Breaking the “hard-to-abate” bottleneck in China’s path to carbon neutrality

Xi Yang
Harvard University
Chris Nielsen
Harvard University
Shaojie Song
Harvard University
Michael McElroy (mbm@seas.harvard.edu)
Harvard University https://orcid.org/0000-0002-1354-167X
Xiaoyang Wang
Ministry of Information and Industry Technology, China

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Title

Breaking the "hard-to-abate" bottleneck in China's path to carbon neutrality

Authors

Xi Yang[1]*, Chris P. Nielsen[1], Shaojie Song[1], Michael B. McElroy[1]*, Xiaoyang Wang[2]

Affiliations

[1]Harvard-China Project on Energy, Economy and Environment, John A. Paulson School of Engineering and Applied Sciences, Harvard University, Cambridge, MA, 02138, USA

[2] Ministry of Information and Industry Technology of the People's Republic of China, Beijing, 100804, China

*Corresponding author. Email: mbm@seas.harvard.edu; xiyang@seas.harvard.edu

Abstract

Countries such as China are facing a bottleneck in paths to carbon neutrality: abating emissions in heavy industries and heavy-duty transport. There are few in-depth studies of the prospective role for clean (green/blue) hydrogen in these "hard-to-abate" (HTA) sectors. Are current mitigation technologies in HTA sectors effective? What are the roles for clean hydrogen towards carbon neutrality? We carry out an integrated modeling analysis to answer these questions. Results show that, first, clean hydrogen as both energy carrier and feedstock can significantly reduce heavy industry emissions. Second, clean hydrogen can fuel up to 50% of China's heavy-duty truck and bus fleets by 2060 together with significant shares of shipping. As a side benefit, a realistic hydrogen scenario, reaching 65.7 Mt of production in 2060, could avoid \$1.72 trillion new investment cost compared to a no-hydrogen scenario. This study provides strong evidence for countries facing challenges similar to China in addressing requirements to reduce emissions from their recalcitrant HTA sectors towards carbon neutrality.

Teaser

Decarbonizing hard-to-abate industrial and heavy transport emissions in major developing countries like China is one of the central challenges of climate change.

Title:

Breaking the "hard-to-abate" bottleneck in China's path to carbon neutrality with clean hydrogen

MAIN TEXT

Introduction

Achieving carbon neutrality is an urgent global mission but there is no "one-size-fits-all" pathway for major emitting nations to meet this objective[1,2]. Most developed nations, such as the US and those of Europe, are pursuing decarbonization strategies focused especially on large light-duty vehicles fleets, electric power generation, industrial processes, and commercial and residential buildings, four sectors that together account for vast majorities of their carbon emissions[3,4]. Major developing-country emitters such as China, by contrast, have very different economies and energy structures, requiring different decarbonization priorities not only in sectoral terms but also in strategic deployment of emerging zero-carbon technologies.

Key distinctions in China's carbon emission profile compared to those of western economies are much larger emission shares for heavy industries and much smaller fractions for light-duty vehicles and energy use in buildings (Fig. 1). China ranks first in the world by far in terms of production of cement, iron & steel, chemicals, and building materials, consuming huge amounts of coal for industrial heat and production of coke. Heavy industry contributes 31% of China's current total emissions, a share that is 8% higher than the world average (23%), 17% greater than that of the US (14%) and 13% higher than that of the EU (18%)[5]. The carbon emissions from China's Baowu Iron & Steel Group in 2018 alone equaled half of those for the entire residential & commercial building sectors of both China and the collective 28 nations of the EU[6], equal also to 65% of emissions from China's light-duty vehicles[7].

Unfortunately for China, its carbon emissions profile includes comparatively large contributions from processes regarded as "hard-to-abate" (HTA). HTA processes include those that will be difficult or impossible to electrify and to thus make the transition to renewable power. Such processes include high-temperature heavy industrial production in basic oxygen steelmaking furnaces, cement kilns, and chemical refineries, as well as heavy-duty transport modes such as shipping, long-distance trucking, and aviation. HTA processes include also industrial production that generates non-combustion ("process") emissions of CO_2, notably calcination during cement making and reduction of iron ore in steelmaking.

As of 2021, more than 100 countries have pledged to reach carbon neutrality before 2050[8]. Since HTA processes play lesser roles in the emission profiles of developed western countries, they can advance towards mid-century carbon neutrality by first prioritizing electrification of their larger non-HTA sectors (e.g., light-duty transportation), coupled with transformation of expanded power systems to zero-carbon generation. Capitalizing on technologies that are rapidly maturing, this prioritization can effectively buy time to develop strategies for mitigation of smaller and inherently more challenging HTA emissions in later years.

China's technology pathway to carbon neutrality is more daunting, however; addressing the emission shares of its HTA sectors are too large to postpone. China surprised the world in September 2020, pledging to peak its carbon emissions before 2030 and achieve carbon neutrality before 2060. This climate pledge earned widespread praise, reigniting hopes for global progress towards the goals of the UN Paris Agreement. But it also raised questions about its feasibility[9], in no small part because of the critical roles of HTA processes in China's economy. Actionable and effective low-cost mitigation plans will be needed for all major carbon-emitting processes in China. These plans must consider solutions that diverge from assumptions of analyses of western energy systems that dominate experience and the literature, since both the scale and time pressure for mitigation of China's HTA emissions are so different. And as a result, how to employ emerging technologies, including notably clean hydrogen as introduced in the next section, may also diverge. There are many debates but relatively few robust studies to date on emission mitigation in HTA sectors in China, the likeliest bottleneck for it to achieve a carbon-neutral future.

Rethinking the potential for clean hydrogen with an expanded perspective on demand

In this study we use "clean" hydrogen to encompass both "green" and "blue" hydrogen, the former produced by water electrolysis using renewable power, the latter sourced from fossil fuels but decarbonized with carbon capture combined with either reuse or storage (CCUS). "Grey" hydrogen, produced from fossil fuels without CCUS, is the dominant current source of hydrogen, employed primarily as an industrial feedstock. China is the world's largest producer, accounting for about 22 Mt per year, sourced almost entirely from coal or as a by-product of other fossil-based chemical production processes.

The existing literature on clean hydrogen is focused largely on production technology options, extended in some cases to consider storage and transport, with analyses of supply-side costs[10]. Discussion of demand is focused largely on the transportation sector in developed countries, on hydrogen fuel-cell vehicles in particular[11,12]. These emphases are perhaps unsurprising given the economic and political influence of powerful incumbent industries in developed nations facing escalating decarbonization pressures, the influence of oil and gas companies advocating fossil-based blue hydrogen as a substitute for petroleum transport fuels, and vehicle manufacturers investing in zero-carbon alternatives to battery electric vehicles. There are fewer studies evaluating the potential demands for clean hydrogen in heavy industries, especially in developing countries. Pressures for decarbonization have lagged in these sectors reflecting probably in part the economic and political influence of the relevant industries, in part the fact that the related emissions may have been seen as too hard to abate pending development of new cost-effective low emission options for production. Understanding the potential of clean hydrogen to advance global carbon neutrality, however, will be inherently biased if analyses are limited largely to the costs for its production, its consumption by a single favored sector, and its application primarily in developed economies.

Clean hydrogen has potential roles for decarbonization throughout the energy system and chemical industry, but its cost effectiveness in all imaginable applications is far from clear and must be evaluated. systematically. One expert but informal evaluation ranks the market potentials for many applications of clean hydrogen, concluding for example that its use in fuel cell vehicles is uncompetitive compared with battery powered electric alternatives but that its use in decarbonized shipping and in production of fertilizer, methanol, and steel[13] may be "unavoidable". These latter applications rank prominently among China's HTA sectors.

China is the world's largest producer and consumer of energy-intensive industrial products. Fig. 2 shows the carbon emissions and regional production capacities of key industries in China. Its iron & steel, cement, and chemical industries together emitted 4384 Mt CO_2 in 2019, accounting for

32.1% of total CO_2 emissions[14]. China's steel production in 2020 was 1.05 billion tons (Fig. 2A), accounting for 56.5% of total global production. China has made strong efforts on energy efficiency improvements and fuel substitution, with the carbon intensity of its economy declining 48.1% over the past 14 years[15]. However, there is little conventional mitigation potential left in HTA processes and further reduction of combustion emissions in these sectors is likely to require entirely new forms of energy inputs. Reducing industrial process emissions of CO_2 will require innovative approaches, with hydrogen-based direct reduction of iron in steelmaking a comparatively mature example. In short, there may be opportunities to use clean hydrogen throughout HTA heavy industries, especially in developing economies such as China that are disproportionately dependent on these activities.

Regarding transportation, the increasing cost-competitiveness of light-duty battery electric vehicles suggests that the potential for clean hydrogen to decarbonize this sector may more likely rest in HTA freight modes, especially long-distance trucking and shipping[16,17]. While this is increasingly acknowledged, less recognized is that combustion of zero-carbon fuels derived from clean hydrogen might be as competitive as hydrogen fuel cells in these modes, especially for shipping. And clean hydrogen has potential uses in other sectors, including as a storage medium in the power sector than could enhance system flexibility as the capacity share of variable renewable electricity increases and risks for curtailment grow due to mismatches between electricity supply and demand.

Evaluating opportunities for clean hydrogen depends on reassessing prospective demands for clean hydrogen not in narrow analyses of particular uses in individual sectors but as an alternative fuel and chemical feedstock across the entire economy and energy system, including consideration of differing national circumstances. Here, we build a model for an integrated energy system including both supply and demand across sectors to analyze the prospective cost-effectiveness and role of clean hydrogen in China's entire economy, with emphasis on the underemphasized HTA sectors (Fig. 1C). There is no in-depth study to date on the role of clean hydrogen in China's net zero future. Filling this research gap will help draw a clearer roadmap for China's CO_2 emission reduction and allow evaluation of the feasibility of its 2030 and 2060 decarbonization pledges.

We seek to answer three key questions in the study:

(1) Different from developed countries, what are the key challenges for HTA sectors decarbonization in developing countries such as China? Are current mitigation technologies in HTA sectors (especially for heavy industry) effective enough to achieve net-zero?;

(2) Does China's cost-effective mitigation pathway to carbon neutrality include clean hydrogen? As an important energy carrier and feedstock, what are the roles for clean hydrogen in HTA sectors, especially for countries such as China that have just begun to develop its production and use?;

(3) As a fossil fuel-dominated country, will green hydrogen be cost competitive with other types of hydrogen in China's net zero future? The answers can provide strong support for China's decarbonization pathway but also a good reference for other countries facing similar challenges.

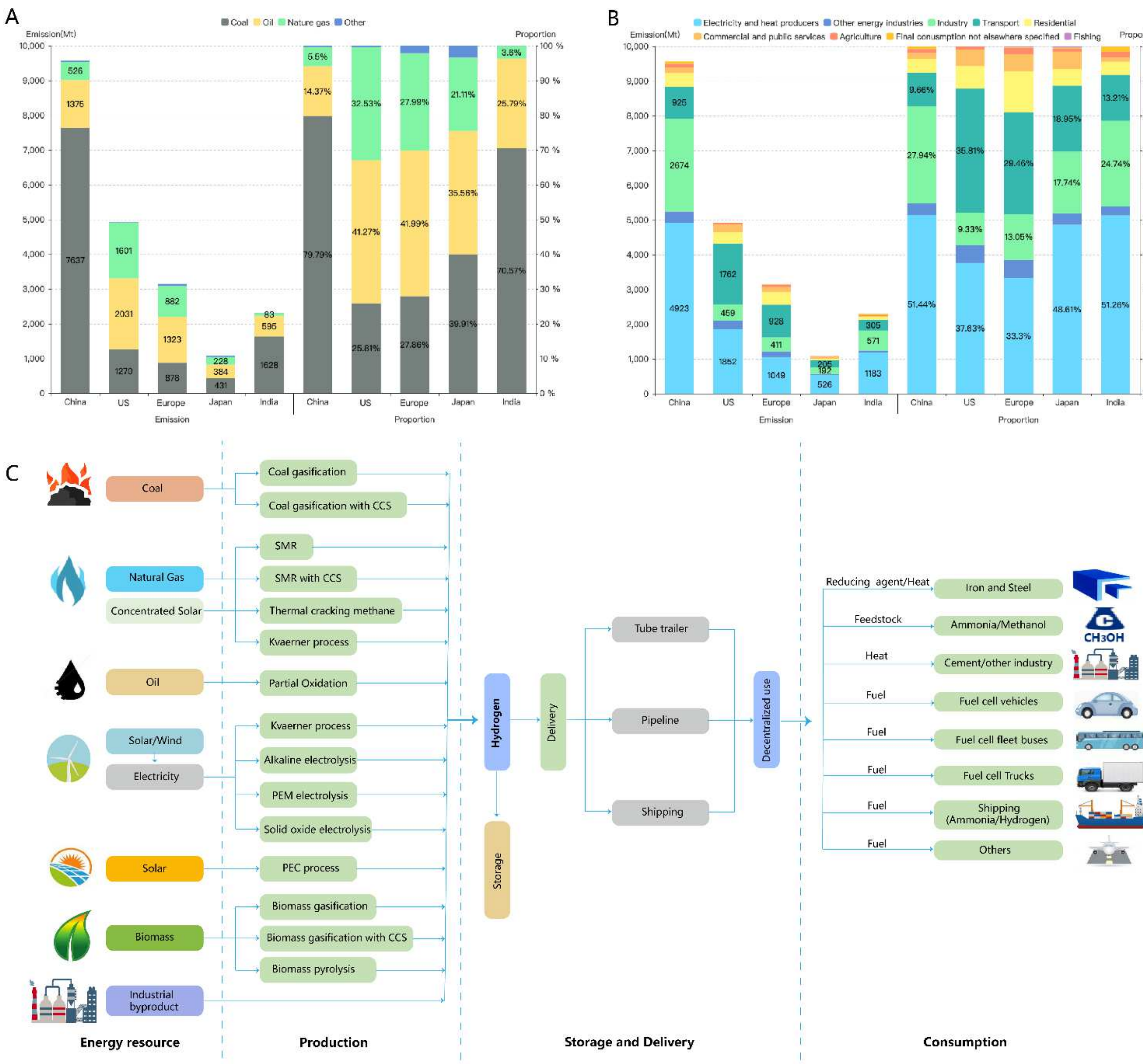


Fig. 1. Carbon emissions of key countries and analytical mechanism for hydrogen in energy system. (**A**) China's carbon emission in 2018 compared to the US, Europe, Japan, and India, by fuels. (**B**) China's carbon emission in 2018 compared to the US, Europe, Japan, and India, by sectors. (**C**) Technical pathway with hydrogen technologies applied in the HTA sectors.

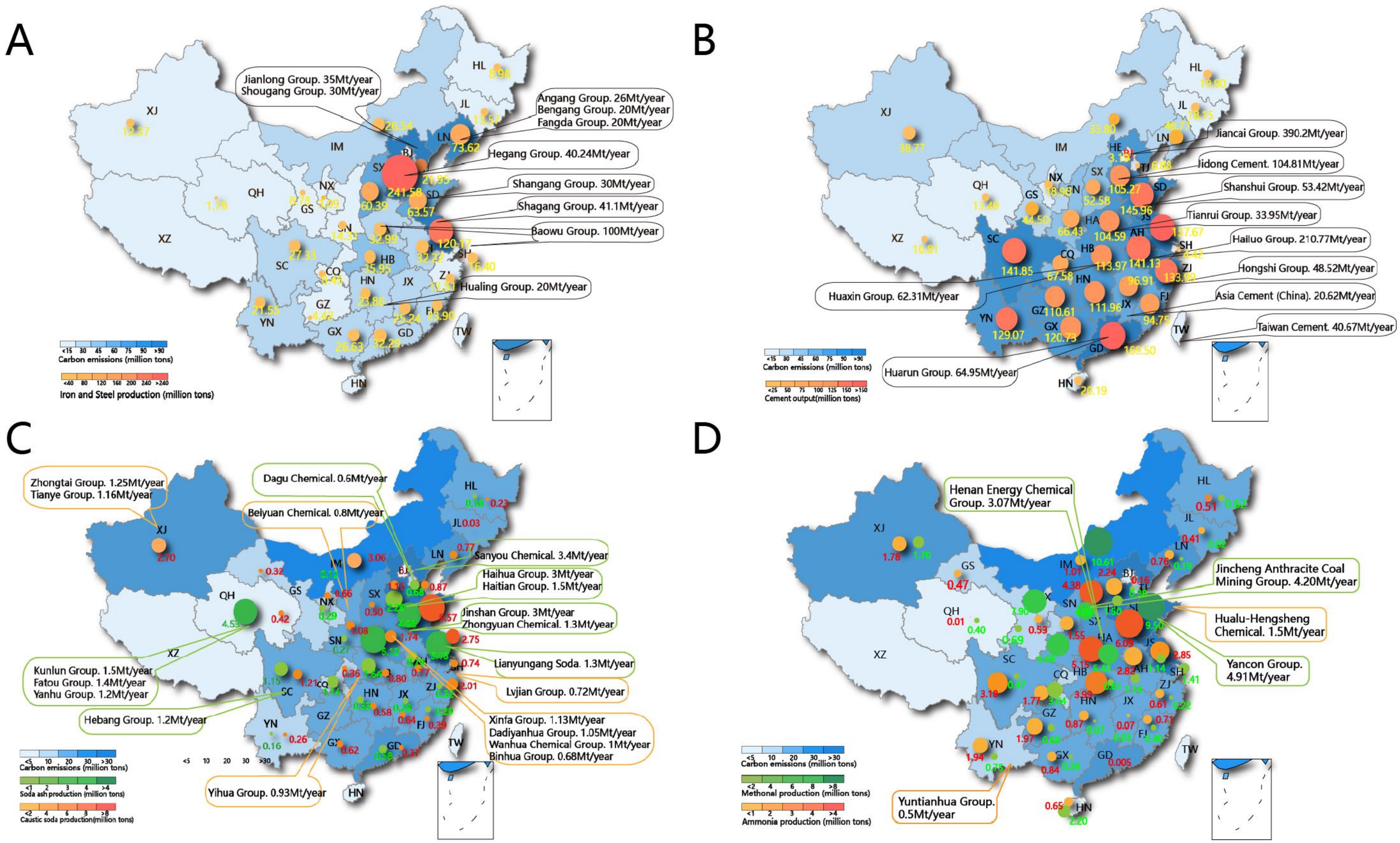


Fig. 2. Production and carbon emissions of key industries in China by region in 2019. (**A**) Iron & steel, (**B**) cement, (**C**) ammonia and methanol, (**D**) soda and caustic soda.

Results

Mitigation opportunities in China's HTA industrial sector

We carry out an integrated optimization analysis of mitigation pathways to carbon neutrality for China in 2060. HTA sectors in this study include industrial production of cement, iron & steel, and key chemicals (including ammonia, soda, and caustic soda); and heavy-duty transport including trucking, domestic shipping and aviation. We develop a technology-rich model to analyze HTA mitigation technologies with and without clean hydrogen applications (see methodology and SI). Besides hydrogen-based technologies, the additional zero-carbon technology of CCUS and the negative-carbon option of bioenergy with carbon capture and storage (BECCS) are also considered. Four scenarios are designed: BAU (business-as-usual), NDC (China's Nationally Determined Contributions under the Paris Agreement), ZERO-NH (net-zero emissions without hydrogen applications) and ZERO-H (net-zero emission with clean hydrogen). Detailed description of the scenarios is given in Table 1.

Table 1. Scenario design (2020-2060)

Scenario	Brief summary	CO_2 levels	Clean H_2?	HTA sector constraints	Mitigation policies/technologies in HTA sectors
BAU	Business as usual	No limits	No	No constraints	No mitigation policy
NDC	Achievement of China's NDC targets around 2030	CO_2 emission peak around 2030, with no further carbon emission constraint after 2030; carbon intensity reduced by 60-65% in 2030 compared to 2005.	No	No constraints for sectoral emissions	NDC targets (at least 20% non-fossil energy supply) HTA: Efficiency improvement measures; combustion fuel replacement; CCUS.
ZERO-NH	Achievement of net-zero before 2060	CO_2 emission peak before 2030 and net-zero before 2060	No	All sectors achieve net-zero in 2060	HTA: Best available efficiency improvement technologies; combustion fuel replacement, CCUS, BECCS.
ZERO-H	Achievement of net-zero before 2060	The same as ZERO-NH	Yes	All sectors achieve net-zero in 2060	HTA: all measures in ZERO-NH plus Hydrogen-DRI process in iron & steel, hydrogen fuel cells in trucking, shipping and aviation; hydrogen-based heat supply.

As noted above, measures to improve energy efficiency and substitute fuels have contributed a great deal to achieving mitigation targets of China's NDCs under the Paris Agreement, including in the HTA sectors. At this point, however, there is less conventional mitigation potential left to be realized, and China has now raised its ambitions since Paris to achievement of full carbon neutrality by 2060. Based on our model simulations, further CO_2 reduction from improved energy efficiency and fuel switching in key sectors can only remove 10-24% of the total industry carbon emissions by 2060. Major HTA sectors, currently accounting for 30% of the world's and 42% of China's annual CO_2 emissions, pose the largest mitigation challenge to China's carbon neutral future.

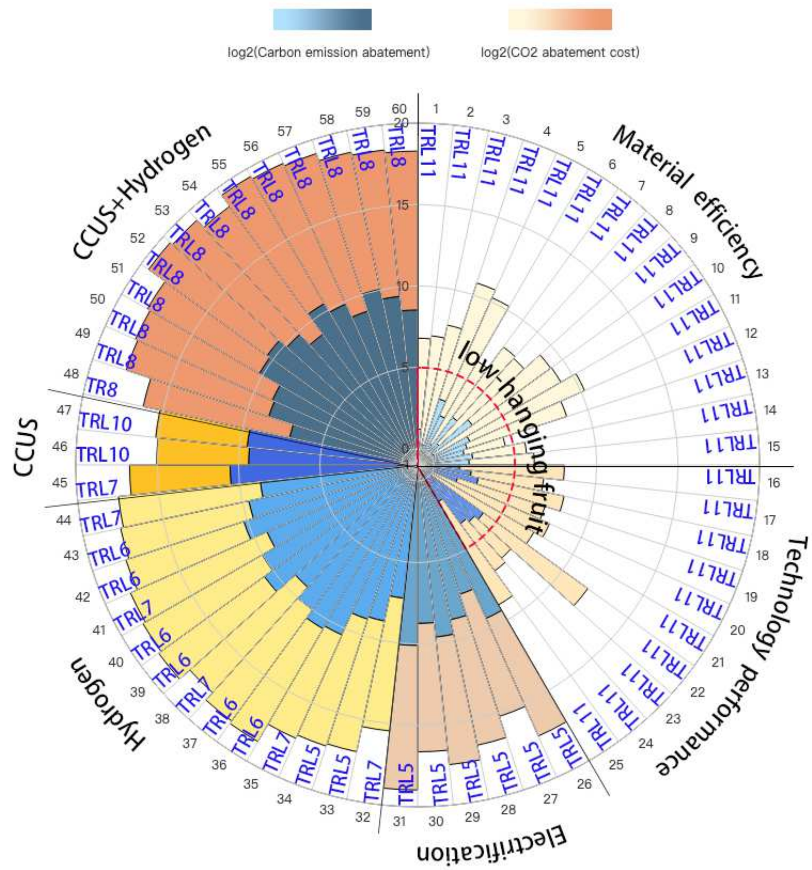
China's current primary hot metal (HM) steel production process is the long process, which includes coking, sintering, pelletizing, operation of a basic oxygen blast furnace (BF-BOF), and conversion. The key input materials are coke, iron ore, quicklime, scrap steel and fluorite (CaF_2). In this process, for every ton of HM steel production, an average of 2.2 kg of CO_2 is emitted[18]. Another method to produce primary HM steel is the direct reduced iron-electric arc furnace (DRI-EAF) route. DRI-EAF mainly uses natural gas to generate reducing agents such as carbon monoxide and hydrogen, with emissions of 1.4 tCO_2/t HM steel. A fully scrap-based EAF production route emits only 0.3 tCO_2 per ton of steel HM production, but comprises only a tiny albeit growing share of total production and is limited by scrap availability. The DRI-EAF process comprised 10.4% of total production in China in 2019, which is 17.5% less than the world average share and 59.3% less than that for the US[18]. The dominant share of existing production in China is by the BF-BOF process (89.6%), a key challenge for deep decarbonization of its iron & steel industry.

We analyzed 60 key steelmaking emission mitigation technologies in the model and classified them into 6 categories (fig 3A): improvement of material efficiency, advanced technology performance, electrification, CCUS, green hydrogen, and blue hydrogen. Material efficiency improvements mainly include coking coal efficiency, recycling of raw materials and reuse of waste heat (Table S1).

In the NDC and ZERO-NH scenarios, hydrogen-based technologies are not included. In the NDC scenario, current mitigation technologies focused on material efficiency and technology performance are sufficient to reduce steelmaking emissions by 15-20% by 2030 compared to the 2020 level, with CCUS contributing another 10-13% reduction. Note that in the NDC scenario, low-carbon power generation is the main source of decarbonization. However, to achieve near-zero emissions in HTA sectors in the ZERO-NH scenario, the emission reductions of the NDC scenario are far from sufficient. Considering emission reduction potentials and costs, the reduction effect of current technologies is insignificant and cannot drive the iron & steel sector towards net-zero emissions. We assume 100% market penetration in 2050 for the best available technologies (BATs) in the ZERO-NH scenario, and find that it reduces CO_2 by only 20.8-24.3% (without CCUS). China cannot rely only on conventional technologies, especially energy efficiency improvements (Fig. 3A), to achieve carbon neutrality in the HTA iron & steel sector. Innovative technologies with high mitigation potentials will need to be developed and applied.

With hydrogen technologies introduced in the ZERO-H scenario, hydrogen-DRI processes in steelmaking will promote significant carbon reduction. Hydrogen can be used as an auxiliary reducing agent in the BF-BOF process and 100% in the hydrogen-DRI route. The 100% hydrogen-DRI process can reduce up to 98% of CO_2 compared to BF-BOF. Hydrogen-DRI units have been built but not yet at commercial scale, so the mitigation potential and abatement costs are taken from the standard routes in the pilot HYBRIT[1] and GrInHy2.0[2] projects. The current production cost of hydrogen-based reduced iron is 40-47% higher than that of for conventional steelmaking. However, with an anticipated continuous decline in hydrogen cost, hydrogen-DRI will become cost-effective in China's steelmaking market after 2045. In the ZERO-H scenario with system cost optimization, the share of BF-BOF would be reduced to 34%, with 45% EAF and 21% hydrogen-DRI. In the ZERO-H scenario, hydrogen would provide 29% of total final energy demand in the iron & steel sector (Fig. 4). As the grid price for solar and wind power declines to 38-40 $/MWh in 2050[19], the 100% hydrogen-DRI route will play a more important role than widely assumed.

[1] HYBRIT project is a hydrogen-DRI project developed by Swedish Steel AB(SSAB), Luossavaara-Kiirunavaara AB (LKAB) and Vattenfall. https://www.hybritdevelopment.se/en/.
[2] GrInHy2.0 project is a hydrogen-DRI project developed by Salzgitter AG. https://salcos.salzgitter-ag.com/en/index.html.



1—Coke dry quenching device of high temperature and high pressure
2—Sintering waste heat power generation technology in the iron and steel industry
3—Dry recovery technology of converter gas
4—Moisture Control and Air Separation Technology for Coking Coal
5—Waste heat utilization technology of flue gas in mineral furnace
6—Unsteady waste heat recovery and saturated steam power generation technology
7—High-temperature flue gas dry purification and recycling technology of fully enclosed submerged arc furnace
8—Sintering waste heat recycling technology
9—Recovery and utilization of sensible heat of coke oven waste gas
10—Regenerative combustion technology: Regenerative rotary hearth furnace treatment of metallurgical dust and recovery of iron and zinc technology
11—Energy saving technology of rotary cutting type high air temperature top burning hot blast stove
12—New energy-saving technology of high thermal conductivity and high density silica bricks for large coke ovens
13—Integral optimization of cold ramming and paste forming furnace energy saving technology
14—High-emissivity coating technology
15—Energy-saving technology of heat storage combustion without induced draft fan and directional valve
16—Screw expansion power drive energy-saving technology
17—Application technology of coaxial unit for energy recovery of metallurgical waste heat and pressure
18—Recovering waste heat by direct heat exchange with blast furnace slagging water
19—Blast furnace blast dehumidification and energy-saving technology
20—Liquid sealing technology of annular cooler
21—Technology of waste gas recovery and pressure automatic regulation in coke oven carbonization chamber
22—Intelligent energy-saving technology for large-scale blast furnace based on optimization of gas volume index
23—Energy management and control technology in the iron and steel industry
24—Energy Saving Technology of Blackbody Enhanced Radiation in Heating Furnace
25—Intermediate and low temperature solar energy industrial thermal application system technology
26—BF-BOF(H2+Zero-C elec)
27—BF-BOF(Zero-C elec)
28—EAF-scrap(Zero-C elec)
29—DRI-coal(Zero-C elec)
30—DRI-gas(Zero-C elec)
31—DRI-gas (H2+Zero-C elec)
32— DRI-NG H2: Green H2-30% injection
33—DRI-NG H2: Green H2-90% injection
34—DRI-NG H2: Green H2-100% injection
35—Hydrogen as auxiliary reduction (BF-BOF)-Hydrogen green
36—HYBRIT- carbon abatement 1575kg/ton-large scale 60Mt/yr-hydrogen green
37— HYBRIT- carbon abatement 1575kg/ton-Middle scale 23Mt/yr-hydrogen green
38—HYBRIT- carbon abatement 1575kg/ton-Small scale 7Mt/yr-hydrogen green
39—GrlnHy2.0- carbon abatement 1600kg/ton-large scale 60Mt/yr-hydrogen green
40—GrlnHy2.0- carbon abatement 1600kg/ton-Middle scale 23Mt/yr-hydrogen green
41—GrlnHy2.0- carbon abatement 1600kg/ton-Small scale 7Mt/yr-hydrogen green
42—GrlnHy2.0- carbon abatement 1200kg/ton-large scale 60Mt/yr-hydrogen green
43—GrlnHy2.0- carbon abatement 1200kg/ton-Middle scale 23Mt/yr-hydrogen green
44—GrlnHy2.0- carbon abatement 1200kg/ton-Small scale 7Mt/yr-hydrogen green
45—SR-BOF with CCUS
46—DRI-gas(CCS)
47—DRI-coal(CCS)
48—DRI-NG H2: Blue H2(SMR+89%CCS)-30% injection
49—DRI-NG H2: Blue H2(SMR+89%CCS)-90% injection
50—DRI-NG H2: Blue H2(SMR+89%CCS)-100% injection
51—Hydrogen as auxiliary reduction(BF-BOF)-hydrogen blue: SMR89%
52—HYBRIT- carbon abatement 1575kg/ton-large scale 60Mt/yr-hydrogen blue: SMR89% CCUS
53—HYBRIT- carbon abatement 1575kg/ton-Middle scale 23Mt/yr-hydrogen blue: SMR89% CCUS
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55—GrlnHy2.0- carbon abatement 1600kg/ton-large scale 60Mt/yr-hydrogen blue: SMR89% CCUS
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60—GrlnHy2.0- carbon abatement 1200kg/ton-small scale 7Mt/yrhydrogen blue: SMR89% CCUS

TRL5—Large prototype
TRL6—Full prototype at scale
TRL7—Pre-commercial demonstration
TRL8—Demonstration
TRL10—Early adoption
TRL11—Mature

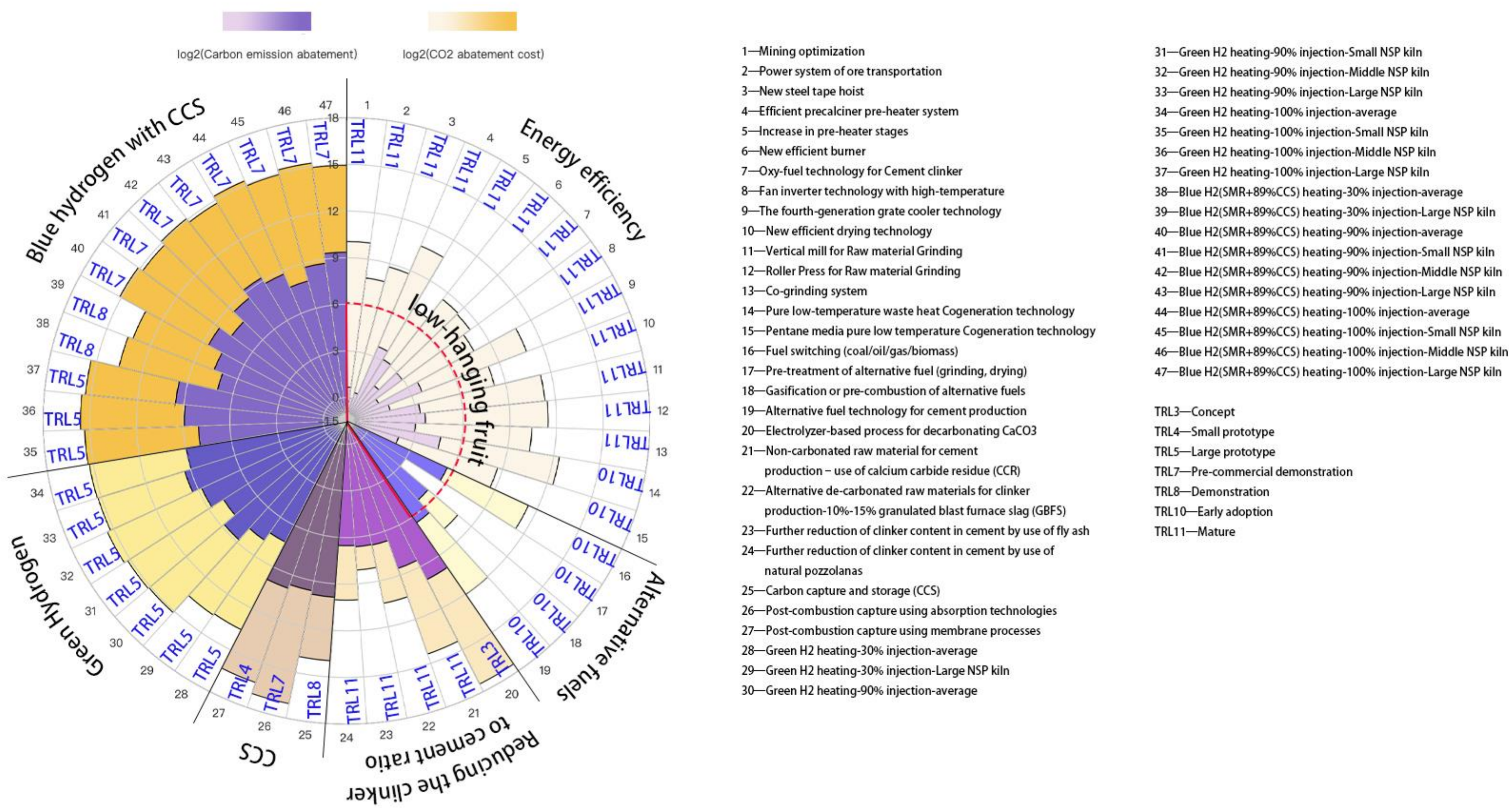


Fig. 3. Carbon mitigation potential and abatement costs of key mitigation technologies. (**A**) 6 categories of 60 key steelmaking emission mitigation technologies, (**B**) 6 categories of 47 key cement emission mitigation technologies.

Regarding cement production, we consider both shaft kiln and new dry processes in this study. New dry cement production refers mainly to application of advanced new suspension pre-heaters and pre-calciners (NSP). China's cement making consists of quarrying, grinding and homogenization of raw materials, pre-heating, kiln processes, clinker grinding, and cement blending and packaging. We analyzed in the model 55 key mitigation technologies across the production processes and classified them into 6 categories: energy efficiency, alternative fuels, reducing the clinker-to-cement ratio, CCUS, green hydrogen, and blue hydrogen (Fig. 3B). The technology set includes highly innovative proposed technologies, e.g., an electrolyzer-based process for decarbonizing $CaCO_3$, producing hydrogen (and other gas streams) that can be used to generate electricity or combusted in the kiln (Fig. 3B, technology 20)[20]. The process has a powerful mitigation potential of 979 kg CO_2/ton but with high mitigation cost. Detailed description of the mitigation technologies is in Table S2.

Results show that improved energy efficiency technologies can only reduce 8-10% of the total CO_2 emissions in the cement sector, and waste-heat cogeneration and oxy-fuel technologies will have limited mitigation effect (4-8%). CCUS can significantly reduce both the process- and combustion-related emissions, but with relatively high costs per ton of CO_2 reduction. Technologies to reduce the clinker-to-cement ratio can yield relatively high carbon mitigation (50-70%), mainly including decarbonized raw materials for clinker production using granulated blast furnace slag (GBFS), although critics question if the resulting cement will retain its essential qualities. But current results indicate that utilization of hydrogen together with CCUS could help the cement sector achieve near-zero CO_2 emissions in 2060. This again suggests limited remaining decarbonization benefits of conventional energy efficiency improvements and material switching.

In the ZERO-H scenario, 20 hydrogen technologies out of 47 mitigation technologies come into play. Note that a key technology, hydrogen injection firing as a heating source, is only in a pilot stage in China and its abatement potential is based only on consultations with experts from the cement industry. In the ZERO-NH scenario, by comparison, CCUS is the only method for large CO_2 emission reductions. We find that the average carbon abatement cost of hydrogen-based technologies is lower than typical CCUS and fuel-switching technologies (Fig. 3B). Furthermore, green hydrogen is expected to be cheaper than blue hydrogen after 2030, at around \$0.7-\$1.6/kg H_2[16]. Therefore, green hydrogen applications can bring significant CO_2 reductions in the provision of industrial heat and help reduce the need for CCUS investments projected in the ZERO-NH scenario. In the ZERO-H scenario, the penetration of hydrogen mainly plays an important role in kiln firing, where its carbon mitigation potential is competitive with CCUS. Current results show that it can reduce 89-95% of the CO_2 in the heating process in China's cement industry (Fig. 3B, technology 28-47), which is consistent with the Hydrogen Council's estimate of 84-92%[21].

We also simulate use of hydrogen as a feedstock in production of ammonia (NH_3), methane (CH_4), methanol (CH_3OH), and other chemicals listed in the model description. Ammonia production routes can be divided into two stages, hydrogen production and an electrochemical process. Gaseous hydrogen and nitrogen are introduced into the electrochemical system, with H_2 converted into protons at the anode and transferred electrochemically to the cathode. They react with N_2 to obtain ammonia, involving both Haber-Bosch and solid-state synthesis processes. In the model, the average hydrogen consumption as feedstock is 178.18-182.44 kgH_2/ton of ammonia. In addition, hydrogen can be an important source of combustion heat to replace that based on fossil fuels. In the ZERO-H scenario, gas-based ammonia production with hydrogen heat will gain a 20% share of total production in 2060 (Fig. 4). The model includes four kinds of methanol production technologies: coal to methanol (CTM), coke gas to methanol (CGTM), natural gas to methanol (NTM), and CGTM/NTM with hydrogen heat. Five sub-stages including air separation, coal milling and drying, syngas production, methanol synthesis and onsite power generation are described for each type of technology. In our model, the average hydrogen consumption as feedstock is 125.12-126.45 kgH_2/ton ammonia. In the ZERO-H scenario, CGTM/NTM with hydrogen heat can achieve a 21% production share in 2060 (Fig. 4). Chemicals are also potential energy carriers of hydrogen. Methane and ammonia are easier to transport and store than gaseous or liquid hydrogen, and their use can potentially take advantage of existing natural gas and chemical transport and storage infrastructure. Based on our integrated analysis, hydrogen can comprise 17% of final energy consumption for heat provision in the chemical industry by 2060. Along with bioenergy (18%) and electricity (32%), hydrogen has a major role to play in decarbonization of China's HTA chemical industry (Fig 5A).

Mitigation opportunities in the HTA transport sector

Based on the modeling results, hydrogen has large potential to decarbonize China's transport sector, although it will take time. According to the International Energy Agency (IEA), currently only 0.01% of produced pure hydrogen is used by fuel-cell electric vehicles[16]. Note that China's transport sector emitted 925 Mt CO_2 in 2018, of which heavy-duty modes emitted 601 Mt, or 65%[22]. In other countries, heavy-duty modes are responsible for smaller shares of total transport emissions: 38% in the US, 52% in the EU, 49% in Japan, and 51% in India[23]. With transportation demands in developing countries such as China accelerating due to swift urbanization and economic growth, decarbonizing heavy-duty transport is a growing challenge which like HTA industries will require innovative abatement measures. Clean hydrogen provides a number of prospective options, for use in fuel cells but also potentially as a feedstock for low- or non-carbon combustion fuels.

Our model suggests that hydrogen can gain large market penetration in China's transport sector chiefly in HTA heavy-duty modes. In addition to light-duty vehicles (LDVs), other transport modes analyzed in the model include fleet buses, trucks (light/small/medium/heavy), domestic shipping, railways and aviation, covering most transportation in China. For LDVs, electric vehicles look to remain cost competitive in the future. In the ZERO-H scenario, hydrogen fuel cell penetration of the LDV market will reach only 5% in 2060 (Fig. 4). For fleet buses, however, hydrogen fuel cell buses will be more cost competitive than electric alternatives in 2045 and comprise 61% of the total fleet in 2060 in the ZERO-H scenario, with the remainder electric (Fig. 4). As for trucks, the results vary by load rate. Light-duty trucks (LDTs) in China are currently fueled by gasoline, CNG and ethanol. Electric LDTs will comprise more than half of the total LDT fleet by 2035 in the ZERO-NH scenario. But in the ZERO-H scenario, hydrogen fuel cell LDTs will be more competitive than electric LDTs by 2035 and comprise 53% of the market by 2060. Regarding heavy-duty trucks (HDTs), hydrogen fuel cell HDTs would reach 66% of the market in 2060 in the ZERO-H scenario. Diesel/bio-diesel/CNG HDVs will quit the market after 2050 in both ZERO-NH and ZERO-H scenarios (Fig. 4). Details about the results in Fig. 4 are shown in Table S3, illustrating further the advantages and higher penetration of hydrogen vehicles in the truck market. Hydrogen consumption of trucks per 100 km ranges in our model from 1.12 kg (equivalent to 4.23 L gasoline) to 10.8 kg according to the load rate, showing the promise for long-distance freight transport. Hydrogen fuel cell vehicles have an additional advantage over electric vehicles in their better performance in cold conditions, important in wintertime in northern and western China.

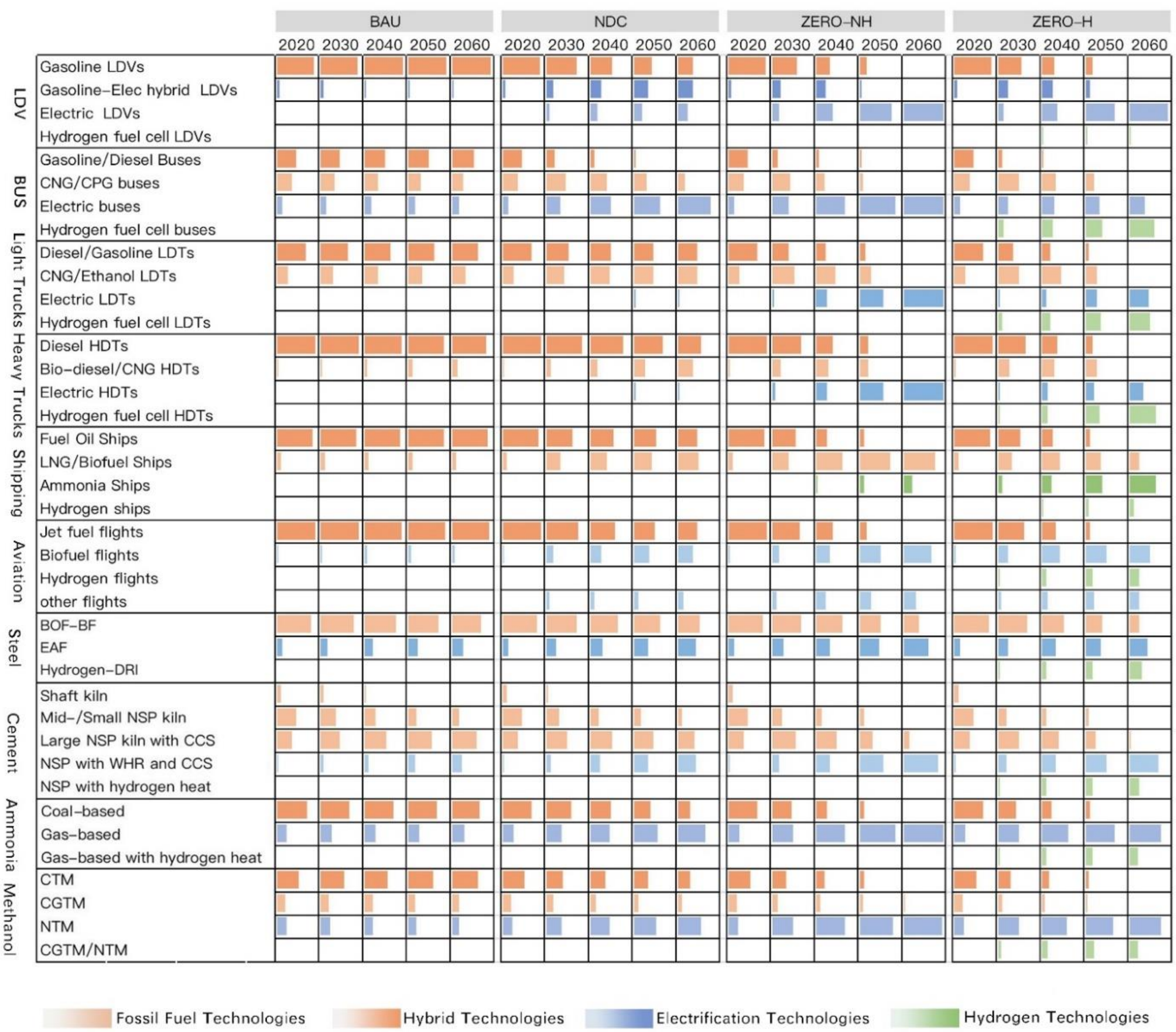


Fig. 4. Technology penetration in typical HTA sectors in BAU, NDC, ZERO-NH, and ZERO-H scenario (2020-2060).

Beyond road transport, the model shows widespread adoption of hydrogen technologies in shipping and aviation in the ZERO-H scenario. China's domestic shipping is very energy-intensive and an especially difficult decarbonization challenge. Ships burning fuel oil have a 90% share in 2020, with the remainder powered by LNG and/or biofuel (Fig. 4). Clean hydrogen, especially as a feedstock for ammonia, provides an option for shipping decarbonization. The model results show that shipping can approach carbon neutrality by 2060 in the ZERO-NH scenario, with ships electrified with rechargeable batteries. A lower-cost solution is represented in the ZERO-H scenario: 65% penetration of ammonia-fueled and 12% hydrogen-fueled ships in 2060 (Fig. 4). In the ZERO-H scenario, hydrogen will account for an average of 56% of final energy consumption of the entire transport sector in 2060.

Besides the key applications of hydrogen in HTA industries and heavy-duty transport, we also modeled hydrogen use in residential heating and energy storage. North China has huge heat demands in winter. In the 2017-2018 winter, policies to encourage "coal-to-gas" and "coal-to-electricity" transitions in residential heating were vigorously promoted in 28 cities of north China (the so-called "26+2" program), to achieve both carbon mitigation and air quality targets. In the carbon neutral future, however, there will be neither coal nor gas in residential heating. The ZERO-NH scenario results in a very high share of electrification (97%). However, dramatic expansion of electrified heating demand will create major pressures for the national grid in the winter, putting the heating system at risk due to unanticipated power outages. A larger share of hydrogen-fueled heating could help to reduce this risk. In the ZERO-H scenario, electricity will still account for the largest proportion (72%) of the final energy demand for residential heating in 2060, but with a notable share of hydrogen-based heating (25%).

Clean hydrogen production in China

In this study, multiple hydrogen production technologies are considered (Table 2), including both hydrogen production from fossil fuels and electrolysis of water. The hydrogen production from fossil fuels includes coal or biomass gasification and natural gas reforming, with and without CCUS. Steam reforming of methane accounts for the largest proportion of this production, mainly because of its low investment cost and high efficiency (up to 76%)[24]. Gasification of coal to produce hydrogen, also common in China, has lower efficiency (55%) and higher cost

(2,670$/kW). For the electrolytic production of (green) hydrogen from water, three kinds of electrolyzers are analyzed in the model: alkaline electrolysis cells (AEC), solid oxide electrolysis cells (SOEC) and proton exchange membrane electrolyis cells (PEMEC). The current efficiency of AEC is up to 61% and SOEC reaches 68%, both expected to be further improved in the long term. With carbon emission constraints in the model, water electrolysis has obvious advantages. Compared to fossil-fuel based hydrogen production without CCUS (grey hydrogen), around 1,517 Mt CO_2 could be saved in 2060 using electrolysis powered by renewables (green hydrogen). About 262 Mt CO_2 could be reduced using green hydrogen compared to blue hydrogen in 2060, due to the electricity consumed in CCUS required for the latter. When taking account of the curtailment of wind and solar power, the cost of green hydrogen may be further reduced with higher renewable penetration. China's national wind power curtailment rate reached as high as 21% in 2016[25], and while curtailment rates have declined since then, investment in renewable power has been affected. Our previous study indicated that the levelized cost of hydrogen (LCOH) could drop to as low as 0.5 $/kg in Western Inner Mongolia, using otherwise-curtailed wind power in the region[26]. AEC and SOEC are identified as the most cost-effective electrolyzer technologies in 2020 and 2030, respectively. We consider transportation of hydrogen mainly by trailer trucks, with efficiencies of 75%-85% and average delivered costs around 0.65-1.73 $/kg H_2 (gas) and 3.87-6.70 $/kg H_2 (liquid)[16]. To simplify the analysis, all hydrogen storage is assumed to occur in tanks, with an average cost of 0.4-0.5 $/kg[27].

In addition to production from water electrolysis and fossil fuels, hydrogen is also produced as an industrial by-product, an important further source of hydrogen supply in China. By-product hydrogen comes largely from steam cracking (mainly ethane and naphtha), chlor-alkali processes, and other processes such as styrene production. Globally, about 30 Mt of hydrogen is produced each year as by-product[17]. In this study, each ton of steel production in China also produces 187.3 m^3 of hydrogen by-product. Similarly, each ton of caustic soda produces 146.5 m^3 of hydrogen. China's total industrial by-product hydrogen reached 6.6 Mt in 2020, accounting for 30% of its hydrogen supply, with a notably low production cost[23]. The key hydrogen production modes up to 2060 are shown in Fig. 5B. In the ZERO-H scenario, results show that hydrogen by-product will increase from 0.78 Mt in 2030 to 14.50 Mt in 2060. However, the by-product hydrogen will retain the same production share in 2060 as in 2020 (32%), as grey hydrogen is replaced with increasing commercialization of green hydrogen as the main supply. Blue hydrogen from coal or methane gasification with CCUS (large scale, centralized) dominates hydrogen production until 2040 in ZERO-H. Green hydrogen will significantly grow after 2030 with increasing cost-effectiveness, especially for SOEC-based production. In this scenario, hydrogen production from SOEC and PEMEC (large size, centralized) will increase to 19.36Mt and 18.10Mt in 2060 (Fig. 5B), comprising more than half of the total hydrogen production (56.9%).

Table 2 Hydrogen production technologies and costs

Technology description	Efficiency (LHV) [%]				Investment cost [$/kW]				Fixed O&M [$/kW]				Lifetime
	2015	2020	2030	2050	2015	2020	2030	2050	2015	2020	2030	2050	Years
AEC electrolysis, centralized	61.2%	63.6%	65.9%	69.2%	1281.86	718.8	658.9	599	64.09	35.94	32.95	29.95	25
PEMEC electrolysis, centralized	54%	58%	62%	67%	2276.2	1317.8	718.8	479.2	113.81	65.89	35.94	23.96	15
SOEC electrolysis, centralized	68%	76%	79%	79%	4552.4	2635.6	718.8	479.2	227.62	79.07	21.56	14.38	20
Biomass gasification, medium-large scale, centralized	56%	60%	63%	70%	3168	2497	1550	997	158.3	124.6	77.5	49.7	20
Coal gasification, medium size, centralized	55%	60%	60%	60%	689	689	689	689	17.2	17.2	17.2	17.2	25
Coal gasification, large size, centralized	40%	45%	50%	55%	556	507	422	271	33.0	30.4	26.9	16.3	25
Coal gasification + CCUS, medium scale, centralized	55%	58%	58%	58%	794	794	794	794	33.0	33.0	33.0	33.0	25
Coal gasification + CCUS, large scale, centralized	40%	43%	48%	48%	686	590	436	281	49.3	41.3	27.3	19.6	25
Natural gas reforming, small size, centralized	76%	76%	76%	76%	519	481	414	266	19.7	19.2	15.3	10.6	25
Natural gas reforming, large size, centralized	62%	66%	66%	66%	242	223	190	122	11.8	11.2	9.2	6.1	25
Natural gas reforming + CCUS, small size, centralized	69%	69%	69%	69%	709	648	541	348	35.5	32.4	28.6	17.4	25
Natural gas reforming + CCUS, large size, centralized	57%	57%	57%	57%	342	300	230	148	17.1	15.0	13.8	7.4	25

Data source: IRENA report et al. [28-31]

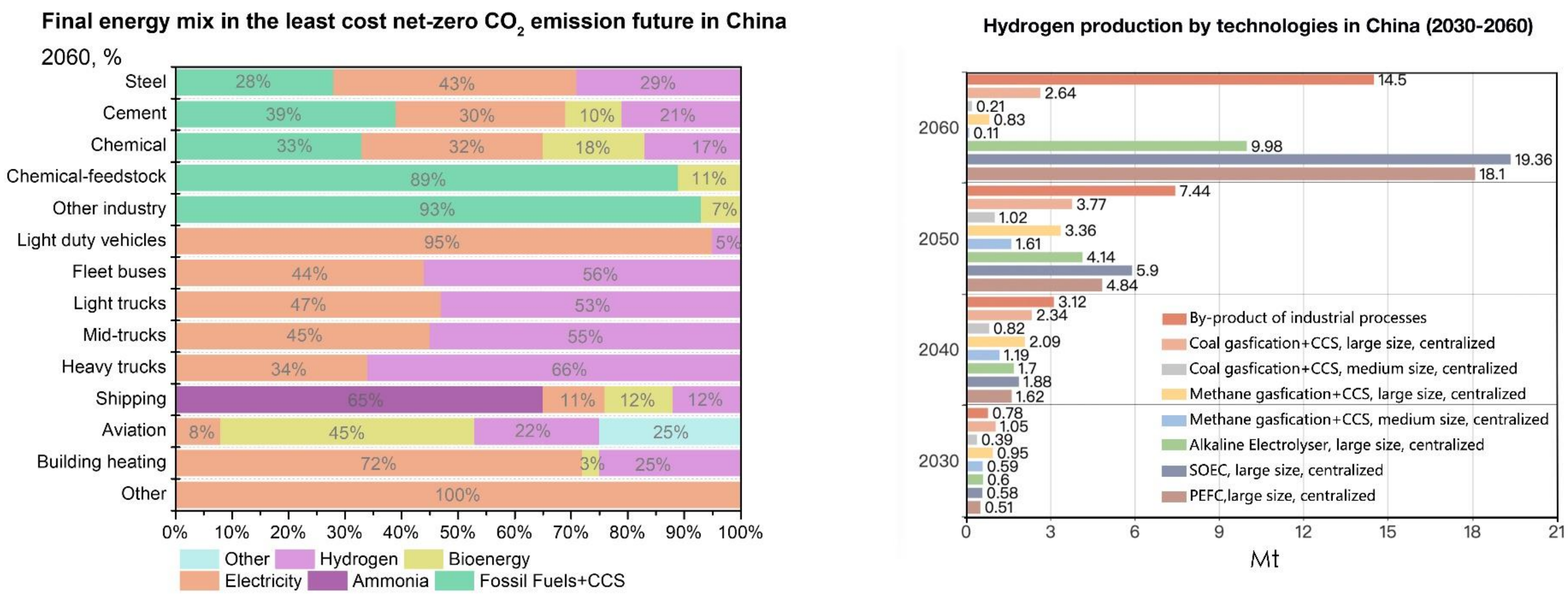
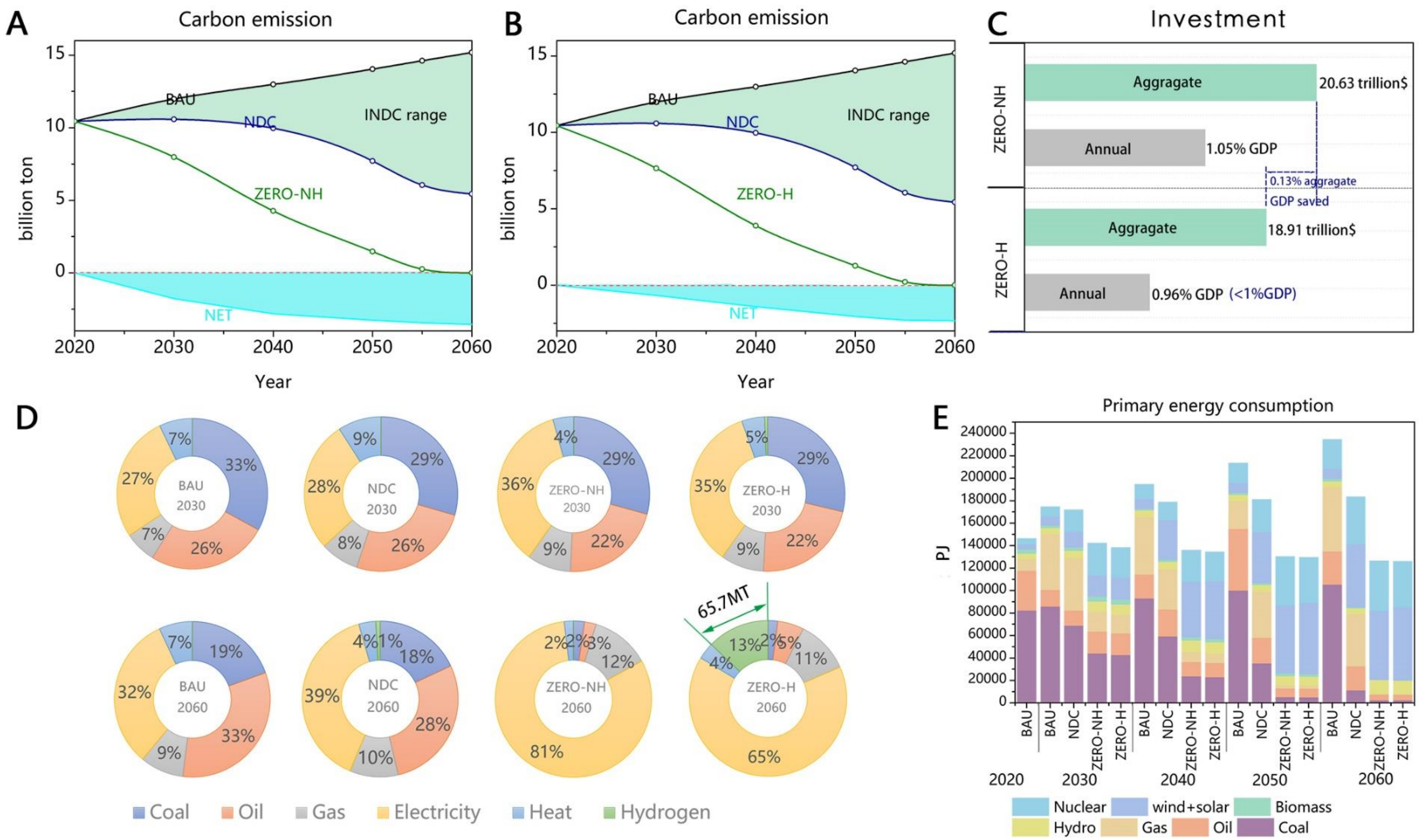


Fig. 5 The contribution of hydrogen as energy carrier and energy storage medium. (A) Final energy mix in the least cost hydrogen-inclusive net-zero CO_2 (ZERO-H) scenario (2060), **(B)** Key hydrogen production technologies in the ZERO-H scenario (2020-2060).

Hydrogen in China's carbon-neutral future

Results of the ZERO-NH and ZERO-H scenarios show that to achieve a carbon neutral 2060, China must make additional efforts beyond its NDC commitments (Fig. 6A). An additional 5.43 billion tons of CO_2 reduction annually compared to China's NDC emission level in 2060 will need to be realized, or 15.18 billion tons annually compared to the BAU scenario (Fig. 6D). In the ZERO-H scenario, an early CO_2 emission peak around 2025 (vs. the NDC target of 2030) could be achieved. In 2050, China's per capita CO_2 emissions will reach 1.02 tons/per capita. China's carbon-neutral future will be characterized by renewable energy dominance, with a phasing out of coal in its primary energy consumption (see Fig. 6D). Non-fossil fuels comprise 88% of the primary energy mix in 2050 and 93% in 2060. Wind and solar will supply half of primary energy consumption in 2060. In China, existing coal plants operate over a minimum lifetime of 20–30 years. More than 90% of conventional coal plants will retire by 2040. In our study, coal consumption will comprise less than 18% of the primary energy demand in 2040 and will be almost fully phased out in 2060 (leaving only 2%-3%, offset by negative carbon technologies).



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424 **Fig. 6. China's net-zero carbon emissions future.** (**A**) CO_2 trajectory in BAU, NDC and ZERO-NH (2020-2060); (**B**) CO_2 trajectory in BAU, NDC and ZERO-H (2020-2060); (**C**) carbon mitigation costs in 2060, compared to BAU scenario; **(D)** Primary energy consumption in BAU, NDC, ZERO-NH, ZERO-H scenarios (2020-2060); **(E)** Primary energy mix in BAU, NDC, ZERO-NH, ZERO-H scenarios (2030-2060).

Although clean hydrogen has only begun to be developed in China, its introduction into the country's energy system would be cost-saving compared to a no-hydrogen scenario achieving carbon neutrality in 2060, even taking into consideration all of the related infrastructure that would be needed (production, storage and transportation). In the ZERO-NH scenario, the cumulative investment cost to achieve carbon neutrality up to 2060 would be \$20.63 trillion, or 1.58% of the aggregate GDP for 2020-2060[32]. The average additional investment on an annual basis would be around \$516 billion per year, or 1.05% of GDP in 2060. This result is consistent with China's \$15 trillion mitigation plan up to 2050, an average annual new investment of \$500 billion[33]. However, introducing clean hydrogen options into China's energy system in the ZERO-H scenario results in a significantly lower cumulative investment by \$18.91 trillion by 2060 and the annual investment would be reduced to 0.96% of GDP in 2060 (Fig. 6C). Regarding the HTA sectors, the annual investment cost in those sectors would be around \$392 billion per year in the ZERO-NH scenario, which is consistent with the projection of the Energy Transition Commission (\$400 billion)[34]. However, if clean hydrogen is applied in the energy system and chemical industry, the ZERO-H scenario indicates the annual investment cost in HTA sectors could be reduced to be \$359 billion. Carbon reduction in HTA sectors under the non-hydrogen scenario would rely heavily on negative emission technologies (NETs) to achieve carbon neutrality, and the associated infrastructure would be more expensive than that to deploy clean hydrogen. Our results suggest that clean hydrogen can save a \$1.72 trillion investment cost which avoid a 0.13% the aggregate GDP (2020-2060) loss compared to the option without hydrogen in 2060.

These results show that clean hydrogen can play an important role in China's carbon neutral future. In the least-cost pathway, consumption of hydrogen increases continually to 12.8% of the total final energy consumption in 2060. This is a remarkably high share, amounting to 65.7 Mt in annual hydrogen demand. For comparison, the projection of the China Hydrogen Energy Alliance is that hydrogen (including grey, blue and green) will account for 10% of energy consumption in 2050[35]. Our analysis shows that in 2050 around 9.8% of the total final energy demand would be supplied by clean hydrogen (i.e., blue and green but not grey). We believe this target in 2050 is achievable as renewable energy costs continue their decline, possibly accelerated further by government subsidies.

Green hydrogen advantages over blue hydrogen

Clean hydrogen is essential for decarbonizing the HTA sectors. The question then is which type of hydrogen is most cost-competitive for a fossil fuel-dominated country like China? Currently, grey hydrogen has the lowest LCOH globally according to IEA (~1.69 \$/kg H_2) and the Hydrogen Council (~1.5 \$/kg H_2). However, global hydrogen production from fossil fuels emits 830 Mt of CO_2 per year[16], equivalent to the annual emissions from energy used by 100 million U.S. homes. Under carbon constraints, grey hydrogen must add CCUS to become blue hydrogen. The LCOH of blue hydrogen globally is 1.5 \$/kg H_2 to 3.5 \$/kg H_2[36]. In contrast, the projected LCOH of green hydrogen is more contentious. At the global level, Cloete et al. (2021) and Zhao et al. (2019) project that costs will remain high in a 10- to 30-year long term (4.47-15.83 \$/kg H_2)[37]. Some previous studies of China have also indicated high costs of green hydrogen (4-7 \$/kg H_2) compared to other regions[38].

However, our results and those of other sources indicate that green hydrogen can be cost competitive with blue hydrogen before 2040, even in fossil fuel-dominated China. The International Renewable Energy Agency (IRENA), Offshore Wind Industry Council, and other authoritative sources are similarly optimistic about green hydrogen, with cost estimates of 1.6-3.3 \$/kg H_2 in 2050[39]. Bloomberg New Energy Finance (BNEF) projects that the cost of green hydrogen will reach even lower levels (0.7-1.6 \$/kg H_2), another optimistic estimate. The US Department of Energy (US DOE) estimates that green hydrogen will be economically competitive only when it costs less than 2 \$/kg H_2[40]. Our results indicate that the average cost of China's green hydrogen can be reduced to 2 \$/kg H_2 by 2037 and by 2050, green hydrogen (1.2 \$/kg H_2) will be much more cost-effective than blue hydrogen (1.9 \$/kg H_2). China has rich untapped resources of solar and wind energy (both onshore and offshore), as demonstrated in our previous studies[41,42]. For these reasons China has huge advantages in production of green hydrogen and could be positioned to take a global lead in exploring large-scale applications.

The debates on the costs of clean hydrogen concern not only LCOH. A fuller cost accounting of clean hydrogen and its impact on other sectors will make the case more conclusive. Most studies focus on the production costs of clean hydrogen, and only sometimes consider transportation and storage costs. Few researchers have also considered the cost of hydrogen end uses[43]. This study seeks to fill this gap in clean hydrogen cost analysis, taking as its scope the entire energy system as well as major chemical industries.

We further evaluate the effects if only green or blue hydrogen is allowed in the ZERO-H scenario. If only blue hydrogen is permitted, the aggregate investment cost will be around \$19.54 trillion, which is \$0.63 trillion higher than green hydrogen enabled. Several factors favor green hydrogen in the market. First, the costs of renewables in China are increasingly competitive. If electrolyzers use otherwise-curtailed (i.e., effectively costless) wind and solar power instead of grid electricity, the total cost will be even lower. Second, China's renewable sources are geographically concentrated, with onshore wind and solar concentrated in the north and northwest, while offshore wind is concentrated along the southeast coast. Hydrogen production, storage and transport are advantaged when the needed infrastructure can also be concentrated, i.e., co-located in renewable-rich areas, further bringing the total costs down compared to a more distributed hydrogen system. Third, blue hydrogen might be cheaper than green hydrogen at the pilot stage and in the short term, but without innovative technologies that can significantly cut the CCUS cost will become uncompetitive over the long run. A take-away conclusion is that green hydrogen is likely to be a more cost-competitive option than blue hydrogen in achievement of China's carbon neutrality in 2060, on the basis of both LCOH and total system cost. This result is a rejoinder to concerns that lower costs of blue hydrogen could lock China into another round of fossil fuel investments if it pursues clean hydrogen. From the perspectives of both emission reduction potentials and costs, green hydrogen appears to be China's strongest option as a centerpiece of a long-term hydrogen strategy for decarbonization.

Discussion

Among the most vexing challenges to achievement of a carbon neutral world is the decarbonization of high-emission HTA sectors, which lack the increasingly mature solutions available for the power and light-duty transportation sectors and are disproportionately large in major developing economies such as China. Based on an integrated modeling analysis, this study makes the case that clean hydrogen, and especially green hydrogen, could provide a basis for prospective decarbonization solutions over a wide array of HTA applications in China, helping the country meet its 2060 carbon neutrality target. In cement, iron & steel, and chemical sectors, clean hydrogen could account for 21-34% of final energy consumption by 2060, replacing fossil fuel-based industrial heat and feedstocks. Clean hydrogen could also help decarbonize China's heavy transport. By fueling 53-67% of trucks, 52% of fleet buses, and 77% of shipping (12% from hydrogen and 65% from hydrogen-derived ammonia), a carbon-free heavy transport sector appears attainable in 2060.

Yet compared to developed countries, China is lagging in development of technologies and policies to encourage clean hydrogen deployment. The EU has made this a priority in its post-COVID-19 economic recovery package[44], which is guided by the European Green Deal which aims to make Europe the world's first carbon-neutral continent by 2050. The US DOE has supported fuel-cell transportation research and development for a long time[45], with the Hydrogen at Scale (H2@Scale) initiative widely cited with recently released targets for hydrogen long-haul trucks encouraging HDV applications[46]. Japan and South Korea have set particularly ambitious hydrogen targets adding to the clean hydrogen initiatives already underway in the US, UK, Germany, and Australia.

Why are countries such as China slow to embrace clean hydrogen? First, this is often assumed to be an inherently expensive energy carrier. This view, however, is increasingly open to question. Recent studies from the IEA, IRENA and BNEF concluded that the LCOH for green hydrogen will decline by 2030 to competitive levels in the US (under 2.0 $/kg), EU (under 2.8 $/kg) and Japan (under 3.3$/kg)[35,47]. Others suggest that despite the low LCOH in richer economies, countries such as China and India are starting from scratch and the needed new investment in clean hydrogen production facilities and transport and storage infrastructure would imply yield higher levelized costs. Assessing that assumption is one of the reasons why we established an integrated analysis model taking account of all processes required for clean hydrogen production and use in China. Our results do not support this negative position, indicating rather a net $1.72 trillion new investment cost that could be avoided by exploiting clean hydrogen in 2060 compared to a no-hydrogen scenario. By that time, green hydrogen technologies will be cost-competitive in HTA sectors compared to blue technologies. In short, clean hydrogen can bring aggregate economic benefits, not costs, for a developing country such as China allowing it to achieve cost competitively its aspirations for a carbon neutral future.

Some have argued that in countries with large existing fossil fuel resources and imbedded infrastructure, production of grey and blue hydrogen may help to lock-in reliance on a fossil fuel-based hydrogen industry, impeding thus benefits that green hydrogen could provide[48]. With no prior study of this topic for China, we have indicated here that the LCOH for green hydrogen may be lower than that for blue hydrogen after 2040. This evidence can help China avoid locking in fossil fuel investments resulting from commitments to grey and blue hydrogen. Under the net-zero constraint of our ZERO-H scenario, China's clean hydrogen demand could reach as high as 65.7 Mt by 2060 comprising then 12.8% of final energy demand, a huge market not only for China but also in terms of projected overall international demand. In a carbon neutral future, the energy system will be dominated by renewable energy. Previous studies, including our own, have shown than China has rich renewable resources, sufficient to provide for ambitious green hydrogen development[41,42,49]. Instead of importing fossil fuels, China could develop as a green hydrogen exporter, particularly if its LCOH were to fall below \$2/kg H_2. In the long term, a flourishing clean hydrogen economy may change the current energy trading map, which in turn could help decarbonize industries in other parts of the world.

Our results indicate that clean hydrogen can help countries optimize their energy structures, better exploit their domestic renewable energy sources, and enhance their energy security. In the long-overlooked HTA sectors, clean hydrogen may emerge as the basis for nearly unavoidable solutions for decarbonization to meet the urgency that climate change demands. This argues for enhancement of incentive policies including subsidies for clean hydrogen development, especially in HTA industries. There are also significant and growing emissions from HTA sectors in other major developing countries, most importantly in India given its large and increasing share of global carbon emissions. Industry contributed close to one quarter of India's carbon emissions in 2018, a share that is expected to grow with swift urbanization[5]. Relevant research funding should be encouraged for developing countries. This study provides an instructive reference for developing countries facing challenges similar to those confronting China as they also seek to mitigate emissions from their HTA sectors in the quest for a shared future goal for carbon neutrality.

Materials and Methods

Hydrogen consumption analysis module

Multiple robust studies of hydrogen production have been done, mainly focusing on hydrogen production. However, the size the prospective hydrogen market remains unclear. The hydrogen demand in some studies is simply evaluated based on GDP growth and other socioeconomic assumptions. However, unlike electricity, hydrogen is consumed in final demand sectors both as a feedstock and energy carrier, which is more complex. The total hydrogen demand is calculated based on our energy system optimization model. The hydrogen demand in this paper includes the consumption in industries, transport and other sectors, shown in (1)-(3).

$$DH_t = INDH_t + TRAH_t + OTHH_t \tag{1}$$

$$\begin{cases} INDH_t = \sum_{x=STE}^{OTHIND} DH_{t,x} & (2) \\ TRAH_t = \sum_{y=LDV}^{AVI} DH_{t,y} \\ OTHH_t = \sum_{z=RES}^{OTH} DH_{t,z} \\ DH_t = \sum_p D_{p,t} \times EH_{p,t} \end{cases}$$

(3)

In the above equations, *DH* denotes the demand of hydrogen and *INDH*, *TRAH* and *OTHH* refers to industry hydrogen demand, transport hydrogen demand and other hydrogen demand, respectively. In the set of *x*, the variables *STE*, *CEM*, *AMO*, *MET*, *OILR* and *OTHIND* are steel, cement, ammonia, methanol, oil refinery and other industry, respectively. In the set of *y*, *LTRU*, *MTRU*, *HTRU*, *SHIP* and *AVI* are light-, medium-, and heavy-duty trucks, shipping and aviation. In the *z* set, *RES*, *ELC* and *OTH* represent residential, power generation and other sectors.

Furthermore, the hydrogen consumed in different sectors varies. The hydrogen consumed in key industry sectors serves as both feedstock and combustion fuel for industrial heat.

$$\begin{cases} DH_{t,STE} = (\sum_p ACT_{p,t,STE}) \times SH_{t,HDRI} + \sum_p (ACT_{p,t,STE} \times EFF_{p,heat}) / EFFH_{t,p,STE} \\ \sum_p ACT_{p,t,STE} \geq DM_{t,STE} \end{cases}$$

(4)

$$\begin{cases} DH_{t,CEM} = \sum_{p}(ACT_{p,t,CEM} \times EFF_{p,heat}) / EFFH_{t,p,CEM} \\ \sum_{p} ACT_{p,t,CEM} \geq DM_{t,CEM} \end{cases} \tag{5}$$

$$\begin{cases} DH_{t,AMO} = \sum_{p}(ACT_{p,t,AMO} \times FEEDH_{AMO}) + \sum_{p}(ACT_{p,t,AMO} \times EFF_{p,heat}) / EFFH_{t,p,AMO} \\ \sum_{p} ACT_{p,t,AMO} \geq DM_{t,AMO} \end{cases} \tag{6}$$

$$\begin{cases} DH_{t,HTRU} = (\sum_{p} ACT_{p,t,HTRU}) \times SH_{t,H-HTRU} / EFFH_{t,p,HTRU} \\ \sum_{p} ACT_{p,t,HTRU} \times DIS_{p,t,HTRU} \times LOAD_{p,t,HTRU} + \\ \sum_{p} ACT_{p,t,MTRU} \times DIS_{p,t,MTRU} \times LOAD_{p,t,MTRU} + \\ \sum_{p} ACT_{p,t,LTRU} \times DIS_{p,t,LTRU} \times LOAD_{p,t,LTRU} \geq DM_{t,RoadF} \end{cases} \tag{7}$$

Functions (4)-(7) define hydrogen demand in key industry sectors and the heavy-duty transport sector, where t denotes time; p represents technology process; DM_t represents energy service demand in year t; *ACT* in industry sectors (4)-(6) denotes industrial production activity; *ACT* in heavy transport sector (7) mainly refers to vehicle stock; $EFF_{p,\ heat}$ represent heat efficiency of technology process p; and $EFFH_{t,\ p}$ is hydrogen combustion efficiency of technology process p in year t.

Specifically, in the steel sector equation (4), in addition to combustion fuel for heat supply, hydrogen is also an important reducing agent in the hydrogen-DRI process; $SH_{t,\ HDRI}$ is the share of hydrogen-DRI technology, which is decided by the energy system optimization based on cost analysis; $DM_{t,\ STE}$ denotes crude steel demand in year t. In the ammonia sector equation (6), the hydrogen consumption includes two parts, as feedstock and combustion fuel for heat, of which $FEEDH_{AMO}$ represents hydrogen consumed as feedstock. The hydrogen consumption in the methanol sector follows the same structure as in the ammonia equation (6). In the heavy-duty transport sector, we take heavy-duty trucking as an example. In equation (7), $SH_{t,H\text{-}HTRU}$ refers to the share of hydrogen fuel-cell heavy-duty trucks; $DIS_{p,t}$ is distance traveled in year t of vehicle type p; $LOAD_{p,t}$ is the load rate of vehicle type p in year t (i.e., tons of freight per vehicle); $HTRU$, $MTRU$, $LTRU$ represent heavy-, medium-, and light-duty trucks respectively. The trucks in operation together in year t should meet the road freight transport service demand in year t, which is shown as $DM_{t, Road}$.

Note that most models simulate only green hydrogen, based on renewables. However, there is considerable potential for blue hydrogen production, based on coal with CCUS in China and on natural gas with CCUS in US. Therefore, we consider fossil-fuel based hydrogen production technologies with different efficiencies and scales, including natural gas reforming and coal gasification with CCUS in this study. Regarding hydrogen delivery, some existing model studies assume the delivery cost is zero while in this study we consider both gaseous and liquid road transport. Long-distance oversea transoceanic transportation for ammonia is not considered in this study.

Final energy service demand prediction module

The mainstream methods of forecasting future terminal service demand involve econometric regression analysis, historical data statistical analysis and elasticity coefficient analysis. The final energy demand forecasts are differentiated by sectors in this paper. The prediction of the transport sector's future passenger and freight turnover, and the construction sector's future residential and public building area are based on an elastic equation method. In order to prevent the overestimation of the future demand forecast, the impact of actual development level and energy services price changes are fully considered.

The transportation sector is divided into road, railway, shipping, and aviation based on transport mode, and is further classified into freight and passenger transportation. The passenger final service demand unit is MPKM (million person-kilometers), and the unit of freight service demand unit is MTKM (million ton-kilometers). The division of the construction sector in the model includes urban residential, rural residential, large commercial buildings, and general commercial buildings. The main factors affecting the demand for energy services in the transportation sector are population, GDP growth rate and final service prices, which are classified by passenger and freight transportation modes. The influence factors for construction energy services demand mainly include population, urbanization rate, and per capita income. The driving factor is a variable that is added to the demand of different final services and used to predict the final service demand in the calculation year of the model.

$$Demand_t = Demand_{t-1} \times k \times driver^{elasticity} \tag{8}$$

where k is a constant as adjustment. The driving factor acts on the final service demand changes through demand elasticity, as shown in formula equation (8). The corresponding driving factors are different in sectoral energy service demand. The driving factors of passenger transportation service demand are per capita income, energy service price and population, for freight demand are income and energy service price, for the construction sector are GDP growth, urbanization rate, population, and changes in energy intensity. In the industrial sector, according to the final industrial products, the prediction is modeled and analyzed separately. The methods of combination model comparison and expert surveys are used to determine future energy service demand. For example, the raw steel demand prediction function is shown in equation (9):

$$\mathrm{DM}_{steel} = RF_1 \times c_1 + RF_2 \times c_2 + CF \times c_3 + \sum_i T_i \times c_{4i} + AP \times c_5 + E_x \tag{9}$$

where DM_{steel} is the demand for steel; RF_1 and RF_2 represent the increase in building area of urban and rural residential buildings respectively; *CF* defines the increase in commercial building area; *T* denotes the increase in transportation products increase, including passenger car, bus, truck, and ship; *AP* is increase in the number of household electricity appliances; increase. E_{xX} refers to other steel demand (export and import are considered); *c* represents steel intensity of products in construction, transportation, household appliances and other products, which units of which are t steel/m^2, t steel/ vehicle, t steel/ appliance; i means denotes transportation types, including passenger car, bus, truck, shipping and aviation.

Energy system optimization model

The energy system optimization model built in this study is the MAPLE-China (Multi-Abatement Planning and Long-term Energy system optimization in China) model. The model framework is shown in Fig. S1. It provides a technology-rich basis to estimate how the energy system operates over a long-term, multiple-period time horizon. It follows a techno-economic bottom-up approach to describe the energy-related sectors in detail through a variety of specific technologies defined by their technical and economic parameters. It offers thus a detailed representation of energy sectors, which includes extraction, transformation, distribution, end uses, and trade of various energy forms and materials. It computes an equilibrium on energy markets (partial equilibrium) and determines an optimal configuration of the energy systems to satisfy service demands at a minimum cost over a long-term horizon, while respecting greenhouse gas emission constraints.

The MAPLE model simulates the investment and operation of major energy technologies under constraints of emissions reductions in China. The model can project and simulate future energy use trends in multiple scenarios and varying degrees of mitigation action. The calculation objective of the model is that the total cost of the energy system must reach the minimum while exogenously given energy demand and any other major constraints on the energy system (e.g. technology availability and growth rates) are satisfied.

Objective functions:

$$C = \sum_t [(CINV_t + CFOM_t + CFU_t + CD_t) / (1 + d_t)^{t-2020}] \tag{10}$$

$$CINV_t = CP_{p,t} + CNP_{p,t} + CS_{p,t} \quad (11)$$

Most current bottom-up models in China do not consider hydrogen and associated technologies, and most existing hydrogen studies for China do not consider blue hydrogen. In (10), t is the year or time period; p denotes technology process, and the variables C, $CINV$, $CFOM$, CFU, CD, and d_t represent total cost, investment cost, fixed O&M cost, fuel cost, delivery cost and discount rate respectively. In the investment cost formula (11), CP, CNP, CS refer to production capacity cost, new pipeline infrastructure cost and storage cost respectively.

The constraints in this paper incorporate resource constraints and emission constraints (equations 12-14). In the constraints, TE is total emissions. Other constraints in the model include those related to inter-period capacity transfer constraints, technical activity constraints, and flow balance equation. MAPLE-China follows the integrated MARKAL/EFOM system (TIMES) energy planning modeling platform principles, detailed instruction and functions could be found in the documentation for the TIMES Model.

$$RS_t \geq \sum_p DF_{t,p} \quad (12)$$

$$TE_t = \sum_{p,i} (DF_{p,t,i} \times ef_{i,p}),\ i = [coal; oil; gas] \quad (13)$$

$$\begin{cases} TE_{2030} \geq TE_t \ (if\ t \geq 2030) \\ TE_{2060} \leq 0 \end{cases} \quad (14)$$

The model performs calculations from 2015/2020 to 2060. The base year calibration mainly includes the following aspects: (i) total energy consumption and category-based energy consumption of various sectors and sub-sectors; (ii) energy consumption per unit of end-use demand of major divisions; (iii) CO_2 emissions. The main data sources of the MAPLE-China model are energy balance tables available from China's Energy Yearbook. For energy consumption in the industrial sub-sectors and technologies, we used several sources such as the China Statistical Yearbook, Industrial Statistical Yearbook, China Steel Statistics, China Chemical Industry Yearbook, China Nonferrous Metals Industry Yearbook, and China Energy Statistical Yearbook. Cost and energy parameters for technologies at an early stage of development are obtained from the Chinese Ministry of Information and Industry Technology and in consultation with industry experts. We also use technical parameter documents on production lines of major industrial sectors, as well as calculation and collation from related literature, internal reports from enterprises, and interview with experts.

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