



## **A quantitative roadmap for China towards carbon neutrality in 2060 using methanol and ammonia as energy carriers**

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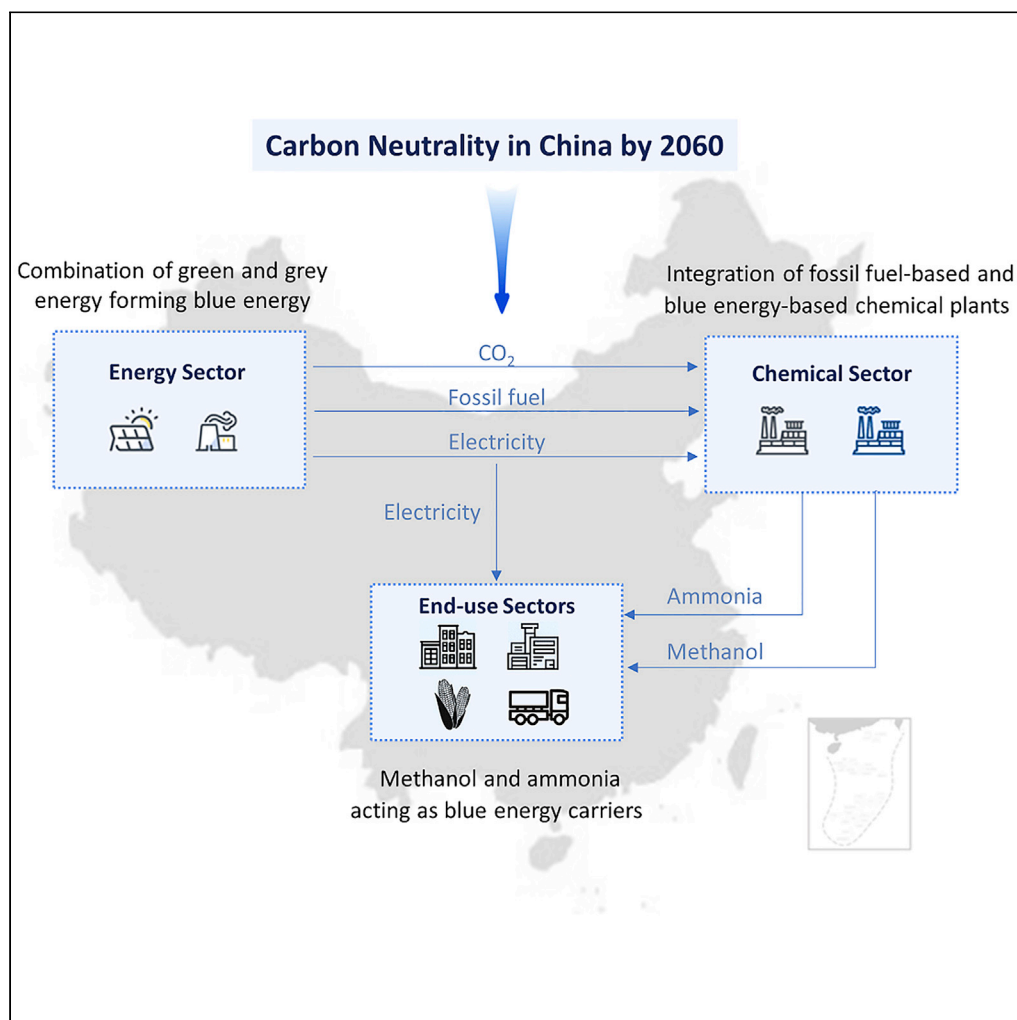
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## Article

## A quantitative roadmap for China towards carbon neutrality in 2060 using methanol and ammonia as energy carriers



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**Highlights**

Roadmap toward carbon neutral supply of electricity, methanol, and ammonia is designed

Potential of methanol and ammonia working as energy carriers in China is investigated

An energy-chemical nexus optimization model with regional cooperation is developed

The absolute sustainability is assessed with planetary boundaries of climate change

## Article

## A quantitative roadmap for China towards carbon neutrality in 2060 using methanol and ammonia as energy carriers

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## SUMMARY

**Carbon neutrality by 2060 is the recent expression of China's international commitment to reduce its carbon dioxide emissions. Energy and chemical sectors, the two main contributors for carbon dioxide emissions in China, are the biggest bottlenecks for reaching the objective of carbon neutrality. Moreover, coal-to-ammonia production and coal-to-methanol production are the major CO<sub>2</sub> emission process contributors in China's coal chemical sector. Herein, a possible route to the carbon neutral target based on energy-chemical nexus for electricity generation as well as methanol and ammonia production is proposed in this study. The most cost-effective solution for meeting the commitment is identified by considering regional variations in renewable and non-renewable resources and adopting an optimized regional cooperation. According to the roadmap presented in this study, an optimized combination of fossil fuels and renewable energies forming "blue energy economy" is feasible and promising.**

## INTRODUCTION

Facing the urgent need to deal with climate change, "Copenhagen Accord" and "Paris Agreement" propelled governments to establish domestic targets to reduce greenhouse gas (GHG) emissions. To compliance with international commitments, China has established its national goal to peak carbon dioxide (CO<sub>2</sub>) emissions by 2030 and cut its GHG emissions per unit of gross domestic product by 60–65% in 2030 compared with the 2005 levels, known as the Intended Nationally Determined Contributions (State Council, 2016). In September 2020 at the United Nations General Assembly, China has not only reaffirmed its national goal of peaking CO<sub>2</sub> emissions before 2030 but also announced the target of carbon neutrality by 2060. Such commitment is an ambitious goal, as China has been the largest annual CO<sub>2</sub> emitter worldwide since 2006. The news of China's carbon neutrality target has been described as a "game changer" for the global climate (European External Action Service, 2020). This significant step in the fight against climate change by China will encourage other countries to take similar actions. In the wake of the announcement, many organizations and research groups have developed models to simulate various future development pathways (Energy Foundation, 2020; Mallapaty, 2020). Although these plans are different in details, they all agree that developing renewable energy is a crucial measure in reducing CO<sub>2</sub> emissions from fossil fuel combustion. However, it is impossible to shift completely to "green energy" (e.g., hydro, wind, solar, and biomass) from its coal-dominated "gray energy" (e.g., coal, oil, and gas) within a short period. Therefore, the continued use of fossil fuels coupled with the carbon capture and storage (CCS) technologies is identified as another potential pathway to achieve the GHG emission reduction target (Wang et al., 2020). The concept of blue energy, defined as a combination of renewable and non-renewable resources, is widely accepted by many researchers (Pattle, 1954; Ramon et al., 2011; Zhou and Jiang, 2020). As demonstrated in our study, an optimized combination of green and gray energy forming a "blue energy economy" is the future direction for the sustainable development of China to achieve its 2060 carbon neutrality goal.

Currently, coal is the most important gray energy carrier in China. It is widely used to provide heat and electricity and as a raw material for the production of chemicals. Consequently, around 75% of China's GHG emissions come from coal consumption (China Power, 2019). For this long-term coal-dominated structure, the energy and chemical sectors are the two main CO<sub>2</sub> emitters, which together account for about 45% of China's total CO<sub>2</sub> emissions in 2015 (IEA, 2016). It is clear that both energy and chemical sectors are pivotal for reaching the objective of carbon neutrality by 2060. Therefore, controlling CO<sub>2</sub> emissions from the

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largest emitting sectors should be regarded as one of the most effective methods when designing the carbon neutrality plan. Moreover, coal-to-ammonia production and coal-to-methanol production are the major CO<sub>2</sub> emission process contributors, which, respectively, share 41.3% and 21.0% of total CO<sub>2</sub> emission process from the coal chemical sector in China (Huang et al., 2019). Therefore, upgrading and diversifying their production methods could significantly contribute to the carbon neutrality target. A roadmap of departing from the independent sectoral development pattern and forming a sectoral nexus is proposed in this study. The relevant concepts including energy-chemical nexus (Li et al., 2020) and methanol economy (Shih et al., 2018) are becoming increasingly appealing. In the nexus of energy and chemical sectors, renewable resources are used in chemical production, which returns chemical products widely applied in the conversion, transportation, and trade of renewable energy. In this regard, the potential of “renewable methanol”, which is produced from CO<sub>2</sub>, water, and renewable resources, was investigated by many pioneering studies (Abate et al., 2015; Chen et al., 2019; Li et al., 2020; Robinus et al., 2017). It is noteworthy that most studies exploring the renewable methanol concept are limited to industrial scope by simply assuming abundant renewable energy and large demand of chemical products (Al-Qahtani et al., 2020; Chen et al., 2019; Zhang et al., 2020). However, the impact of feedstock availability, technology transfer and penetration, and market structure are not taken into consideration. Our previous paper (Li et al., 2020), as a pioneer study, analyzed the energy-chemical nexus for renewable methanol production in China from the perspective of geography, sectoral development, environment, and economic cost. Many studies have also excessively emphasized extending the use of renewable energy and replacement of fossil fuel for both energy and chemical sectors (Al-Qahtani et al., 2020; Kauw et al., 2015), which overlooks that a smooth and effective transition toward the energy-chemical nexus needs conjunctive use of both renewable energy and fossil fuels. The blue energy concept has not been intensively studied in the literature for energy-chemical nexus. The potential of such integrated systems attributed to the national carbon neutrality target is of great significance but rarely mentioned.

Considering the productions of methanol and ammonia are the major CO<sub>2</sub> emission process contributors in China, we propose the concept of a blue energy economy formed by the energy-chemical sectoral nexus, which converts both gray and green energy into methanol and ammonia as energy carriers. The “methanol economy” presented previously (Li et al., 2020) is further enriched to “blue energy economy”, which considers a more smooth and effective transition toward the energy-chemical nexus. To our best knowledge, it is the first time that the potential of methanol and ammonia working together as blue energy carriers has been investigated with quantitative methods in the context of China. The novelty of this work has been largely widened by attributing the energy-chemical nexus concept to the China 2060 carbon neutrality target. To favor policymaking toward the carbon neutrality target by 2060, this study provides an analytical assessment of the blue energy economy development through the energy-chemical nexus. We developed a regional cooperation model that optimizes the regional development of China’s energy and chemical sectors under a 2060 carbon neutrality policy scenario at minimal cost. The results provided novel and detailed information to the nexus patterns that determine changes in CO<sub>2</sub> emissions of the national energy-chemical nexus from 2018 to 2060, providing insights on China’s future energy mix and chemical production. With the natural decay of major atmospheric greenhouse gases explicitly modeled, the dynamic evolvement of climate change related to planetary boundaries is also assessed in detail.

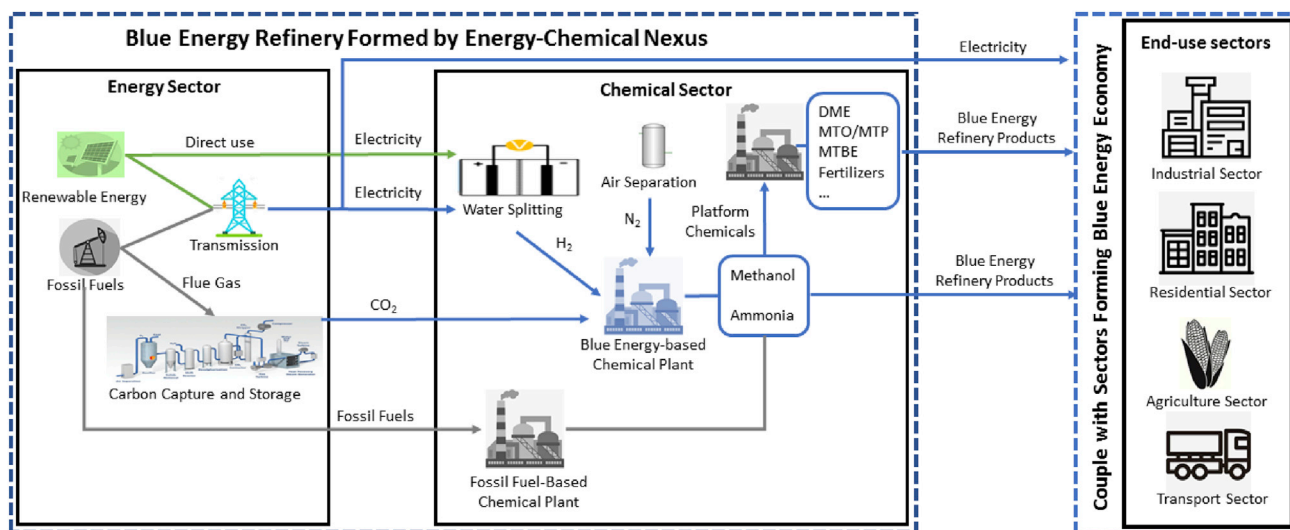
## Concepts of blue energy refinery and blue energy economy

### *Blue energy refinery*

The nexus of energy and chemical sectors forms a blue energy refinery through sharing resources. As it can be seen from Figure 1, the energy sector supplies electricity, CO<sub>2</sub>, and fossil fuels simultaneously to the chemical sector. Fossil fuel-based and blue energy-based chemical plants produce methanol and ammonia from fossil fuels and non-fossil fuel sources, respectively. Apart from using finished chemical products, methanol and ammonia are also important and versatile platform chemicals for fuels, agricultural fertilizers, and other chemicals, which largely expand the products of the blue energy refinery.

### *Blue energy economy*

Forming a blue energy economy would require the blue refinery coupled with other sectors. Suitable blue energy carriers are the key for this holistic transformation across all sectors. Methanol and ammonia, which are stable liquids at ambient conditions and suitable for storage, transportation, and distribution, have been proposed as blue energy carriers. The possibilities of methanol and ammonia production from both fossil and non-fossil sources can offer a smooth and effective transition from the conventional gray



**Figure 1. Concepts of blue energy refinery and blue energy economy**

Figure 1 depicts the concepts of blue energy refinery formed by energy-chemical nexus and its integration with end-use sectors forming the blue energy economy. Through energy-chemical nexus, both gray and green energy are used to produce methanol and ammonia, which act as energy carriers substantiating the blue energy economy.

energy economy to the more sustainable blue energy economy future. The wide applications of methanol and ammonia, from the component of fuel mix to upstream products for fertilizers, provide a variety of sector coupling methods of forming a blue energy economy.

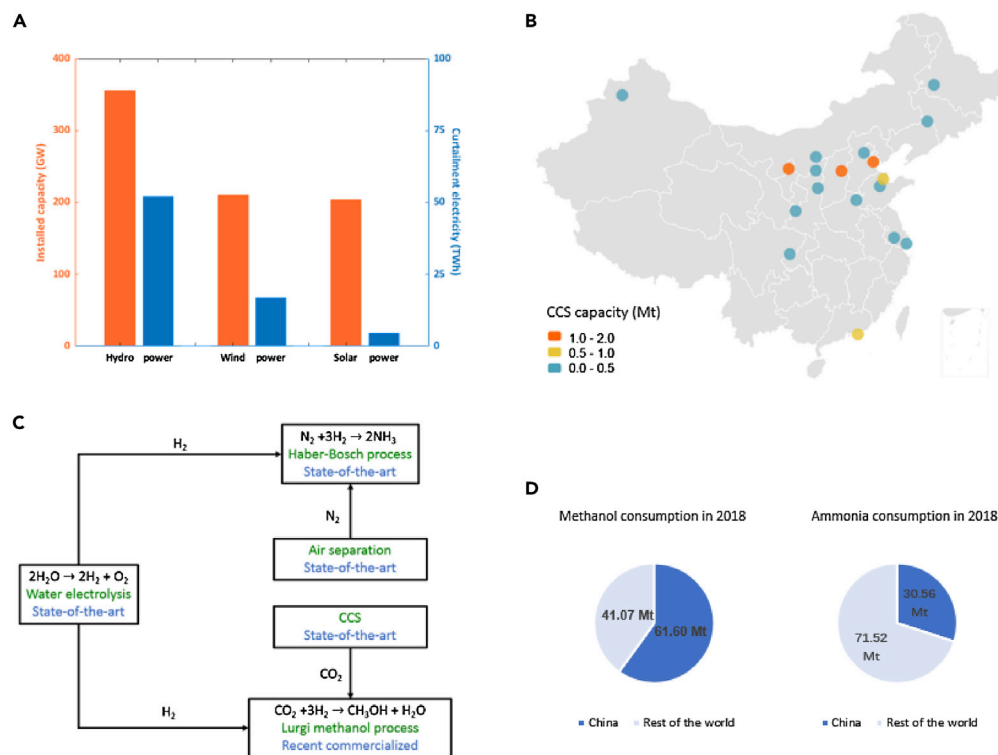
### Feasibility analysis of forming blue energy economy in China

#### *Oversupply of electricity from large-scale deployment of renewable energy*

The biggest challenge for the blue energy refinery is large-scale commercialized hydrogen production. Electrolysis is a promising method for hydrogen production, which could be zero emissions depending on the source of the electricity used. Stimulated by the policy incentives, China has made significant progress in deploying renewable energy power plants, having the world's largest installed capacity of renewable energy. Hydro, wind, and solar energy are the three major renewable energy sources in China, and their total installed capacity in 2019 reached 770 GW<sup>23</sup> as shown in Figure 1. Compared with these major renewable energies, biomass energy in China has also been developing rapidly, which increased by 26.6% and reached 22.4 GW in 2019<sup>23</sup>. Although the installation expands rapidly in China, the utilization of renewable energy is limited because of its discontinuous and fluctuating nature. Renewable electricity can dynamically change with time and affects the stability of power grids (Lew et al., 2013). Therefore, a significant amount of renewable electricity has to be abandoned to ensure the safety of power grids. As shown in Figure 2A, the curtailment of hydro, wind, and solar power in 2019 reached 52 TWh, 16.9 TWh, and 4.6 TWh, respectively (Liu et al., 2018; National Energy Administration, 2020). The total curtailed renewable electricity in China in 2019 was 73.5 TWh, which was equivalent to the total electricity consumption in Chile in 2019 (Enerdata, 2020). Instead of connecting to the power grids, this intermittent electricity from renewable energy can be directly applied to water electrolyzers for hydrogen production, which can be used for methanol and ammonia syntheses. In this way, the renewable energy is stored in these blue energy carriers, which can decrease the curtailment of electricity and increase the efficiency of renewable power utilization.

#### *Large amount of captured CO<sub>2</sub> from the development of CCS*

Apart from hydrogen, CO<sub>2</sub> is another important feedstock for methanol synthesis in the blue energy chemical plants. CCS is a technology that can effectively capture CO<sub>2</sub> from coal-fired thermal power plants and other emission sources. The speed of CCS deployment in China has been rapid with a series of policies proposed by the government. As shown in Figure 2B, by 2018, China has 18 CCS facilities in 15 provinces, involving power, coal, and oil industries. The total maximum CO<sub>2</sub> capture capacity of these 18 CCS facilities in China can reach 5.2 Mt per year. China may become the largest market for CCS technologies in the future



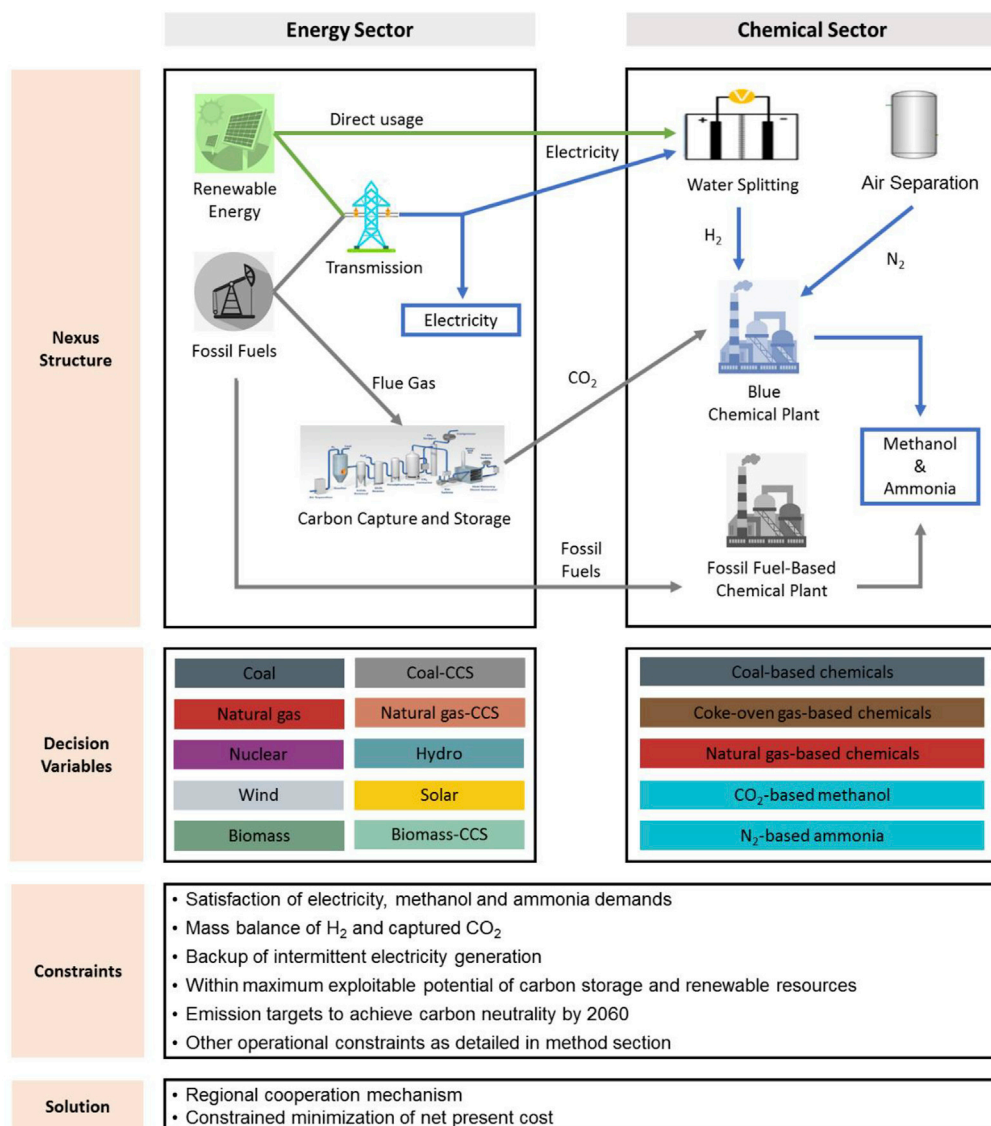
**Figure 2. Feasibility analysis of forming blue energy economy in China**

- (A) Oversupply of electricity from large-scale deployment of renewable energy.  
 (B) Distribution of CCS facilities.  
 (C) High technology readiness level of H<sub>2</sub>-mediated chemical synthesis.  
 (D) Largest market for both methanol and ammonia.

(Wang et al., 2020). However, large-scale CCS deployment in China also faces many challenges. Its high cost is claimed as the major obstacle hampering widespread adoption of CCS, especially the cost for the safety guarantee of geological storage (Budinis et al., 2018). Although geological storage is the fastest solution for the captured CO<sub>2</sub>, using captured CO<sub>2</sub> as a raw material for methanol production can significantly improve the economics of CCS. This in return can further enhance the promotion of CCS.

### High technology readiness levels of H<sub>2</sub>-mediated chemical syntheses

The process and technology readiness levels of H<sub>2</sub>-mediated methanol and ammonia production are shown in Figure 2C. The Haber-Bosch process converting nitrogen and hydrogen to ammonia is the main industrial procedure for the ammonia production all over the world. Even though the Haber-Bosch process was developed by Fritz Haber and Carl Bosch in 1913, this century-old process is still the state-of-the-art technology and continues to produce more than 90% of ammonia globally today (Wang et al., 2018a). Currently, two-thirds of the world's ammonia is synthesized from natural gas. While in China, about 97% of ammonia is produced from coal due to its abundant coal resources and limited natural gas reserve (Xiang and Zhou, 2018). Compared to the direct synthesis of ammonia from N<sub>2</sub> and H<sub>2</sub> with the Haber-Bosch process, methanol synthesis from H<sub>2</sub> and CO<sub>2</sub> is a recently commercialized technology. The company named Carbon Recycling International (CRI) in Iceland launched the world's first commercial-scale methanol production plant synthesized directly from H<sub>2</sub> and CO<sub>2</sub>. The plant of CRI has produced approximately 4000 t/year of methanol since 2014, and it actively plans to expand its commercial-scale plants to 50 Mt/year of methanol using the Lurgi methanol processes with H<sub>2</sub> and CO<sub>2</sub> as feedstocks (Graves et al., 2011). By importing this CO<sub>2</sub> hydrogenation to methanol technology from CRI, the first carbon dioxide hydrogenation methanol production plant in China has been under construction in Anyang, Henan Province, since July 2020 (Carbon Recycling International, 2019). With future methanol production capacity of 110,000 t/year, this methanol plant in China will be the world's largest carbon dioxide hydrogenation methanol production plant (Carbon Recycling International, 2019).



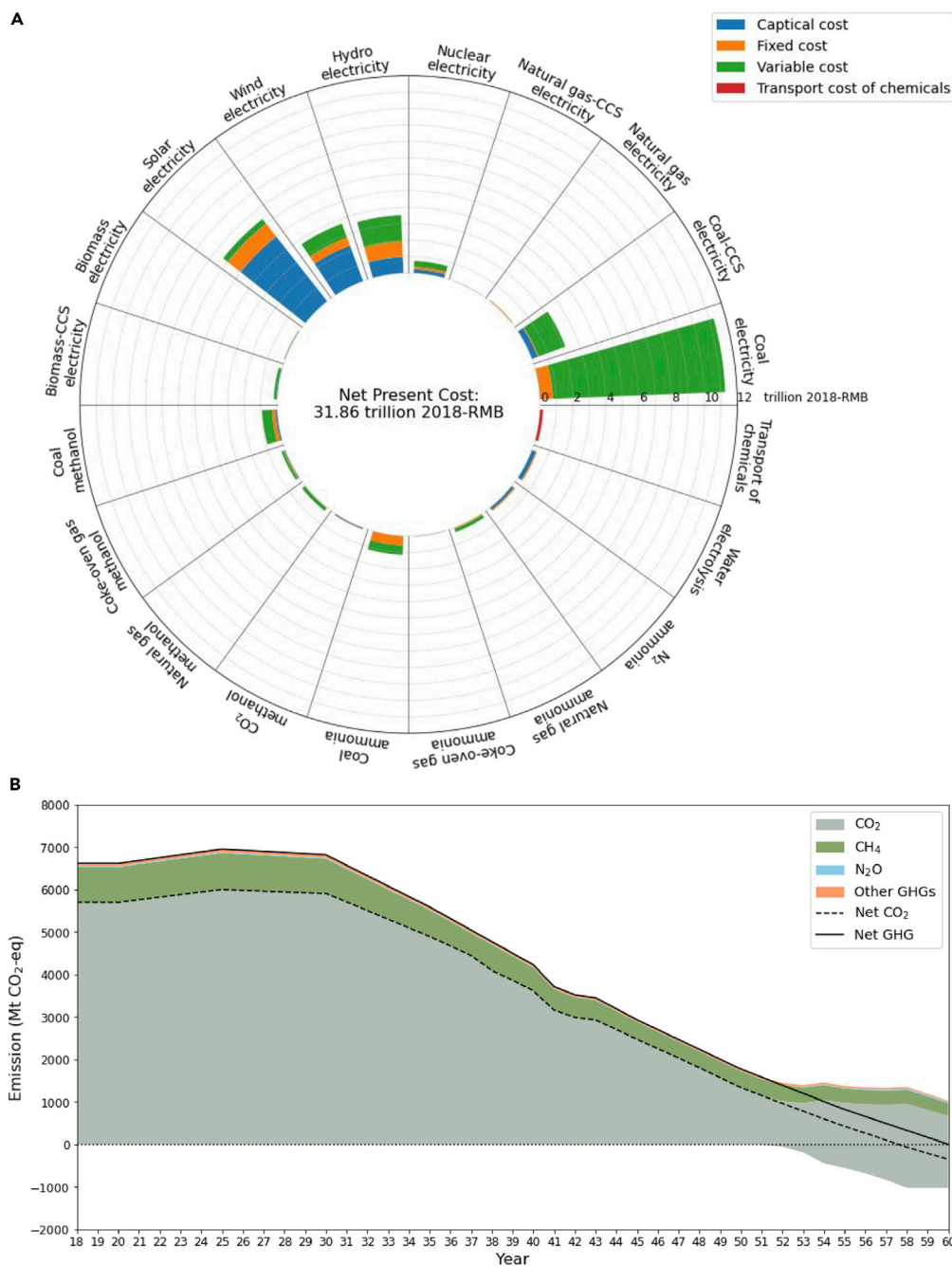
**Figure 3. Energy-chemical nexus model based on optimized regional cooperation**

The energy-chemical nexus model aims to find the optimal solution based on regional cooperation mechanism. The model contains three main elements: decision variables, constraints, and solutions.

### Largest consumer market and policy implications

China is the world's largest producer and consumer for both methanol and ammonia. By 2019, China's methanol and ammonia demands account for 60% and 30% of the global methanol and ammonia consumptions, respectively, as shown in Figure 2D (Statista, 2020; USGS, 2020). The structure of China's fossil resources is characterized by "rich coal, meager oil, and little gas". The proven reserves include 94% coal, 5% crude oil, and 0.6% natural gas (Han et al., 2018). In order to reduce dependence on foreign oil and natural gas and improve national energy security, Chinese government promotes the application of methanol and ammonia as alternatives to imported oil and natural gas. For instance, methanol-fueled vehicles are promoted to replace a portion of fossil-based gasoline (Nami, 2015) and methanol and ammonia are used to replace parts of natural gas for heating (China Energy Net, 2018). It is forecasted that the demand growth rate in China will remain 7% and ammonia demand will remain mostly stable (Forward Business Information Co. Ltd., 2019; Yang, 2020). The production methods for methanol and ammonia in China are mainly coal based currently due to the aforementioned energy structure. These dominated coal-based chemical plants leading to high levels of CO<sub>2</sub> emissions, together with the increasing demand



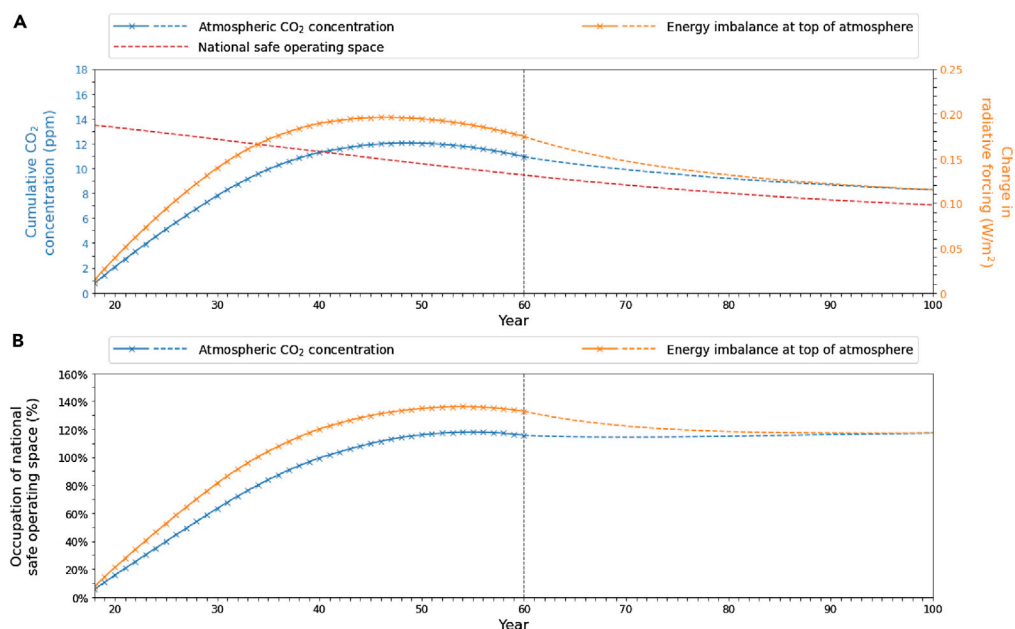


**Figure 4. Net present cost (A) and GHG emission profile (B)**

The contributions from different cost components of different technologies to the net present cost (trillion 2018 RMB) are shown in (A). The term “transport of chemicals” shown in red refers to the total cost of both methanol and ammonia transport during the planning period. The emission (Mt per year) profiles for CO<sub>2</sub>, CH<sub>4</sub>, N<sub>2</sub>O, and other GHGs are shown in (B). All GHGs are converted to CO<sub>2</sub>-eq based on GWP-100a (IPCC, 2013). The positive and negative CO<sub>2</sub> emissions are shown separately above and below the dotted zero line with the net CO<sub>2</sub> and GHG emissions shown in dashed and solid lines, respectively.

for chemical products, would possibly hinder the 2060 carbon neutrality target. Therefore, the penetration of blue energy-based chemical plants is vital for the sustainable development of the methanol and ammonia industries in China. Additionally, most ammonia plants in China are collocated and integrated with methanol plants in order to allow for greater robustness since the process allows for any split in production between methanol and





**Figure 5. Nexus impact scores for climate change related planetary boundaries (A) and their occupation of national safe operating spaces (B)**

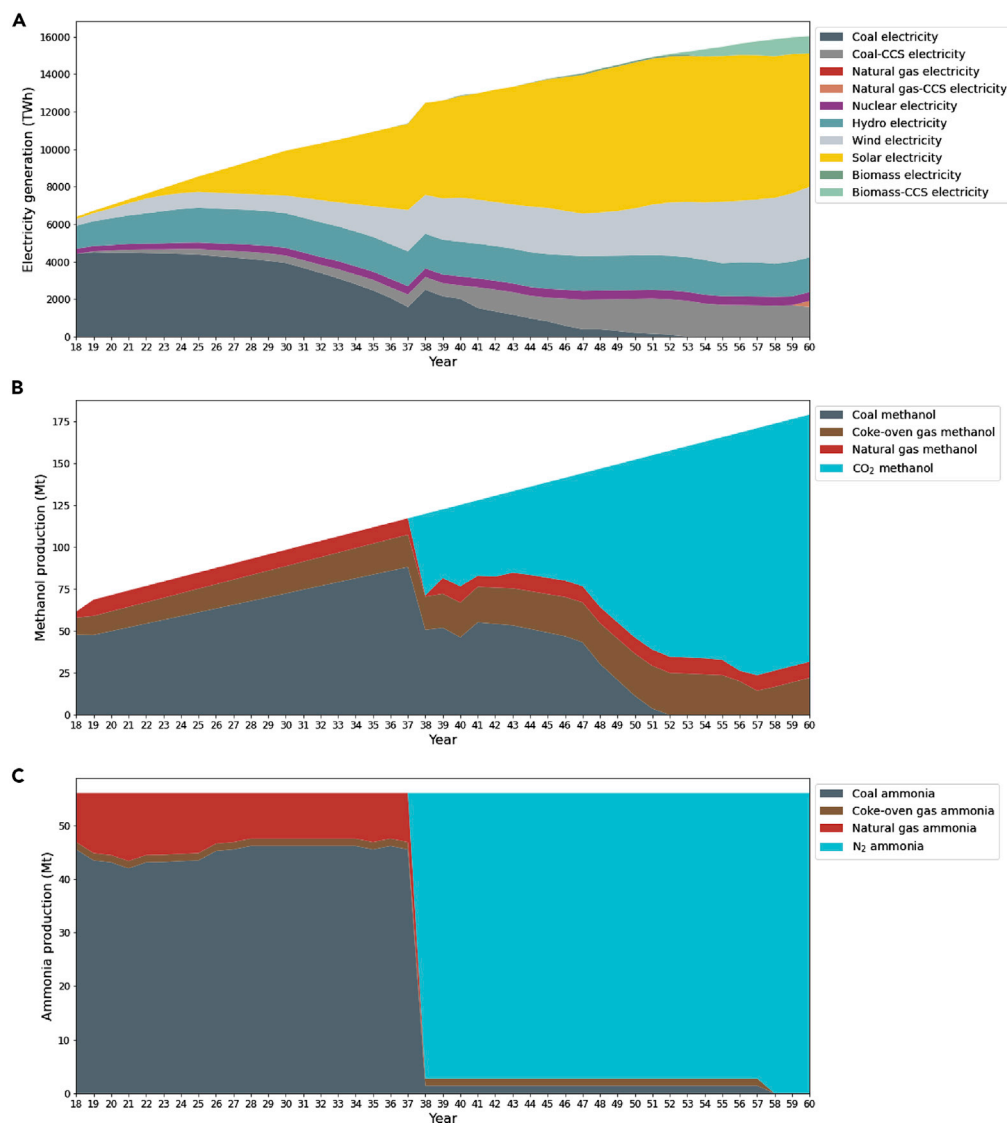
The left y axis in (A) shows the cumulative CO<sub>2</sub> concentration in the atmosphere from 2018 (ppm), which is the control variable for boundary: atmosphere CO<sub>2</sub> concentration. The right y axis in (A) shows the change in radiative forcing from 2018 (W/m<sup>2</sup>), which is the control variable for boundary: energy imbalance at top of atmosphere. Both the emission and natural decay of CO<sub>2</sub>, CH<sub>4</sub>, and N<sub>2</sub>O are considered from 2018 to 2060 while only the natural decay is extrapolated afterward. The two y axes in (A) are adjusted such that the national safe operating spaces of both boundaries align with each other as shown by the single red dotted line. Based on the impact scores, the occupation of national safe operating spaces is plotted in (B). More details on the accumulation of atmospheric GHGs with year can be found in [Figure S1](#).

ammonia in accordance to the market demand ([Xu et al., 2017](#)). Such integrated chemical plants not only enable a smoother integration of adjustment to market demands but also minimize both capital costs and operating expenses, providing greater feasibility of integration into the blue energy economy in China.

## Blue energy economy development based on China's 2060 carbon neutrality target

### *Energy-chemical nexus model based on optimized regional cooperation*

The diagram for energy-chemical nexus model is shown in [Figure 3](#). For the study of energy-chemical nexus in this work, electricity is selected as the representative product for energy sector which can be generated from ten different technologies, namely coal, natural gas, hydro, wind, solar, and biomass, as well as carbon capture and storage integrated generation including coal CCS, natural gas CCS, and biomass CCS. For the chemical sector, methanol and ammonia are considered, and they can both be produced conventionally from coal, natural gas, and coke oven gas. Specially, methanol and ammonia can also be synthesized directly from CO<sub>2</sub> and N<sub>2</sub>, respectively, with H<sub>2</sub> supplied by water electrolysis, which is named as CO<sub>2</sub>-based methanol and N<sub>2</sub>-based ammonia. To study the transition of China from its current energy structure to a future "blue energy" economy under the 2060 carbon neutrality goal, the nexus optimization model minimizes net present cost over a time frame of more than 40 years from 2018 to 2060. For each year, it is required that the generation from all technologies satisfies product (either energy or chemical) demand while production amount not exceeding the existing capacity or exploitable potential. Also, the total annual GHG emissions must stay within the corresponding targets set by the government over the entire planning period. Detailed information for the energy-chemical nexus model can be seen in the [STAR Methods](#) Section. It should be noted that China's political scheme has a top-down structure, such that the provincial legislation cannot be independent of the national system. Once the central government adopts a national strategy to support the blue energy economy, full cooperation among provinces will be established through trading and sharing resources. This inter-provincial cooperation mechanism can exploit regional advantages and identify the most cost-effective pathway for the achievement of a blue energy economy ([Galán-Martín et al., 2018](#)).



**Figure 6. Technology adoption for electricity (A), methanol (B), and ammonia (C)**

The national total amounts of electricity generation (TWh per year), methanol production (Mt per year), and ammonia production (Mt per year) of different technologies from 2018 to 2060 are stack plotted in (A), (B), and (C), respectively. The construction of new facilities and utilizable capacities is plotted in Figures S2–S4.

### Cost and emission assessment

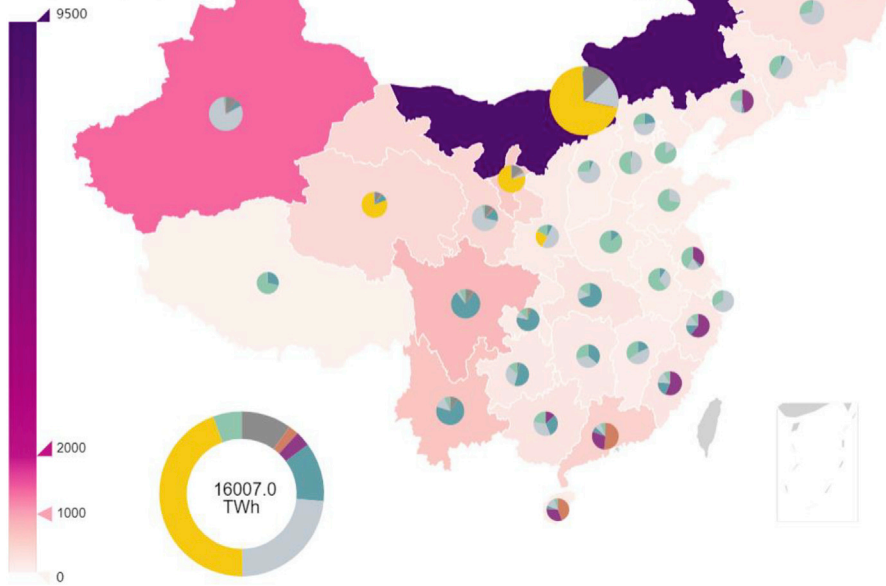
In this work, the emission reduction pathway for China proposed by Zhang (Zhang, 2020) is used considering the fact that it is specially designed for energy system transformation and targeted at the recently announced 2060 carbon neutrality goal. The national emission targets are downscaled proportionally according to the share of GHG emissions induced by the energy-chemical nexus in China's national total GHG emissions in 2018 (*status quo*). Minimizing the net present cost (NPC) of the energy-chemical nexus under a discount rate of 8% subject to those aforementioned operation and emission constraints results in a total cost of 31.86 trillion 2018 Chinese Yuan (Renminbi, or RMB), which converts to about 4.8 trillion 2018 USD under the average exchange rate in 2018 (OECD, 2020). The NPC structure of the optimal solution and its corresponding emissions profile is shown in Figure 4.

From Figure 4A, it can be seen that costs of the energy sector dominate the total NPC, which can be explained from the following two aspects. Firstly, with the demands for chemicals converted to energy unit according to

**A Electricity sector: 2060**

Coal Coal-CCS Natural gas Natural gas-CCS Nuclear  
Hydro Wind Solar Biomass Biomass-CCS

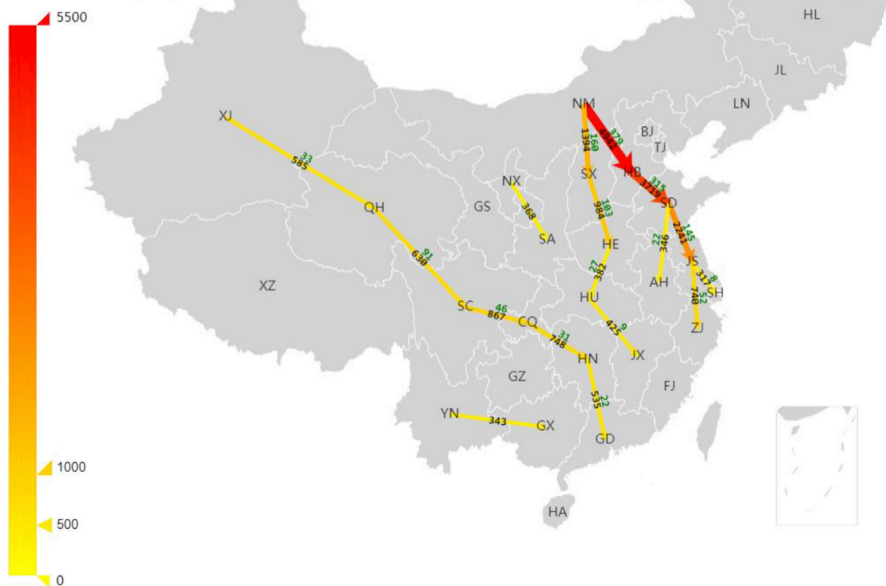
Total generation (TWh)



**B Energy transmission: 2060**

Black number: grid transmission (TWh)  
Green number: equivalent transmission via green chemicals (TWh)

Total transmission (TWh)



**Figure 7. Electricity generation and transmission map of China in 2060**

In (A), the pie charts show the proportions of electricity generation in different provinces. The share of the electricity generation of the whole nation is presented in the donut chart. The background color of provinces shows the amount of power generation (TWh per year). In (B), arrows illustrate the total energy transmission (both electricity and green chemicals) between different provinces, with their color showing the amount of energy transmission. The amounts of transported green methanol and green ammonia are converted to energy based on their heat values and presented by green numbers. The amounts of transmitted electricity are labeled in black numbers. More plots of other years are available in [Figures S5 and S6](#), and interactive versions of map plots in [Figures 7, 8, and 9](#) are provided in [Data S1](#).

heat values, China's national electricity demand far exceeds its demands for methanol and ammonia, especially when the future trend of increasing electrification is concerned. Secondly, under the inter-sectorial nexus, utilities cost along the supply chain from electricity to chemicals with hydrogen as intermediate is partially borne by energy sector, which also explains why the costs of CO<sub>2</sub>-based methanol and N<sub>2</sub>-based ammonia production are not significant in the figure. Within the energy sector, different cost structures can be observed for different technologies. In particular, capital cost is the major component for wind and solar electricity while variable cost dominates the cost of fossil-based generation. Also, it is interesting to note that even though coal-based electricity is gradually replaced in the future, its cost is still significant, which can be explained by the calculation of NPC that costs occurred earlier in future are less discounted when converting to present values. The emission profiles for three typical GHG species, i.e., CO<sub>2</sub>, CH<sub>4</sub>, and N<sub>2</sub>O, together with a lump sum of other GHGs are shown in [Figure 4B](#). All GHGs are converted to CO<sub>2</sub> equivalents (CO<sub>2</sub>-eq) according to their 100-year global warming potential (GWP-100a) from the Fifth Assessment Report of the United Nations Intergovernmental Panel on Climate Change (IPCC) ([Myhre et al., 2013](#)). As it can be seen, the three explicitly considered GHG species account for more than 97% of total positive GHG emissions over the planning period while negative CO<sub>2</sub> emission in the energy-chemical nexus occurs after 2050. Net zero GHG emission is achieved by 2060 in accordance with China's carbon neutrality target.

**Planetary boundaries of climate change assessment**

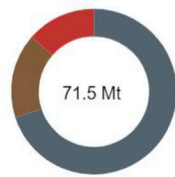
The concept of planetary boundaries provides a set of criteria on absolute sustainability assessment based on Earth system processes. In order to quantify the effects of emission control measures on combating climate change by the end of this century (2100), two relevant planetary boundaries, i.e., atmospheric CO<sub>2</sub> concentration (ppm) and energy imbalance at top of atmosphere (W/m<sup>2</sup>), can be used for assessment. Among the two boundaries, the former one provides an explicit upper bound on CO<sub>2</sub> inventory in the atmosphere, while the latter one is more fundamental and stringent. In this study, the global safe operating spaces of both boundaries are taken from ([Steffen et al., 2015](#)) and then downscaled to the national level according to the share of China's population in the world, where development in population until 2100 was based on the UN's population prospects using the medium fertility variant ([United Nations Department of Economic and Social Affairs Population Division, 2019](#)). Both the emission and natural decay of three major aforementioned GHG species, i.e., CO<sub>2</sub>, CH<sub>4</sub>, and N<sub>2</sub>O, are explicitly modeled from 2018 to 2060. In order to assess the effects of GHGs emitted during the planning period at the end of this century and also considering China's 2060 carbon neutrality goal which requires net zero national GHG emissions after 2060, the natural decay of those three atmospheric GHGs is further extrapolated until 2100.

As shown in [Figure 5A](#), the effects of GHG emissions of the energy-chemical nexus from 2018 to 2060 in terms of atmospheric CO<sub>2</sub> concentration and radiative forcing will peak around year 2045 after which the effects will start to decrease as a result of the reduction in GHG emission toward carbon emission neutrality in 2060. We see that the decrease in effects is slow due to the long atmospheric lifetime of CO<sub>2</sub>, in particular. [Figure 5B](#) shows that the emissions pertaining to the energy-chemical nexus from 2018 to 2060 will occupy up to 140% of China's national safe operating space around year 2050 and about 120% by the end of the century. In principle, this means that the energy-chemical nexus will on its own exceed China's national safe operating space without taking into account the contribution from other sectors. The large occupation is again due to the slow removal rate of CO<sub>2</sub> in the atmosphere and because China's share of global population will decrease in the future due to larger population growths in other countries ([United Nations Department of Economic and Social Affairs Population Division, 2019](#)). Generally, we see that the occupied share of the national safe operating space is decreasing over time. However, the impact of achieving carbon neutrality, in terms of staying with the national safe operating space, will not be realized until after the end of century because of the time lag in the atmosphere. Indeed, this further underlines the importance of striving toward carbon neutrality at the fastest possible pace.

**A** Chemical sector - methanol: 2020

Coal Coke-oven gas Natural gas Carbon dioxide

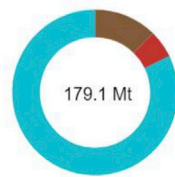
Total production (Mt)



**B** Chemical sector - methanol: 2060

Coal Coke-oven gas Natural gas Carbon dioxide

Total production (Mt)



### Figure 8. Comparison of methanol production between 2020 and 2060

The pie charts show the proportions of methanol production methods in different provinces. The share of the methanol production methods of the whole nation is present in the donut chart. The background color of provinces shows the amount of methanol outputs (Mt per year).

See Figure S7 for plots of other years.

### Technology and sectoral development assessment

Throughout the planning period from 2018 to 2060, different technologies are adopted at different years, showing a clear trend of transformation from the current “gray energy” structure to a future “blue energy” economy as shown in Figure 6. In the electricity sector, renewable energies (i.e., hydro, wind, solar, and biomass) gradually become the main source of power generation while coal-based facilities are being phased out and partially replaced by coal CCS plants. As a negative emission technology, biomass CCS gets adopted after 2050 in order to further push the nexus GHG emission to zero by 2060. For the chemical sector, given the anticipated future increase in methanol demand, an initial increase in fossil-based methanol production can be observed; however, CO<sub>2</sub>-based production appears around 2040 and eventually dominates the technology mix by the end of the planning period. The demand for ammonia is expected to be stable in the future; thus, a sharper phase transition from fossil-based production to N<sub>2</sub>-based process is observed after 2040 when most of the existing plants reach the end of their lifetime.

The proportion of renewable energy would increase dramatically in the energy sector, contributing about 70% of the total China electricity generation in 2060 shown in Figure 7A. National energy production bases at a large scale would be formed in both Xinjiang and Inner Mongolia. Although conventional coal-fired and natural gas power plants would be completely eliminated, coal CCS, biomass, and biomass CCS would be deployed widely throughout the country, which ensure the stability of the whole power system. About 90% of the wind resources, 80% of solar resources, and 80% of the hydro resources of China are distributed in north, northwest, and southwestern regions, respectively (Huang, 2020). However, electricity is mainly consumed in the eastern regions. Therefore, thousands of kilometers of ultra-high voltage electricity transmission lines are needed in order to match this geographical imbalance in China as shown in Figure 7B. The blue energy refinery converts renewable energy to green chemicals. In this way, renewable energy is not only transmitted through the power grids but also transported out of the power grids by green methanol and green ammonia as energy vectors. As is shown in Figure 7B, the power grid has been extended by the transportation of green methanol and green ammonia.

For the chemical sector, the domination of traditional fossil fuel-based methanol and ammonia production methods would fade away, and the blue energy-based chemical production methods, such as CO<sub>2</sub>-based methanol production and ammonia production with H<sub>2</sub> supplied by water electrolysis, will comprise the main approaches. Figures 8 and 9 show the comparison of chemical sectors between 2020 and 2060 at the province level. Although coke oven gas-based and natural gas-based methanol production would be still adopted in many provinces as predominant methods in 2060, their total production outputs only account for approximately 30% of the total national methanol production. Fossil fuel-based ammonia plants would be completely replaced by blue energy-based ammonia plants in 2060. The provinces of Xinjiang, Qinghai, and Inner Mongolia would become national methanol and ammonia production bases. The northwest provinces, which now remain relatively underdeveloped compared to other parts of the country, would become both the energy and chemical production hub in China. These changes would significantly promote the implementation of China’s Western Development Program and Belt and Road Initiative.

### Energy security assessment

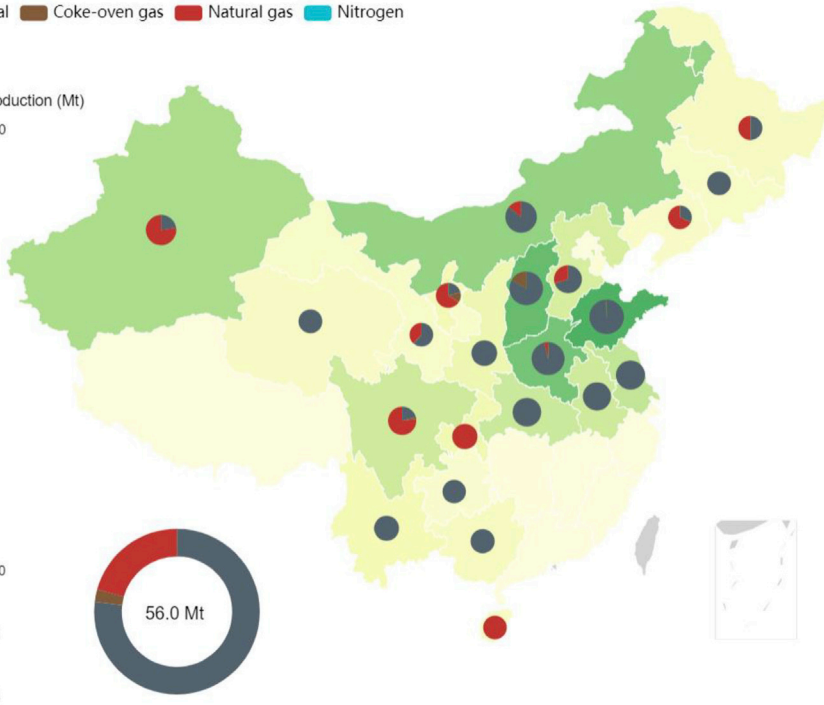
Poor oil reserves and its rapid growth of demand lead to China’s dependency on foreign oil, which has exceeded 70% in 2019 (IEA, 2020), seriously threatening its energy security. The blue energy economy would provide China with an alternative to petroleum-based products and play an important role in ensuring energy security. China has identified methanol as not only a chemical material but also an alternative transportation fuel. China is the first country to start the application of pure methanol (M100) for both passenger cars and trucks (Li et al., 2019). By 2019, the total number of methanol vehicles in China was about 10000 (Zhao, 2019). Even though electric cars far outnumber methanol cars dominating the market of alternative fuel cars, the improved methanol engine offers a new promising direction. On the basis of this framework, the availability of excess methanol production to support the replacement for gasoline is researched in this section.



**A** Chemical sector - ammonia: 2020

Coal   Coke-oven gas   Natural gas   Nitrogen

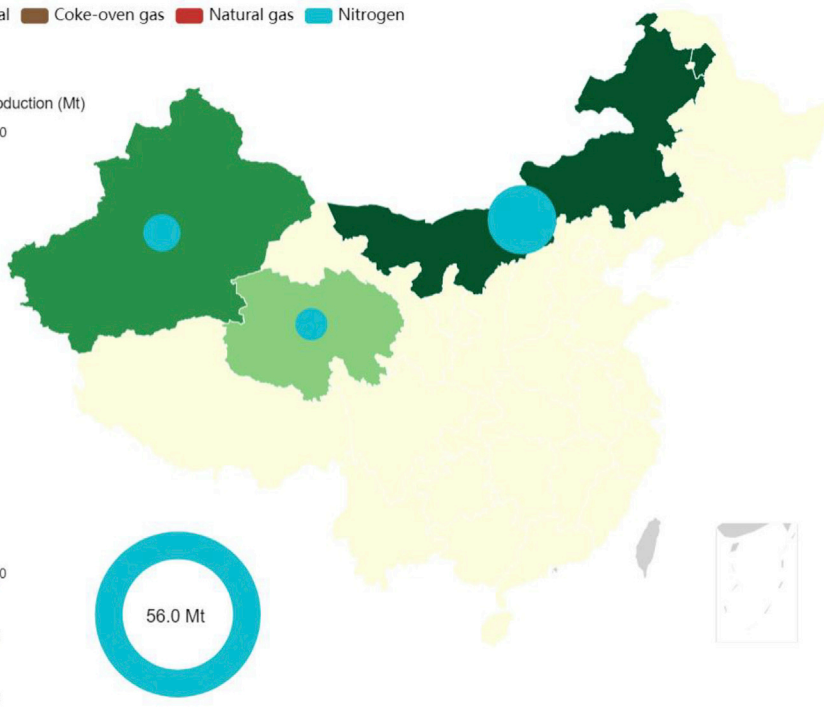
Total production (Mt)



**B** Chemical sector - ammonia: 2060

Coal   Coke-oven gas   Natural gas   Nitrogen

Total production (Mt)



**Figure 9. Comparison of ammonia production between 2020 and 2060**

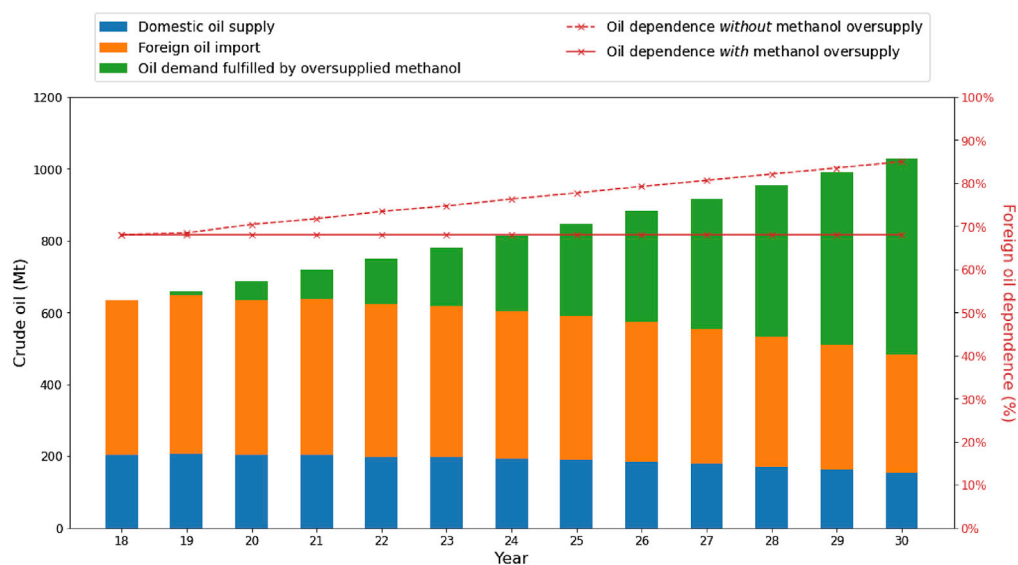
The pie charts show the proportions of ammonia production methods in different provinces. The share of the ammonia production methods of the whole nation is present in the donut chart. The background color of provinces shows the amount of ammonia outputs (Mt per year).

See Figure S8 for plots of other years.

According to a forecast for China's dependency on foreign oil (Wang et al., 2018b), oil consumption in China will rise steadily and peak at 1027 Mt, with the oil foreign dependence ratio exceeding 80% in 2030, as shown as red dotted line in Figure 10. It is assumed that methanol can provide an alternative to gasoline and enhance energy security. Methanol burns more efficiently than gasoline in engines, even though its heat content is only half of gasoline. Therefore, around 1.4 t methanol can replace 1 t of gasoline (Yang and Jackson, 2012). The substituted amount of gasoline can be further converted to standard crude oil according to the fixed coefficient of 0.83 kg gasoline per kg crude oil (Zhili et al., 2019). Based on the previous model, we add an energy security constraint for the previous model, which requires foreign oil dependence to remain around 70%, as shown as the red line in Figure 10. Under this energy security constraint, an extra amount of methanol would be produced to provide an alternative to crude oil shown in green color in Figure 10. It can be seen that the substitution of gasoline with methanol is an effective approach for alleviating the pressures connected with energy security. To keep China's dependency on foreign oil remaining below 70% in 2030, the original oil demand can be reduced to half through the substitution of gasoline with methanol.

### Limitations of the study

In this study, there are several aspects that could be further developed in future studies. Firstly, to achieve the 2060 China carbon neutrality target, efforts from all the sectors are required. However, the herein presented sector-based study in those two largest emitting sectors is considered as one of the most important issues when prompting and designing the carbon neutrality plan. Therefore, our work presents an emission pathway for the energy and chemical sectors by applying the emission share across sectors as of today. The roadmap for other sectors is beyond the scope of this paper. Both the technologies and applications for renewable electricity to chemicals (hydrogen, methanol, ammonia, etc.) are competing at this stage and predicting the future trend is not straightforward. In this research, we focus on methanol and ammonia as they are the leading contributors of CO<sub>2</sub> emission accounting for over 60% in coal chemical sectors in China. Other possible alternative technologies such as electric or hydrogen fuel vehicles are not discussed in this paper.



**Figure 10. Energy security analysis for substitution potential of methanol for gasoline**

The left y axis shows crude oil supply, import, and fulfillment by methanol with stacked bar plots. The right y axis shows China's oil dependence with (solid line) and without (dotted line) methanol oversupply from 2018 to 2030.

Although this study focuses on energy and chemical sectors in China, the findings presented in this work might provide some insights for deploying the concept of sectoral nexus in other sectors. For any sectors that would like to contribute to the carbon neutrality target, the results of this study can be used as benchmarks for estimating and understanding the China's future energy mix and technology development. Achieving the 2060 carbon neutrality target needs efforts from all sectors with effective cooperation. Further work could be concentrated on a system-wide nexus including all sectors, where all sectors are closely linked and cooperated in different levels by sharing both the emission targets and resources.

### Resource availability

#### Lead contact

Further information and requests for resources and reagents should be directed to and will be fulfilled by the Lead Contact, Xiaonan Wang ([chewxia@nus.edu.sg](mailto:chewxia@nus.edu.sg)).

#### Materials availability

This study did not generate new unique reagents.

#### Data and code availability

The input data are available in the [Key Resources Table](#), and the code associated with this article is available from the Lead Contact on reasonable request.

## STAR★METHODS

Detailed methods are provided in the online version of this paper and include the following:

- [KEY RESOURCES TABLE](#)
- [METHOD DETAILS](#)
  - Nomenclature
- [EXTENSION OF THE MODEL FOR SHORT-TERM ENERGY SECURITY](#)

## SUPPLEMENTAL INFORMATION

Supplemental information can be found online at <https://doi.org/10.1016/j.isci.2021.102513>.

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## AUTHOR CONTRIBUTIONS

Y.L. and L.S. collected the data. Y.L. wrote the code, ran the simulations, and visualized the results with contributions from M.R. Y.L., S.L., M.R., and X.W. analyzed the results. Y.L., S.L., and X.W. wrote the paper with contributions from J. P.-R and M.R. X.W. and J. P.-R led the research. All authors contributed to the research concept and paper content.

## DECLARATION OF INTERESTS

The authors declare no competing interests. All affiliations are listed on the title page of the manuscript. All funding sources for this study are listed in the "Acknowledgments" section of the manuscript. The authors and their immediate family members (1) have no financial interests to declare; (2) have no positions to declare and are not members of the journal's advisory board; and (3) have no related patents to declare.

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## STAR★METHODS

### KEY RESOURCES TABLE

REAGENT or RESOURCE	SOURCE	IDENTIFIER
<b>Deposited data</b>		
The current values of CAPEX <sub>t,i,j</sub> for coal, natural gas, nuclear, wind, solar and biomass-electricity	Market information	<a href="https://news.bjx.com.cn/html/20180725/915587.shtml">https://news.bjx.com.cn/html/20180725/915587.shtml</a>
The current values of CAPEX <sub>t,i,j</sub> for coal-CCS, natural gas-CCS and biomass-CCS-electricity	Morris et al.	<a href="https://doi.org/10.1016/j.ijggc.2019.05.016">https://doi.org/10.1016/j.ijggc.2019.05.016</a>
The current values of CAPEX <sub>t,i,j</sub> for hydro-electricity	National Energy Administration	<a href="https://news.bjx.com.cn/html/20171024/857253-2.shtml">https://news.bjx.com.cn/html/20171024/857253-2.shtml</a>
The current values of FOPEX <sub>t,i,j</sub> for coal, coal-CCS, natural gas, natural gas-CCS, nuclear, wind, solar, biomass and biomass-CCS-electricity	Morris et al.	<a href="https://doi.org/10.1016/j.ijggc.2019.05.016">https://doi.org/10.1016/j.ijggc.2019.05.016</a>
The current values of FOPEX <sub>t,i,j</sub> for hydro-electricity	IRENA	<a href="https://www.irena.org/publications/2019/May/Renewable-power-generation-costs-in-2018">https://www.irena.org/publications/2019/May/Renewable-power-generation-costs-in-2018</a>
The current values of VOPEX <sub>t,i,j</sub> for coal and coal-CCS-electricity	China Electricity Council	<a href="https://www.cec.org.cn/detail/index.html?3-172335">https://www.cec.org.cn/detail/index.html?3-172335</a>
The current values of VOPEX <sub>t,i,j</sub> for natural gas and natural gas-CCS-electricity	Huaneng Power International, Inc.	<a href="https://www.hpi.com.cn/_layouts/15/WopiFrame.aspx?sourcedoc=%7B8068a9b6-ebf7-42f7-9a92-da32a83b4069%7D&amp;action=interactivepreview">https://www.hpi.com.cn/_layouts/15/WopiFrame.aspx?sourcedoc=%7B8068a9b6-ebf7-42f7-9a92-da32a83b4069%7D&amp;action=interactivepreview</a>
The current values of VOPEX <sub>t,i,j</sub> for nuclear and hydro electricity	IEA	<a href="https://www.iea.org/reports/projected-costs-of-generating-electricity-2015">https://www.iea.org/reports/projected-costs-of-generating-electricity-2015</a>
The current values of VOPEX <sub>t,i,j</sub> for wind and solar-electricity	Morris et al.	<a href="https://doi.org/10.1016/j.ijggc.2019.05.016">https://doi.org/10.1016/j.ijggc.2019.05.016</a>
The current values of VOPEX <sub>t,i,j</sub> for biomass and biomass-CCS-electricity	Market information	<a href="https://www.sohu.com/a/271751001_422316">https://www.sohu.com/a/271751001_422316</a>
The future values of CAPEX <sub>t,i,j</sub> and FOPEX <sub>t,i,j</sub> for all electricity technologies	Cheng et al.	<a href="https://doi.org/10.1016/j.apenergy.2014.10.023">https://doi.org/10.1016/j.apenergy.2014.10.023</a>
The future values of VOPEX <sub>t,i,j</sub> for all electricity technologies	U.S. Energy Information Administration	<a href="https://www.eia.gov/outlooks/aeo/data/browser/">https://www.eia.gov/outlooks/aeo/data/browser/</a>
The current values of CAPEX <sub>t,i,j</sub> , FOPEX <sub>t,i,j</sub> and VOPEX <sub>t,i,j</sub> for coal, coke-oven gas and natural gas-methanol	Li et al.	<a href="https://doi.org/10.1039/d0se01337d">https://doi.org/10.1039/d0se01337d</a>
The current values of CAPEX <sub>t,i,j</sub> , FOPEX <sub>t,i,j</sub> and VOPEX <sub>t,i,j</sub> for CO <sub>2</sub> -methanol	Pérez-Fortes et al.	<a href="https://doi.org/10.1016/j.apenergy.2015.07.067">https://doi.org/10.1016/j.apenergy.2015.07.067</a>
The current values of CAPEX <sub>t,i,j</sub> , FOPEX <sub>t,i,j</sub> and VOPEX <sub>t,i,j</sub> for coal-ammonia	Habgood et al.	<a href="https://doi.org/10.1016/j.cherd.2015.06.008">https://doi.org/10.1016/j.cherd.2015.06.008</a>
The current values of CAPEX <sub>t,i,j</sub> , FOPEX <sub>t,i,j</sub> and VOPEX <sub>t,i,j</sub> for coke-oven gas and natural gas-ammonia	Lee Pereira et al.	<a href="https://doi.org/10.1016/j.apenergy.2020.115874">https://doi.org/10.1016/j.apenergy.2020.115874</a>
The current values of CAPEX <sub>t,i,j</sub> , FOPEX <sub>t,i,j</sub> and VOPEX <sub>t,i,j</sub> for N <sub>2</sub> -ammonia	Morgan	<a href="https://doi.org/10.7275/11kt-3f59">https://doi.org/10.7275/11kt-3f59</a>
The future values of CAPEX <sub>t,i,j</sub> and FOPEX <sub>t,i,j</sub> for all methanol and ammonia technologies	Mignard	<a href="https://doi.org/10.1016/j.cherd.2013.07.022">https://doi.org/10.1016/j.cherd.2013.07.022</a>

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REAGENT or RESOURCE	SOURCE	IDENTIFIER
The future values of $VOPEX_{t,i,j}$ for all methanol and ammonia technologies	U.S. Energy Information Administration	<a href="https://www.eia.gov/outlooks/aeo/data/browser/">https://www.eia.gov/outlooks/aeo/data/browser/</a>
The current and future values of $CAPEX_{t,i,j}$ , $FOPEX_{t,i,j}$ and $VOPEX_{t,i,j}$ for hydrogen technology (i.e., water electrolysis)	IEA	<a href="https://www.iea.org/reports/the-future-of-hydrogen">https://www.iea.org/reports/the-future-of-hydrogen</a>
The current and future values of $FREIGHT_t$	Li et al.	<a href="https://doi.org/10.1039/d0se01337d">https://doi.org/10.1039/d0se01337d</a>
$DIST_{i,i'}$	Li et al.	<a href="https://doi.org/10.1039/d0se01337d">https://doi.org/10.1039/d0se01337d</a>
R	Take as 8%	N/A
$CF_{i,j}$ for coal, coal-CCS, natural gas, natural gas-CCS, nuclear, biomass and biomass-CCS-electricity	Morris et al.	<a href="https://doi.org/10.1016/j.ijggc.2019.05.016">https://doi.org/10.1016/j.ijggc.2019.05.016</a>
$CF_{i,j}$ for hydro, wind and solar-electricity	Li et al.	<a href="https://doi.org/10.1039/d0se01337d">https://doi.org/10.1039/d0se01337d</a>
$LT_{i,j}$ for coal, coal-CCS, natural gas, natural gas-CCS, nuclear, hydro, wind and solar-electricity	IEA	<a href="https://www.iea.org/reports/projected-costs-of-generating-electricity-2015">https://www.iea.org/reports/projected-costs-of-generating-electricity-2015</a>
$LT_{i,j}$ for biomass and biomass-CCS-electricity	IRENA	<a href="https://www.irena.org/publications/2019/May/Renewable-power-generation-costs-in-2018">https://www.irena.org/publications/2019/May/Renewable-power-generation-costs-in-2018</a>
$CF_{i,j}$ and $LT_{i,j}$ for coal, coke-oven gas and natural gas-methanol	Li et al.	<a href="https://doi.org/10.1039/d0se01337d">https://doi.org/10.1039/d0se01337d</a>
$CF_{i,j}$ and $LT_{i,j}$ for $CO_2$ -methanol	Pérez-Fortes et al.	<a href="https://doi.org/10.1016/j.apenergy.2015.07.067">https://doi.org/10.1016/j.apenergy.2015.07.067</a>
$CF_{i,j}$ and $LT_{i,j}$ for coal-ammonia	Habgood et al.	<a href="https://doi.org/10.1016/j.cherd.2015.06.008">https://doi.org/10.1016/j.cherd.2015.06.008</a>
$CF_{i,j}$ and $LT_{i,j}$ for coke-oven gas and natural gas-ammonia	Lee Pereira et al.	<a href="https://doi.org/10.1016/j.apenergy.2020.115874">https://doi.org/10.1016/j.apenergy.2020.115874</a>
$CF_{i,j}$ and $LT_{i,j}$ for $N_2$ -ammonia	Morgan	<a href="https://doi.org/10.7275/11kt-3f59">https://doi.org/10.7275/11kt-3f59</a>
$CF_{i,j}$ and $LT_{i,j}$ for water electrolysis	IEA	<a href="https://www.iea.org/reports/the-future-of-hydrogen">https://www.iea.org/reports/the-future-of-hydrogen</a>
$CAPEM_{i,j,k}$ for coal, coal-CCS, biomass, biomass-CCS-electricity	Ecoinvent: market for hard coal power plant	<a href="https://v37.ecoquery.ecoinvent.org/Details/LCI/654d160a-d72a-4fff-9668-83a40058e235/290c1f85-4cc4-4fa1-b0c8-2cb7f4276dce">https://v37.ecoquery.ecoinvent.org/Details/LCI/654d160a-d72a-4fff-9668-83a40058e235/290c1f85-4cc4-4fa1-b0c8-2cb7f4276dce</a>
$CAPEM_{i,j,k}$ for natural gas and natural gas-CCS-electricity	Ecoinvent: market for gas power plant, combined cycle, 400MW electrical	<a href="https://v37.ecoquery.ecoinvent.org/Details/LCI/b93c924a-15a8-414f-af2d-ea6520799d29/290c1f85-4cc4-4fa1-b0c8-2cb7f4276dce">https://v37.ecoquery.ecoinvent.org/Details/LCI/b93c924a-15a8-414f-af2d-ea6520799d29/290c1f85-4cc4-4fa1-b0c8-2cb7f4276dce</a>
$CAPEM_{i,j,k}$ for nuclear-electricity	Ecoinvent: nuclear power plant construction, pressure water reactor 1000MW	<a href="https://v37.ecoquery.ecoinvent.org/Details/LCI/40179ee2-96a1-4ef2-825e-1d2aa8e511a4/290c1f85-4cc4-4fa1-b0c8-2cb7f4276dce">https://v37.ecoquery.ecoinvent.org/Details/LCI/40179ee2-96a1-4ef2-825e-1d2aa8e511a4/290c1f85-4cc4-4fa1-b0c8-2cb7f4276dce</a>
$CAPEM_{i,j,k}$ for hydro-electricity	Ecoinvent: market for hydropower plant, run-of-river	<a href="https://v37.ecoquery.ecoinvent.org/Details/LCI/ab1f031b-306f-4672-8732-079e887c3fd5/290c1f85-4cc4-4fa1-b0c8-2cb7f4276dce">https://v37.ecoquery.ecoinvent.org/Details/LCI/ab1f031b-306f-4672-8732-079e887c3fd5/290c1f85-4cc4-4fa1-b0c8-2cb7f4276dce</a>
$CAPEM_{i,j,k}$ for wind-electricity	Ecoinvent: market for wind turbine, 4.5MW, onshore,	<a href="https://v37.ecoquery.ecoinvent.org/Details/LCI/58d9935d-7ffe-4643-afa9-b06353adf99b/290c1f85-4cc4-4fa1-b0c8-2cb7f4276dce">https://v37.ecoquery.ecoinvent.org/Details/LCI/58d9935d-7ffe-4643-afa9-b06353adf99b/290c1f85-4cc4-4fa1-b0c8-2cb7f4276dce</a>
$CAPEM_{i,j,k}$ for solar-electricity	Ecoinvent: market for photovoltaic plant, 570kWp, multi-Si, on open ground	<a href="https://v37.ecoquery.ecoinvent.org/Details/LCI/58a36f1c-7006-47f5-baaa-dc291b647f95/290c1f85-4cc4-4fa1-b0c8-2cb7f4276dce">https://v37.ecoquery.ecoinvent.org/Details/LCI/58a36f1c-7006-47f5-baaa-dc291b647f95/290c1f85-4cc4-4fa1-b0c8-2cb7f4276dce</a>

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REAGENT or RESOURCE	SOURCE	IDENTIFIER
CAPEM <sub>ij,k</sub> for all methanol technologies	Ecoinvent: market for methanol factory	<a href="https://v37.ecoquery.ecoinvent.org/Details/LCI/37d1cacf-a73b-4d3b-91c3-166f261b3a69/290c1f85-4cc4-4fa1-b0c8-2cb7f4276dce">https://v37.ecoquery.ecoinvent.org/Details/LCI/37d1cacf-a73b-4d3b-91c3-166f261b3a69/290c1f85-4cc4-4fa1-b0c8-2cb7f4276dce</a>
CAPEM <sub>ij,k</sub> for all ammonia technologies	Ecoinvent: market for chemical factory, organics,	<a href="https://v37.ecoquery.ecoinvent.org/Details/LCI/314014d9-87eb-4227-a8b9-c78dc0f15620/290c1f85-4cc4-4fa1-b0c8-2cb7f4276dce">https://v37.ecoquery.ecoinvent.org/Details/LCI/314014d9-87eb-4227-a8b9-c78dc0f15620/290c1f85-4cc4-4fa1-b0c8-2cb7f4276dce</a>
CAPEM <sub>ij,k</sub> for water electrolysis	Icelandic New Energy	<a href="https://www.researchgate.net/publication/288874663_Generation_of_the_energy_carrier_HYDROGEN_in_context_with_electricity_buffering_generation_through_fuel_cells">https://www.researchgate.net/publication/288874663_Generation_of_the_energy_carrier_HYDROGEN_in_context_with_electricity_buffering_generation_through_fuel_cells</a>
POPEM <sub>ij,k</sub> together with ELEC <sub>ij</sub> , METH <sub>ij</sub> , AMMO <sub>ij</sub> , HYDO <sub>ij</sub> , CARB <sub>ij</sub> and NOPEM <sub>ij,k</sub> for coal-electricity	Ecoinvent: electricity production, hard coal	<a href="https://v37.ecoquery.ecoinvent.org/Details/LCI/f3e04ca2-4833-483d-92ef-5d2bb9c5ee64/290c1f85-4cc4-4fa1-b0c8-2cb7f4276dce">https://v37.ecoquery.ecoinvent.org/Details/LCI/f3e04ca2-4833-483d-92ef-5d2bb9c5ee64/290c1f85-4cc4-4fa1-b0c8-2cb7f4276dce</a>
POPEM <sub>ij,k</sub> together with ELEC <sub>ij</sub> , METH <sub>ij</sub> , AMMO <sub>ij</sub> , HYDO <sub>ij</sub> , CARB <sub>ij</sub> and NOPEM <sub>ij,k</sub> for coal-CCS, biomass and biomass-CCS-electricity	Yang et al.	<a href="https://doi.org/10.1016/j.apenergy.2019.113483">https://doi.org/10.1016/j.apenergy.2019.113483</a>
POPEM <sub>ij,k</sub> together with ELEC <sub>ij</sub> , METH <sub>ij</sub> , AMMO <sub>ij</sub> , HYDO <sub>ij</sub> , CARB <sub>ij</sub> and NOPEM <sub>ij,k</sub> for natural gas-electricity	Ecoinvent: electricity production, natural gas, combined cycle power plant	<a href="https://v37.ecoquery.ecoinvent.org/Details/LCI/8cf408b9-05b3-4313-a8aa-dd45d035c554/290c1f85-4cc4-4fa1-b0c8-2cb7f4276dce">https://v37.ecoquery.ecoinvent.org/Details/LCI/8cf408b9-05b3-4313-a8aa-dd45d035c554/290c1f85-4cc4-4fa1-b0c8-2cb7f4276dce</a>
POPEM <sub>ij,k</sub> together with ELEC <sub>ij</sub> , METH <sub>ij</sub> , AMMO <sub>ij</sub> , HYDO <sub>ij</sub> , CARB <sub>ij</sub> and NOPEM <sub>ij,k</sub> for natural gas-CCS-electricity	Singh et al.	<a href="https://doi.org/10.1016/j.ijggc.2010.03.006">https://doi.org/10.1016/j.ijggc.2010.03.006</a>
POPEM <sub>ij,k</sub> together with ELEC <sub>ij</sub> , METH <sub>ij</sub> , AMMO <sub>ij</sub> , HYDO <sub>ij</sub> , CARB <sub>ij</sub> and NOPEM <sub>ij,k</sub> for nuclear-electricity	Ecoinvent: electricity production, nuclear, pressure water reactor	<a href="https://v37.ecoquery.ecoinvent.org/Details/LCI/0907b6d0-4f40-4f0a-a2d4-2b1340b879a6/290c1f85-4cc4-4fa1-b0c8-2cb7f4276dce">https://v37.ecoquery.ecoinvent.org/Details/LCI/0907b6d0-4f40-4f0a-a2d4-2b1340b879a6/290c1f85-4cc4-4fa1-b0c8-2cb7f4276dce</a>
POPEM <sub>ij,k</sub> together with ELEC <sub>ij</sub> , METH <sub>ij</sub> , AMMO <sub>ij</sub> , HYDO <sub>ij</sub> , CARB <sub>ij</sub> and NOPEM <sub>ij,k</sub> for hydro-electricity	Ecoinvent: electricity production, hydro, run-of-river	<a href="https://v37.ecoquery.ecoinvent.org/Details/LCI/5bac713a-07eb-4d62-9920-3c2c0cca33c6/290c1f85-4cc4-4fa1-b0c8-2cb7f4276dce">https://v37.ecoquery.ecoinvent.org/Details/LCI/5bac713a-07eb-4d62-9920-3c2c0cca33c6/290c1f85-4cc4-4fa1-b0c8-2cb7f4276dce</a>
POPEM <sub>ij,k</sub> together with ELEC <sub>ij</sub> , METH <sub>ij</sub> , AMMO <sub>ij</sub> , HYDO <sub>ij</sub> , CARB <sub>ij</sub> and NOPEM <sub>ij,k</sub> for wind-electricity	Ecoinvent: electricity production, wind, >3MW turbine, onshore	<a href="https://v37.ecoquery.ecoinvent.org/Details/LCI/4e531afb-1240-4457-9c89-7022b5133ea1/290c1f85-4cc4-4fa1-b0c8-2cb7f4276dce">https://v37.ecoquery.ecoinvent.org/Details/LCI/4e531afb-1240-4457-9c89-7022b5133ea1/290c1f85-4cc4-4fa1-b0c8-2cb7f4276dce</a>
POPEM <sub>ij,k</sub> together with ELEC <sub>ij</sub> , METH <sub>ij</sub> , AMMO <sub>ij</sub> , HYDO <sub>ij</sub> , CARB <sub>ij</sub> and NOPEM <sub>ij,k</sub> for solar-electricity	Ecoinvent: electricity production, photovoltaic, 570kWp open ground installation, multi-Si	<a href="https://v37.ecoquery.ecoinvent.org/Details/LCI/66f4a404-f4f6-41d9-bcf7-c43f87d23742/290c1f85-4cc4-4fa1-b0c8-2cb7f4276dce">https://v37.ecoquery.ecoinvent.org/Details/LCI/66f4a404-f4f6-41d9-bcf7-c43f87d23742/290c1f85-4cc4-4fa1-b0c8-2cb7f4276dce</a>
POPEM <sub>ij,k</sub> together with ELEC <sub>ij</sub> , METH <sub>ij</sub> , AMMO <sub>ij</sub> , HYDO <sub>ij</sub> , CARB <sub>ij</sub> and NOPEM <sub>ij,k</sub> for coal and coke-oven gas-methanol	Li et al.	<a href="https://doi.org/10.1016/j.jclepro.2018.04.051">https://doi.org/10.1016/j.jclepro.2018.04.051</a>
POPEM <sub>ij,k</sub> together with ELEC <sub>ij</sub> , METH <sub>ij</sub> , AMMO <sub>ij</sub> , HYDO <sub>ij</sub> , CARB <sub>ij</sub> and NOPEM <sub>ij,k</sub> for natural gas-methanol	Ecoinvent: methanol production	<a href="https://v37.ecoquery.ecoinvent.org/Details/LCI/282e1d3f-4724-43d1-a5a5-168fb3866e03/290c1f85-4cc4-4fa1-b0c8-2cb7f4276dce">https://v37.ecoquery.ecoinvent.org/Details/LCI/282e1d3f-4724-43d1-a5a5-168fb3866e03/290c1f85-4cc4-4fa1-b0c8-2cb7f4276dce</a>
POPEM <sub>ij,k</sub> together with ELEC <sub>ij</sub> , METH <sub>ij</sub> , AMMO <sub>ij</sub> , HYDO <sub>ij</sub> , CARB <sub>ij</sub> and NOPEM <sub>ij,k</sub> for CO <sub>2</sub> -methanol	Pérez-Fortes et al.	<a href="https://doi.org/10.1016/j.apenergy.2015.07.067">https://doi.org/10.1016/j.apenergy.2015.07.067</a>

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REAGENT or RESOURCE	SOURCE	IDENTIFIER
POPEM <sub>ij,k</sub> together with ELEC <sub>ij</sub> , METH <sub>ij</sub> , AMMO <sub>ij</sub> , HYDO <sub>ij</sub> , CARB <sub>ij</sub> and NOPEM <sub>ij,k</sub> for coal-ammonia	Ecoinvent: ammonia production, partial oxidation	<a href="https://v37.ecoquery.ecoinvent.org/Details/LCI/c652d909-53c1-41fb-b7ef-cb30f3db2140/290c1f85-4cc4-4fa1-b0c8-2cb7f4276dce">https://v37.ecoquery.ecoinvent.org/Details/LCI/c652d909-53c1-41fb-b7ef-cb30f3db2140/290c1f85-4cc4-4fa1-b0c8-2cb7f4276dce</a>
POPEM <sub>ij,k</sub> together with ELEC <sub>ij</sub> , METH <sub>ij</sub> , AMMO <sub>ij</sub> , HYDO <sub>ij</sub> , CARB <sub>ij</sub> and NOPEM <sub>ij,k</sub> for coke-oven gas-ammonia	First-hand survey, see (Li et al., 2020) for procedure details	N/A
POPEM <sub>ij,k</sub> together with ELEC <sub>ij</sub> , METH <sub>ij</sub> , AMMO <sub>ij</sub> , HYDO <sub>ij</sub> , CARB <sub>ij</sub> and NOPEM <sub>ij,k</sub> for natural gas-ammonia	Ecoinvent: ammonia production, steam reforming, liquid	<a href="https://v37.ecoquery.ecoinvent.org/Details/LCI/264ee04e-4093-41a8-840b-49dc47e7e93c/290c1f85-4cc4-4fa1-b0c8-2cb7f4276dce">https://v37.ecoquery.ecoinvent.org/Details/LCI/264ee04e-4093-41a8-840b-49dc47e7e93c/290c1f85-4cc4-4fa1-b0c8-2cb7f4276dce</a>
POPEM <sub>ij,k</sub> together with ELEC <sub>ij</sub> , METH <sub>ij</sub> , AMMO <sub>ij</sub> , HYDO <sub>ij</sub> , CARB <sub>ij</sub> and NOPEM <sub>ij,k</sub> for N <sub>2</sub> -ammonia	Morgan	<a href="https://doi.org/10.7275/11kt-3f59">https://doi.org/10.7275/11kt-3f59</a>
POPEM <sub>ij,k</sub> together with ELEC <sub>ij</sub> , METH <sub>ij</sub> , AMMO <sub>ij</sub> , HYDO <sub>ij</sub> , CARB <sub>ij</sub> and NOPEM <sub>ij,k</sub> for water electrolysis	Icelandic New Energy	<a href="https://www.researchgate.net/publication/288874663_Generation_of_the_energy_carrier_HYDROGEN_in_context_with_electricity_buffering_generation_through_fuel_cells">https://www.researchgate.net/publication/288874663_Generation_of_the_energy_carrier_HYDROGEN_in_context_with_electricity_buffering_generation_through_fuel_cells</a>
TREM <sub>ij,k</sub>	Ecoinvent: market for transport, freight, lorry >32 metric ton, EURO4	<a href="https://v37.ecoquery.ecoinvent.org/Details/LCI/21a13e95-2e8f-407f-a64e-f0d352a860f6/290c1f85-4cc4-4fa1-b0c8-2cb7f4276dce">https://v37.ecoquery.ecoinvent.org/Details/LCI/21a13e95-2e8f-407f-a64e-f0d352a860f6/290c1f85-4cc4-4fa1-b0c8-2cb7f4276dce</a>
FR <sub>τ,τ,k</sub>	Ryberg et al.	<a href="https://doi.org/10.1016/j.procir.2017.11.021">https://doi.org/10.1016/j.procir.2017.11.021</a>
RE <sub>k</sub>	Myhre et al.	<a href="https://www.ipcc.ch/site/assets/uploads/2018/02/WG1AR5_Chapter08_FINAL.pdf">https://www.ipcc.ch/site/assets/uploads/2018/02/WG1AR5_Chapter08_FINAL.pdf</a>
LOSS	Galán-Martín et al.	<a href="https://doi.org/10.1039/c7ee02278f">https://doi.org/10.1039/c7ee02278f</a>
BACKUP	Morris et al.	<a href="https://doi.org/10.1016/j.ijggc.2019.05.016">https://doi.org/10.1016/j.ijggc.2019.05.016</a>
CSPT	Wei et al.	<a href="https://doi.org/10.1016/j.jcou.2014.12.005">https://doi.org/10.1016/j.jcou.2014.12.005</a>
The current values of ELDM <sub>t,i</sub>	China Electric Power Yearbook	<a href="https://data.cnki.net/trade/Yearbook/Single/N2019060101?z=Z025">https://data.cnki.net/trade/Yearbook/Single/N2019060101?z=Z025</a>
The future values of ELDM <sub>t,i</sub>	State Grid	<a href="https://www.sohu.com/a/212053367_418320">https://www.sohu.com/a/212053367_418320</a>
The current values of MEDM <sub>t,i</sub>	Li et al.	<a href="https://doi.org/10.1039/d0se01337d">https://doi.org/10.1039/d0se01337d</a>
The future values of MEDM <sub>t,i</sub>	Argus	<a href="https://www.columbiariverkeeper.org/sites/default/files/2018-08/Credit%20Paper%20on%20NWIW%20Request%20for%20Loan%20Guarantee.pdf">https://www.columbiariverkeeper.org/sites/default/files/2018-08/Credit%20Paper%20on%20NWIW%20Request%20for%20Loan%20Guarantee.pdf</a>
The current values of AMDM <sub>t,i</sub>	First-hand survey, see (Li et al., 2020) for procedure details	N/A
The future values of AMDM <sub>t,i</sub>	Yang	<a href="https://www.ccr.com.cn/c/2020-03-24/623994.shtml">https://www.ccr.com.cn/c/2020-03-24/623994.shtml</a>
EXCAP <sub>t,i,j</sub> for all electricity technologies	China Electric Power Yearbook	<a href="https://data.cnki.net/trade/Yearbook/Single/N2019060101?z=Z025">https://data.cnki.net/trade/Yearbook/Single/N2019060101?z=Z025</a>
EXCAP <sub>t,i,j</sub> for all methanol technologies	Li et al.	<a href="https://doi.org/10.1039/d0se01337d">https://doi.org/10.1039/d0se01337d</a>
EXCAP <sub>t,i,j</sub> for all ammonia technologies	First-hand survey, see (Li et al., 2020) for procedure details	N/A
POT <sub>t,i,j</sub> for coal, coal-CCS, natural gas, natural gas-CCS and nuclear-electricity	Assumed to increase with demand	N/A
POT <sub>t,i,j</sub> for hydro, wind and solar-electricity	Li et al.	<a href="https://doi.org/10.1039/d0se01337d">https://doi.org/10.1039/d0se01337d</a>

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REAGENT or RESOURCE	SOURCE	IDENTIFIER
POT <sub>t,i,j</sub> for biomass and biomass-CCS-electricity	Kang et al.	<a href="https://doi.org/10.1016/j.rser.2020.109842">https://doi.org/10.1016/j.rser.2020.109842</a>
POT <sub>t,i,j</sub> for coal and coke-oven gas-methanol	Assumed to increase with demand	N/A
POT <sub>t,i,j</sub> for natural gas-methanol	National Development and Reform Commission	<a href="http://www.chemchina.com.cn/portal/xwymt/hyxw/webinfo/2012/11/1352683957825442.htm">http://www.chemchina.com.cn/portal/xwymt/hyxw/webinfo/2012/11/1352683957825442.htm</a>
POT <sub>t,i,j</sub> for CO <sub>2</sub> -methanol	Unconstrained	N/A
POT <sub>t,i,j</sub> for coal, coke-oven gas and natural gas-ammonia	Assumed constant due to stable demand	N/A
POT <sub>t,i,j</sub> for N <sub>2</sub> -ammonia	Unconstrained	N/A
POT <sub>t,i,j</sub> for water electrolysis	Unconstrained	N/A
AGR <sub>t</sub> for coal, coal-CCS, natural gas, natural gas-CCS, nuclear, biomass and biomass-CCS-electricity	Unconstrained	N/A
AGR <sub>t</sub> for hydro, wind and solar-electricity	Energy Foundation	<a href="https://www.efchina.org/Reports-zh/china-2050-high-renewable-energy-penetration-scenario-and-roadmap-study-zh">https://www.efchina.org/Reports-zh/china-2050-high-renewable-energy-penetration-scenario-and-roadmap-study-zh</a>
AGR <sub>t</sub> for all methanol and ammonia technologies	Li et al.	<a href="https://doi.org/10.1039/d0se01337d">https://doi.org/10.1039/d0se01337d</a>
AGR <sub>t</sub> for water electrolysis	Unconstrained	N/A
RGR <sub>t</sub> for coal, coal-CCS, natural gas, natural gas-CCS, nuclear, biomass and biomass-CCS-electricity	Unconstrained	N/A
RGR <sub>t</sub> for hydro, wind and solar-electricity	Realmonte et al.	<a href="https://doi.org/10.1038/s41467-019-10842-5">https://doi.org/10.1038/s41467-019-10842-5</a>
RGR <sub>t</sub> for all methanol and ammonia technologies	Li et al.	<a href="https://doi.org/10.1039/d0se01337d">https://doi.org/10.1039/d0se01337d</a>
RGR <sub>t</sub> for water electrolysis	Unconstrained	N/A
TGT <sub>t</sub>	Zhang	<a href="https://www.enerarxiv.org/page/thesis.html?id=2464">https://www.enerarxiv.org/page/thesis.html?id=2464</a>
MEOS <sub>t</sub>	Wang et al.	<a href="https://doi.org/10.1016/j.energy.2018.08.127">https://doi.org/10.1016/j.energy.2018.08.127</a>
<b>Software and algorithms</b>		
Python v3.7.9	Python Software Foundation	<a href="https://www.python.org/">https://www.python.org/</a>
Gurobi v9.0.2	Gurobi Optimization	<a href="https://www.gurobi.com/">https://www.gurobi.com/</a>
ECharts v2	Apache Software Foundation	<a href="https://echarts.apache.org/en/index.html">https://echarts.apache.org/en/index.html</a>

## METHOD DETAILS

### Nomenclature

The definitions of all symbols appearing in the optimization model above are summarized in the following table.

Symbol	Definition
<b>Sets:</b>	
$t \in T$	Period of time from 2018 to 2060
$i \in I$	Provinces in China excluding Hong Kong, Macao and Taiwan

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**Continued**

Symbol	Definition
$j \in J$	Technologies, i.e., Coal-electricity, Coal-CCS-electricity, Natural gas-electricity, Natural gas-CCS-electricity, Nuclear-electricity, Hydro-electricity, Wind-electricity, Solar-electricity, Biomass-electricity, Biomass-CCS-electricity, Coal-methanol, Coke-oven gas-methanol, Natural gas-methanol, CO <sub>2</sub> -methanol, Coal-ammonia, Coke-oven gas-ammonia, Natural gas-ammonia, N <sub>2</sub> -ammonia and Water electrolysis
$k \in K$	Greenhouse gases, i.e., CO <sub>2</sub> , CH <sub>4</sub> and N <sub>2</sub> O. GHG stands for all greenhouse gas converted to CO <sub>2</sub> -eq according to GWP-100a.

*Independent decision variables:*

$x_{t,i,j}$	Capacity expansion of technology $j$ in province $i$ in year $t$
$y_{t,i,j}$	Operation of technology $j$ in province $i$ in year $t$
$z_{t,i,i'}^E$	Transfer of electricity from province $i$ to $i'$ in year $t$
$z_{t,i,i'}^M$	Transfer of methanol from province $i$ to $i'$ in year $t$
$z_{t,i,i'}^A$	Transfer of ammonia from province $i$ to $i'$ in year $t$

*Dependent variables:*

$u_{t,i,j}$	Usable capacity of technology $j$ in province $i$ in year $t$
$e_{t,k}^P$	Positive emission of GHG $k$ in year $t$
$e_{t,k}^N$	Negative emission of GHG $k$ in year $t$
$e_{t,k}^C$	Equivalent emission of GHG $k$ in year $t$ due to GHG species conversion
$m_{t,k}$	Cumulative mass of GHG $k$ in the atmosphere in year $t$
$c_{t,k}$	Cumulative concentration of GHG $k$ in the atmosphere in year $t$
$r_t$	Change in radiative forcing in year $t$

*Parameters:*

$CAPEX_{t,i,j}$	Capital cost of technology $j$ in province $i$ in year $t$
$FOPEX_{t,i,j}$	Fixed operating cost of technology $j$ in province $i$ in year $t$
$VOPEX_{t,i,j}$	Variable operating cost of technology $j$ in province $i$ in year $t$
$FREIGHT_t$	Road transportation freight rate in year $t$
$DIST_{i,i'}$	Distance between province $i$ and $i'$
$R$	Future cash flow discount rate
$CF_{i,j}$	Capacity factor of technology $j$ in province $i$
$LT_{i,j}$	Lifetime of technology $j$ facility in province $i$

(Continued on next page)

**Continued**

Symbol	Definition
$ELEC_{i,j}$	Electricity produced from unit operation of technology $j$ in province $i$ , negative for consumption
$METH_{i,j}$	Methanol produced from unit operation of technology $j$ in province $i$ , negative for consumption
$AMMO_{i,j}$	Ammonia produced from unit operation of technology $j$ in province $i$ , negative for consumption
$HYDO_{i,j}$	Hydrogen produced from unit operation of technology $j$ in province $i$ , negative for consumption
$CARB_{i,j}$	Carbon dioxide captured from unit operation of technology $j$ in province $i$ , negative for consumption
$CAPEM_{i,j,k}$	Emission of GHG $k$ from capacity expansion of technology $j$ in province $i$
$POPEM_{i,j,k}$	Positive emission of GHG $k$ from operation of technology $j$ in province $i$
$NOPEM_{i,j,k}$	Negative emission of GHG $k$ from operation of technology $j$ in province $i$
$TREM'_{i,i',k}$	Emission of GHG $k$ from road transportation from province $i$ to $i'$
$FR_{\tau,t,k}$	Fraction of GHG $k$ emitted in year $\tau$ that remains in the atmosphere in year $t$
$RE_k$	Radiative efficiency of GHG $k$
LOSS	Electricity transmission loss rate
BACKUP	Intermittent electricity backup rate
CSPOT	Carbon storage potential
$ELDM_{t,i}$	Electricity demand of province $i$ in year $t$
$MEDM_{t,i}$	Methanol demand of province $i$ in year $t$
$AMDM_{t,i}$	Ammonia demand of province $i$ in year $t$
$EXCAP_{t,i,j}$	Existing capacity of technology $j$ in province $i$ constructed in year $t$ , which is before 2018
$POT_{t,i,j}$	Potential of technology $j$ in province $i$ in year $t$
$AGR_j$	Maximum absolute growth rate of capacity for technology $j$
$RGR_j$	Maximum relative growth rate of capacity for technology $j$
$TGT_t$	GHG emission target in year $t$
$MEOS_t$	Oversupply of methanol in year $t$

For the study of energy-chemical nexus in this work, electricity is selected as the representative product for energy sector which can be generated from coal, natural gas, hydro, wind, solar and biomass, as well as carbon capture and storage (CCS) integrated technologies including coal-CCS, natural gas-CCS and biomass-CCS. For the chemical sector, methanol and ammonia are considered and they can both be produced conventionally from coal, coke-oven gas and natural gas. Specially, methanol and ammonia can also be synthesized directly from  $CO_2$  and  $N_2$ , respectively, with  $H_2$  supplied by water electrolysis. To study the transition of China from its current energy structure to a future “blue energy” economy under the 2060



carbon neutrality goal, the nexus optimization model minimizes net present cost over a time frame of more than 40 years from 2018 to 2060.

$$\min_{x, y, z} \sum_t \frac{1}{(1+R)^t} \left( \sum_{i,j} (\text{CAPEX}_{t,i,j}) x_{t,i,j} + \sum_{i,j,\tau < t \wedge \tau + \text{LT}_{i,j} \geq t} (\text{FOPEX}_{\tau,i,j}) \right. \\ \left. \times (x_{\tau,i,j} + \text{EXCAP}_{\tau,i,j}) + \sum_{i,j} (\text{VOPEX}_{t,i,j}) y_{t,i,j} + \sum_{i,i'} (\text{FREIGHT}_t) (\text{DIST}_{i,i'}) (z_{t,i,i'}^M + z_{t,i,i'}^A) \right) \quad (\text{Equation 1})$$

where  $t$ ,  $i$  and  $j$  are the indices of years from 2018 to 2060, provinces in China (excluding Hong Kong, Macao and Taiwan) and technologies, respectively. As decision variables,  $x_{t,i,j}$  and  $y_{t,i,j}$  represent capacity expansion and operation of technology  $j$  in province  $i$  in year  $t$ , respectively.  $z_{t,i,i'}^E$ ,  $z_{t,i,i'}^M$  and  $z_{t,i,i'}^A$  are the transfer of electricity, methanol and ammonia from province  $i$  to an adjacent province  $i'$  in year  $t$ , respectively. In terms of model parameters,  $R$  is the future cash flow discount rate for calculating net present cost which is taken as 8% in this work.  $\text{LT}_{i,j}$  represents the lifetime of technology  $j$ 's facility in province  $i$  and  $\text{EXCAP}_{\tau,i,j}$  is the existing capacity of technology  $j$  in province  $i$  constructed in year  $\tau$ , which is before the planning period.  $\text{CAPEX}_{t,i,j}$ ,  $\text{FOPEX}_{\tau,i,j}$  and  $\text{VOPEX}_{t,i,j}$  are the capital cost, fixed operating cost and variable operating cost of technology  $j$  in province  $i$  in year  $t$ , respectively.  $\text{FREIGHT}_t$  is the road transportation freight rate of chemicals in year  $t$  while  $\text{DIST}_{i,i'}$  denotes inter-provincial distance between province  $i$  and  $i'$ . The nexus optimization model is solved subject to various operation and emission constraints. Firstly, product demands in both energy and chemical sectors should always be satisfied.

$$\sum_j (\text{ELEC}_{i,j}) y_{t,i,j} - \sum_{i'} z_{t,i,i'}^E + \sum_{i'} (1 - (\text{LOSS}) (\text{DIST}_{i',i})) z_{t,i',i}^E \geq \text{ELDM}_{t,i} \quad \forall t, i \quad (\text{Equation 2})$$

$$\sum_j (\text{METH}_{i,j}) y_{t,i,j} - \sum_{i'} z_{t,i,i'}^M + \sum_{i'} z_{t,i',i}^M \geq \text{MEDM}_{t,i} \quad \forall t, i \quad (\text{Equation 3})$$

$$\sum_j (\text{AMMO}_{i,j}) y_{t,i,j} - \sum_{i'} z_{t,i,i'}^A + \sum_{i'} z_{t,i',i}^A \geq \text{AMDM}_{t,i} \quad \forall t, i \quad (\text{Equation 4})$$

where  $\text{ELEC}_{i,j}$ ,  $\text{METH}_{i,j}$  and  $\text{AMMO}_{i,j}$  denote electricity, methanol and ammonia produced from unit operation of technology  $j$  in province  $i$ , respectively, which take negative values for consumption.  $\text{LOSS}$  is the electricity transmission loss rate while  $\text{ELDM}_{t,i}$ ,  $\text{MEDM}_{t,i}$  and  $\text{AMDM}_{t,i}$  represent electricity, methanol and ammonia demand of province  $i$  in year  $t$ , respectively. In order to have sufficient supply of  $\text{H}_2$  and captured  $\text{CO}_2$  for chemical synthesis,

$$\sum_j (\text{HYDO}_{i,j}) y_{t,i,j} \geq 0 \quad \forall t, i \quad (\text{Equation 5})$$

$$\sum_j (\text{CARB}_{i,j}) y_{t,i,j} \geq 0 \quad \forall t, i \quad (\text{Equation 6})$$

where  $\text{HYDO}_{i,j}$  and  $\text{CARB}_{i,j}$  are hydrogen produced and carbon dioxide captured from unit operation of technology  $j$  in province  $i$ , respectively, with negative values for consumption. Due to the anticipated vast deployment of CCS-integrated technologies in the future, a significant amount of  $\text{CO}_2$  would be captured and permanently sequestered underground, which should not exceed the national storage potential.

$$\sum_{t,i,j} (\text{CARB}_{i,j}) y_{t,i,j} \leq \text{CSPOT} \quad (\text{Equation 7})$$

where  $\text{CSPOT}$  denotes the potential of carbon storage in China. Given the intermittent nature of hydro, wind and solar-based power generation, unless consumed immediately on the spot, a certain amount of backup generation from conventional technologies is required.

$$(\text{BACKUP}) \left( \sum_{j \in J_1} (\text{ELEC}_{i,j}) y_{t,i,j} + \sum_{j \in J_2} (\text{ELEC}_{i,j}) y_{t,i,j} \right) \leq \sum_{j \in J_3} (\text{ELEC}_{i,j}) y_{t,i,j} \quad \forall t, i \quad (\text{Equation 8})$$

where  $\text{BACKUP}$  is the intermittent electricity backup rate and technology sets  $J_1 = \{\text{Hydro-electricity, Wind-electricity, Solar-electricity}\}$ ,  $J_2 = \{\text{CO}_2\text{-methanol, N}_2\text{-ammonia, Water electrolysis}\}$ ,  $J_3 = \{\text{Coal-electricity, Coal-CCS-electricity, Natural gas-electricity, Natural gas-CCS-electricity, Biomass-electricity, Biomass-CCS-electricity}\}$ . Considering existing capacities as well as the construction and retirement of facilities, technology capacity can be computed and operation should always be kept within capacity.

$$u_{t,i,j} = \sum_{\tau < t \wedge \tau + LT_{i,j} \geq t} x_{\tau,i,j} + EXCAP_{\tau,i,j} \quad \forall t, i, j \quad (\text{Equation 9})$$

$$y_{t,i,j} \leq (CF_{i,j})(1 \text{ year})u_{t,i,j} \quad \forall t, i, j \quad (\text{Equation 10})$$

where  $u_{t,i,j}$  denotes the usable capacity of technology  $j$  in province  $i$  in year  $t$  and  $EXCAP_{\tau,i,j}$  is the existing capacity of technology  $j$  in province  $i$  constructed in year  $\tau$ , which is before the planning period.  $LT_{i,j}$  and  $CF_{i,j}$  are the facility lifetime and capacity factor of technology  $j$  in province  $i$ , respectively. Technology capacities are also subject to the limit of natural resources, especially for hydro, wind, solar and biomass, which is captured by technology exploitable potentials.

$$u_{t,i,j} \leq POT_{t,i,j} \quad \forall t, i, j \quad (\text{Equation 11})$$

where  $POT_{t,i,j}$  is the potential of technology  $j$  in province  $i$  in year  $t$ . In the real world, the national growth rate of new capacities (i.e., construction speed) should also be constrained within a reasonable range.

$$\sum_i x_{t,i,j} \leq AGR_j \quad \forall t, j \quad (\text{Equation 12})$$

$$\sum_i x_{t,i,j} \leq (RGR_j) \sum_i u_{t,i,j} \quad \forall t, j \quad (\text{Equation 13})$$

where  $AGR_j$  and  $RGR_j$  are the maximum absolute and relative growth rate of capacity for technology  $j$ , respectively. In order to realize the carbon neutrality commitment by 2060, regulations on greenhouse gas (GHG) emissions need to be enforced.

$$e_{t,k}^P = \sum_{i,j} (CAPEM_{i,j,k})x_{t,i,j} + (\text{POPEM}_{i,j,k})y_{t,i,j} + \sum_{i,i'} (\text{TREM}_{i,i',k}) (z_{t,i,i'}^M + z_{t,i,i'}^A) \quad \forall t, k \quad (\text{Equation 14})$$

$$e_{t,k}^N = \sum_{i,j} (\text{NOPEM}_{i,j,k})y_{t,i,j} \quad \forall t, k \quad (\text{Equation 15})$$

where  $k$  is the index of GHG species. In particular, three GHGs, i.e.,  $\text{CO}_2$ ,  $\text{CH}_4$  and  $\text{N}_2\text{O}$ , are explicitly modeled in this work and a fourth index (written as GHG) representing all GHGs converted to  $\text{CO}_2$  equivalents ( $\text{CO}_2\text{-eq}$ ) according to 100-year global warming potential (GWP-100a) from the Fifth Assessment Report (AR5) of the United Nations Intergovernmental Panel on Climate Change (IPCC) (Myhre et al., 2013) is included to account for total GHG emissions.  $e_{t,k}^P$  and  $e_{t,k}^N$  denote the positive and negative emission of GHG  $k$  in year  $t$ , respectively. Since positive emission occurs in the construction phase for all technologies in this work,  $CAPEM_{i,j,k}$  represents the (positive) emission of GHG  $k$  from capacity expansion of technology  $j$  in province  $i$ .  $\text{POPEM}_{i,j,k}$  and  $\text{NOPEM}_{i,j,k}$  are the positive and negative emission of GHG  $k$  from operation of technology  $j$  in province  $i$ , respectively.  $\text{TREM}_{i,i',k}$  is the (positive) emission of GHG  $k$  from road transportation from province  $i$  to  $i'$ .

$$e_{t,\text{GHG}}^P + e_{t,\text{GHG}}^N \leq \text{TGT}_t \quad \forall t \quad (\text{Equation 16})$$

where  $\text{TGT}_t$  is the GHG emission target in year  $t$ . For planetary boundaries assessment, two relevant boundaries on climate change, i.e., atmospheric  $\text{CO}_2$  concentration and energy imbalance at top of atmosphere, are analyzed in this work. Positive emissions are emitted directly to the atmosphere, so their natural decay is considered while negative emissions are sequestered underground and their natural decay is ignored. The mass of GHG in the atmosphere can be estimated as Equation 17. Note that for  $\text{CO}_2$ , the conversion (i.e., decay) of  $\text{CH}_4$  to  $\text{CO}_2$  in the atmosphere is also included as input while for other GHGs, that special term ( $e_{t,k}^C$ ) equals zero.

$$m_{t,k} = \sum_{\tau \leq t} (\text{FR}_{\tau,t,k}) (e_{\tau,k}^P + e_{\tau,k}^C) + e_{\tau,k}^N \quad \forall t, k \in \{\text{CO}_2, \text{CH}_4, \text{N}_2\text{O}\} \quad (\text{Equation 17})$$

where  $m_{t,k}$  is the cumulative mass (starting from the beginning of the planning period) of GHG  $k$  in the atmosphere in year  $t$  and  $\text{FR}_{\tau,t,k}$  is the fraction of GHG  $k$  emitted in year  $\tau$  that remains in the atmosphere in year  $t$ .  $e_{t,k}^C$  is the equivalent emission of GHG  $k$  in year  $t$  due to GHG species conversion in the atmosphere, which is specially included for  $\text{CO}_2$  after the beginning of the planning period (i.e.,  $e_{t,k}^C = 0$  otherwise). In particular, the input of atmospheric  $\text{CO}_2$  from conversion of  $\text{CH}_4$  in the atmosphere is calculated as follows.

$$e_{t,\text{CO}_2}^C = \left( \frac{M_{\text{CO}_2}}{M_{\text{CH}_4}} \right) \sum_{\tau \leq t-1} (\text{FR}_{\tau,t-1,\text{CH}_4} - \text{FR}_{\tau,t,\text{CH}_4}) e_{\tau,\text{CH}_4}^P \quad \forall t > 2018 \quad (\text{Equation 18})$$

where  $M_{\text{CO}_2}$  and  $M_{\text{CH}_4}$  are the molar mass of  $\text{CO}_2$  and  $\text{CH}_4$ , respectively. The natural decay of atmospheric GHGs, as reflected by  $\text{FR}_{\tau,t,k}$ , can be calculated as follows. For GHGs other than  $\text{CO}_2$ ,

$$FR_{\tau,t,k} = \exp\left(-\frac{t-\tau}{\alpha_k}\right) \quad \forall \tau, t \geq \tau, k \in \{\text{CH}_4, \text{N}_2\text{O}\} \quad (\text{Equation 19})$$

where  $\alpha_k$  is the atmospheric lifetime of GHG  $k$ . In particular, from IPCC AR5 (Myhre et al., 2013),  $\alpha_{\text{CH}_4} = 12.4$  years and  $\alpha_{\text{N}_2\text{O}} = 121$  years. For  $\text{CO}_2$ ,

$$FR_{\tau,t,\text{CO}_2} = a_0 + \sum_{n=1}^3 a_n \exp\left(-\frac{t-\tau}{\alpha_n}\right) \quad \forall \tau, t \geq \tau \quad (\text{Equation 20})$$

where  $a_0 = 0.212$ ,  $a_1 = 0.244$ ,  $a_2 = 0.336$ ,  $a_3 = 0.207$ ,  $\alpha_1 = 336.4$  years,  $\alpha_2 = 27.89$  years and  $\alpha_3 = 4.055$  years. The coefficients are based on Joos et al. and were used for fitting model responses in  $\text{CO}_2$  related to a  $\text{CO}_2$  emission pulse of 100 GtC added to an existing  $\text{CO}_2$  concentration of 389 ppm, without climate feedback (Joos et al., 2013). A unit conversion gives atmospheric GHG concentration.

$$c_{t,k} = \frac{1/M_k}{m_{\text{air}}/M_{\text{air}}} (10^6 \text{ ppm}) m_{t,k} \quad \forall t, k \in \{\text{CO}_2, \text{CH}_4, \text{N}_2\text{O}\} \quad (\text{Equation 21})$$

where  $c_{t,k}$  is the cumulative concentration (starting from the beginning of the planning period) of GHG  $k$  in the atmosphere in year  $t$ .  $M_k$  is the molar mass of GHG  $k$ ,  $m_{\text{air}} = 5.15 \times 10^{18}$  kg is the mass of the atmosphere and  $M_{\text{air}} = 28.97$  g/mol is the molar mass of air. The change in radiative forcing is a function of GHG concentrations.

$$r_t = \sum_{k \in \{\text{CO}_2, \text{CH}_4, \text{N}_2\text{O}\}} (\text{RE}_k) c_{t,k} \quad \forall t \quad (\text{Equation 22})$$

where  $r_t$  denotes the change in radiative forcing in year  $t$  and  $\text{RE}_k$  is the radiative efficiency of GHG  $k$ . In particular, from IPCC AR5 (Myhre et al., 2013),  $\text{RE}_{\text{CO}_2} = 1.37 \times 10^{-5} \text{ W m}^{-2} \text{ ppb}^{-1}$ ,  $\text{RE}_{\text{CH}_4} = 3.63 \times 10^{-4} \text{ W m}^{-2} \text{ ppb}^{-1}$  and  $\text{RE}_{\text{N}_2\text{O}} = 3.00 \times 10^{-3} \text{ W m}^{-2} \text{ ppb}^{-1}$ . For planetary boundaries analysis, both the emission and natural decay of the three GHGs (i.e.,  $\text{CO}_2$ ,  $\text{CH}_4$  and  $\text{N}_2\text{O}$ ) are explicitly modeled from 2018 to 2060. In order to assess the effects of GHGs emitted during the planning period at the end of this century, and also considering China's 2060 carbon neutrality goal which requires net zero national GHG emissions after 2060, the natural decay (i.e.,  $FR_{\tau,t,k}$ ) of those three atmospheric GHGs is further extrapolated until 2100.

## EXTENSION OF THE MODEL FOR SHORT-TERM ENERGY SECURITY

China's foreign oil dependence has already reached 64.4% by 2016 and the number is anticipated to continuously increase until exceeding 80% by 2030 (Wang et al., 2018b), which poses the problem of short-term energy security to the country. Thus, the model can be extended to explicitly focus on China's dependence on crude oil import in the near future from 2018 to 2030. In order to over-produce a certain amount of methanol (i.e., above demand) to substitute for gasoline, a new constraint can be added.

$$\sum_{i,j} (\text{METH}_{i,j}) y_{t,i,j} \geq \sum_i \text{MEDM}_{t,i} + \text{MEOS}_t \quad \forall t \leq 2030 \quad (\text{Equation 23})$$

where  $\text{MEOS}_t$  is the methanol oversupply in year  $t$ , which is targeted at stabilizing foreign oil dependence at the level of 2018 in this work. Since the growth rate of methanol facilities is calculated from historical data, which is rather conservative, the optimization model can be solved again with exactly the same objective and constraints as stated previously except the constraint on methanol growth rate together with the additional Equation 23 to assess the feasibility of the energy-chemical nexus in mitigating the issue of short-term energy security for China.