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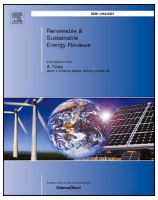

Energy modelling challenges for the full decarbonisation of hard-to-abate sectors

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ABSTRACT

Many Countries have set extremely ambitious targets to speed up the energy transition and reach zero emission by 2050. This has gained even more important motifs in light of the recent geo-political events and the energy crisis that have been shaking the world balance and messing with the energy agendas of many Countries, especially those with a high reliance on imported fossil fuels. Thus, it has become ever more important to find solutions for the decarbonisation of every economic sector including also the "hard-to-abate" ones. Different solutions have been identified for the decarbonisation of such sectors that for their heterogeneity and specific requirements need sometimes unique technologies. Most proposed solutions entails a tighter connection to the power system either through direct or indirect electrification. This research wants to shade light on the most promising technologies, their impact and potential synergies with the entire energy system thus supporting Sustainable Development Goals 7, 8, 9 and 13. Furthermore, this review also discuss how the decarbonisation of hard-to-abate sectors is analysed in energy system modelling for energy planning purposes, what are the most used approaches and what each of them entails, critically discussing and analysing the main challenges while offering potential solutions to tackle them.

ABBREVIATIONS

Alcohol-to-jet synthetic paraffinic kerosene	ATJ-SPK
Aqueous phase reforming	APR
Basic oxygen furnace	BOF
Blast furnace	BF
Carbon capture	CC
Carbon capture & storage	CCS
Carbon capture utilisation & storage	CCUS
Direct air capture	DAC
Direct reduced iron-electric arc furnace	DRI-EAF
Electric arc furnace	EAF
Electro fuels	e-fuels
Global change analysis model	GCAM
Global energy and climate	GEC
Greenhouse gas	GHG
Heat pumps	HPs
HtA	hard-to-abate
Hydrothermal liquefaction	HTL
Integrated assessment model	IAM
Iron & steel	I&S
liquid hydrogen	LH2
Liquid natural gas	LNG
Natural gas	NG
One Earth Climate Model	OECM
PEM	
Power-to-liquid through fischer-tropsch synthesis	PtL-FT
Pulp & paper	P&P
Renewable energy sources	RES
Sustainable aviation fuels	SAFs
Synthesised isoparaffins from hydroprocessed fermented sugars	HFS-SIP
Synthetic paraffinic kerosene from hydroprocessed esters and fatty acids	HEFA-SPK

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Technology readiness level	TRL
World Energy Model	WEM

1. Introduction

As the whole World is proceeding towards a decarbonised economy, there are still some sectors that are lacking behind and that still pose significant doubts and questions [1]. These are the so called hard-to-abate (HtA) sectors that are widely accepted to be the most challenging ones and these are some subcategories of the industrial and transportation (aviation, maritime and road-freight) sectors [2].

These sectors currently account for almost 50 % of total global CO_2 emissions [3], but, on current trends, their emissions could account for a much larger share by 2050 considering they are set to slowly transition while the rest of the economy decarbonizes [4]. Accelerating the transition of hardest-to-abate sectors could impact a large part of the whole system. For instance, 70 % of the whole industrial sector's emissions and energy consumption are produced by energy-intensive, and HtA, industries, and is thus crucial to achieve climate change goals [5]. This is especially worrisome considering that several national strategies – as declared in Nationally Determined Contributions – pay extremely little attention to HtA sectors [4].

A reason for the lack of attention to the decarbonisation of these sectors lies mostly on technical and economic reasons but also on social and political ones. Indeed, the decarbonisation process will translate in new investment and technologies that might not be market ready and thus will lead to a price increase for consumers [6]. Nevertheless, there are studies that prove that the increase of prices for consumers would be limited. The most significant overprice would be found in aviation-related activities, mostly tourism, because of a 10–20 % increase in ticket prices [4]. Additionally, the indirect impact on related economic sectors as well as unemployment in specific areas are reason for concerns.

Nevertheless, the EU Commission and Parliament agreed on clear and ambitious targets for all of those sectors as well. For instance the ReFuelEU Aviation initiative aims at boosting the decarbonisation of the aviation sector by affecting both the demand and supply of sustainable fuels [7].

From a technical point of view the main challenge can be simplified by stating that the specific requirements and necessities of each industries and of each of the three sub-transport sector as it will be specified in the next sections. That means that each sub-sector needs to identify its specific solution that can hardly be replicated and scaled to other sectors needs.

Regarding the industrial sector for instance, there is a dizzying array of processes that make decarbonizing each individual sector independently extremely complex. Indeed, developing any single solution will not guarantee the replicability to other industries and processes. Nevertheless, it is possible to find an important commonality within industries that could help a generalised analysis. Indeed, about 7.5 Gt of CO_2, equivalent to 21 % of global CO_2 emissions in 2016, result from generation of over 100 EJ_{th} of heat [8]. This is the reason why, in this research we decided to focus on the shared challenge and opportunity that is represented by the decarbonisation of heat in industries.

Even though all the technical, economic and social challenges posed by the decarbonisation of HtA sectors, some of them are already experiencing relevant reduction of both emissions and energy intensity, e.g. the steel industry reduced the energy consumption per ton of steel by 61 % since 1960 [9]; nevertheless, the road ahead is still long and in many cases it is not clear what will be the best solution. Electrification is seen as the best option for all those end-uses where it is technically possible [10]. For the remaining demands, switching to biomass/biofuels can be the solution for many technologies [11]. Nevertheless, when proposing bioenergy as the solution to HtA decarbonisation, it is important to consider all other sectors at the same time since there are limits to the amount of biomass that may be sustainably produced [12] thus creating competition and policy concerns with agriculture and biodiversity needs [13]. Indeed, a biomass feedstock crunch is foreseen as early as 2027 [14]. The most used, and in risk of experiencing a feedstock crunch, are wastes and residues that are currently the highest demanded since they satisfy greenhouse gas (GHG) and feedstock policy objectives in Europe and the United States. Differently than wastes and residues, sugars and starches as well as sugar cane and maize are under lower pressure. Another set of possible solutions are based on hydrogen and hydrogen-based fuels and thus power-to-fuel options [15]. This is the case for the so-called synthetic [16] or electro fuels (e-fuels) that also need carbon dioxide (CO_2) as feedstock and thus carbon sequestration technologies to capture it [17].

This brief introduction about the decarbonisation of HtA sectors and the main technologies immediately shows how strong the interconnection with the power sector is and how important a conscious and comprehensive modelling is when planning the transition of the energy system that must be able to cope with the demands and requirements of all sectors [18]. Furthermore, it is also important to embed the analysis of HtA sectors when analysing the energy systems since the decarbonisation solutions and technologies also have a flexibility potential that could support the power grid in hosting high penetration of Renewable Energy Sources (RES) [19], and thus potentially decreasing the need for alternative, and more costly, technologies [20].

In light of the identified needs and current gaps, the novelty of this review study is that it aims at summarising the most promising technologies to decarbonise the industry and transport sectors focusing on those branches that are considered hard-to-abate. Such novelty is believed to support the development of Sustainable Development Goals (SDGs) 7, 8, 9 and 13. An additional novelty of this review is to identify the energy models that are adopted to analyse these sectors, how they approach the challenge and what are the main issues and strengths of each approach so as to help future energy modellers and other interested parties.

2. Analysis of technologies for the decarbonisation of hard-to-abate sectors

In this chapter, the technologies and solutions that are considered viable candidates for the decarbonisation of the industry and transport sectors are briefly reviewed.

2.1. Industry

The first step of this research consisted in identifying the most relevant industry sub-sectors and identify the main technologies to decarbonise such sectors. Industries worldwide in 2021 consumed 169 EJ accounting for 38 % of the overall final energy use and about 9.4 Gt of CO_2 [21].

The Iron & Steel (I&S) sector is the most polluting with 2.7 Gt of CO_2 in 2021 (7 % of global CO_2 emissions), followed by the 2.52 Gt of the cement subsector, 1.37 Gt of the chemical & petrochemical, 0.28 Gt from the Aluminium industry, 0.19 Gt from Pulp & Paper (P&P) and 2.31 Gt from other industries [22].

Regarding the I&S industry, for energy supply it relies for the 75 % on coal that is the major reason for its negative record of highest emitter. Indeed, 27 EJ for I&S production come from coal, 3 EJ from gas and only 5 EJ from electricity and 1 EJ from external heat sources [23].

In terms of trends, cement industry has seen a gradual decline thanks to energy efficiency improvements especially in the use of thermal energy that indeed remained constant in the last years [24].

The emissions from chemical and petrochemical industry has seen an increase in the last years [25]. This sector is the highest energy consumer but only the third highest emitter because the energy input is used as feedstock and not for energy production [25]. The highest emissions for produced chemicals derive from Ammonia, followed by high-level chemicals such as ethylene, propylene and benzene, and then Methanol. Regarding process energy for primary chemical production in 2021, 3.2 EJ came from Coal, 0.1 EJ from Oil, 4.9 EJ from Gas, 0.7 EJ from electricity.

Regarding aluminium production, the process of refining and smelting lead to about 90 % of the whole emissions while the remaining 10 % is due to casting, anode production and recycled production [26].

The energy need in P&P production is mostly the thermal energy for drying purposes, in 2021 it has been estimated to be equal to 8.59 EJ [27].

As previously mentioned, this review focuses only on emissions that are linked to heating purposes thus neglecting all emissions related to other industrial processes.

Thus, solutions such as reduced material use, additive manufacturing, industry ecology and circular economy have not been considered since they are considered out of the scope of this research. Nevertheless, these solutions should somehow be considered when planning the decarbonisation of the future energy system since it would influence the need for production [28]. Also energy efficiency measures will not be analysed even though those are considered essential to reach the full decarbonisation by decreasing the overall energy demand.

Furthermore, the choice to consider only the thermal energy demand has been taken since this is considered the most interesting topic in relation to the whole energy systems and also being the most generic and inclusive to most industries while focusing on the decarbonisation of industry specific processes does not possess any replicability potential being extremely specific. The thermal energy is mostly supplied by coal, natural gas or oil and it is used for different purposes such as distillation, drying or chemical reactions with an extremely wide range of temperatures [29].

Rissman et al. [29] estimated that direct and indirect energy-related emissions would cover the largest part of industrial-related emissions since they represent about 81 % of the overall value.

In Table 1, technologies and solutions for the full decarbonisation of the main energy-intensive industries are summarised.

Generally the solutions that are considered can be classified in four different clusters 1) switching to bio- or electro-fuels, 2) using clean and sustainable heat from renewables (e.g. solar, geothermal) or even nucelar, 3) direct electrification of the heating process and 4) Carbon Capture [8]. Following, a brief focus on each of the 4 clusters is presented.

Fuel switching might be the only solution for some processes that require higher temperatures or some chemical compound that is necessary within the process. Traditional biofuels can be generally employed for low to medium temperatures [30] while biomethane and hydrogen could be used for higher temperatures together with solid biomass [5]. Indeed, hydrogen and biomethane are considered to be extremely suitable for all technologies currently adopting natural gas thanks to the physical and chemical similarities between the mentioned fuels [31]. The main barrier to fuel switching is the lack of a reliable supply chain ensuring continuous supply at viable costs. Another barrier is considered to be the product quality for all those processes that adopt direct heat applications [31]. On the other hand, one of the major strengths would be the potential involvement of companies currently involved in the fossil fuel industry. Indeed, the similarities between the old and new business models and for the needed infrastructures and

Table 1
Technologies for the decarbonisation of energy-intensive industries.

Industry	Energy-related process	Source of emission	Technology/Solution for decarbonisation
Cement	Heat precalciner and rotary kiln 30–40 % of direct emission. Usually $T > 1400$ °C [35]	Mostly coal (70 %), then oil and Natural Gas (NG) (24 %) and biomass & waste heat (6 %) [54]	Fuel switching [29] Carbon Capture & Storage (CCS) [29] Heat electrification through: - electric furnaces & thermal plasma for the cement sector not yet fully developed [5]) - electric kilns [24] Biomass in the kiln and calciner burners [46]
Iron & Steel	- Blast furnace/Basic oxygen furnace (BF/BOF) covers 71 % of all stell production (of which 6 % use direct reduced iron-electric arc furnace (DRI-EAF)) [29] – 20–25 % uses electric arc furnace (EAF) [29] - 4–9% Induction furnaces (Secondary steel production from scrap) [29]	- Coal is used as process heat and as chemical agent - Iron ore and coke (purified coal) are the input of the blast furnace - energy mix for electricity	Carbon Capture (CC) [29] Hydrogen (through electrolysis) [29] (e.g., Ulcolysis) [5] Renewable supplied EAF [29] BF/BOFs (biocharcoal as fuel and reducing agent) [29] Electrowinning [5,35]
Chemicals (Except hydrogen)	Combustion for [29]: - steam crackers ca 850 °C (break hydrocarbons in smaller molecules) - distillation, drying and evaporation (for chemical separations)	Fossil fuels	for steam crackers: electrical naphtha or electrical steam crackers (under study [55]) Carbon capture, utilisation and storage (CCUS) and electrolytic hydrogen [25]
Pulp & Paper	CHP, fossil fuel supplied boilers	Gas	- Direct electric heating (i.e. electric boiler or heat pump) [5] - biomass with or without CC (mainly wood or derivative) [56,57] - microwave drying [5] - solar thermal energy [58]
Aluminium	- Refining bauxite to produce alumina mainly through the Bayer chemical process (70 %) [59] is the major energy consumption due to the high temperature (7–21 GJ/tonne) [60] - smelting (refining alumina to pure aluminium) through the Hall-Hèroult electrolytic process at about 1000 °C [61]	- Aluminium Smelting: Coal 56.9 %, Hydro 31.3 %, NG 9.7 %, renewables 1.3 %, others 0.8 %; - Alumina refining: Coal 51.5 %, Gas 31.4 %, Electricity 8.2 %, Oil 7.9 %, Others 1 % [62]	- Fuel switching (e.g. biofuels and hydrogen) [26] - Electrification [26]
Glass and Lime industry	High Temperature (usually $T > 1400$ °C [35]).	Mostly natural gas and coal	- glass: e-methane or electric furnaces [29] - lime: fuels will be changed upstream to high temperature electro-thermal processes [29]

components for fuels treatment and storage make this transition easier. Moreover, it might also lead to an easier shift of the workforce so as to enable a smoother transition from a social point of view.

A particular focus is required for hydrogen that is experiencing an incredible attention both from the public and private sectors. Indeed, hydrogen thanks to the possibility to be used for combustions with temperatures higher than 1000 °C is considered a solution for several industries such as I&S and Cement [29]. Hydrogen also presents invaluable benefits for the I&S industry since it can work as a substitute of methane in the iron reduction process and in combination with the use of electric arc furnaces [29]. Vogl et al. [32] estimated that using hydrogen in a DRI process would consume around 3.5 MWh and 51 kg of hydrogen per ton of produced steel. Fichedick et al. [33] suggests that the use of hydrogen in the steel industry might be competitive if a carbon tax is in place (with a cost of 40–75 $/t of CO_2) and with electricity prices lower than 50 $/MWh. Sweden is also betting on hydrogen steel production aiming at Technology Readiness Level (TRL) 6. Indeed, HYBRIT and H2 Green Steel projects aim at developing a hydrogen-based DRI process at industrial scale [23]. Rio Tinto announced a project for the use of hydrogen instead of natural gas in the calcination process for alumina production [26,34].

In addition to the afore-mentioned industries and proposed solutions, hydrogen is also used for the production of different electro-fuels (e-fuels) that might represent the optimal solution for other HtA sectors such as transport. Several projects are already ongoing for ammonia; methane; methanol but also Fischer-Tropsch-naptha (FT-naphta) [35].

Nowadays, hydrogen-based technologies' success seems to be mostly reliant on clean hydrogen. Given the fact that hydrogen represents a potential option for the future decarbonisation of many sectors, it is very likely that investment will arrive and this will surely lead to an improvement in technologies' efficiency and a decrease in their cost. This is especially important for electrolysers that, as hydrogen production technologies, are at a lower TRL and can thus benefit from such investments. Furthermore, the interest in electrolysers is also strong for their potential role as flexibility providers for a grid that will need an increasing level of flexibility in order to properly manage non-dispatchable RES.

Regarding electrification, electricity is already used in some industrial processes for heat generation, indeed it accounts for 27 % of the demand while fossil fuels cover the remaining 73 % [36]. The process of electrification is the foreseen solution for several demands and sectors, in terms of heating demand this is surely true for residential heating (low temperature) thanks to Heat Pumps (HPs). HPs can also represent the optimal solution for the decarbonisation of industries for low temperature processes, this might be the case for the food processing industry [37]. For instance, a Kraft Foods plant in Iowa adopted a HP to substitute natural gas saving up to 250000$ per year and about 50 ML of water [29]. Nevertheless, low temperature processes are not considered HtA; indeed, most of the processes require either medium or high temperatures thus respectively, between 100 and 400 °C or above 400 °C [35] and electrification is considered to be key for the decarbonisation of this processes [38]. Electric furnaces represent the most ready technology to provide medium-to-high temperature [35] but other technologies are also available such as those based on microwaves, radio frequency [39], ultra-violet light and infrared radiation, induction, electric arc and plasma, resistive heating or laser sintering [40]. Some technologies are considered to be already mature for medium temperatures demand such as microwaves, infrared, or even electric boilers [41] or some HPs technologies specifically developed for medium temperatures [35]. Some of these are already used as is the case for microwave and infrared technologies for drying purposes and curing paints. Also electric arcs are already adopted in the I&S industry for steel production from scrap [42] while plasma technologies are used in waste treatment plants.

The major barrier against the development of electrification in industry is usually cost [43]. Other barriers are the specificity of application and of equipment [43] that hinders the development of technologies that indeed are not considered mature and market-ready yet [44]. In the I&S industry, electrowinning is considered to be one of the most energy efficient solutions for electrification [45]. Regarding cement industry, the most heat intensive processes are in the precalciner (about 900 °C) and the kiln (about 1400 °C), in this industry around 20–30 % of the demand is already electrified [46]. VTT Decarbonate announced a project for producing a prototype electric kilns for the production of clinker [24,47]. Alcoa presented their project to switch to electric demands in alumina refining processes [26].

The major hidden potential drawback of electrification of the industrial demand could be the very high electricity demand for a grid that will already have to face many challenges for renewing its infrastructure to provide secure and stable electricity with the growing RES production as well as the electrification of other sectors. Nevertheless, industries represent relatively stable and easy-to-deal-with users since they are usually already strategically located in well-supplied places. Thus, an improvement of the supply-capacity should not represent an issue. Nevertheless, the added need for RES electricity production should be considered in terms of added investment and potentially even in terms of land usage.

Carbon Capture (CC) is considered to be a promising solution to decarbonise the industrial sector especially for those industries that requires emitting processes such as I&S and cement [48] but it is also a feasible solution for power and heat production. Indeed, CC can be clustered in four categories pre-combustion, post-combustion, oxyfuel combustion process and direct air capture (DAC) [49]. Different techniques for the separation of carbon are available and/or under study based on chemical absorption, physical, membrane, calcium looping [5]. Aside from the high cost, the main barriers common to most CC methods and technologies are the high energy demand required to obtain an acceptable carbon purity [50], and the lack of a proper infrastructure to transport the captured CO_2 for its use or for long-term storage [51]. Currently, the most productive usage of captured CO_2 is that of pumping it in the same reservoir where oil and gas are extracted so as to increase the reservoir pressure and make the fossil fuel extraction cheaper and efficient. At the same time, the reservoir is also used for long-term storage making this method a Carbon Capture Utilisation and Storage (CCUS) [52]. Nevertheless, in the future, different industries could benefit from the captured CO_2 as a feedstock, this is true for chemical industries as well as for the production of e-fuels as it will be discussed further in the next section.

Some ongoing projects are the Longship in which CC is applied to waste-to-energy [53], the LEILAC-2 and the Norcem Brevik projects that aim at using CC for cement production [24].

Within the chemical sector, the e-methanol plant to be installed in Norway is an example of a carbon-to-fuel project, thus a Carbon Capture Utilisation (CCU), using the captured CO_2 and renewable hydrogen from electrolysis [25]. Moreover, a CC plant in the I&S industry in France is able to capture 0.4 kt of CO_2 per year and aims at reaching 1 Mt in the next years [23].

CC is also considered to be offsetting industrial emission (in general HtA sectors) even in the case it is applied at biomass power plants or with DAC since these are considered to be negative emissions. Considering the very challenging targets that some Countries identified, and the low-speed at which the energy transition is unfolding, CC might not just be a viable and feasible solution but it might simply be necessary especially when leading to negative emissions.

Another fact that can be considered is that CC in the power sector might represent the clean solution for the fossil industry that could thus maintain its business model unaltered; for this to be true though, the cost must experience a significant drop. Nevertheless, investment in CC in the power sector might also boost the technology development in the industry-sector where the competition is much more open.

2.2. Transport

In this section, the possible and foreseeable pathways for the decarbonisation of the HtA sub-sectors of aviation, maritime and road-freight transport are discussed.

2.2.1. Aviation

The aviation sector experienced abrupt growth from 2000 to 2019, increasing the number of flights by 140 % [63]. The sector is also expected to continue growing at an annual rate of 3.5 % over the next two decades [64]. The usual carbon number in a jet fuel is between 8 and 16 and kerosene is currently the most widely used aviation fuel [65].

So-called Sustainable Aviation Fuels (SAFs), are alternatives to conventional fuels in the short-to medium-term, which have already found application in conventional engines. Already today, SAFs are used in aviation. In 2019, there were more than 250,000 flights with blended fuels, however the current SAF consumption remains at 0.1 % in relation to fossil fuel consumption [66]. The application of blended SAFs is characterised in the various national and international regulations by blending limits ranging from 5 % to 50 % depending on the country and the SAF production process [67].

Renewable drop-in kerosene can be produced by means of diverse methodologies, each contingent upon different feedstock and technological alternatives.

Synthetic Paraffinic Kerosene produced from Hydroprocessed Esters and Fatty Acids (HEFA-SPK) represents the most mature and commercial technology [68]. The process consists of the hydrotreatment of vegetable oils and animal fats. This solution is similar to the production of hydrotreated vegetable oil. However, there is an additional isomerisation step in order to reduce the freezing point of the fuel. Notably, the conversion efficiency is very high, above 75 % [69]. HEFA-SPK is the only currently commercial solution and the cost currently ranges between 1100 € and 1350 € per tonne [68]. The disadvantage of this process is mainly the limited feedstock availability.

Another innovative method is the Alcohol-to-Jet Synthetic Paraffinic Kerosene (ATJ-SPK) production process, which entails the conversion of alcohols into jet fuel through a sequence of reactions including dehydration, oligomerisation, hydrogenation, isomerisation and distillation [70]. The alcohol can be derived from conventional processes involving the fermentation of sugar or starch cultures, or through advanced routes from lignocellulosic feedstock and waste. A notable advantage of this process is its versatility in accommodating various alcohol typologies from different feedstocks [71]. However, the production cost of jet fuel through ATJ-SPK is relatively high compared to HEFA-SPK.

The production process of Synthesised Isoparaffins from Hydroprocessed Fermented Sugars (HFS-SIP) is based on the conversion of sugar into hydrocarbons or lipids by means of genetically modified microorganisms [72]. This methodology, known as the direct sugars to hydrocarbons process is presently limited to small-scale installations for the chemical, pharmaceutical and food industries. The large-scale development of the process could make this option interesting also for the jet fuel production. However, such process is complex and characterized by low efficiency, resulting in high costs and high energy consumption [73].

The gasification process coupled with Fischer-Tropsch synthesis for Synthetic Paraffinic Kerosene involves the transformation of lignocellulosic biomass or solid waste into fuels [74]. The process consists of the following key steps: feedstock pre-treatment, gasification, syngas cleaning and conditioning, FT catalysis, distillation, and hydrocracking. Supplementary procedures, including isomerisation and catalytic reforming are required to process the jet fuel [75].

The pyrolysis and upgrading process offer versatility in terms of feedstocks, accommodating lignocellulosic biomass or solid waste. Pyrolysis results in the production of a bio-crude oil, and is a TRL 8 process, with first commercial applications [76]. However, upgrading pyrolysis oils into a finished fuel product is still not a commercial process. The main obstacles for the deployment of this process are the materials and catalysts used [77].

The Aqueous Phase Reforming (APR) process employs a catalyst to convert oxygenates derived from different feedstocks present in an aqueous solution into a blend of hydrogen, CO_2 and alkanes, acids, ketones and aromatics [78]. Different condensation reactions are then used to elongate the carbon chains in the hydrocarbon mixture, which is then subjected to hydrotreatment, isomerisation and distillation. Unlike other reforming techniques, APR works under humid conditions, mitigating the expense associated with removing moisture from specific feedstocks such as sugars. However, its limited selectivity for liquid hydrocarbons results in high gas yields and a short catalyst lifetime [79]. These features increase the cost of APR in terms of both capital and operating expenditure.

Hydrothermal liquefaction (HTL) is a process that involves heating biomass and water at extremely high pressures to produce a bio-crude oil. The high-pressure water serves as both a reactant and catalyst, breaking down the biomass into smaller molecules [80]. Similar to the pyrolysis process, the bio-crude oil produced by HTL can be refined. The higher molecular weight distribution of the HTL oil makes it more suitable for diesel production, though it is also feasible to produce gasoline and jet fuel by introducing hydrocracking stages. HTL is an ideal choice for processing extremely wet biomass, however, the high pressure and corrosive conditions this process employs are the main obstacles to its widespread use [81].

Power-to-Liquid technology using Fischer-Tropsch synthesis (PtL-FT) produces liquid fuels by catalytically combining a stream of hydrogen generated by electrolysis with a carbon source [82]. Green hydrogen from renewable electricity is combined with a concentrated source of CO_2. The maturity of the PtL-FT method depends on the maturity of the individual components and the chosen design configuration [83]. In the PtL process, solid oxide electrolysers are used, which are more efficient but less developed than other electrolysis technologies [84]. Different concentrated CO_2 sources, such as biogas upgrading, ethanol production or CO_2 waste streams from industrial processes, can be used. An important advantage consists in the maturity of the FT synthesis process, however it is applied on a large scale, but its application in small-scale settings remains in the demonstration phase [85].

The use of direct hydrogen for aircraft propulsion present certain advantages, but is accompanied by notable drawbacks. While hydrogen has three times the energy density of kerosene, its substantially larger specific volume necessitates significantly larger storage tanks to contain equivalent energy, resulting in considerable storage challenges [86]. Cryogenic hydrogen or liquid hydrogen (LH2) requires cryogenic storage ($-253\,^{\circ}C$; 20K) to maintain hydrogen in liquid form [87]. This is due to the high specific volume of hydrogen at standard atmospheric pressure and temperature. Implementing cryogenic hydrogen storage requires substantial redesign of existing aircraft configurations.

Hydrogen propulsion systems have been demonstrated in both combustion and fuel cell modes. The hydrogen use is expected mainly for the commuter to short-haul categories. For the former, fuel-cells are envisaged, while hybrid solutions are more suitable for the latter. The use of LH2 introduces concerns regarding leakage because to the high boiloff rate and small size of hydrogen molecules. Consequently, the use of hydrogen mandates strict adherence to safety protocols and standards, encompassing safety certification at airports, production and storage facilities, transportation, distribution, and aircraft operations to prevent and manage potential leaks in case of an incident [88].

The electrification of air transport faces several limitations related to the battery energy density and the limited number of charging cycles [85]. Moreover, this technological solution requires adaptations spanning individual components to entire infrastructures. Although small all-electric aircraft already exist, the weight and reliability of electric propulsion systems and energy storage have hindered the spread of electric propulsion in aircraft for long-distance commercial flights [89]. Realistically, all-electric propulsion systems may find application in commuter routes, and turbo-electric hybrid systems in various configurations could be suitable for short-haul routes [90]. One of the main barriers is the high power-to-weight ratio of the different electrical components in this kind of aircraft. High-performance lithium-ion batteries have a specific energy of 250 Wh/kg, while the specific energy of jet fuel is 12000 Wh/Kg. An energy density of 800–1200 Wh/kg would make the technology competitive for commercial flights. However, it can be seen as a milestone that is unlikely to be realised before the mid-century, considering the current trajectory of energy density trends [91]. Furthermore, such a solution would require a radical change in the charging infrastructure at the airports. Table 2 summarises the solutions and barriers that have been identified in the aviation sector.

In energy planning studies of 100 % renewable energy systems, various approaches have been used showing a heterogeneity of solutions adopted. However, a common trend in long-term planning concerns the adoption of biofuels and electro-fuels.

For instance, according to the work of Connolly et al. [97], half of fuel for air transport can be replaced with bio-electrofuels and half with CO_2-electrofuels.

Mathiesen et al. [98] assessed solutions for heavy-duty transport decarbonisation. Accordingly, both electrification and the direct application of hydrogen are solutions to be ruled out due to the cost of aircraft. In that work, the solution adopted is the development of e-fuels produced from bio-based CO_2.

In Ref. [99], ethanol has been applied to supply all the jet fuel demand.

Jacobson et al. elaborated a roadmap to decarbonise California [100]. In their work, the strategy adopted for the aviation sector involves various technologies, both direct electrification and cryogenic hydrogen systems.

Table 2
Technologies for the decarbonisation of aviation.

Reference	Promising technology	Range of application	Main advantages	Identified barriers
Siew Ng et al. [92]	Biofuels	No limitation of range	- Application of fuel without modification to aircraft or airport infrastructure	- Feedstock availability - High production costs
Pio et al. [93]	E-fuels	No limitation of range	- Application of fuel without modification to aircraft or airport infrastructure	- High production costs - Current high costs of hydrogen
Ortega et al. [96]	Synthetic paraffinic fuels	No limitation of range	- Application of fuel without modification to aircraft or airport infrastructure	- High production costs
Sahoo et al. [94]	Electrification	Short range	- No emissions during flight	- Current high costs of batteries - Change of airport infrastructure - High power-to-weight ratio of electric components
Clarke et al. [95]	Cryogenic hydrogen	Short-medium range	- No emissions during flight - No further synthesis of hydrogen respect to electro-fuel	- Current high costs of hydrogen - Change of airport infrastructure

Also in Ref. [101] electric and hybrid electric/hydrogen-fuel-cell aircrafts have been adopted. In that work, the authors highlighted how such technologies are not yet commercially available. However, they are confident in such technologies, predicting that all short-haul commercial flights can be electrified that long-haul flights can be served by hydrogen fuel cell-electric hybrid aircrafts.

2.2.2. *Maritime*

Maritime transport is a vital component of the global economy, but also a significant and expanding contributor to greenhouse gas emissions. In the year 2018, emissions from global shipping accounted for approximately 2.9 % of worldwide emissions attributable to human activities [102]. In addition, the continuous growth in global trade will result in a rising demand for the maritime transportation [103]. Its substantial dependence on heavy fuel oil and diesel has made decarbonisation a substantial challenge and a HtA sector [104]. As such, the development and implementation of sustainable and renewable technologies to decarbonise this sector is of paramount importance [105]. In this sub-chapter, we delve into the most promising technologies that can aid in substantially reducing the maritime sector's carbon footprint.

1. Electrification: The electrification of short sea shipping routes is a promising avenue to pursue, given the progress in battery technology. Fully electric vessels have a limited range, making them most suitable for short-distance travel, such as ferries or small cargo vessels in coastal areas. Battery technology is rapidly advancing, and with increases in energy density and decreases in cost, electrification may become feasible for longer routes in the future [106].
2. Hydrogen and Fuel Cells: Hydrogen, particularly green hydrogen produced through electrolysis powered by renewable energy, is a zero-carbon fuel that can be used in fuel cells to generate electricity for propulsion. High energy density and relatively quick refuelling times make hydrogen a compelling candidate for longer voyages. However, the storage of hydrogen on ships presents significant challenges due to its low density, requiring high-pressure or cryogenic storage systems. Additionally, the development of a hydrogen supply infrastructure at ports is a prerequisite for the large-scale adoption of this technology. Ustolin et al. [107] provides an extensive overview of the potential use of hydrogen as a clean and renewable fuel to power ships and boats. They emphasize the need for storing hydrogen in the cryogenic liquid phase, which is one of the best options for large long-range ships with high energy demands and conclude that liquid hydrogen can replace fossil fuels in the maritime industry only if some identified challenges are surmounted, which involves addressing the high costs of LH2 and the infrastructure necessary for its management and storage.
3. Ammonia and Methanol: Ammonia and methanol, produced from renewable hydrogen, are another viable option for maritime transport due to their higher energy density and easier storage conditions compared to hydrogen [108]. While ammonia is a carbon-free fuel, it poses issues due to its toxicity and the challenge of NO_x emissions during combustion. Methanol, on the other hand, is less toxic and easier to handle but is not entirely carbon-free, although it produces fewer emissions than conventional marine fuels. E-Methanol can be produced by combining electrolytic hydrogen with carbon oxides [109] and it represents a promising alternative to diesel in maintaining a high engine efficiency with lower emissions [110].
4. Wind-Assist and Sail Propulsion: Incorporating wind-assist technologies and sail propulsion into ship design can significantly reduce fuel consumption and associated emissions. These technologies include Flettner rotors, wing sails, and kite sails [111]. Although not a standalone solution, when used in conjunction with other clean technologies, they can contribute to the overall reduction of GHG emissions.
5. Energy Efficiency Measures: enhancing the energy efficiency of ships through improved hull design, propulsion efficiency, waste heat

recovery, and optimised operational procedures can result in substantial fuel savings and emission reductions.

Gore et al. [112] analysed the use of LNG, methanol, green hydrogen, and green ammonia as alternative fuels to mitigate CO_2 emissions in shipping. The combination of green hydrogen and green ammonia with PEM fuel cells showed the highest potential for emission reduction (100 %), followed by dual-fuel engines for LNG (37 %) and methanol (14 %). LNG was the most profitable option with the highest net present value, followed by methanol and green hydrogen. Green ammonia resulted in a negative net present value due to its high operational costs and lower net calorific value.

From a regulatory point of view, the research conducted by Dong et al. [113] indicates that the implementation of laws aimed at decarbonizing the transport sector may inadvertently raise the cost of international maritime transport. This could have an unequal impact, particularly burdening developing countries. Their study also highlighted challenges in synchronizing individual and collective regulations. It was found that ports imposing local pollution taxes could inadvertently drive business to their rivals and experience increased secondary pollution.

Table 3 shows different studies that present the identified promising technologies to decarbonise the maritime shipping sector. While no single technology currently offers a silver bullet solution, the combination of these technologies, tailored to specific applications and complemented by energy efficiency measures, could pave the way towards a more sustainable maritime sector. It is also crucial to address the identified barriers, including technological, infrastructural, economic, and regulatory challenges, to accelerate the transition towards a decarbonised maritime sector. Future research and policy efforts should focus on overcoming these barriers and fostering the development and deployment of these promising technologies.

2.2.3. Road freight transport

The transportation of goods by road plays a crucial role in driving economic activity and is a significant contributor to the demand for energy, particularly oil. Oil-based fuels are the primary source of energy for trucks. In terms of global oil demand, trucks rank as the second-largest consumer after passenger cars and are on par with the entire industry sector [119]. When it comes to diesel consumption, road freight stands out as the largest contributor globally, accounting for approximately half of the total diesel demand. However, this heavy reliance on oil raises concerns about the environment. Road freight transport is responsible for over one-third of CO_2 emissions related to transportation worldwide and contributes 7 % to the total energy-related CO_2 emissions [120]. Various approaches to improve vehicle efficiency, enhance logistics and supply chain operations, and explore alternative fuels are currently considered. In the future, the availability of certain transport biofuels for heavy-duty road freight could increase depending on advancements in technology and higher production levels. These biofuels are not widely commercially accessible at present but hold potential for the future.

- ED95 ethanol, derived from conventional crop-based or cellulosic feedstocks, which consists of 95 % fuel ethanol along with lubricants and additives to enhance ignition and protect against corrosion. ED95 can be utilized in appropriately modified diesel engines for heavy-duty transport. However, the availability of vehicles compatible with ED95 is still relatively limited [121].
- Biofuels produced through thermochemical processes like gasification and pyrolysis. These processes can generate fuels suitable for heavy-duty transport using various biomass feedstocks such as forestry and agricultural residues, as well as municipal solid waste. The syngas produced from gasification can be upgraded to biomethane for use in a similar manner as biomethane derived from anaerobic digestion. Alternatively, syngas can undergo conversion

Table 3
Technologies for the decarbonisation of maritime shipping.

Reference	Promising technology	Best application	Identified barriers
Campillo et al. [106]	Electrification	short-distance travel, such as ferries or small cargo vessels in coastal areas	- Range and autonomy limitations - Batteries costs
Anwar et al. [114]	Electrification	short-distance travels	- Range and autonomy limitations - Batteries costs
Ustolin et al. [107]	Liquid hydrogen	Long-range ships	- High production cost and emissions depending from primary energy source - High costs of specific storage equipment - Low available infrastructure
Panic et al. [115]	Hydrogen	Long-range ships	- High production cost
Al-Aboosi et al. [108]	Ammonia	Deep-sea cargo ships	- High cost of water electrolysis (Electrochemical synthesis of ammonia is attractive and can potentially be more competitive)
European Maritime Safety Agency (2022) [116]	Ammonia	Deep-sea cargo ships	- Toxicity and related risks
Machaj et al. [117]	Ammonia	Deep-sea cargo ships	- Low efficiency. From RES electricity through to powering a ship using ammonia as a hydrogen carrier – is estimated at around 18 % - Ammonia requires about 1.5 times the storage space of LNG, potentially reducing cargo space and raising transport costs. - Limitations of current legal regulation
Zincir et al. [110]	Methanol	Deep-sea cargo ships	- There is no need for special storage tanks for methanol as it can be stored in conventional fuel tanks after minor modifications. However, similar fuel supply and safety equipment as needed for LNG are necessary for methanol - Methanol is biodegradable and less harmful to the environment in case of spillages, but it is toxic to humans if ingested, absorbed through the skin, or inhaled. Methanol is also odorless below 2000 ppm in air, necessitating completely closed-off fuel systems and proper ventilation on ships to ensure safety

(*continued on next page*)

Table 3 (*continued*)

Reference	Promising technology	Best application	Identified barriers
Traut et al. [111]	Wind-Assist and Sail Propulsion	Small vessels, Cargo ships only in oceans (better wind conditions)	- Weather dependency - Limited applicability (to small vessels) - Operational complexity
Angelini et al. [118]	Wind-Assist and Sail Propulsion	Small vessels, Cargo ships only in oceans (better wind conditions)	- High maintenance costs

processes to produce biomethanol, dimethyl ether [122], and Fischer-Tropsch (FT) diesel. Pyrolysis oils can also be refined into diesel-like substitutes. Collectively, these fuels are known as biomass-to-liquid fuels.

- Power-to-X (PtX) synthetic fuels, which involve combining hydrogen (produced through processes like electrolysis) with carbon or nitrogen to generate gaseous or liquid fuels. PtX fuels can be produced with or without renewable electricity and carbon streams [123]. However, the interest in PtX technologies has primarily emerged from policies aiming to reduce the carbon intensity of fuels. As a result, production pathways based on renewable energy and carbon sources are gaining momentum. PtX technologies can also produce ammonia (using hydrogen and nitrogen) as an energy carrier.

If the electrification of the sector is to be considered, the main issues are related to the infrastructure to charge the vehicles.

- The implementation of electric road systems involves significant upfront costs. The installation expenses are approximately USD 1 million or more per lane-km when designed to accommodate traffic flows on the core sections of the road network, handling around 250 trucks per hour [124]. However, over the long term, these costs may reduce by half, approaching the scale of infrastructure upgrades seen in rail electrification projects. Electric road systems technology is based on a widely adopted and commercialized system used for buses in many cities.

When considering inductive charging infrastructure, the cost per kilometer is comparable to that of electric road systems on new roads, approximately USD 0.8 million/km. However, on existing roads, the costs can be up to four times higher, exceeding USD 3.1 million/km [125]. To optimize investment requirements while catering to the majority of heavy-duty traffic, focusing on motorways and major trunk roads for infrastructure development could be a strategic approach. Table 4 summarises the identified technologies and their barriers and best applications.

3. Energy modelling examples & challenges

This section focuses on how the HtA sectors and the previously identified decarbonisation solutions and technologies have been modelled, what are the adopted methods and the criticalities that can be found from these analyses.

Different methods have been used to imagine the future energy system considering the HtA sectors. The EnergyPLAN software is able to analyse this sectors [126]; e.g. in Ref. [127], HtA sectors' decarbonisation is considered by a scenario analysis with different sources used as a basis for the uptake of different technologies.

The Global Change Analysis Model (GCAM) is a global integrated assessment model (IAM) able to consider HtA sectors [128]. These are considered as demands of feedstock and energy and allow for scenario-based analysis considering different decarbonisation pathways [129]. For instance in Ref. [130], GCAM is adopted to study the decarbonisation of the US economy under different assumptions on water availability proving that water scarcity might impact availability and affordability of bioenergy. Also, in Ref. [131], the GCAM-USA (v4.2) is adopted considering industry as a single demand sector and the same approach is used in GCAM-LA [132]. Nevertheless, in later versions of the model the industrial sectors have been divided. In Ref. [133], the P&P industry is analysed; in Ref. [134] Durga et al. analysed the I&S sector adopting GCAM v7; while Lee et al. [135] analysed all industrial sub-sector in their GCAM-KAIST 2.0 model.

Table 4
Technologies for the decarbonisation of road freight transport.

Reference	Promising technology	Best application	Identified barriers
Hagman et al. [121]	Ethanol ED95	heavy duty transport	- Required adjustments to existing vehicles - Need for Additives supply chain
Landalv et al. [122]	Dimethyl ether	heavy duty transport	- Required new generation refineries - Carbon management
Ramboll [123]	Ammonia	Long-distance journey	- High production cost and emissions depending from primary energy source - High costs of specific storage equipment - Low available infrastructure
McKinsey [124]	Electrification	Electric Road Systems	- High construction cost
CODOT [125]	Electrification	Inductive charging infrastructures	- High cost on existing roads

Lechtenböhmer et al. [35] analysed the decarbonisation of the European industrial sector in 2050 through a scenario analysis without a specific model or tool. Scenarios are developed based on a forecast of future productions, assumptions on the development of new technologies and then a simple calculation of emissions and energy consumption. The resulting scenario end up suggesting the electrification of most energy-intensive industries leading to an industrial electricity consumption of about 1700 TWh/y against an approximate current demand of 1000 TWh/y.

The set of scenarios developed by Shell Global are also a valid example. It can be noticed that one of the first challenges is that of assuming the political, societal and economic background. In the set of scenarios developed by Shell Global, this is mirrored by the 3 main scenarios call Mountains, Oceans and Sky [136]. The Oceans scenario is based on the assumption of a weak leadership where the common interest of climate change is translated into an economic opportunity. The Mountains scenario assumes that the leadership is very influential and as such the system stability is extremely valued thus creating an extremely cautious and moderated transition. Sky relies on an in-between perspective that accepts both the pushes from the established leadership as well as accepting the share of responsibilities and benefits in order to tackle the wide complexities and interests that are in place [137]. The scenarios were then tested with the Shell's World Energy Model (WEM) [138] able to match different demands and supplies considering different drivers (e.g. economic, technical, social, political and geopolitical) and constraints due to resources availability, technology constraints (technical and social) and prices applying a mixed approach that comprehends both top-down and bottom-up features. WEM is a partial equilibrium model with a yearly time-resolution that enables analysis up until 2100. Mountains and Oceans scenarios are not target-oriented, thus the results do not reach the ambitious goal of limiting the temperature increase below 2 °C while the Sky scenario instead applying a defined target so as to provide useful insights to policy-makers. As a result, Sky foresees that hydrogen covers 10 % of the overall final energy demand covering 25 % of the overall demand in the transportation sector and 10 % of the industrial one. Specifically, the sectors of aviation and maritime transport shift to liquid or gaseous (depending on the development of the conversion into methane) synthetic-fuels obtained from biomass starting in 2030. Later on in the transition hydrogen takes over, particularly in the aviation sector. The road freight transport sector shifts partly to hydrogen, biodiesel and also electrification. Regarding the industrial sector, the so-called light-industry is for the most part electrified but it also sees a limited use of hydrogen as a substitute of gas. Heavy industry requires a slower transition and indeed hydrogen, biomass and electrification arise by 2050 and the real solution is the adoption of CCS and with a limited Utilisation mainly for e-fuels that gains economic relevance only by the end of the century due to delays to develop the needed infrastructure.

The analysis developed by the Energy Transitions Commission is also another example of how HtA sectors can be included in long-term energy analysis [139]. The Mission Possible report was developed through a literature review and expert opinion method thanks to stakeholders engagement. The Energy Transitions Commission reached similar conclusions to other research but no model nor simulation was adopted.

IEA's reports and researches are some of the most considered long-term energy analysis. The currently adopted model is the Global Energy and Climate (GEC) model that integrates the capabilities of the previously used models that were the World Energy Model (WEM) and the Energy Technology Perspectives [140]. The World Energy Outlook 2022 was, for instance, developed thanks to the GEC model [141]. GEC is a bottom-up and technology-rich model based on partial-optimisation that is of course applicable at large scale, dividing the whole world energy system into 26 regions. It relies on the integration of several dedicated models to properly analyse the final energy and material demand in different sectors (e.g. agriculture, industry, transport, buildings), also considering biofuels and e-fuels production processes, and energy supply. Each demand is supplied by both existing and new technologies but only considering technologies that have already been tested and for which a prototype is also available so as to better assess cost and performance status and future trends. GEC is implemented in Vensim and integrates also many other software and tools (e.g. TIMES).

In the latest World Energy Outlook [141] obtained by IEA's GEC model, the main driver of the energy transition is, as expected, electrification that in 2050 supplies about 50 % of the overall final consumption and around 66 % of useful energy. The only sectors that are not electrified are transport and industry, with the transport sector (50 % of the whole demand is electrified, even 3 % of the aviation one) that represents 85 % of the non-electrified demand pushed by the shift for light-duty vehicles. The steel industry switches to 60 % rate of electrification for secondary production (possible only thanks to a higher recycling rate) and by means of Hydrogen-based DRI and thus in-loco production of hydrogen through electrolysers (i.e. 25 % of the sectoral electricity demand). The cement industry reaches a 20 % of electrification through the use of electric kilns from 2040 onwards. The chemical industry is expected to switch 35 % of its total demand to electricity through the use of electrolysers and the use of hydrogen as feedstock (mainly for ammonia, methanol and e-fuels). Hydrogen and e-fuels cover about 10 % of the overall final consumption while bioenergy reaches a value of 15 %. Indeed, sustainable fuels (i.e. bio-energy, hydrogen and e-fuels) correspond to 65 % of all fuels by 2050. Hydrogen and e-fuels cover about 30 % of the transport sector demand; namely, 25 % of the aviation demand is met by e-kerosene and 8 % by hydrogen (hydrogen-fuelled planes are assumed to enter the market in 2035). Regarding biofuels, these are used in the power sector as well as in residential and industry (about 10 % of steel industry, 30 % in the cement one) and transport (15 % of the overall demand for transportation, namely 45 % of the aviation energy demand is met by biojet kerosene). E-fuels use about 25 % of the whole hydrogen production mainly for e-kerosene, that covers 25 % of the aviation demand, and ammonia, which supply about 45 % of the maritime shipping industry. CC technologies are envisaged to sequestrate 6.2 $GtCO_2$ by 2050, 60 % of which are expected to be captured in the industrial sector (more than 20 % of the overall demand in the steel industry). Oil and derivatives are still used in 2050, some in the power sector but mostly in aviation (20 % of the overall demand), maritime (about 15 % of the total demand) and cement industry even though, a great part of this use do not lead to any emissions being power plants equipped with CC or applications that do embody CO_2 in their final product (e.g. asphalt and other chemical feedstocks) or it is offset through DAC or bio-energy production with CC.

There are then software and models tailored to some specific sectors such as the industrial one. In 2018, Fleiter et al. [142] stated that the FORECAST model is the only tool to analyse the decarbonisation of the industry sector adopting a bottom-up approach. The FORECAST model has been developed to investigate the decarbonisation of the industrial sector together with the services and residential sectors [143]. In FORECAST, several technologies and decarbonisation strategies are considered with high detail considering the most energy-intensive industries as separated sub-sectors for higher detail so as to better mirror heterogeneous data and information. The model works with a mix of exogenous inputs and discrete simulation while some are endogenous such as energy efficiency and fuel-switching solutions. Overall, the model can be divided in 6 modules to consider decarbonisation solutions that entails energy efficiency, CC, recycling (and circular economy), material efficiency and the option to switch to sustainable fuels.

Another, more recent, tool able to analyse the decarbonisation of the industrial sector is IndustryPLAN. Implemented as a combination of Visual Basic for Application and Excel is available online and open-access [144], IndustryPLAN aims at filling the gap between single industry specific analysis and aggregated models [145]. IndustryPLAN disaggregates the demands of different industries and for each one of them identifies the mitigation strategies following a pre-defined priority list that always begin with material and energy efficiency followed by electrification and fuel-switching with a higher priority to hydrogen and then biomass as last opportunity since the authors believe that biomass should be prioritised in other sectors such as transport and power sector [146].

In [147], IndustryPLAN is adopted to analyse the decarbonisation of industries in all 27 European member states plus United Kingdom. Results show that in all scenarios electrification takes the lion's share while the hydrogen is adopted only for processes at high and very high temperature and it is favoured only if biomass is used in other sectors since hydrogen increases the overall cost and energy losses.

TransportPLAN is a tool for modelling national transport decarbonisation scenarios. Like IndustryPLAN, such a model allows interfacing with EnergyPLAN. This allows users to assess the impact of the decarbonisation of transportation on the national energy system. TransportPLAN has been used in Ref. [148] in order to assess a potential pathway towards full decarbonisation of the Danish transport sector. According to their findings, light transport is almost completely electrified, while e-fuels are the best choice for decarbonising aviation, shipping and heavy-duty road transport.

Teske and Guerrero [149] introduced the One Earth Climate Model (OECM) 2.0, a MATLAB-based IAM with a high technical resolution on industries (it currently includes 12 different industry sectors) with the additional possibility of analysing the transport sector. Furthermore, the OECM 2.0 allows different temporal resolution, from years to hours, for scenarios with high shares of variable power generation. The required energy services are three: electricity, heat (divided into four levels depending on the temperature), and fuels for other processes. Synthetic fuels and hydrogen are considered both as demands and supply. In the same way, technologies for heat generation are defined by the temperature levels they can supply.

The GEM-E3 model is a global model using partial-equilibrium and has the ability to analyse the decarbonisation paths of HtA sectors. Different examples can be found in literature such as [150] in which authors analyse the rebound effect of energy efficiency measures in the industrial sector and particularly they use as case study the automotive sector and the rebound effects on the I&S industry. Charalampidis et al. [151] adopted the GEM-E3-R extended version of the model with a focus on the transport sector adopting a nested scheme. Fragkos et al. [152] adopted the GEM-E3-FIT version in order to focus on energy-intensive industries in Europe and how European-only policies could affect the global picture. In all scenarios, European GHG reduction is mainly driven by the energy sector followed by the industrial one thanks to energy efficiency, electrification and fuel switching to biomass and green hydrogen. In scenarios where EU is the only region that applies carbon policies the rest of the world increases their emissions because of the industrial relocation with the sectors being most vulnerable being Chemicals, Metals and Non-metallic minerals. It is worth-noting that carbon leakage can also be indirect and connected to relocation in regions that are outside the scope of simulation. This is mirrored by a reduction in domestic EU production driven by a lower international competitiveness caused by unilateral application of carbon pricing. Indeed when EU and China jointly develop decarbonisation policies, carbon leakages are largely reduced to about 6 % over 2025–2050.

In [153], the authors integrate the WILIAM and the EnergyPLAN models to properly consider the variability of RES and thus size storage and flexibility options such as storages and electrolysers. Here, the industrial demand is at first considered to be decarbonised through hydrogen-based e-fuels in EnergyPLAN in order to obtain the first set of results that are then inputted in WILIAM to obtain the final results.

The MESSAGE model is a combination of five models focusing on energy (MESSAGE), land use (GLOBIOM), air pollution and GHG emissions (GAINS), economy (MACRO), and climate model (MAGICC). In terms of HtA sectors, the model is able to analyse both the transportation and industry [154].

The most applied transport decarbonisation strategy includes fuel switching and electrification with a price-elastic demands (through iteration with the MACRO module) due to energy price and climate policy. Constraints on the fuel switching options depend on infrastructure availability and technology (e.g. the electrification of the aviation demand is not enabled). The same approach is also used for international shipping. The decarbonisation of transport in EU is analysed in Ref. [155].

As far as the industry is concerned, this is divided into two demands: specific and thermal. The thermal demand is divided into temperature levels and each level can be supplied by specific energy carriers depending on the technology. The specific demand instead, can be either supplied as electricity or can be supplied as another energy carrier that is then converted to electricity (e.g. fuel cell).

Table 5 summarises the main information on the previously discussed models and their capabilities. It must be noted that other integrated assessment models have the capabilities to analyse HtA and power sectors even though no relevant publications or reports have been found; thus, for the sake of completion the IAM consortium website is suggested for a more detailed analysis [156].

4. Discussion of results

Different models and approaches to including HtA sectors in energy models have been discussed. What is clear is that a detailed industry and transport-sector-specific model necessitates a complex and data-intensive model architecture. Some models tend to include them as exogenous demands and thus tend to apply a scenario-based analysis to study how different paths would impact the energy sector. Other models analyse these sectors in high-technical detail by means of sub-modules or external models that are able to grasp their specific requirements. Nevertheless, the approach of separate modules for different energy sectors is not recommended due to the high level of sector coupling, since the interactions between sectors cannot be fully captured [149] unless an iterative approach is applied. Only the OECM 2.0 model and MESSAGE seem to be able to include HtA sectors without using external modules (even though MESSAGE constitutes of five modules). Table 6 shows an in-depth analysis of different approaches.

Fig. 1 shows a graphical representation of the different approaches to model HtA sectors in energy models for a more immediate understanding.

Another interesting insight on the adopted approaches to model HtA sectors. The following discussions will take for granted the need to somehow cluster the demands. Indeed, it does not seem reasonable to model each single industry and it would be impossible for the transport sector to model each means of transport.

The main approaches can be categorised as follows.

1. Subdivision at macro-level
2. Subdivision on the characteristics of demand
3. Integration of approach 1 and 2

For instance, adapted to the industry sector, it would translate as.

1. Subdivision for industry type (e.g. I&S, P&P, Cement etc.);
2. Subdivision based on temperature of the required services;
3. Subdivision based on industry type and for each industry type the demand is divided based on temperature.

Using the first approach, each industry sector would represent a different bus for which a supply-demand equilibrium constraint would be required. The number of industry types would depend on the specific case study and the importance that each sector has in the analysed economy. By doing this, it is possible to define different technologies that are able to “supply” only certain type of industries in which such solutions are actually feasible. This would enable the modeller the freedom to indicate different costs and efficiencies (and all the

Table 5
Models analysing hard-to-abate sectors: main features, methodologies, sectors coverage and type of integration.

Authors [Ref]	Model name	Methodology		Energy sectors covered			HtA solutions type	HtA sectors integration	
		Simulation	Optimisation	power	industry	transport		embedded	Soft-link
[126,127]	EnergyPLAN	X		X	X	X	Exogenous	X	
[128–130]	GCAM		X	X	X	X	Endogenous	X	
[138]	WEM	X		X	X	X	Exogenous	X	
[140,141]	GEC		X	X	X	X	Endogenous		X
[142,143]	FORECAST		X		X		Endogenous	N.C.	
[144,145], [146]	IndustryPLAN		X		X		Mixed	N.C.	
[148]	TransportPLAN	X				X	Exogenous	N.C.	
[149]	OECM 2.0		X	X	X	X	Endogenous		X
[150–152]	GEM-E3			X	X[a]	X[a]	Endogenous		
[153]	WILIAM-EnergyPLAN		X	X	X	X	Hybrid		X
[154,155]	MESSAGE		X	X	X	X	Endogenous	X	

[a] Different extended versions are available to include different sectors. For instance Ref. [151], focuses on transportation while [152] focused on energy-intensive industries.

Table 6
Critical analysis of different approaches to model hard-to-abate sectors.

Main Approach	Details	Strengths	Weaknesses
Exogenous information for technology (energy vector) usage per sector	Different scenarios are built assuming a different, fixed, usage of certain technologies and energy vectors.	Enables flexibility in building scenarios analysing different pathways. Facilitates the model since the hard-to-abate sectors are only an added demand of energy vector and/or cost. Fast solution and limited computational effort; this also enables to adopt a higher time and technical resolution.	It completely rely on the experience of the modeller in order to build plausible scenarios. It strongly relies on external sources of data.
Endogenous information for technology (energy vector) usage per sector	When analysing the energy sector, the different options for the decarbonisation of hard-to-abate sectors are analysed and selected within the model itself.	The model is able to analyse the interactions between sectors and optimize considering such synergies and sector coupling solutions. External sources are limited to economic and technical data of technologies. Able to analyse competitive technologies.	If optimisation model, the flexibility in scenario is limited to prices and efficiencies. Higher complexity of the model.
Soft-link to external models	Hard-to-abate sectors are analysed (optimised or not) in external tailored models that receives and send information to the main model whose aim is that of analysing the energy system	Freedom to use different, tailored methods and approach to model the different sectors since models are separated. If an iterative process is used, it is possible to grasp synergies and analyse competitive technologies.	Complexity is considered high since different models are needed. Especially, if an iterative approach is modelled

parameters used to describe technologies) per technology per industry type.

With the second approach, each range of temperature would represent a different "bus". In this case, the number of additional buses would depend on the technologies instead of the energy demand. In this case, for each technology it should be specified which thermal levels could be supplied. This approach would not enable different performance and costs in different industries.

By adopting the third approach for each industry type different thermal demand categories would be defined; thus, creating different energy buses for each industry type. This approach is the most complex and time consuming both to model and to solve but it combines the strengths of both approaches.

Those approaches adapted to the transport sector would translate as.

1. Subdivision for the transport type (e.g. maritime, aviation, road freight terrestrial transport)
2. Subdivision based on the distance and/or peak power of the transportation mean
3. Integration of approaches 1 and 2

Subdivision based on the transport type in this case needs a deeper classification since within each category there are different requirements. Indeed, for maritime transportation some solutions (e.g. electrification) are feasible only for short-distance transport while others that are viable and feasible for long-distance travelling might not be a solution for short-distances because of economies of scale. For terrestrial transport this is even more crucial since a classification could be made considering 1) heavy-duty long-distance, 2) heavy-duty short-distance. As it can be noticed, the proposed classification already adopts a subdivision of type 2) based on the distance travelled and thus the needed autonomy, weight, etc. Thus, the authors think that for the transport sector an approach of type 3) is the only feasible one.

As far as flexibility of HtA sectors and sector coupling opportunities, as mentioned in the Introduction, the enabling solutions can be summarised in the strategies of 1) direct electrification and 2) indirect electrification through hydrogen-based solutions. The synergies and interactions between the different solutions and the power sector can be better analysed with endogenous models or through soft-linking with external models as shown in Table 6. Exogenous models can also analyse the impact of sector coupling through scenario analysis, but it might be hard to properly develop such scenarios based on externally produced assumptions. As far as the flexibility that is considered to be available from HtA sectors, this is not considered to be relevant since this are high added-value sectors so their operation should not be based on flexibility but on stability of operation and security of supply. Thus, flexibility can only be offered through storage solutions. In this framework, hydrogen-based solution offer more opportunities thanks to the longer storage time.

Another encountered challenge is due to the unclear development of critical technologies to decarbonise both industry and transport. Indeed, it is possible to include only existing solutions thus neglecting new technologies that might arise in the future. This adds up to further uncertainty connected to the projections of industrial production volumes and potential relocation. Indeed, material demand variation is due to a multitude of factors such as behavioural changes, population and economic growth. Furthermore, it is hard to consider future relocation of industry so global models present an intrinsic advantage to avoid such problem. Otherwise, when analysing specific areas, modellers should either consider different scenarios or make proper assumptions to take into account potential relocation. The same approach should also be taken for energy efficiency measures, future material usage projections and other sustainable solutions to decarbonise the industry and transport sectors; unless this is properly modelled as done by the IndustryPLAN, FORECAST and TransportPLAN models for the industrial and transport sectors, respectively, different scenarios assuming different uptakes of alternative decarbonisation measures should be considered since they might largely impact energy and material consumption.

Models are considered to be the best tool to estimate potential effects of different solutions and to predict indicators to describe the energy system performance. Nevertheless, it must be remembered that models are simplifications of reality and one cannot predict the future but, at best, outputs of energy models can be considered uncertain. Indeed, it is considered crucial to account for uncertainties in energy system planning, particularly in long-term plans [157]. For HtA sectors, given the even higher level of uncertainty, it is considered of utmost importance to include a sensitivity or even an uncertainty analysis. Indeed, it is important to envision the system of solutions that could represent the future energy system and the range in which the outputs could fall since for HtA sectors it is even more unpredictable. Thus, the authors believe that this type of analysis should be embedded in the energy planning process. Furthermore, another line of research would be to investigate the differences that could be encountered when applying a sensitivity

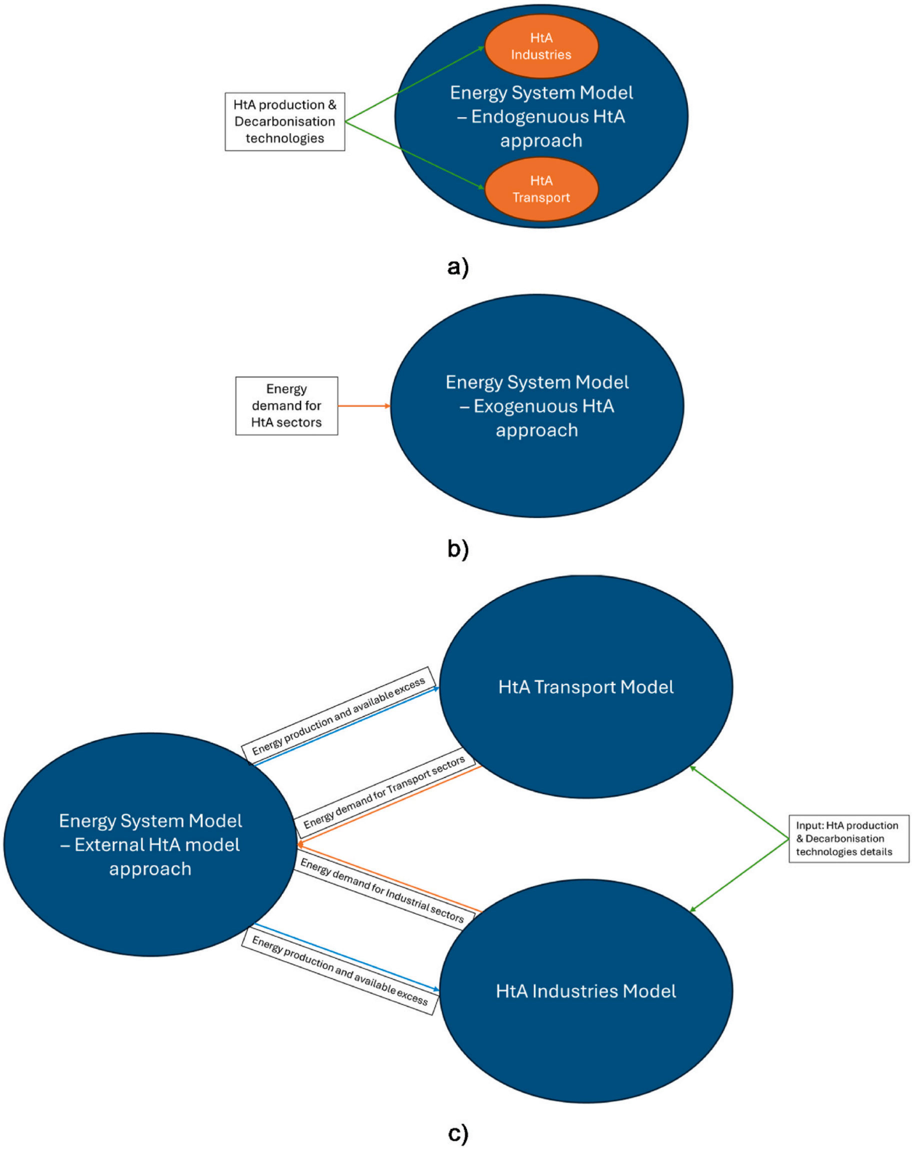

Fig. 1. Graphical representation of the main modelling approaches.

analysis to a model with perfect foresight against one using a rolling-horizon approach. Indeed, rolling-horizon models could represent in a better way the current situation since they can embed within the model the uncertainty of technological development and thus the stall-situation that investors are experiencing.

Even though there is such a high-level of uncertainty in inputs and thus results, the possibility that policymakers and investors could be misled does not seem to be a real possibility.

Another major challenge is the amount of data and information that are needed for an all-around analysis that does include all industries and transportation. This is particularly challenging since some of this information are not available, confidential or very hard to come by. The most used data come either from the IEA database or directly from reports or databases developed by or for sectoral associations. Another source of official data is represented by either local or national plans. Here, an additional challenge presents itself and that is of either selecting National Datasets, with a kind of aggregated top-down approach, or a bottom-up approach based on local data for building the dataset. Indeed, several times national documents are not based on the sum of local data and thus issues of coherence and consistency may arise. Furthermore, EuroStat also represents a valid source of inputs for Europe and European Countries. Otherwise, national specific energy plans might represent another reliable, and official, source when available. To this regard, the "Energy and Industry Geography Lab" [158] represents a very powerful tool to gather some of the needed information but it must be integrated with other data about energy consumption since it only provides information on location, type of industry and specific process-technology adopted as well as the transport infrastructure instead of the energy or feedstock demands or emissions. As regards reliable sources of energy-related data for industry and transport, it must be noticed that EuroSTAT [159] represents a very broad and exhaustive source. Regarding difficulties linked to data gathering and reliability, it is expected that more sources will gradually appear as attention to HtA sectors continues growing and thus more studies and analysis are produced. Nevertheless, funding and effort at Country-level should be increased so as to increase the reliability and precision of data and to boost the development of such databases. Moreover, alternative solutions based on artificial intelligence could prove to be useful for filling data gaps.

5. Conclusions

The research has summarised the most promising technologies to decarbonise the industry and transport sectors focusing on those branches that are considered hard-to-abate showing how most of the identified solutions will require a stronger connection with the power sector and thus require to be included in energy models that aim at analysing complete decarbonisation pathways. Then, different models and approaches to including hard-to-abate sectors in energy models have been found and discussed pinpointing potential strengths and weaknesses of each one of them. Additionally, possible classification and clustering methods have also been proposed so as to support the discussion of the issue as well as future modellers. What is clear, and it is mentioned in many of the analysed studies, is that to develop a detailed industry and/or transport-sector-specific solution requires a highly complex and data-intensive model architecture.

Some models tend to include them as exogenous demands while other analyse these sectors in high-technical detail by means of submodules or even external models that are able to grasp the specific requirements of each sub-sectors. Only the OECM 2.0 model seems to be able to include the hard-to-abate sectors in an energy model without relying on external modules. MESSAGE also seems to offer the same option even though it actually uses five separate but interlinked models internally.

Another major challenge is due to the unclear development of critical technologies to decarbonise both industry and transport that is to some extent a limitation, since many technologies may arise in the future but the absolute potential for implementation remains uncertain and hard, if not impossible, to model today. This adds up to further uncertainty connected to the projections of industrial production volumes and potential relocation and thus transportation, an issue that global models intrinsically avoid. These criticalities suggest that sensitivity or even uncertainty analysis are of utmost importance when hard-to-abate sectors are analysed.

Another major challenge is the amount of data and information that are needed for an all-around analysis that does include all industries and transportation. This is particularly challenging since some of this information are not available, confidential or very hard to come by. Some of the most used sources have been pinpointed.

Future research should thus focus on developing a more holistic approach able to properly model both the energy sector and the hard-to-abate ones to fully grasp the optimal development of different economic sectors that strongly influence each other and that might use the same resources creating a competition between different sectors.

CRediT authorship contribution statement

Daniele Groppi: Conceptualization, Investigation, Writing – original draft. **Lorenzo Mario Pastore:** Conceptualization, Investigation, Writing – original draft. **Benedetto Nastasi:** Conceptualization, Investigation, Writing – original draft. **Matteo Giacomo Prina:** Conceptualization, Investigation, Writing – original draft. **Davide Astiaso Garcia:** Supervision, Writing- Reviewing and Editing. **Livio de Santoli:** Supervision, Writing- Reviewing and Editing.

Declaration of competing interest

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests: *Professor Benedetto Nastasi, author on this paper is a guest editor, he was blinded during the review process and the paper was handled by another editor.*

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Data availability

No data was used for the research described in the article.

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