the UK MARKAL model is ongoing and the model will be gradually improved. Within this process, changes to the handling of energy storage, variable demands and inflexible energy generation will be incorporated, which will substantially improve the model's capability to represent to potential role of hydrogen in energy storage. In particular the model's temporal disaggregation will be radically improved.

Furthermore, a parallel model will be developed to run alongside, and interact with, MARKAL to provide spatial optimisation of H₂ infrastructure development via a geographic information systems depiction of the UK energy system. By running the two models iteratively, it is hoped that the results will produce insights that depict detailed driver forces and potential outcomes of optimal and feasible H₂ infrastructure development.

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Appendix: UK Markal Model Hydrogen Technology Data

Technologies that explicitly define the H₂ network system are listed below. They are presented in the following four groups: resource, process, transmission, and distribution technologies. End-use technologies are further broken out into electricity (and heat) conversion technology and transport technologies (by mode). Large-scale conversion technologies are poly-generation (electricity and hydrogen) plants that include CO₂ capture and are vintaged. Small scale conversion plants are micro-generation plants utilizing distributed hydrogen to produce electricity (and heat for CHP options) which can be distributed to the residential, commercial and residential energy carriers. Transport hydrogen technologies cover a wide range of modes and are vintaged every 10 years to reflect improvements in efficiencies, capital and operational costs. The main technology classes are: bus H₂ ICEs, bus H₂ FCVs, bus methanol FCVs, car H₂ ICEs, car H₂ FCVs, car methanol ICEs, car methanol FCVs, HGV H₂ ICEs, HGV H₂ FCVs, HGV methanol FCVs, LGV H₂ ICEs, LGV H₂ FCVs, LGV methanol ICEs, LGV methanol FCVs, air domestic H₂, air international H₂, rail (freight) H₂ FCVs, rail (passenger) H₂ FCVs, 2-wheel H₂ FCVs, 2-wheel methanol FCVs. Further details for the complete technology dataset is given in Strachan et al (2006).

Table 3: H₂ resource technologies

No	Technology description	First year	Cost (£2000/GJ) (note 1p/kWhr = £2.78/GJ)
1	Imported liquid hydrogen	2000	23.33 falling to 15.41 by 2050 ⁷

Table 4: H₂ process technologies

No	Technology description	Year	Efficiency (%)	Invest cost (£/GJ/yr)	Variable costs (£/GJ)	Lifetime (years)
3	Current coal gasification	2000	60%	11.44	0.71	30
4	Current coal gasification plus CO ₂ sequestration	2000	50%	11.69	0.71	30
5	Future coal gasification	2015	70%	8.62	0.51	30
6	Future coal gasification plus CO ₂ sequestration	2030	60%	8.62	0.51	30
7	Future membrane coal gasification	2030	70%	6.16	0.51	30
8	Future membrane coal gasification plus CO ₂ sequestration	2030	65%	6.19	0.51	30
9	Current large SMR	2000	80%	4.05	1.37	30
10	Current large SMR with CO ₂ sequestration	2000	65%	7.61	1.37	30
11	Future large SMR	2015	80%	5.85	0.71	30
12	Future large SMR with CO ₂ sequestration	2015	75%	6.20	0.71	30
13	Current small SMR	2000	65%	46.07	1.37	20
14	Future small SMR	2015	70%	32.03	0.71	20
15	Electrolysis – small current	2000	75%	70.98		15
16	Electrolysis – small future	2020	85%	15.87		20
17	Electrolysis – large current	2000	60%	42.08		15
18	Electrolysis – large future	2020	75%	4.89		25
19	Biomass gasification to hydrogen - current	2000	50%	32.05	0.71	30
20	Biomass gasification to	2020	50%	19.23	0.71	30

⁷ Combination of solar electricity, electrolysis and liquefaction annualized over 30 years, plus operating liquefaction plant costs and second step for international LNG, includes learning economies of solar PV (commercial)

	hydrogen - future					
21	Biomass pyrolysis to hydrogen	2010	50%	11.20	0.71	25
22	Waste gasification - hydrogen	2000	65%	22.80	0.71	30
23	Liquefaction of hydrogen	2000	70%	18.37	0.78	30

Table 5: H₂ transmission technologies

No	Technology description	Year	Efficiency (%)	Invest cost (£/GJ/yr)	Variable costs (£/GJ)	Lifetime (years)
24	Hydrogen tube trailer	2000	89%			
25	Hydrogen pipeline	2000	98.7%	11.97		
26	Liquid H ₂ transmission	2000	98%			

Table 6: H₂ distribution technologies

No	Technology description	Year	Efficiency (%)	Invest cost (£/GJ/yr)	Variable costs (£/GJ)	Lifetime (years)
27	Hydrogen pipeline (SD,HF)	2000			1.57	
28	Hydrogen pipeline (SD,LF)	2000			4.70	
29	Hydrogen pipeline (LD,HF)	2000			3.13	
30	Hydrogen pipeline (LD,LF)	2000			16.84	
31	Hydrogen tube trailer (SD,HF)	2000			3.13	
32	Hydrogen tube trailer (SD,LF)	2000			3.52	
33	Hydrogen tube trailer (LD,HF)	2000			11.75	
34	Hydrogen tube trailer (LD,LF)	2000			12.13	
35	Liquid H ₂ by road (SD,HF)	2000			0.39	
36	Liquid H ₂ by road (SD,LF)	2000			0.39	
37	Liquid H ₂ by road (LD,HF)	2000			1.17	
38	Liquid H ₂ by road (LD,LF)	2000			1.17	
39	On-site liquefaction (SD,HF)	2000	70%	18.37	0.78	30
40	On-site liquefaction (SD,LF)	2000	70%	43.04	0.78	30
41	On-site liquefaction (LD,HF)	2000	70%	18.37	1.17	30
42	On-site liquefaction (LD,LF)	2000	70%	43.04	1.17	30

* As distribution technologies are defined to reflect the impacts of distribution distance and flow rates on the cost of these technologies, they are presented explicitly here where SD: short distance, LD: long distance, HF: high flow and LF: low flow. The costs follow Yang and Ogden (2006), and efficiency losses are accounted in the transmission technologies that were listed in the previous table.