Master's thesis

NTNU
Norwegian University of Science and Technology
Faculty of Engineering
Department of Energy and Process Engineering

Francis Isidore Barre

The global cycle of Graphite

A dynamic Material Flow Analysis (2020-2050) of the natural, synthetic and recycled graphite value chains to understand the supply of LIB anodes

Master's thesis in Industrial Ecology
Supervisor: Daniel Beat Müller (NTNU)
Co-supervisor: Romain Guillaume Billy (NTNU), Fernando Aguilar Lopez (NTNU), Gunstein Skomedal (VIANODE)
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Preface

This master's thesis was conducted during the spring semester of 2023 as the final step of my Master of Science in Industrial Ecology at the Norwegian University of Science and Technology in Trondheim and builds on a semester project carried on during the fall semester in 2022.

I would like to thank my supervisors at NTNU, Daniel B Müller, Romain G. Billy and Fernando Aguilar Lopez, for supporting me throughout the semester, showing me the right direction, and always keeping the expectations high. I also want to thank my external co-supervisor from Vianode, Gunnstein Skomedal, for his time, dedication, and his extended knowledge about graphite, and Robin Hansson for his always interesting input on graphite recycling. The different experts that agreed to take some of their time to discuss with me were also key in my understanding of graphite.

I am grateful to have been surrounded by amazing people at IndEcol, which I greatly thank for their support throughout the semester, both motivating me to keep focus and determination and also putting emphasis on the importance of breaks and free time. I also thank my family, which has kept me motivated from a distance, and always reminded me of what mattered most.

Francis Isidore Barre

Abstract

The decarbonisation of the transportation sector is expected to rely on electric vehicles (EV), mainly equipped with Lithium Ion Batteries (LIB). The primary anode material for these batteries is graphite. Graphite is either mined and called natural graphite or graphitised from a carbon precursor, usually needle coke, and called synthetic graphite. There are concerns that the rapid penetration of LIBs could disrupt the natural and synthetic graphite value chains.

A parametric model was developed to quantify the flows in the graphite value chain and its use in electric vehicles between 2020 and 2050 in several scenarios. This model provides the amount of needle coke and graphite ore needed to ensure the supply of the value chains. The scenarios comprise vehicle ownership, size of vehicles, EV penetration, battery chemistries, recycling technologies and the share of natural versus synthetic graphite in batteries. Parallely, a model of petroleum refineries was developed to quantify the maximum supply of needle coke in the different penetration scenarios and compare it with the demand. On the natural graphite side, an analysis of the current situation was conducted to understand the geographical origin of the supply as well as potential barriers to its expansion. Significant attention has been paid to the importance of uncertainty in the model, using Monte Carlo simulation to assess the uncertainty of results.

A parametric model of the demand for graphite was developed. The results can be visualised online at http://129.241.153.120:8052. The range of the demand for graphite ore and needle coke varies greatly between the scenarios, with 1312 to 25673 ktons of graphite ore and 3945 to 22301 ktons of needle coke in 2050 in the six selected scenarios. The maximum supply for needle coke varies from 3596 to 39123 ktons depending on EV penetration and flexibility in refineries. The study revealed the dependence of LIB production on the extraction of hydrocarbons leads to supply constraints for synthetic graphite. In scenarios with fast EV penetration, less petroleum is required by the transportation sector, and the supply of needle coke is constrained as a consequence. By replacing conventional vehicles, electric vehicles cut their own supply of needle coke and synthetic graphite. On the other side, graphite ore is abundant, but the lack of infrastructure and development time makes it unlikely to see its supply keep up with the galloping demand.

Only the combination of the most efficient recycling techniques with societal changes, such as lower vehicle ownership and smaller vehicles, can mitigate the risk of graphite supply shortages. However, such recycling rates are impossible to implement today, as the ageing mechanisms of graphite in LIBs are still not fully understood. Therefore, sobriety has a crucial role in decreasing the demand for graphite. It would also bring co-benefits, as smaller vehicles could use alternative battery chemistries and reducing the overall production of EVs would limit environmental impacts related to graphite production.

Sammendrag

Dekarboniseringen av transportsektoren forventes å være avhengig av elektriske kjøretøy (EV), hovedsakelig utstyrt med litiumionbatterier (LIB). Det primære anodematerialet for disse batteriene er grafitt. Grafitt utvinnes enten fra gruver og kalles naturlig grafitt, eller grafittiseres fra en karbonforløper, vanligvis nålekoks, og kalles syntetisk grafitt. Det er bekymring for at den raske veksten i markedsandelen til LIB-er kan forstyrre naturlige og syntetiske grafitt-verdikjeder.

En parametrisk modell ble utviklet for å kvantifisere strømmene i grafittverdikjeden og bruken i elektriske kjøretøy mellom 2020 og 2050 i flere scenarioer. Denne modellen gir mengden nålekoks og grafittmalm som trengs for å sikre forsyningen av verdikjedene. Scenariene omfatter kjøretøyets eierskap, størrelse på kjøretøy, EV-markedsandel, batterikjemi, gjenvinningsteknologier og andelen naturlig kontra syntetisk grafitt i batterier. Samtidig ble det utviklet en modell for petroleumraffinerier for å kvantifisere maksimal tilførsel av nålekoks i ulike markedsandelscenarier og sammenligne det med etterspørselen. Når det kommer til naturlig grafitt ble det gjennomført en analyse av den nåværende situasjonen for å forstå geografisk opprinnelse for forsyningen, samt potensielle hindringer for utvidelse. Det er blitt lagt betydelig vekt på betydningen av usikkerhet i modellen ved å bruke Monte Carlo-simulering for å vurdere usikkerheten i resultatene.

En parametrisk modell for etterspørselen etter grafitt ble utviklet. Resultatene kan visualiseres online på http://129.241.153.120:8052. Behovet for grafittmalm og nålekoks varierer betydelig mellom scenarioene, med 1312 til 25673 kton grafittmalm og 3945 til 22301 kton nålekoks i 2050 i de seks valgte scenarioene. Maksimal tilførsel av nålekoks varierer fra 3596 til 39123 kton avhengig av EV-markedsandelen og fleksibilitet i raffinerier. Studien avdekket at LIB-produksjonen er avhengig av utvinning av hydrokarboner, noe som fører til begrensninger i tilførselen av syntetisk grafitt. I scenarioer med rask EV-markedsandelen kreves det mindre petroleum av transportsektoren, og tilførselen av nålekoks begrenses som en konsekvens. Ved å erstatte konvensjonelle kjøretøy reduserer elektriske kjøretøy sin egen tilførsel av nålekoks og syntetisk grafitt. På den andre siden er grafittmalm rikelig, men mangelen på infrastruktur og utviklingstid gjør det usannsynlig å se at tilførselen holder tritt med den galopperende etterspørselen.

Bare kombinasjonen av de mest effektive gjenvinningsteknikkene med samfunnsmessige endringer, som lavere kjøretøyomsetning og mindre kjøretøy, kan begrense risikoen for mangel på grafittforsyning. Imidlertid er slike gjenvinningsrater umulig å implementere i dag, da aldringsmekanismene til grafitt i LIB-er fortsatt ikke er fullt ut forstått. Derfor spiller nøkternhet en avgjørende rolle for å redusere etterspørselen etter grafitt. Dette ville også ha medfølgende fordeler, da mindre kjøretøy kan bruke alternative batterikjemier, og begrensning av produksjonen av EV-er generelt ville begrense miljøpåvirkningen knyttet til grafittproduksjonen.

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1 Introduction

1.1 Motivation

According to the Intergovernmental Panel on Climate Change, the transport sector accounts for 23% of all energy-related emissions [53]. The transition towards low-carbon transportation is expected to happen thanks to the electrification of means of transportation. The political targets at an international scale, such as the recent ban on thermal vehicles in the European Union from 2035 show this ambition [33]. This shift towards electrification results in fundamental changes in energy demand, material use, and infrastructure needs globally. Lithium Ion Batteries (LIB) are the favourite technology for all types of electric vehicles thanks to their high capacity, high reversibility and long cycle life as well as no memory effect. LIBs are composed of a cathode, an anode as well as an electrolyte, a binder, current collectors, plastic and steel. Due to its excellent performance and affordability, graphite has become the preferred material for battery anodes, leading to an anticipated surge in its demand in the coming decades. This study focuses on establishing a material flow analysis of graphite production to identify any potential disruptions in the supply chain of this crucial material for green transportation.

1.2 Background

1.2.1 Origin and uses of graphite

Graphite is a natural occurrence of the carbon atom, number 8 in the periodic table. It is one of two allotropes of carbon, the other being diamond. Graphite is the most thermodynamically stable form of carbon under room temperature and pressure. Carbon materials are often not described as either graphitic or non-graphitic but present a degree of graphitisation [47]. Graphite has a highly anisotropic structure composed of stacked layers of graphene, as shown in figure 1. Its geometry gives graphite some useful properties, such as high thermal stability and thermal and electrical conductivity.

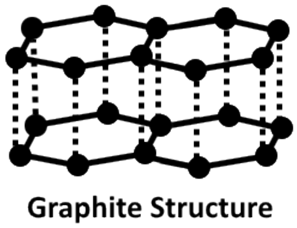


Figure 1: Graphite structure [23]

Graphite naturally occurs in metamorphic deposits such as marble, schists and gneisses. Uses of graphite have been reported since as far as the 4th millennium BCE. Its use as refractories began during the 16th century, but it started to expand during the 19th century when it became popular for uses in foundries, lubricants, paints, and pencils [12]. The development of flotation in the 19th century allowed for the purification of graphite, spreading its use to more industries[73][56]. Once extracted from the soil, graphite ore undergoes several treatments to remove impurities, such as potassium, sodium, calcium, magnesium, and aluminium silicate minerals [55]. Based on its morphology and crystallinity, natural graphite can be classified into three categories: amorphous graphite, vein (or lump) graphite, and flake graphite. Amorphous graphite is characterized by its microcrystalline structure, with grains smaller than 4 μm and an ore grade ranging between 50% and 90% carbon. This type of graphite finds its use primarily in recarburizers, lubricants, and pencils. Vein graphite, on the other hand, is the most crystalline form of graphite with a purity level higher than 90% graphite. It is exclusively available in Sri Lanka and is considered to be the most expensive option among the three. Finally, flake graphite comprises large crystal platelets, with grain sizes ranging from 40μm to 4cm [72].

Synthetic graphite was discovered in the 1890s by Edward G. Acheson when he accidentally graphitized carborundum. Initially used as a lubricant, it quickly found its primary application in the steel industry for Electric Arc Furnaces. To produce synthetic graphite, a carbon precursor undergoes pre-processing steps before being heated at temperatures above 3000°C to enable the carbon atoms to rearrange in a graphitic structure, a process known as graphitization [47]. Refining steps follow to make the graphite suitable for its intended use. Although many different precursors can be used to produce synthetic graphite, the quality of the precursor is the primary driver of the quality of the end product [47]. The most commonly used carbon precursor is coke, specifically calcined petroleum coke, which is derived from the calcination of green coke, a byproduct of the refining of crude oil. As a result, synthetic graphite production depends on the extraction of crude petroleum. Depending on the precursor, synthetic graphite can exhibit a microcrystalline to crystalline structure with various particle sizes.

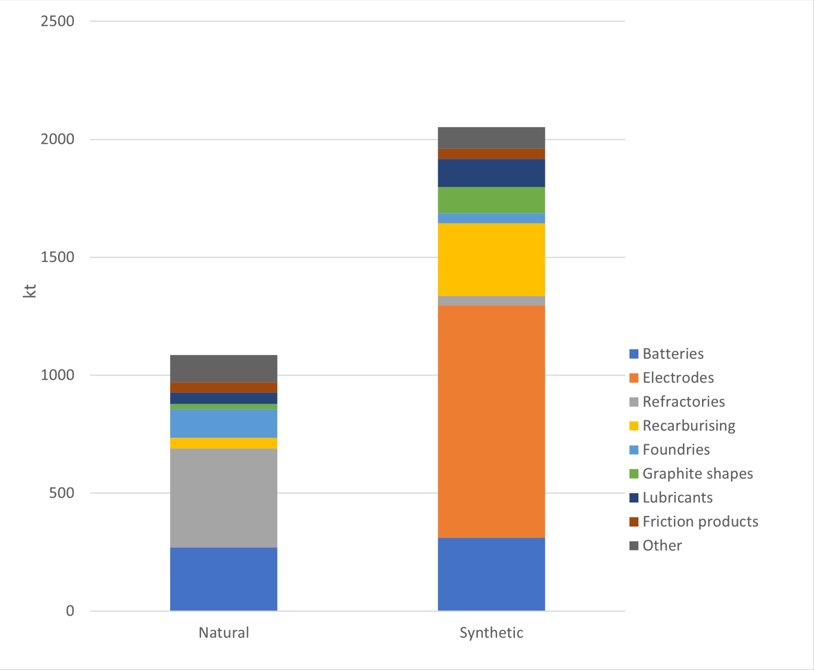


Figure 2: Applications of graphite in 2022, adapted from Wood Mackenzie, 2022 [108]

Graphite's properties explain its various uses, which are presented in figure 2 for the year 2022.

Today, the production of synthetic graphite has exceeded that of natural graphite with respective productions of 2128 and 1266 ktons in 2022 [100][28]. Synthetic graphite finds its largest application as electrodes in the steel industry, along with recarburizing and batteries. Natural graphite is primarily used in refractories for metal smelting, batteries, and foundries. It is interesting to note that apart from the battery sector, sectors are usually distributed between mostly synthetic graphite or mostly natural graphite users as shown in figure 3 [29]. Although the battery sector may not currently be the main consumer of graphite, it is expected that the demand for both natural and synthetic graphite will increase significantly in the coming years, largely driven by the expanding battery industry. The demand for natural graphite in the battery sector is predicted to increase by 15% per year, while synthetic graphite for batteries is expected to grow by 20% per year [27]. By 2040, the demand for graphite is expected to grow 25 times by 2040 according to the International Energy Agency (IEA), to ensure sustainable development targets [51].

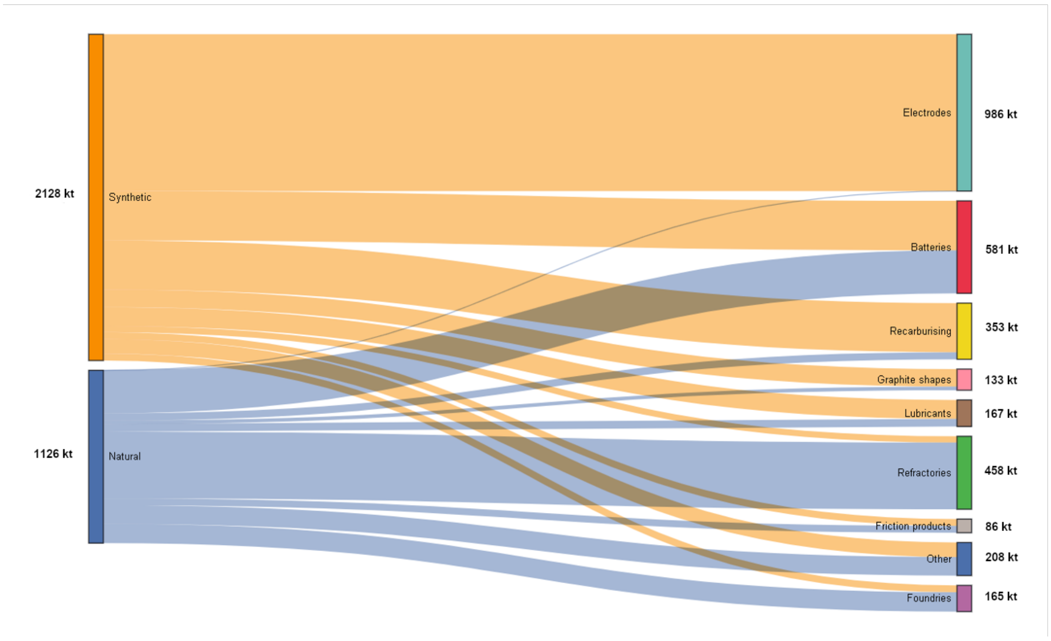


Figure 3: Final consumption of Natural and Synthetic graphite in 2022, data from the ECGA [28]

1.2.2 Graphite's importance for sustainable transport

The predominance of graphite as an anode material is explained by its electrical and thermal conductivity, its capacity to intercalate lithium, its stability but also its availability and low cost [48][76][72]. Silicon is also a promising anode material, as its theoretical capacity is 10 times higher than graphite. Still, it undergoes dramatic volume changes during cycles, making it unsuitable for EVs [48]. As a result, graphite is currently the main industrial option for LIB anodes, sometimes blended with a small amount of silicon, usually less than 10% [5].

The quantity of graphite in EV batteries varies greatly, depending on the size of the vehicle and the chemistry of the battery. According to the IEA, electric vehicles contain, on average, 66.3kg of graphite [51]. Natural and synthetic graphite are usually blended in battery anodes to combine their properties, decrease the price and diversify the supply. The ratio between natural and synthetic graphite largely depends on the manufacturer but also on demand from the client, whether they focus on high performance or lowering the prices [87]. Table 1 outlines the advantages of using synthetic graphite for battery anodes, including longer battery life, shorter charging times, and reduced volume expansion. However, the cost of synthetic graphite is a major disadvantage, as it is 2 to 3 times more expensive than natural graphite, which also has a higher theoretical capacity. Recycled graphite from end-of-life (EOL) batteries could relieve the pressure on the natural and synthetic graphite supply chains but faces technical issues to retrieve battery grade graphite [89].

Type of graphite	**Natural graphite**	**Synthetic graphite**
Price ($/kg) [72]	4-8	8-12
Longevity [49]	ca 1000 cycles	ca 1500 cycles
Charging time [49]	/	faster charging
Volume expansion (for safety) [49]	Low	Very low
Theoretical capacity (mAh/g) [49]	340-370	310-360
Carbon footprint (kg CO2/kg Gr)	2.1-7.75	4.86-13.8
Other environmental impacts	Hydrofluoric acid	unknown
Human health impact	Graphite dust	unknown
Development time (years) [11][87]	8-10	1-2

Table 1: Comparison between natural and synthetic graphite, from various sources [72][49][11][87]

To understand the challenges and opportunities in the supply of battery anode material (BAM), it is crucial to understand the material cycle of graphite as well as the supply of raw materials required for its production.

1.3 Previous studies and research gap

1.3.1 Availability of graphite

Despite the large reserves of graphite, which are currently 320 times higher than the annual production, graphite is still considered a critical and strategic resource in the US, EU, and China [21] [101]. This is due to its crucial role in decarbonizing the transport sector and the heavy reliance on a few suppliers, mainly China. The absence of an industrial substitute for LIB anodes adds to its criticality. Nonetheless, there has been a diversification of the supply in recent years, particularly with the increase in natural graphite production in Eastern Africa, such as Mozambique, which accounted for 9% of the global production in 2018 [100]. The concentration of graphite production in a few countries (China, Brazil, Mozambique) raises concerns about potential supply tensions for Western industries, as 99% of the natural graphite used in the EU is imported [31]. It is worth noting that only certain fractions of natural graphite flakes, i.e., those with low heavy metal concentrations, can be used for the production of battery anodes [11]. A major issue facing natural graphite production in the next decade is development time. With the demand for graphite expected to explode in the coming decades, it is possible that the supply may not keep up with demand. Betz et al. report that geological surveys, feasibility studies for opening a new mine, and establishing natural graphite production typically take between 8 and 10 years [11]. The production of natural graphite has already shown its first signs of shortages due to a lack of mining sites and refining infrastructure [9].

Studies show that synthetic graphite has the advantage of established and readily available raw materials for its production [11]. The competitive edge of synthetic graphite manufacturers lies in their technology for producing battery anode material. These processes might take time to develop for new producers [87]. Once the technology is developed, production can be easily scaled up within 1-2 years due to faster licensing procedures and technical realization time compared to natural graphite [11]. Unlike graphite ore, petroleum coke is globally available, as many countries refine crude oil within their territory. Therefore, the development of synthetic graphite infrastructure is not constrained geographically. Additionally, the production of synthetic graphite can offer independence from the Chinese production of natural graphite, despite China also being the primary synthetic graphite producer today, accounting for 78% of the production [79].

1.3.2 Social and environmental impacts of graphite production

Previous studies have approached the production of graphite with a life cycle approach to determine the impacts of the production of battery anodes through different production routes (natural or synthetic graphite). These studies often focus on the global warming potential of such production, concluding in higher emissions for synthetic graphite, with 4.86-13.8kg CO2-eq/kg Graphite, compared to that of natural graphite, with 2.1-7.75kg CO2-eq/kg graphite [11][67][82][93][113][30]. Synthetic graphite production emits high amounts of greenhouse gases due to energy-intensive processes, especially the graphitization process, production of raw materials, such as petroleum coke and coal pitch, and release of volatiles during coke transformation [93]. The most extensive study is probably the one conducted by Engels et al., with a thorough description of the processes in cooperation with EV and battery manufacturers, allowing for a deeper understanding of the natural graphite value chain [30].

The recycling of graphite material has also been subject to extensive investigation to understand the different recycling processes, their potential and limitations [11][65][71][89][111] as well as the environmental impact of natural graphite, which is responsible for relatively low emissions compared to that of natural and synthetic graphite, with 2.4 kg CO2-eq/kg graphite [85].

Environmental impacts which are not included in these studies may include impacts associated with the extraction and beneficiation of natural graphite. Graphite itself is inert and non-toxic, but graphite purification typically involves the use of hydrofluoric acid, which is harmful to the environment and human health [56]. Research is being conducted to develop less damaging purification methods, but the use of hydrofluoric acid remains common due to its low cost and effectiveness. Grinding graphite ore can also release harmful graphite dust, which can cause respiratory problems [17]. These health concerns have led to temporary mine closures in China due to local protests [107]. Concerning social issues, Mancini et al. analyzed the main graphite producers and companies operating mines in China, Mozambique, India, and Tanzania. The authors expressed concern about issues such as child labour, poor governance, and the lack of environmental regulations in some of these countries [66].

These studies help broaden the understanding of the supply chains of graphite, the different processes, raw materials and the associated environmental impacts. However, they only focus on the analysis of processes and do not consider the availability of essential raw materials. They have not dealt with a global approach to the production of graphite, which is crucial to study the supply of critical materials to the LIB industry.

1.3.3 Quantification of graphite flows

Material flow analysis (MFA) has been extensively used to obtain fresh perspectives and quantify the cycles of numerous materials, including battery components. However, graphite has been somewhat neglected in comparison to cathode materials, which are generally considered more critical due to their higher costs and scarcity. Recent studies have nevertheless shown interest in using MFA to understand the flows in the graphite system and how this impacts anode supply. Rui et al. showed the importance of landfill stocks compared to in-use stocks by performing a material flow analysis in China from 2001 to 2018 for natural graphite [82]. Ciacci et al. conducted a similar study in the EU between 2012 and 2016 to evaluate the performance of the supply chains of manganese, nickel and natural graphite on efficiency and recycling indicators [18]. Song et al. studied the use of Lithium, cobalt, nickel and graphite using material flow analysis (MFA) in the 2013-2025 period in China [90]. Finally, Zhang et al. provide a complete MFA of graphite flows in the US economy for 2018, including all sectors, both natural and synthetic graphite and with more detail on the different life stages of the material [112]. These studies bridge the lack of systematic understanding of the graphite cycle. However, there are limited to subsets of graphite production, often including only natural or synthetic graphite, or do not include all relevant processes and are focused on specific regions. With the notable exception of Song et al.'s paper, these studies are also backwards looking and therefore do not to address potential future issues with the supply of graphite. To thoroughly study the future supply and recycling of graphite, it is necessary to have a future-oriented global model, including both natural and synthetic graphite, as well as competition from other graphite-using sectors. Sofia Genovesi paved the way for such a study, combining both natural and synthetic graphite for the global production of LIBs [41]. This study provides a complete description of the graphite production routes but is limited to the LIB sector and lacks information on the supply of raw resources.

1.4 Research questions

The purpose of this thesis is to quantify the graphite cycle between 2020 and 2050, including natural, synthetic and recycled graphite and all graphite-using sectors. Further attention will be given to the battery sector, as it is expected to drive the demand in the near future and also presents the largest recycling opportunities. A large part of the study is also dedicated to quantifying the need for key raw resources for graphite production, namely natural graphite ore and petroleum needle coke, to understand what amount can be supplied in the future and the potential limitations to their supply.

From this are derived the following research questions:

- How is the demand for graphite expected to grow in the future?
- What are the bottlenecks in the supply of natural graphite ore and petroleum needle coke?
- What strategies can be put in place to ensure that the supply of graphite meets the growing demand?

To answer these research questions, several tasks covering different parts of the system of graphite production have been carried out.

First, the current state of the global graphite system is described and quantified. This system is a simple representation of the graphite cycle that allows for deeper investigation in the following steps.

The second step involves diving into graphite production and describing the processes involved. The different data sources for both the parameters describing the processes as well as the demand for graphite from different sectors are also described. Based on the work previously done in the master project in the fall semester [7], a dynamic model is developed to quantify flows in graphite production. The model is parametric and allows for easy scenario development. Using six example scenarios built on this model, an uncertainty analysis is conducted to visualize the range of the demand for raw materials for a given end-use demand.

The third step is to investigate the results of the previous model for natural graphite and analyse the limitations and opportunities in graphite mining to provide sufficient amounts of natural graphite for the demand scenarios. This step consists of analysing the current geographic distribution of mining and the potential evolution of this distribution.

The fourth step is analogue to the third one, focusing this time on synthetic graphite. Diving into the refining of crude oil, the extent of petroleum coke that can be provided to synthetic graphite production is modelled. A strong focus will also be dedicated to the quality of the coke, analysing its main limitation, the sulfur content.

Finally, the last step is a literature review of the potential of recycling to relieve pressure on the supply of natural and synthetic graphite value chains. This step describes the different recycling processes, the limitations of recycled graphite as an anode material, and what barriers need to be overcome for recycling to provide high-quality anode material.

2 Methodology

2.1 Global system definition and quantification

2.1.1 Global system definition

This thesis employs Material Flow Analysis (MFA) to study the global graphite cycle. MFA applies the principle of mass balance to identify and measure the flows and stocks of a material within a specific space and time frame [15].

The system considered in this paper includes all steps of graphite production for both natural and synthetic graphite. Synthetic and natural graphite production include several steps to produce and refine the graphite, as it is usable by different industries. The refining steps are sector-specific; the graphite required by the battery industry differs significantly from the graphite needed for refractories. The system also includes the production of needle coke, which originates from petroleum refineries, as a byproduct of the production of diesel and gasoline. Once a finished product, graphite is distributed to various sectors, including the battery one. The system definition only includes the battery (and EV) sector to take into account recycling from EOL vehicles. For batteries, natural, synthetic and recycled graphite are blended and then manufactured into the EV. When electric vehicles exit the use phase, batteries can be recycled. Depending on the recycling method, graphite can be extracted from the batteries, purified, and reintroduced into batteries.

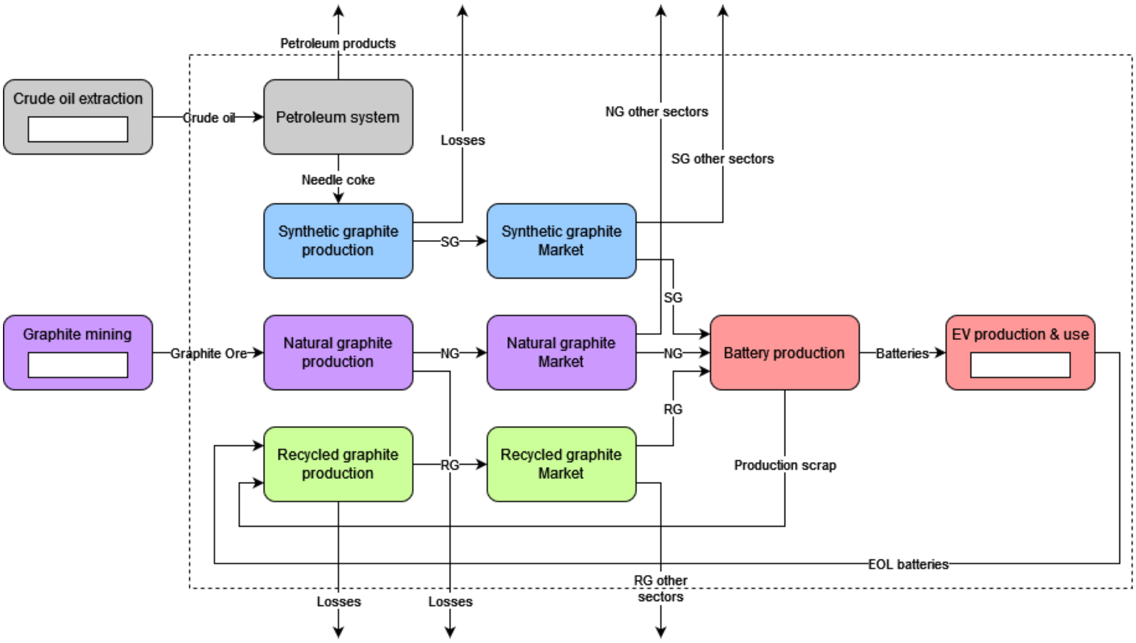


Figure 4: Global system of the graphite cycle

To define the system of graphite production, interviews were conducted with both synthetic graphite manufacturers [87], natural graphite producers [10][35] as well as needle coke specialists [20]. Figure 4 presents the global system and shows the link between the different parts. Later sections will focus on subsystems of the global one. The demand side corresponds to all processes following the flows of needle coke and graphite ore. In contrast, the supply side looks into how to provide these resources, as well as recycled graphite. On the demand side, the value chain of graphite production is further studied to calculate the demand for needle coke and graphite ore in different scenarios. Accordingly, the petroleum system is studied to provide the supply of needle coke in the scenarios and check if enough material can be produced or if there is a mismatch between supply and demand. A qualitative study of the supply has also been conducted for graphite ore and recycled graphite.

2.1.2 Quantification

To get a first overview of the graphite system, the global system has been quantified for the year 2022. This quantification is based on the work done during the MSc project, with modifications to include the petroleum system as well as recycling [7]. The quantification of the global system is a simplification of the quantification of the different subsystems, the data sources and methods used to quantify them are described in the relevant sections. This global quantification allows for an overview of the system to understand the key flows and processes.

To quantify the demand for graphite in batteries in 2022, the number of electric vehicles sold in 2022 was combined with the average content of graphite in batteries from the IEA [51][102]. It is also assumed that no graphite is yet recycled for the year 2022, as most recycling processes use pyrometallurgy, which burns the graphite. Graphite is mainly recovered at lab scale in 2022.

2.2 Demand - Detailed graphite value chain system

2.2.1 System definition

A major aspect of the thesis was the description of the so-called demand model, which is a subset that includes both natural graphite, synthetic graphite and recycled graphite production, the markets for all sectors and the production and use of batteries and EVs, as shown on figure 5. The production and use of EVs are included to track the availability of recycled material. It is assumed that only graphite from EV batteries is recycled and that recycled graphite is only used for the EV sector. This system includes all the major processes in the natural and synthetic graphite value chains, whereas the recycled graphite value chain is simplified as it is not the main scope of this study and is already described in previous works such as Hansson [46], Sommerville et al. [89] and Moradi et al. [71].

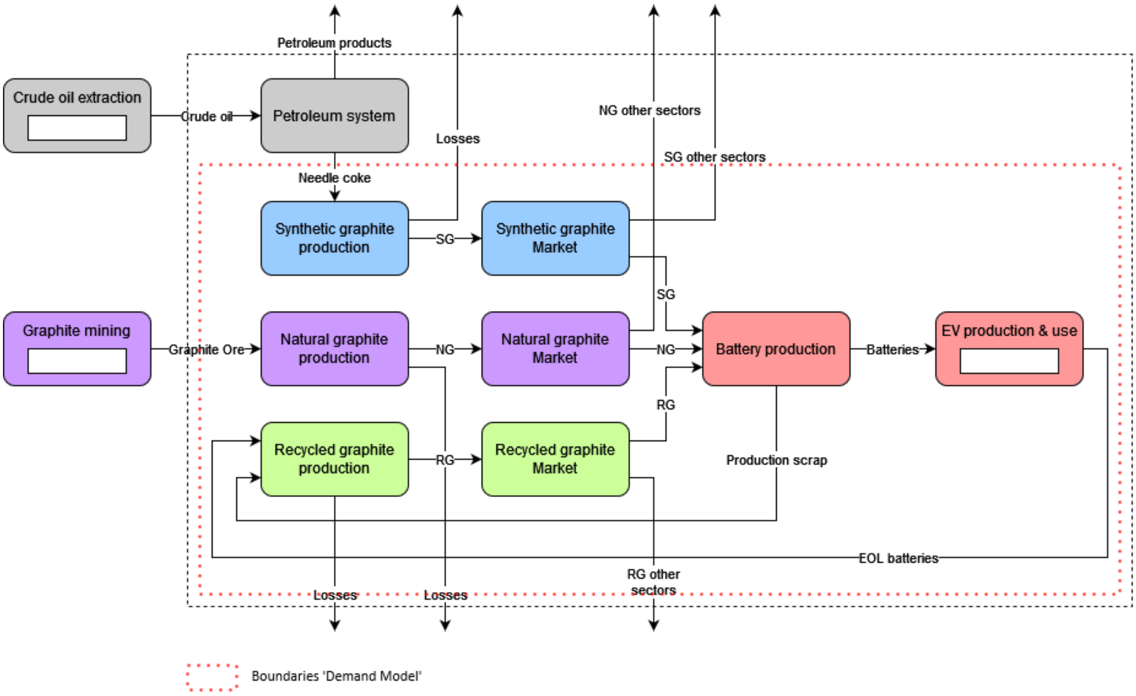


Figure 5: Global system of the graphite cycle, with boundaries for the demand model

The demand model describes all three production routes in more detail to account for losses and production of byproducts along the value chain. Even though it is not the main scope of the study, having a detailed description of the processes also allows a deeper understanding of the key processes in terms of energy use and emissions. The value chains of the different graphite production routes have been described using a literature review, especially LCIs and LCAs of graphite production, which require listing all processes. This description of value chains was improved through expert interviews, both on the natural and synthetic sides, mostly to understand what processes are required for which graphite products. The graphite used in the various sectors indeed presents very important variations in quality and price, and it is important to point out that if one sector consumes less graphite in the future, it does not necessarily mean that more will be available for the battery sector. Not all types of graphite are equal. The system which has been studied and quantified in this section is present in figure 6.

The model has then been quantified using a parametric approach for the time frame 2020-2050.

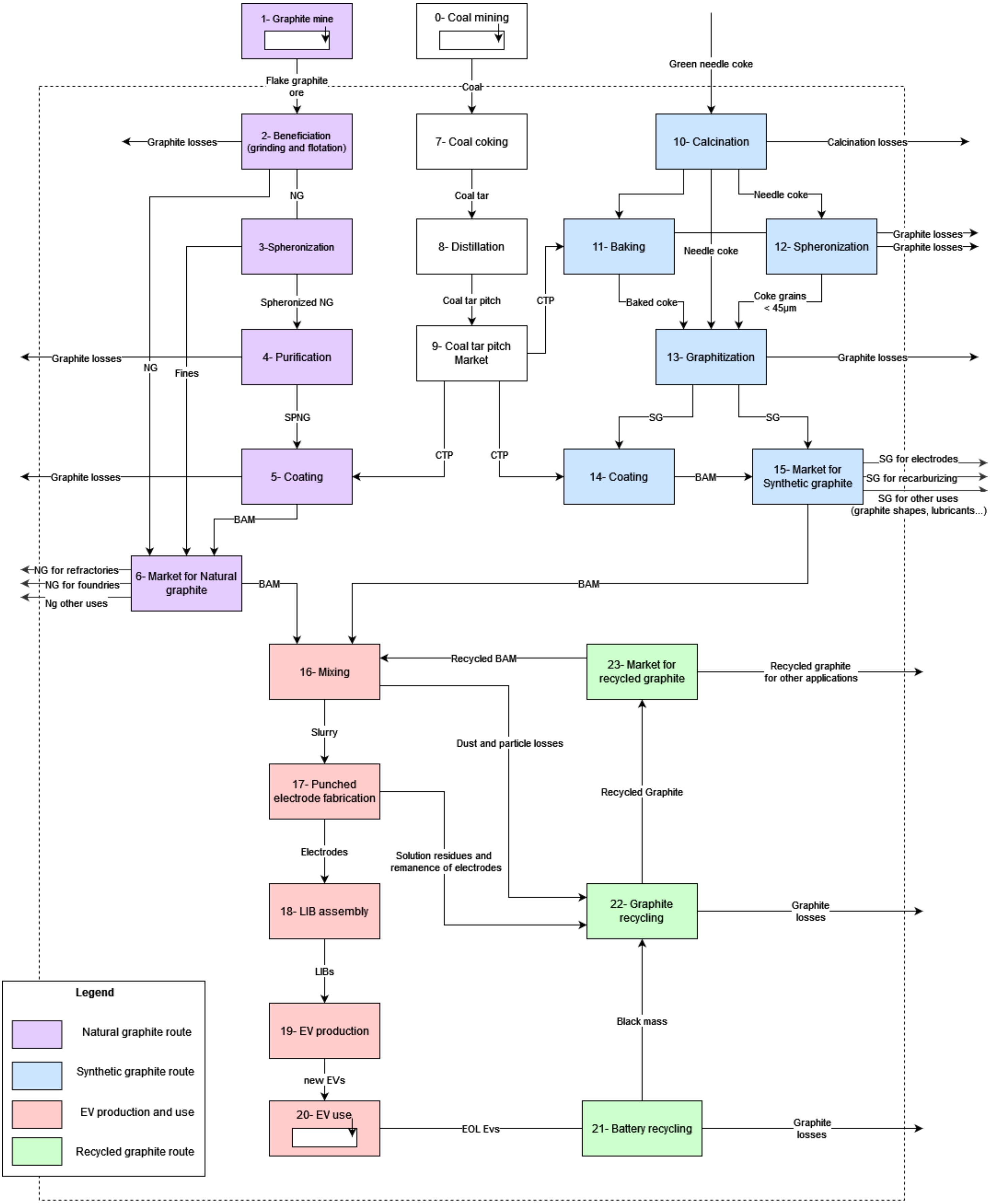


Figure 6: Detailed system definition of demand model

Natural graphite route

Natural graphite production is composed of 5 processes (plus a market) and corresponds to processes 1 to 6 in figure 6. The production comprises the extraction of the graphite ore, its beneficiation, the spheronization of the graphite, its purification and finally, a coating step. Then the graphite is sold to the different sectors which require natural graphite.

Graphite mining (process 1) can be carried out by either open pit or underground methods. The open pit method is commonly employed when the graphite ore is close to the surface with only a thin layer covering the deposit. This method is ideal for extracting flake graphite (the type used for batteries) since the deposits are typically situated close to the surface. Graphite ore has a content of graphite which ranges from 3% to 52% [101] and therefore requires processing before it can be used by industries. Battery anodes, for example, require a graphite grade of around 99.95% [93].

The process of producing high-grade graphite from its ore involves multiple steps grouped in the beneficiation process (process 2), which vary depending on the ore grade, impurities present, and desired final product grade. Typically, the ore is subjected to flotation and grinding to separate the graphite, which has low density and floats, from impurities that sink. However, the graphite often coats the surrounding rock, also causing it to float. To overcome this, repeated grinding and flotation steps are necessary. Although these mechanical methods can yield graphite that is 97-98% pure, additional purification is necessary to achieve higher purity levels required for specific applications such as battery anodes [64][73]. The graphite produced from this process is, however, of sufficient quality to be used in most non-battery industries.

To ensure that graphite possesses sufficient electrochemical properties for batteries, it must undergo several operations, such as conditioning, grinding, classifying, and coating. The sequence of these operations can vary, and some, such as product coating, may be optional. The spheronization process (process 3) comprises grinding and classifying the graphite product to reach and select particles of an optimal round shape and size, around 15 to 30 μm [35]. The performance of graphite in LIBs is highly dependent on the shape and size of the graphite particles [87]. A byproduct, graphite fines, originates from the grinding of graphite flakes. This material consists of a powder of high-quality graphite but with grains smaller than the required size for the battery sector.

To further remove impurities, the two main types of purification methods for graphite are hydrometallurgical and pyrometallurgical purification (process 4). The hydrometallurgical methods, which include acid-based and hydrofluoric acid methods, are the most common due to their affordability and ease of small-scale development. On the other hand, pyrometallurgical methods, such as chlorination roasting or high-temperature purification, require high energy consumption and large-scale infrastructure. Although high-temperature purification is highly efficient in boiling off impurities, it is very rarely used by graphite producers, mainly due to its price [56].

Graphite material for the battery sector usually also undergoes coating (process 5), which corresponds to surrounding the graphite grains with coal tar pitch. The purpose of the coating is to prevent graphite from ageing during its use by avoiding any reaction between the electrolyte and the graphite. This coating helps to limit the irreversibility of the first charge/discharge cycle, as reported by Nozaki et al. in their study [75].

As illustrated in Figure 3, natural graphite finds diverse applications, including refractories, batteries, foundries, recarburising, lubricants, and more. These different sectors do not require the same type of graphite (flake or amorphous) or the same purity. They also require different refining steps, and only the battery sector requires the spheronization, purification and coating steps. Graphite fines can also be used for non-battery sectors. In this study, it is assumed that all non-battery sectors can use graphite fines, this simplification allows us to show that even with this conservative approach, there could be an overproduction of graphite fines.

Synthetic graphite route

The synthetic graphite route is composed of processes 10 to 15 which correspond to the following processes: calcination of coke, the baking of coke for electrode uses, or its spheronization for battery uses, the graphitization of the graphite precursor, the coating and finally a market.

The main precursor for producing synthetic graphite is coke and in particular, petroleum needle coke. Needle coke is a term to describe high-quality coke that can be produced either from coal or crude oil. Petroleum coke is usually preferred due to its higher aromaticity and graphitizable properties [54][87]. The first step is to heat the coke around 1300°C to remove impurities and volatile matter and raise the precursor's carbon content during the calcination process (process 10).

Similarly to natural graphite, synthetic graphite destined for the battery sector has to undergo a series of operations. The spheronization (process 12) is very similar to the natural graphite one, where the aim is to reach coke grains of a specific shape and size. The main difference is that coke grains may be more homogeneously distributed and rounded than natural flakes before the spheronization. Therefore, the losses in the process are lower for synthetic than for natural graphite production.

Alternatively, the precursor has to undergo a baking operation (process 11) to produce electric arc furnace electrodes. To reduce the porosity of the coke, a binder, typically coal tar pitch, is mixed with it. The mixture is then heated to a temperature of 1000/1200°C in the absence of air [93].

The precursor is then graphitized (process 13), which is the main and most crucial step of synthetic graphite production. During graphitization, the precursor's structure is modified in an oxygen-free environment at a temperature of around 2500-3000°C. The precursor undergoes a fluid phase where aromatic molecules align with each other to form a graphitic structure, as depicted in figure 7 [47]. This step is both the longest and most energy-intensive, requiring the material to be heated, maintained at high temperatures, and then cooled down.

Finally, synthetic graphite can be coated with coal tar pitch (process 14) to improve conductivity identically to natural graphite.

The use of synthetic graphite is distributed among various industries, such as electrodes, recarburizing, graphite shapes, and lubricants, as depicted in figure 3. The battery sector, on the other hand, utilizes both synthetic and natural graphite. Today, the electric arc furnace (EAF) industry is the main consumer of synthetic graphite. While all sectors require the calcination and graphitization step, the baking step is exclusive to the electrode sector, while the spheronization and coating steps are exclusive to the battery sector.

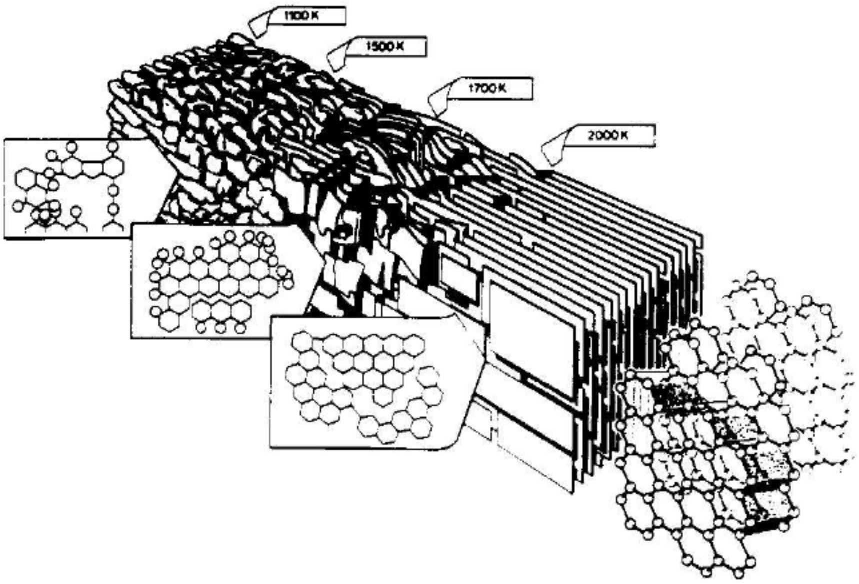


Figure 7: Marsh-Griffiths model of graphitization process [47]

Coal tar pitch production

To enhance the conductivity of graphite material, it is common practice to apply a coating of carbon pitch, usually coal tar pitch (CTP). This coating creates a uniform and isotropic layer around the graphite particles, improving conductivity and reducing resistance at the anode-electrolyte interface [45] [57]. Coal tar pitch can be applied to both natural and synthetic graphite for use in lithium-ion batteries (LIBs) and is also used for the baking stage of electrodes for EAF. Coal tar pitch is a byproduct of coal coking (process 7) used to produce metallurgical coke. Coal is the raw material used to produce that type of coke, and during the process of coking, coal tar is produced as a byproduct. The tar is then distilled to produce coal tar pitch (process 8), which can be used for coating graphite. Coal extraction is an energy-intensive process and generates direct emissions. Additionally, the production of coal tar pitch also generates tar residues [54]. This production corresponds to steps 0, 7, 8 and 9 in the system figure 6.

Battery production and EV use phase

The battery production and EV use phases correspond to processes 16 to 20 in figure 6.

After the different production steps, the natural and synthetic graphite are refined and ready for use as battery anode material. The proportion of each type of graphite used depends on factors such as the end product, market prices, and availability. Historical data shows that natural graphite has been more commonly used than synthetic graphite in batteries. Still, the trend could be reversed depending on quality requirements and the evolution of prices [28].

The mixture is then dried and punched into round electrodes with a diameter of approximately 12 mm (process 17). These electrodes are assembled with lithium chips, the cathode material, the electrolyte, and the separator to form batteries. The batteries are then installed in electric vehicles and used on the roads for a certain lifespan. The scrap from the battery production is of battery grade and is, therefore, a valuable input to the recycling of graphite.

Recycled graphite route

When the electric vehicle exits circulation, batteries are sent to recycling plants to sort out the different valuable materials before sending them to specific recycling processes (processes 21 to 23). Scrap in battery production can also be recycled to provide graphite for batteries. The different recycling routes are pyrometallurgy, hydrometallurgy and direct recycling. Pyrometallurgy does not allow for recovering graphite as it is burnt in the process and used as a fuel [89]. This study also focuses on the techniques for the recycling of batteries and graphite as well as the challenges and limits of recycling.

Once graphite is isolated from other valuable material, it is sent to a dedicated plant to be isolated and to recover a sufficient grade. Both battery recycling and graphite recycling are associated with high losses of graphite and, in many cases, a notable decrease in quality. Therefore, the amount of recycled graphite in new batteries can be limited, or it might be used in other sectors with less stringent grade requirements.

2.2.2 Quantification and data sources

A literature review was conducted to characterize the different processes that were just described. For each process, it is important to know the inflows, outflows, the grade of carbon/graphite of these flows, and the transfer coefficient(s) between them. Life cycle inventories were key in this work, as they usually present an exhaustive description of the processes and flows present in the value chain. The transfer coefficients and the carbon concentration of flows within the system are summarized in table 2. One can notice the important losses in the spheronization process for both natural and synthetic graphite production. It is also important to note that the amount of graphite recovered during recycling can vary from 0 to 90%.

Process	Inflows		Outflows (excluding losses)		Yield DM	Yield Gr	Source
	Type	%C	Type	%C			
1 - Graphite mine			Graphite ore	8,8%	1		[100]
2 - Beneficiation	Graphite ore	8,8%	Natural graphite	95%		0,865	[64][30]
3 - Spheronization	NG	95%	SNG	95%		0,450	[30]
			Graphite fines			0,547	[30]
4 - Purification	SNG	95%	PNG	99,95%		0,931	[30]
5 - Coating	PNG	99,95%	BAM	99,95%		0,990	[30]
	Pitch	60%					
10 - Calcination	Green coke	92,50%	Needle coke	99%	0,74		
11 - Baking	Needle Coke	99%	Precursor	99%		0,996	[13][26][42]
	Pitch	60%					[30][54]
12 - Spheronization	Needle Coke	99%	Ground Needle Coke	99%		0,65	[93]
13 - Graphitization	Precursor	99%	SG	99,95%	0,98		[13]
14 - Coating	SG (95.3%)	99,95%	SG for batteries	99,95%	0,99		[30]
	Pitch (4.7%)	60%					
16 - Mixing	NG	99,95%	BAM	99,95%		0,95	[41]
	SG	99,95%					
17 - PEF	BAM	99,95%	Electrodes	99,95%		0,95	[41]
18 - LIB assembly	Electrodes	99,95%	Batteries	99,95%		1	[41]
19 - EV production	Batteries	99,95%	EV	99,95%		1	[41]
20 - EV use	EV (new)	99,95%	EV (EOL)	99,95%		1	[41]
21 & 22 - Recycling	EV (EOL)	99,95%	BAM recycled	99,95%		0/0,4/0,9*	[4]
	Battery scrap	99,95%					

Table 2: Transfer coefficients and concentrations per process

The yield corresponds to the ratio of output on total input and is given on the Dry Matter (DM) or on the Graphite (Gr) layer. The share of carbon is given for the graphite/carbon material within the flow (The flow of EV corresponds to graphite anodes in EVs)

* *The recycling rate is scenario dependant, depending on the recycling technology. The carbon content applied*

Validation and calibration of parameters

The processes within graphite production have been described thanks to literature and interviews and summarized in table 2. It is, however, important to compare the natural and synthetic graphite value chains with previous work. Many studies present the global efficiency of the value chain, from the raw resource (graphite ore or petroleum coke) to the final product (natural or synthetic graphite). Calculating this overall efficiency of the value chain allows for an easy comparison of different studies.

Natural graphite production

Table 3 summarizes the efficiencies of natural graphite production for various studies. These efficiencies are only calculated for Battery anode material (BAM) and represent the ratio between output BAM and input graphite ore. While the efficiencies are given for both the DM and graphite layer, comparing the graphite content is more informative due to the variation in ore composition across studies.

In their environmental impact analysis, Zhang et al. reported using 19.6 kg of graphite ore with a 7.87% Gr concentration to manufacture 1 kg of BAM. In comparison, our system requires 31.5 kg of graphite ore with an 8.8% Gr content to produce the same amount of BAM. This model requires 2.7 kg of graphite in the ore to produce 1 kg of BAM, while Zhang et al. only need 1.54 kg. The difference could be attributed to the spheronization process, which has a yield of only 45%. Although Zhang et al. also accounts for spheronization and coating in their study, they do not provide the LCIA details, making it difficult to compare the methods and results. In this study, 1 kg of non-anode graphite (without the spheronization and coating step) requires 1.25 kg of graphite in the ore, which is closer to Zhang et al.'s value [113].

Studies that use a similar approach for the spheronization process report similar efficiencies for natural graphite production, with values around 38% on the graphite layer [30][82]. Therefore, with a ratio of 35.92% for natural graphite production, this study is consistent with previous works that used a similar spheronization approach, emphasizing the importance of this process and comprehensive data across the graphite value chain.

Study	Efficiency DM	Efficiency C
Engels et al (2022) [30]	4.11%	37.41%
Zhang et al (2018) [113]	5.1%	64.83%
Rui et al (2022) [82]	2.48%	38.15%
Sofia Genovesi (2021) [40]	50%	56.71%
This study	3.17%	35.92%

Table 3: Literature comparison for the efficiency of natural graphite production

Synthetic graphite production

The table 4 summarizes the efficiencies for the synthetic production route in literature. The efficiency is given as the ratio between the output of BAM and the input of petroleum coke plus coal pitch. As specified in the table, the pitch is not always included in the calculations depending on the paper.

Unlike natural graphite production, the efficiency from this study is lower than any study, whether coal tar pitch is included or not. This difference can be explained as some processes were included in this study, whereas most of the papers did not include them. Dunn et al. [26] only consider the baking and graphitization processes, therefore overlooking the calcination of the coke and the milling and shaping (spheronization) of the particles. Surotseva et al. [93] include the calcination of the coke but still not the spheronization of graphite. These processes have important losses and explain why the ratio observed in this study is significantly lower than for these studies. Using the same system as in the study but excluding spheronization leads to 71.8% efficiency, a lot closer to the value from Surotseva et al. [93]. Excluding the calcination of coke also leads to a 90.3% ratio between input and output, which comes closer to the value from Dunn et al. [26].

This comparison highlights the importance of a thorough understanding of the value chain of synthetic graphite production, from the green coke to the BAM.

Study	Efficiency DM	Efficiency C	Including pitch
Notter et al (2010) [74]	83.3%		No
Dunn et al (2015) [26]	84%		Yes
Surotseva et al (2022) [93]	76,2%		Yes
Sofia Genovesi (2021) [40]	60%	65.9%	Yes
This study	45.2%	49.2%	Yes
This study	46.2%	50.0%	No
This study - without spheronization	71.8%	77.6%	No
This study - without spheronization and calcination	90.3%	98%	No

Table 4: Literature comparison for the efficiency of synthetic graphite production

2.3 Demand - Dynamic model description

2.3.1 Principle

The graphite value chain was quantified from 2020 to 2050 using the processes defined in the previous section and demand data for battery and non-battery sectors. The model is parametric, meaning that all the flows are calculated for all combinations of each parameter, making up for a total of 4050 different ”scenarios”. The different parameters of the model are summarized in the table 5. A schema explaining the structure of the dynamic model is presented in figure 8.

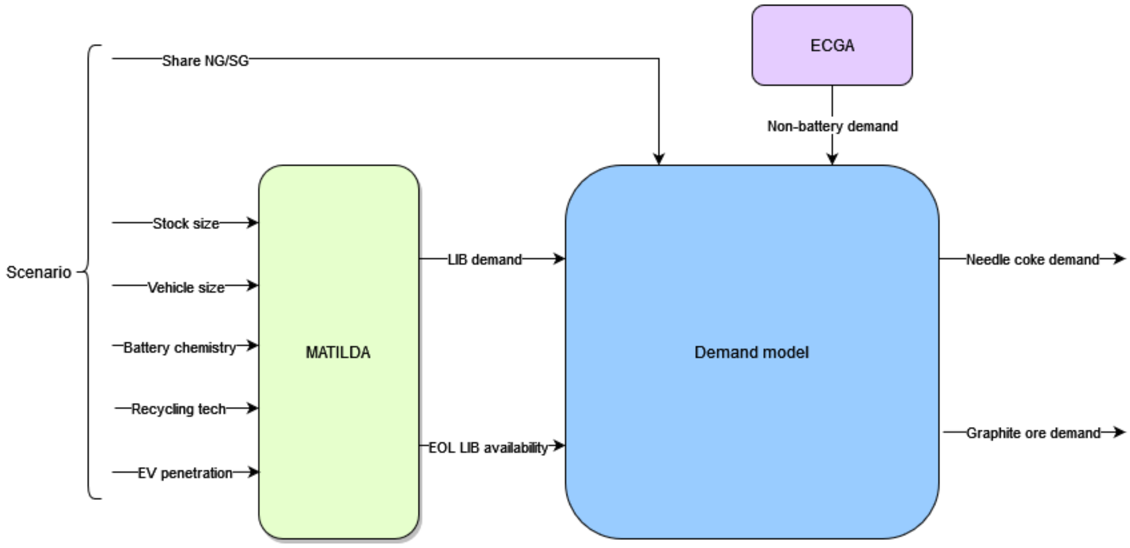


Figure 8: Structure of dynamic model

Demand for the battery sector

For each year, the demand from the different sectors in both natural and synthetic graphite is required as an input. The demand from the battery sector is obtained from the Material Demand and Availability (MATILDA) model [4]. The MATILDA model uses a parametric approach to simulate the electric vehicle system and its components. In particular, the MATILDA model includes a material layer for Graphite, providing, for each year, the amount of total graphite

(A_{19-20} in the system, figure 6) and secondary graphite (A_{23-16}) required by the transportation sector, as well as the stock of graphite contained in EVs in the use phase (M_{20}). The model is parametric, meaning that every parameter can be changed individually and allows for creating a great number of different scenarios. The MATILDA model includes 6 different parameters, 5 of which are included in the present model as shown in table 5. The reuse scenario parameter is not a parameter in this study for simplification purposes. These parameters and their signification are more thoroughly described in the dedicated paper [4].

Demand for non-battery sectors

The demand for non-battery sectors was extracted from the European Carbon and Graphite Association (ECGA) reports. The data is based on outlooks from McKenzie and partially made publicly available by the ECGA, which gives the demand in 2020 as well as the Compound annual growth rate (CAGR) for the periods 2020-2030 and 2030-2050. From this, an estimation of the demand from each sector can be calculated for every year until 2050, assuming constant geometric growth between 2020 and 2030 and then between 2030 and 2050. The share of natural and synthetic graphite for each sector is assumed to be constant over time, reflecting the preference of each sector for a certain type of graphite. The assumptions made here, that the demand grows at a constant rate and that the share of natural and synthetic graphite for non-battery sectors is constant, are assumed to have low consequences on the results of the model because of the predominance of the battery sector in most scenarios.

The quantification of all possible combinations allows anyone to examine the results for a specific scenario of interest. The downside is that this approach poses problems in data management due to the high number of combinations and calculations for each of them. The combination of all the parameters from table 5 makes for 4455 scenarios, with 31 years each. The graphite system, because it is defined for all the graphite sectors, is made up of more than 100 flows, each of them having values on the 2 layers. This totals to more than 31 million data points. To allow for the modelling of this parametric model, a generic MFA recursive python model has been developed, it is described in the annexe 6.1, and the code is available on GitHub (https://github.com/mfa-indecol/graphite-cycle).

Parameter	Description
Stock scenario	The stock scenario describes the potential evolution of the car stock **Options**: Low, Medium, High
EV penetration scenario	The EV penetration scenario characterize the share of electric vehicles in the vehicle stock. The SD scenario is the least ambitious, whereas the Net zero scenario assumes only electric vehicles in the vehicle stock by 2050. **Options**: STEP, SD, Net zero
Vehicle size	Vehicle size allows for simulating the impact of smaller or larger vehicles in the vehicle stock. **Options**: Shift to small cars, Constant, Shift to large cars
Battery chemistry scenario	There are 5 possible chemistry combinations defined based on external literature or specific to the MATILDA model. **Options**: NCX, LFP, Next gen LFP, BNEF, Next gen BNEF
Recycling process	The 3 recycling methods are representative of how batteries are handled at the EOL of electric vehicles. **Options**: Direct, Hydrometallurgy, Pyrometallurgy
Share NG in batteries	The share of natural and synthetic graphite in batteries has important consequences on demand for raw materials and depends on various factors (price, performance, availability). **Options**: Varies from 0 to 100% (10% step).

Table 5: Parameters for the demand model, the 5 first come from the MATILDA model and the last one is specific to this study

2.3.2 Sensitivity analysis

A sensitivity analysis was conducted on the model to gain a deeper understanding of how each of the previous parameters influences the system, especially the demand for needle coke and graphite ore. This analysis was conducted on the demand for graphite ore, looking at how each change in parameter decreases the demand for graphite ore over the years. This analysis consists in starting with the baseline scenario for graphite ore demand, ie medium vehicle stock, medium EV penetration, constant vehicle size, BNEF battery chemistry, Pyrometallurgy as a recycling process and 50% natural graphite in batteries. Shifting each parameter one by one to affect the demand for graphite ore, one can observe the impact of the parameters. It is, however, important to keep in mind that the order in which the parameters are changed has an influence on how much they reduce the demand.

2.3.3 Scenarios

To illustrate the results of the model described above, the demand for graphite for six scenarios is described. These scenarios are only a small subtract of the entire results and are used to illustrate the findings of the paper. These scenarios will also serve in the next section for the uncertainty analysis. The six scenarios are extracted from the MATILDA paper [4]. The six scenarios are the following:

- **EV-MRS 1, Slow transition:** Prices increase fast due to high battery demand, low EV penetration and technology development. Natural graphite is favoured in this scenario to limit the cost of battery anodes.
- **EV-MRS2, Slow transition - technology-oriented:** EVs are expensive and an elite product, turning towards performant batteries for high-end vehicles. Due to its higher performance, synthetic graphite becomes the preferred battery anode material.
- **EV-MRS 3, Baseline:** Moderate EV penetration and technology improvements. The share of natural and synthetic graphite remains equal.
- **EV-MRS 4 - SG, Fast transition – focus on electrification:** High material demand due to high penetration of EVs and size of the vehicle fleet, relying on technology breakthroughs. Synthetic graphite is preferred for higher performance.
- **EV-MRS 4 - NG, Fast transition – focus on electrification:** High material demand due to high penetration of EVs and size of the vehicle fleet, relying on technology breakthroughs. The high material demand raises prices, and natural graphite is preferred to lower costs.
- **EV-MRS 5, Fast transition – diversified portfolio with resource efficiency:** Resource efficient scenario where the fast EV penetration is allowed by technological and social changes. Both natural and synthetic graphite contribute to the transition.

Scenario	Vehicle stock	EV penetration	Chemistry	Vehicle size	Recycling	Share NG
MRS1	Medium	Slow (STEP)	LFP	Constant	Pyrometallurgy	80%
MRS2	Medium	Slow (STEP)	NCX	Shift to large	Pyrometallurgy	20%
MRS3	Medium	Medium (SD)	BNEF	Constant	Pyrometallurgy	50%
MRS4-SG	High	Fast (Net Zero)	Next gen BNEF	Constant	Hydrometallurgy	20%
MRS4-NG	High	Fast (Net Zero)	Next gen BNEF	Constant	Hydrometallurgy	80%
MRS5	Low	Fast (Net Zero)	Next gen BNEF	Shift to small	Direct	50%

Table 6: Scenario description from Lopez et al., with an additional parameter regarding the share of natural graphite [4]

The parameters for the six scenarios are presented in table 6. An extra parameter concerning the share of natural and synthetic graphite has been added for each scenario compared to the MATILDA model. As explained previously, synthetic graphite is preferred for its performance in battery anodes, but the choice between natural and synthetic graphite is mainly cost dependent and, therefore, highly dependent on the availability of both resources. Based on the different storylines, either natural or synthetic graphite is preferred to favour cost or performance. Scenario MRS4 is presented with two variants, based on the share of natural and synthetic graphite, to present the realistic high end of the demand for both materials.

2.3.4 Uncertainty analysis

When developing a parametric model, the main uncertainty regarding the results comes from the choice of parameter itself. But for a given set of parameters, such as for the scenarios, there also is uncertainty about the demand for needle coke and graphite ore. It is not possible to provide the exact amount of graphite ore and needle coke required to produce a given amount of graphite. This uncertainty is due to the fact that the processes described in the system definition can vary from one supplier of graphite to another and might also evolve in the future. The data extracted from the different papers and the expert interviews are subject to caution and might not represent the global production of graphite. To evaluate the robustness of the findings of this study, an uncertainty analysis has been performed for the 5 scenarios. To derive uncertainties, a Monte Carlo analysis has been performed. Monte Carlo analysis has been extensively used in the field of Material Flow Analysis to calculate uncertainties of flows and stocks within a system [25][58][63][99][106]. Each parameter is assigned a distribution and a standard deviation. Then, each parameter is sampled from its probability distribution, and the model is run many times based on these samples to find the distribution of the results.

The Pedigree matrix approach was used to assign a probability distribution to each parameter. This approach, first developed by Funtowicz and Ravetz in 1990, is used to translate pedigree criteria on the quality of data to a quantitative uncertainty [37]. The method was popularized in the field of industrial ecology due to its use for assessing uncertainties in the LCI database Ecoinvent [19]. It has also been used previously in the field of Material Flow Analysis by Laner et al., and the approach for this study is very similar to theirs [59]. The quality of each parameter is characterised by 5 indicators, reliability, completeness, temporal correlation, geographical correlation and other correlation (technological correlation), as shown in the annexe in table 14. Based on the quality of the source, the parameter is attributed a score from 1 to 4 on each indicator. This score is associated with a coefficient of variation in that category, as shown in table 7. The coefficient of variation, or relative standard deviation, corresponds to the ratio of the standard deviation compared to the mean. The total coefficient of variation for the parameter is calculated with the following equation:

$$cv_{tot} = \sqrt{cv_{reliability}^2 + cv_{completeness}^2 + cv_{tempcorr}^2 + cv_{geogcorr}^2 + cv_{othercorr}^2} \tag{1}$$

	Score: 1	**Score: 2**	**Score: 3**	**Score: 4**
Data quality indicator	**CV (in %)**			
Reliability	2.3	6.8	20.6	62.3
Completeness	0	2.3	6.8	20.6
Temporal correlation	0	2.3	6.8	20.6
Geographic correlation	0	2.3	6.8	20.6
Other correlation	0	2.3	6.8	20.6

Table 7: Quantitative coefficient of variation (relative standard deviation) for the different quality indicators, from Laner et al. [59]. The CV for each category and score indicates how this indicator contributes to the total standard deviation of the parameter, calculated with equation 1.

This pedigree matrix allows for a consistent method for assigning uncertainties to parameters and also allows for a variation of the uncertainty with time when dealing with a dynamic model. The temporal correlation parameter indeed rises with the years for each parameter because they have been sourced from papers dating from the 1990s to 2023. This means that the uncertainty of the results in 2050 is systematically higher than in 2020. Because no information is provided, all parameters were assigned a normal distribution for simplification purposes. The pedigree indicators for each indicator are found in the annexe, in table 15.

The uncertainty analysis was run with the help of a Python module developed by Nils Dittrich. This module is a Python-based function that allows for a simple simulation of uncertainty analysis for MFA using Monte Carlo methods, with an emphasis on distribution choices and the sampling of parameters. The module also allows for sensitivity analysis and data reconciliation, but these functionalities were not used for this thesis. The module is available on Zenodo (https://doi.org/10.5281/zenodo.8004730).

2.4 Natural graphite supply

The demand model based on MATILDA described above provides the range of raw resources that will be required in different scenarios to ensure the decarbonisation of the transport sector. To understand the supply of these different raw resources, the thesis presents the limitations and opportunities in the supply of natural graphite, synthetic graphite and recycled graphite. First, it is interesting to understand how much graphite can be mined and treated, focusing for this section on a subset of the global graphite system, including the graphite extraction and natural graphite production, as presented in figure 9.

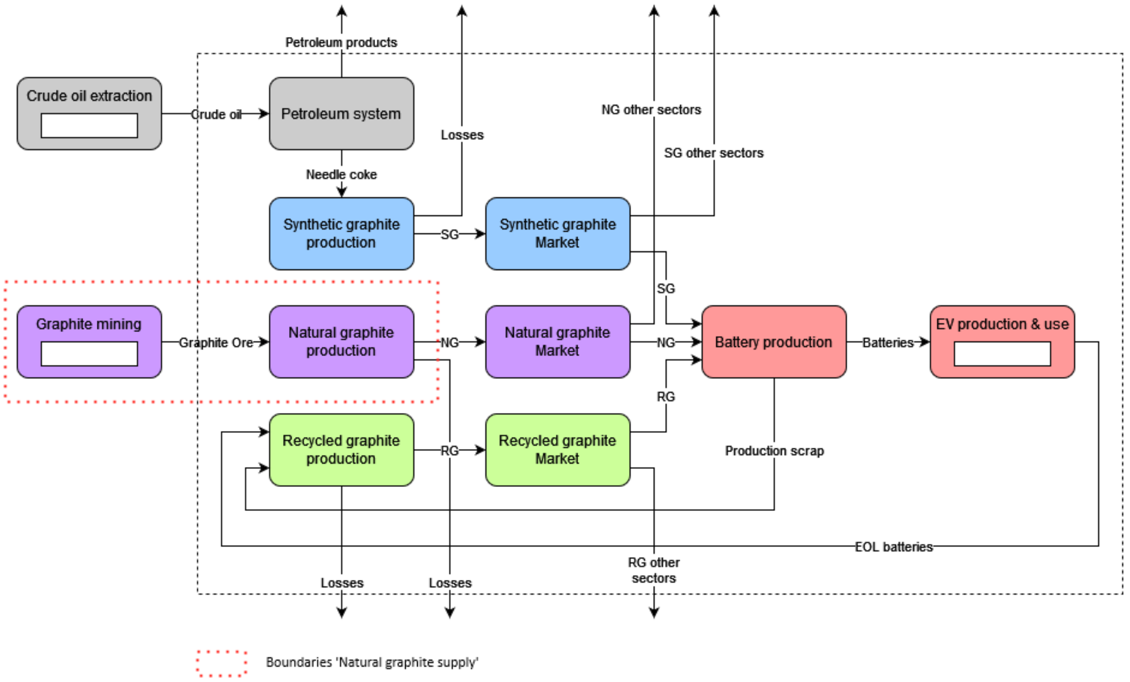


Figure 9: Global system of graphite production, with boundaries for the natural graphite supply

The research regarding the mining and refining of graphite is mainly based on a literature review. Several experts in the domain have been interviewed to understand which factors hinder the development of the natural graphite sector and how the supply could be extended. Among the interviewees were Berit Berbusmel, working as a geologist for the Norwegian graphite producer Skaland and Christoph Frey, the founder of Pro-Graphite, a company specialised in providing expertise around graphite and graphite products. To gain insight into the present status of graphite mining and to assess its potential for future expansion, Geographic Information System (GIS) methods have been used on graphite mines datasets. The application of GIS technology has facilitated the creation of a visual representation of the geographical distribution of natural graphite production.

2.5 Synthetic graphite supply: Petroleum System

The production of synthetic graphite is highly dependent on the supply of needle coke, mostly from petroleum sources. First and foremost, it is crucial to understand the definition of petroleum coke as well as gain an understanding of the petroleum refining system, from which petroleum needle coke is a byproduct. A Material Flow Analysis of the petroleum refinery system was conducted to grasp the dynamics behind needle coke production. The system studied in this section is represented as a subset of the global system in figure 10.

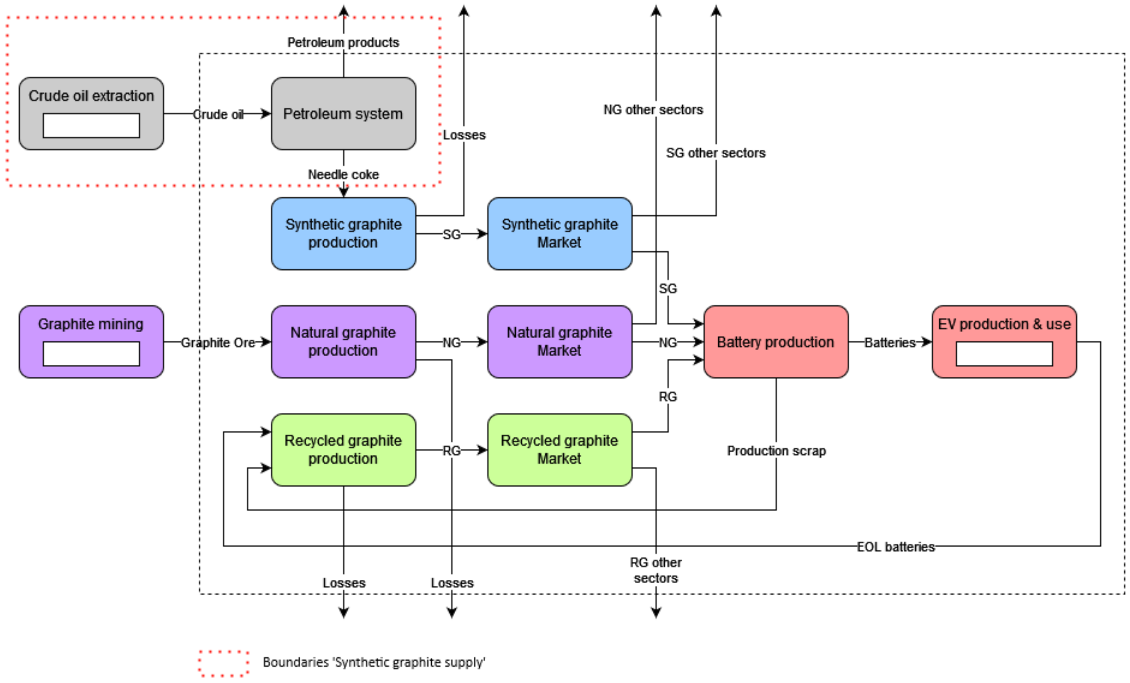


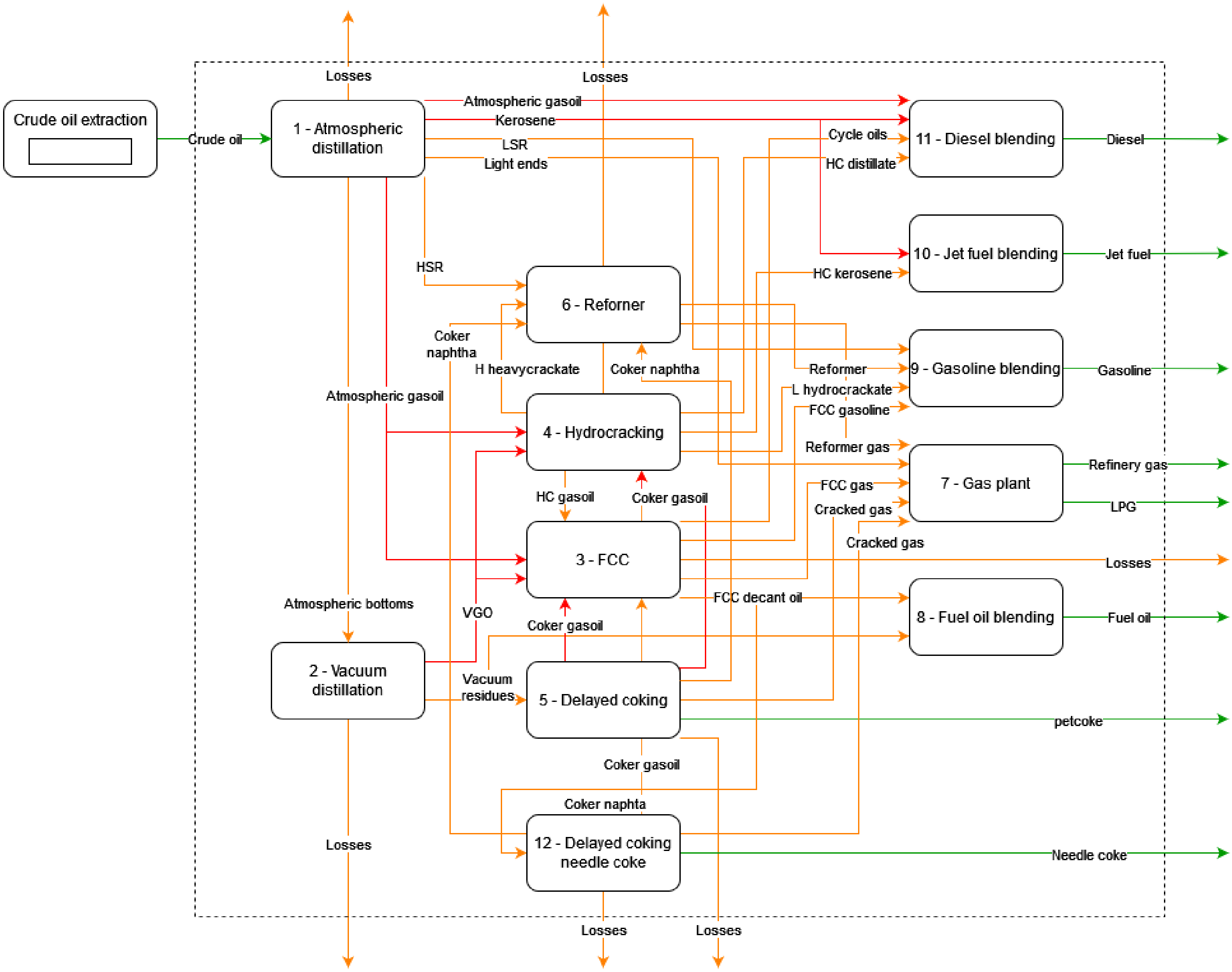
Figure 10: The global system of graphite production, with boundaries for the synthetic graphite supply

2.5.1 System Definition

The petroleum refinery system has been simplified to the essential processes to understand the key dynamics ruling refineries and the trade-offs at stake while keeping the system simple, understandable and easy to model. The goal is to model the current state of refineries to be able to downscale it depending on the forecasted production of crude oil. The transport sector's electrification aims to decrease the production of diesel and gasoline and, therefore, its byproducts, such as needle coke.

On the other hand, this electrification is responsible for a surge in the production of graphite and, therefore, the demand for needle coke. Therefore, this model serves to estimate if the penetration of electric vehicles could have consequences on the supply of this crucial battery material.

Crude oil is a complex blend of hydrocarbons; refineries use different processes to separate the different fractions depending on their physical and chemical properties. The petroleum refinery system is a complex system that converts crude oil (or petroleum) into different products such as gasoline, diesel, jet fuel, and gases. The main goal of a refinery is to maximise the output of valuable products, which are the lighter fractions: diesel and gasoline. The system has been simplified for the sake of this study. It only includes the following processes present in figure 11: atmospheric distillation (AD), vacuum distillation (VD), fluid catalytic cracking (FCC), hydrocracking (HC), reforming, the delayed coking unit (DCU) and the gas plant.



The green flows are directly extracted from the OECD statistics. The orange flows are calculated from the crude oil flow based on transfer coefficients and mass balance. The red flows have several target processes possible and are calibrated in order to mass balance the blending processes on the left of the system

Figure 11: System definition for the petroleum refinery system

The first process in a petroleum refinery is atmospheric distillation (process 1 in the system definition, figure 11), which separates the different distillation cuts of crude oil based on their boiling point. The input of the process is crude oil, and it produces various products, from the lightest to the heaviest, such as refinery gases, light ends, straight run naphtha, kerosene, atmospheric gasoil, and atmospheric bottoms.

The products from atmospheric distillation are either sent further to refining processes or directly blended into the end product pools. The atmospheric bottoms are sent to vacuum distillation (process 2), a second distillation unit for further separation of the distillation cuts. The outputs of vacuum distillation are vacuum gasoil and vacuum resid.

The former is sent to one of the cracking units of the refinery, Fluid catalytic cracking or hydrocracking units (processes 3 and 4), which produce various products that are sent to different end-use pools. These units aim at upgrading gasoil from various refinery processes into lighter products. The main difference is that the FCC has a higher yield of gasoline, while the HC produces more diesel. The refiner uses each unit depending on the economic situation and the output they wish to maximize.

Finally, vacuum resid is sent to the delayed coking unit (process 5) to produce petroleum coke (petcoke), coker naphtha, coker gasoil, and cracked gas. However, it is important to note that petcoke produced by this process is not suitable for the production of graphite due to its low quality and level of impurities. Refiners that aim at producing needle coke need a specific delayed coking process (process 12) that uses FCC decant oil as a feedstock, a highly aromatic output from the FCC unit.

Most types of naphtha, produced from the atmospheric distillation or the cracking units, are sent to the reformer unit (process 6), which produces reformate, a high-quality gasoline blendstock. The gas plant's (process 7) goal is to separate valuable products, such as propane and butane, and send lower-value methane and ethane to the refinery fuel system. Refineries usually have two gas plants, the saturated one and the unsaturated one, but they have been grouped here.

The blending processes (processes 8 to 11) consist of blending different hydrocarbons to produce the desired industrial product, corresponding to a certain density and potentially stringent requirements on the impurities such as sulfur.

Although many flows in the refinery system are also hydrotreated (treated with hydrogen), this process has been ignored as it does not produce a new product, it only decreases the sulfur content. Isomerization is another process that upgrades naphtha to make it a more valuable gasoline blendstock. However, it is not relevant to the production of needle coke and has also been ignored. The processes, their inputs and outputs, as well as the different transfer coefficients and sources, are summarized in Table 8.

Nr	**Process**	**Inputs**	**Outputs**	**Fraction**	**Source**
1	Atmospheric distillation	Crude oil	Refinery gas	0%	[34][1]
			Light ends	1%	[34][1]
			Light straight run naphtha	4%	[34][1]
			Heavy straight run naphtha	12%	[34][1]
			Kerosene	15%	[34][1]
			Atmospheric gasoil	26%	[34][1]
			Atmospheric bottoms	42%	[34][1]
2	Vacuum distillation	Atmospheric bottoms	VGO (light)	44%	[34][1]
			VGO (heavy)		[34][1]
			Vacuum resid	56%	[34][1]
3	FCC	VGO	FCC gasoline	48%	[68][39]
		Coker gasoil	Cycle oils	19,4%	[39][1]
		Atmospheric gasoil	FCC decant oil	7%	[44][39][1]
			FCC gas	26%	[68][39][1]
4	Hydrocracker	VGO	Hydrocracked distillate	41%	[83]
		Coker gasoil	Hydrocracked gasoil	6%	[83][1]
		Cycle oils	Hydrocracked kerosene	27%	[83][1]
		Atmospheric gasoil	Heavy hydrocrackate	7%	[83][1]
			Light hydrocrackate	6%	[83][1]
			Isobutane	5%	[83][1]
5	Delayed coker	Vacuum resid	Coker naphtha	14%	[81]
			Coker gasoil	52%	[81][1]
			Pet coke	25%	[81][1]
			Cracked gas	9%	[81][1]
6	Reformer	HSR naphtha	Reformate	91,95%	[39]
		Hydrotreated naphtha	Hydrogen	1,70%	[39]
		Heavy hydrocrackate	Reformer gas	6,35%	[39]
7	Gas plant	Cracked gas	Propane, butane		
		Reformer gas	Refinery gas		
		Light ends			
		FCC gas			
8	Fuel oil blending	FCC DO, vacuum resid	Fuel oil		
9	Gasoline blending	Naphta, reformer...	Gasoline		
10	Jet fuel blending	Kerosene...	Jet fuel		
11	Diesel blending	Gasoil, kerosene...	Diesel		
12	Needle delayed coker	FCC decant oil	Coker naphtha	9%	[81]
			Coker gasoil	35%	[81]
			Needle coke	50%	[20]
			Cracked gas	6%	[81]

Table 8: Description of processes for the petroleum refinery system

2.5.2 Data sources and calibration

The different processes have been described thanks to different studies on petroleum refineries, mainly the Petroleum Refinery Life Cycle Inventory Model (PRELIM) model developed by the University of Calgary [1]. The system was first quantified for the global production of petroleum in 2017. The inflow and outflows to the system, respectively, crude oil and the different end-use petroleum products, have been quantified directly from OECD statistics. They are shown in green in the system figure 11. The different processes have been described in table 8, but there remains uncertainty on the destination of flows. For example, atmospheric gasoil can be directly used for diesel blending or sent to one of the cracking units, FCC and hydrocracker. The share of that flow that goes to each of the three processes is unknown. The same happens for vacuum gasoil and coking gasoil, which are cracked either by the FCC or the hydrocracking, and kerosene from the Atmospheric distillation that can be blended either in jet fuel or diesel. Figure 11 shows these flows in red in the system definition. To determine these unknown shares, all flows were calculated based on the crude oil input (independently from the different fuel outputs), and the system (the unknown shares) was then calibrated based on mass balance at the different blending processes, using the different fuel outputs (gasoline, diesel...) for the calibration.

The share of the orange flows going to the different processes has been adjusted to do the calibration while minimising the sum of the squared mass balance difference in each blending process. The goal is to minimise the error Err defined by the following equation:

$$Err = \sum_{P \in Blending} (Inflows_P - Outlows_P)^2 \tag{2}$$

Once the model is calibrated, it can be scaled to provide scenarios for the production of needle coke in the future, depending on EV penetration but also taking into account potential adaptations in the refinery system to maximise the production of needle coke. Scenarios from the International Energy Agency (IEA) have been used to scale the refining system. The IEA have three scenarios, which are identical to the EV penetration scenarios used in the MATILDA model. The advantage is that for one demand scenario stating how much needle coke is needed, there is a corresponding supply scenario giving the amount of needle coke that can be produced. The 3 IEA scenarios are the following:

- **Stated Policies (STEP):** Reflect policies currently in place (at the time of the report in 2021) in every sector
- **Announced Pledges Scenario (APS):** Assuming all commitments made by the government are met (This scenario is not identical but close to the Sustainable Development (SD) scenario used in MATILDA in terms of climate goals [98])
- **Net Zero Emissions by 2050 Scenario (NZE):** Scenario where the energy sector reaches 0 emissions by 2050

As explained, these scenarios correspond to the EV penetration parameter in the demand scenarios. The demand and supply scenarios are therefore connected in the following way:

- **Stated Policies (STEP):** MRS1 and MRS2
- **Announced Pledges Scenario (APS):** MRS3
- **Net Zero Emissions by 2050 Scenario (NZE):** MRS4-SG, MRS4-NG and MRS5

For each of the scenarios, two limits for the production of needle coke were calculated, one assuming that the petroleum system remains identical to today, and a second one allowing for flexibility in the different processes, in particular, to maximise the output of needle coke. The yields of the different processes within the petroleum system depend on the physical properties of the oil but also on the economic situation and the products that the refiners try to maximise. The maximum supply of needle coke in an optimised situation for needle coke production takes these two factors into account:

- Economic value of needle coke: Assuming that the transportation sector engages its decarbonisation heavily relying on graphite, the relative price of needle coke compared to gasoline and diesel might increase, raising the benefit for refiners to maximise needle coke output
- Physical properties of crude oil: Over the past few decades, there has been a notable increase in the density of extracted crude oil. This trend is expected to continue, with a shift towards extracting heavier crude oils as lighter oils become less prevalent. Heavier oils have higher yields of heavy products, including petroleum needle coke and its feedstocks.

The new yields for this optimised situation are taken from expert interviews. They are based on refineries that produce heavier oils and producers of needle coke, who already try to maximise their output.

2.6 Recycled graphite supply

The supply potential for graphite ore and needle coke is independent to some extent of the demand for graphite; it depends more on resource limitations and infrastructures for graphite ore and on the amount of extracted crude oil and refinery dynamics for needle coke. For recycled graphite, on the other hand, the supply is tightly linked to the demand. It depends directly on how much scrap from battery production and graphite in EOL batteries is available for recycling. Therefore, the modelling of the recycling flows is largely dependent on the MATILDA model also. This model calculates the in-use stock of EVs, but also the inflows (the demand for new EVs) and the outflows (EOL EVs) of this stock.

In a similar manner to the natural graphite supply, the recycled graphite supply was studied with a more qualitative approach, mainly based on a literature review and expert interviews to understand the processes in the recycling of graphite, the ageing mechanisms of graphite, and the limitation regarding the use of recycling graphite in batteries that could hinder its use and limit the circularity of the graphite value chain. The scope of this section is shown in figure 12. The MATILDA model provided how much graphite was recycled for the different scenarios but without taking into account potential limitations in the recycling value chain or in the reuse of recycled graphite for new batteries. It is important to keep in mind that the efficiency of recycling is multifactorial, technological, economic and industrial challenges have to be overcome to allow for important recycling.

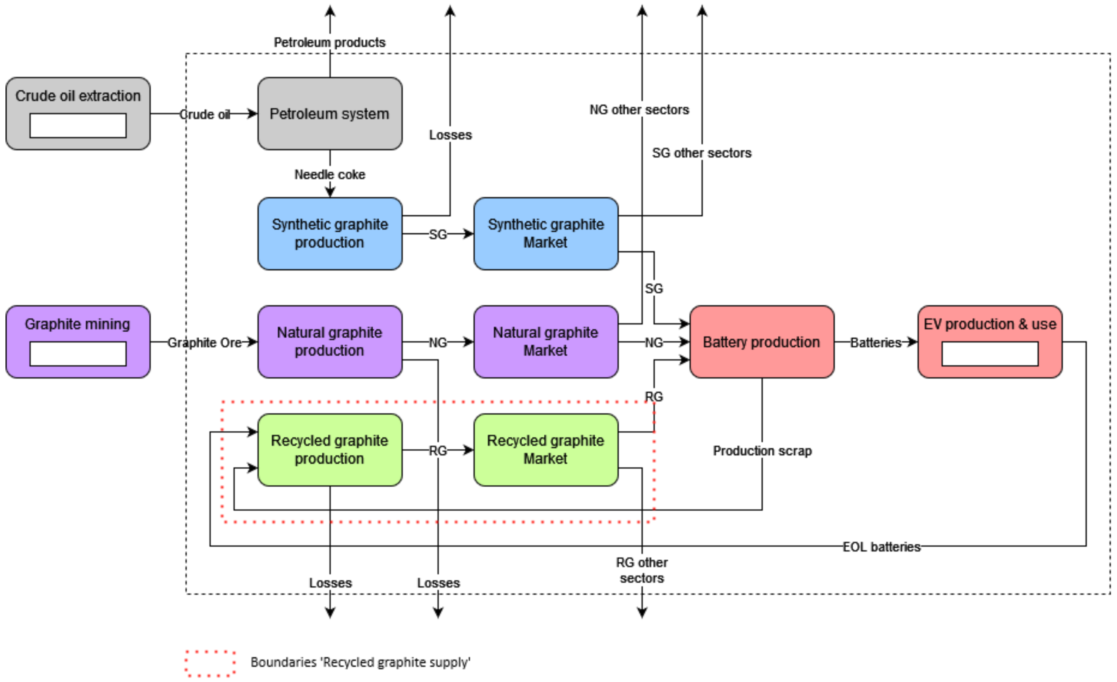


Figure 12: The global system of graphite production, with boundaries for the recycled graphite supply

In the model, three recycling routes are described.

The first one is Pyrometallurgy, which is the most common recycling route currently [72]. With pyrometallurgical recycling, batteries are smelted to retrieve important metals like lithium, cobalt, and nickel [60]. The heating allows the separation of metals from other materials present in the battery, but graphite is burnt and lost in the process. Pyrometallurgy allows for no recovery of graphite material [71][89].

In hydrometallurgical recycling, the batteries are normally crushed or shredded before going through leaching procedures, in which the metals are dissolved in a suitable solvent or acid. The desirable metals, such as lithium, cobalt, and nickel, are subsequently recovered from the leachate by treating and purifying it [60][111]. The advantages of hydrometallurgical recycling include selective metal recovery and support for a variety of battery chemistries. Graphite can be extracted from the black mass through further purification steps [89].

Direct recycling consists of the physical separation and recovery of valuable elements from used batteries. The batteries are disassembled, and numerous mechanical processes, including sieving, magnetic separation, and shredding, are used to separate the various components [60]. The quality of the recovered metals can be increased by further refining procedures. This method allows for the highest rate of recovered graphite as it is the least destructive [89].

3 Results

3.1 Global graphite cycle for 2022

The current system was quantified for the year 2022. However, the petroleum system was quantified for 2017, the last year when high-quality data was available from the OECD. Considering the size of the petroleum system compared to that of the graphite one, it is assumed that this has a minor incidence on the current quantification. The quantification of the current system is displayed in figure 13. In the current system, the battery sector is not yet the predominant driver of the demand for graphite. The other sectors, particularly the electrode sector, show a higher demand for graphite than the battery one.

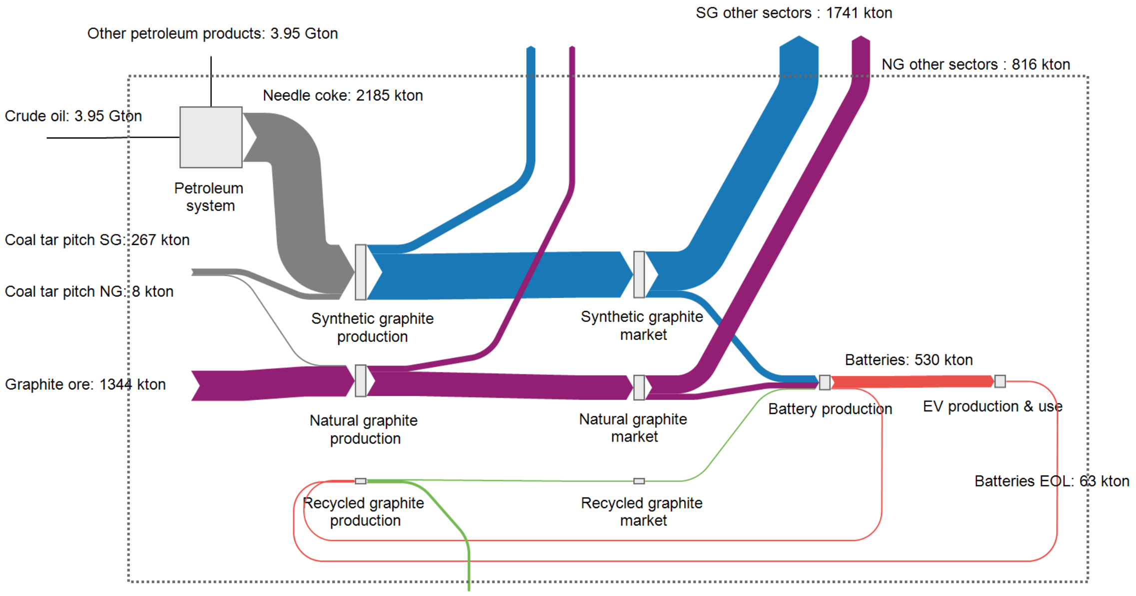
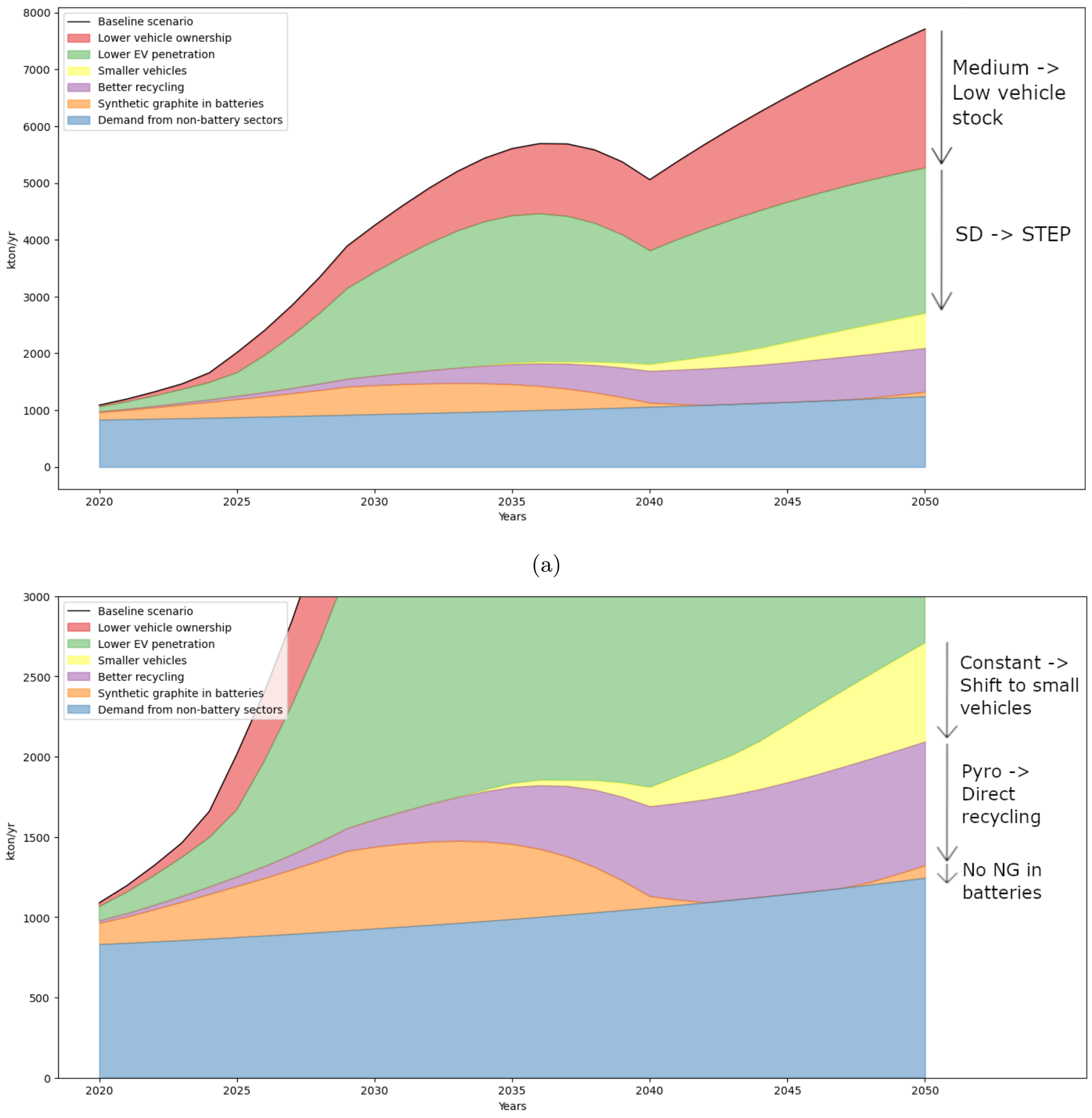


Figure 13: Sankey diagram of the global system for the year 2022.
The arrows representing the flows of crude oil and other petroleum products are not at scale for readability purposes, as these flows are 1800 times larger than the second largest flow in the system.

3.2 Demand Scenarios

3.2.1 Sensitivity analysis

To evaluate the impact of each parameter on the demand for raw resources and understand the consequences of parameter choices in the design of scenarios, the demand for graphite ore was observed starting from the maximal case and changing each parameter one by one, as shown in figure 14.



(a)

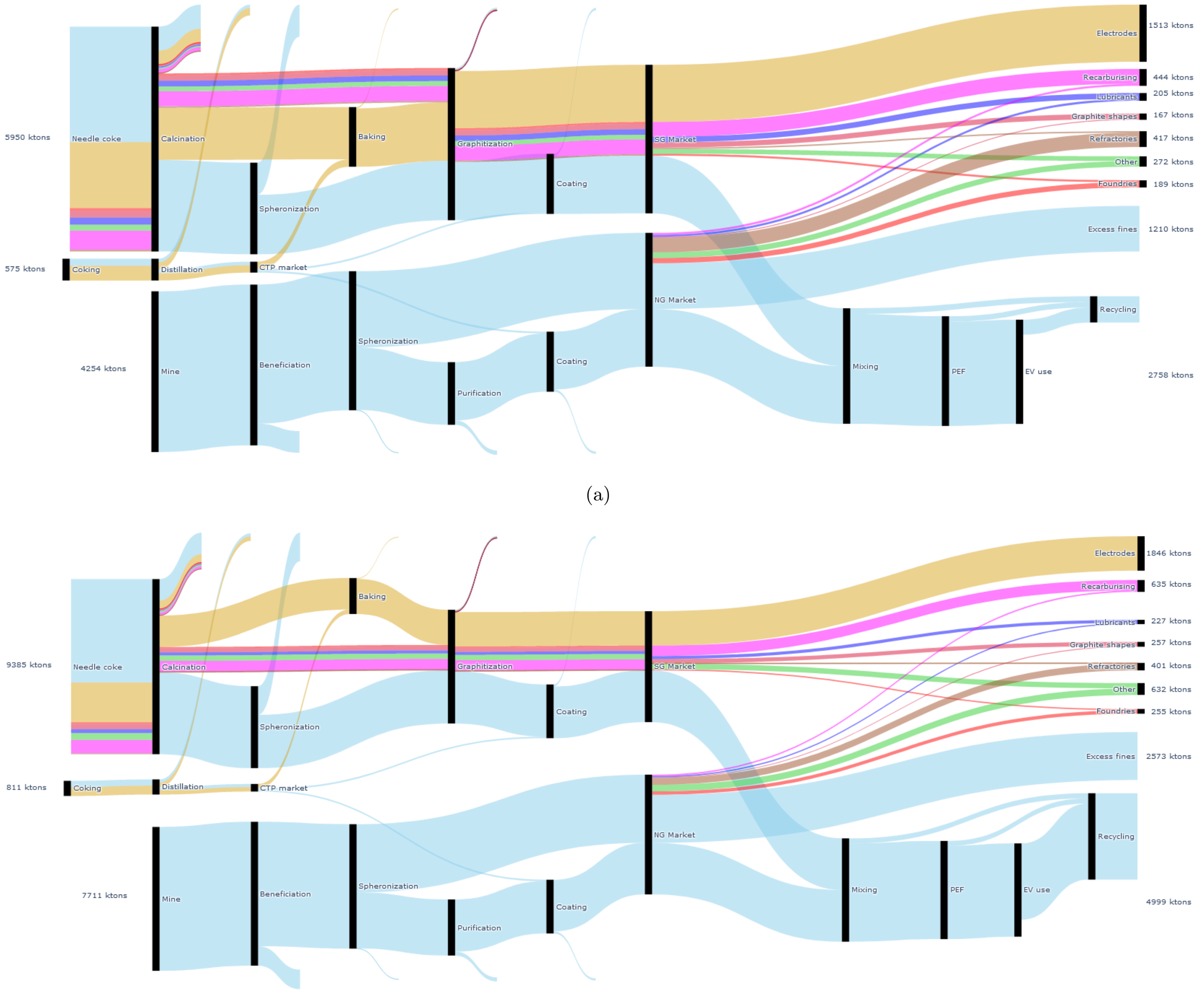
(b)

Figure 14: Sensitivity of the graphite ore demand to the different parameters from the parametric model. The order of the parameters has a great influence on the observed sensitivity. Figure (b) is identical to figure (a) but limited to 3 Mton on the y-axis

The sensitivity analysis shows the broad range of possibilities within the parametric model, with the demand for graphite ore varying from 8000 ktons in the baseline case to around 1000 ktons when only synthetic graphite is used in the batteries. It is also interesting to note how the different parameters impact the demand from a time perspective. For example, the battery recycling shift only affects the demand in the later years when the amount of EOL batteries is sufficient enough. The transition to smaller vehicles also has long-term effects because vehicles are progressively replaced with smaller ones. In contrast, car ownership or EV penetration changes immediately influence the demand for graphite ore.

3.2.2 Value chain of graphite production

By varying the different parameters, 4455 different scenarios can be constructed. The demand system was quantified for each of them. To visualize the full extent of the results, a website was developed and hosted on servers at NTNU at the following address: http://129.241.153.120:8052. This scenario builder tool helps understand the influence of the different parameters on the supply chain of graphite and estimate how much raw resources should be supplied to ensure the electrification of the transport sector for a given situation. The Sankey diagram of the baseline scenario (MRS3) is presented in figure 15, the Sankey diagram for the scenario MRS5 in figure 16, and the Sankey diagrams for the four other scenarios are present in the annexe, in section 6.3.

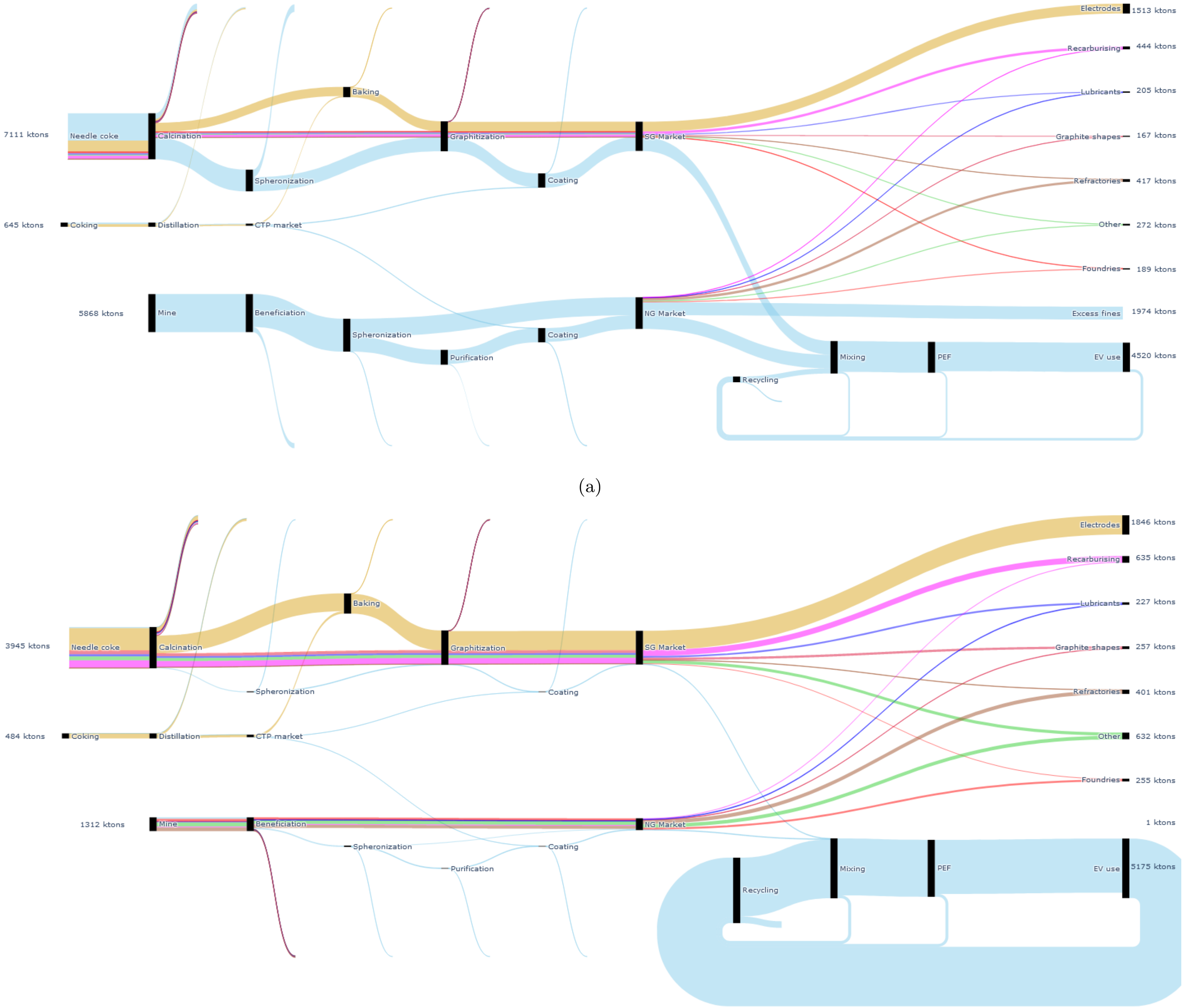


(a)

(b)

(The Sankey diagrams have different scales)

Figure 15: Sankey diagram of the graphite value chain for (a) Baseline scenario (MRS3) in 2030, (b) Baseline scenario (MRS3) in 2050 on the graphite layer in kton. The colors correspond to the different sectors, to understand the origin of the demand for needle coke and graphite ore.



(a)

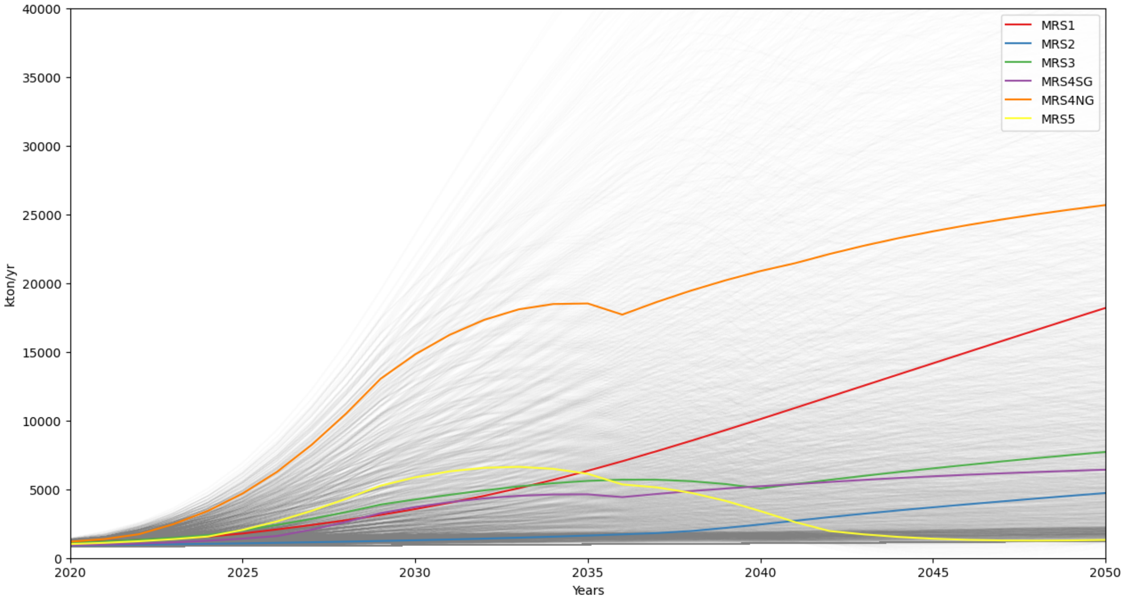
(b)

(The Sankey diagrams have different scales)

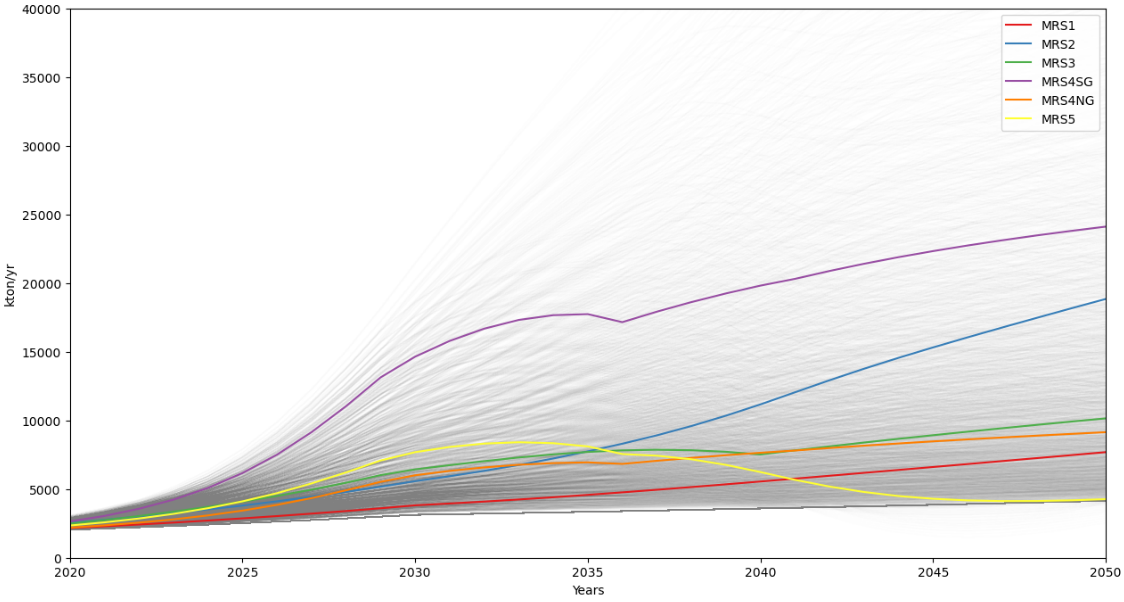
Figure 16: Sankey diagram of the graphite value chain for (a) Scenario MRS5 in 2030 and (b) Scenario MRS5 in 2050 on the graphite layer in kton. The colors correspond to the different sectors, to understand the origin of the demand for needle coke and graphite ore.

The Sankey figures look very different between the baseline scenario and scenario MRS5 because the latter includes graphite recycling, whereas, in the baseline scenario, batteries are recycled using Pyrometallurgy. As a reminder, graphite is not recovered during the pyrometallurgical process but is instead burnt and used as fuel. The recycling loop is, therefore, not present for the baseline visualization. In both scenarios (and in the four others), the system is subject to drastic changes between today, 2030 and 2050, with a demand for graphite in batteries that increases rapidly, even for the slower penetration scenario. For scenarios using Pyrometallurgy as the recycling process, the need for raw materials explodes and reaches up to 10 times the current production levels for needle coke in scenario MRS4-SG and up to 25 times for graphite ore in MRS4-NG (the two high-end demand scenarios). These scenarios show how broad the range of the demand for raw resources can be depending on technological changes, such as recycling techniques, battery chemistry, and the choice of graphite but also on societal changes, such as vehicle ownership, the size of vehicles and most importantly the penetration of EV in the vehicle stock.

3.2.3 Raw material demand in the scenarios



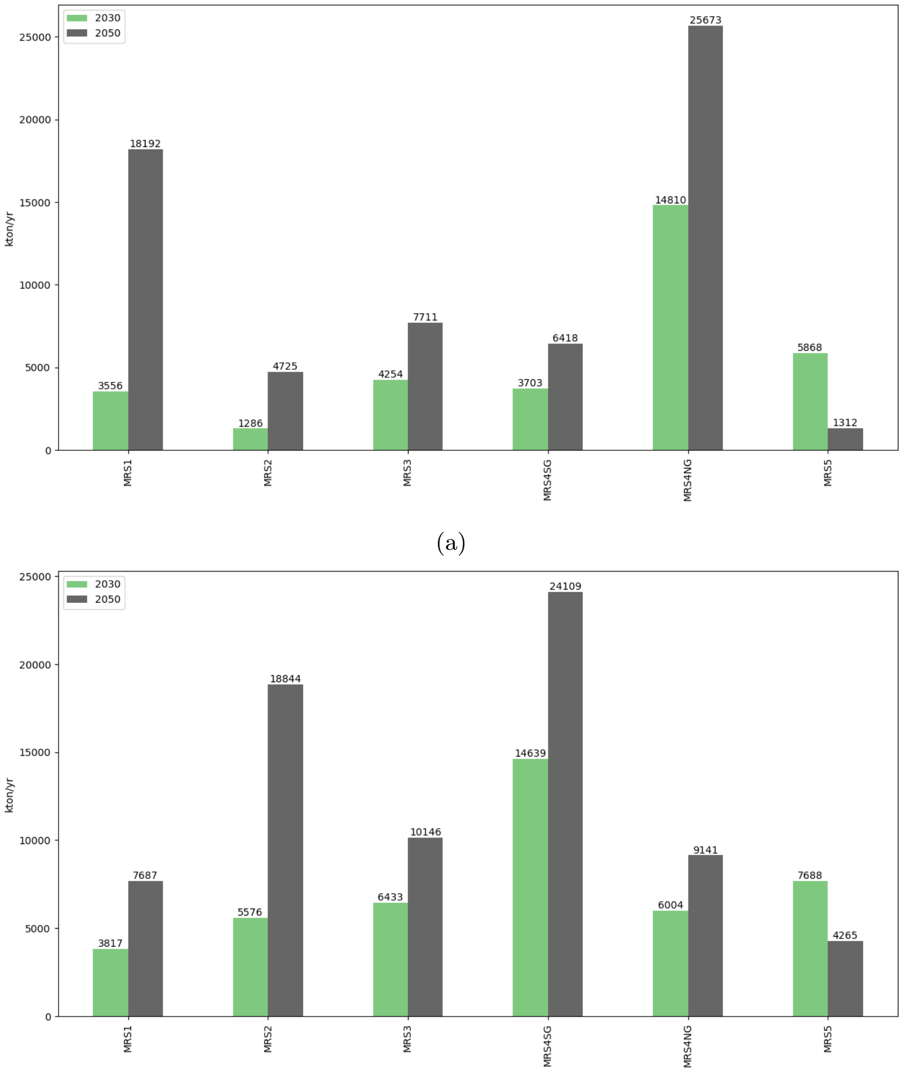
(a)



(b)

Figure 17: Raw material demand for all scenarios, with the 6 MSR scenarios highlighted. The figures show the demand for (a) graphite ore and (b) needle coke. For Needle coke, the demand is given on the DM layer, whereas for graphite ore, it is given on the graphite layer to match reports and articles on the respective topics.

The main goal of quantifying the value chain of graphite production was to quantify the raw material demand in the different scenarios to understand how much needle coke and graphite ore should be supplied to ensure the transition of the transportation sector. The demand for both graphite ore and needle coke for the scenarios is displayed over time in figure 17. The bar chart in figure 18 shows the demand in 2030 and 2050 while the values are summarized in the table 16. The technological, societal and political changes drastically affect the demand for these two resources, as shown in figure 17.



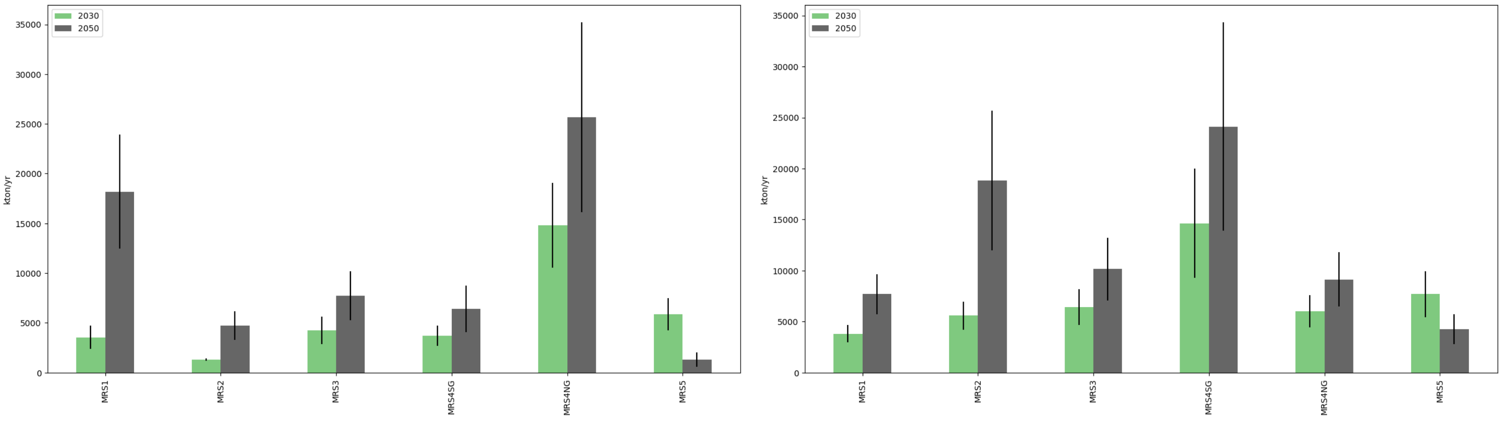
(a)

(b)

Figure 18: Demand for (a) graphite ore and (b) needle coke in the six scenarios in 2030 and 2050

3.2.4 Uncertainty analysis on scenarios

For each scenario, an uncertainty analysis was conducted to evaluate the level of uncertainty on the demand for raw materials due to uncertainty in the processes and the concentrations of the flows within the system in figure 6. Figure 20 shows the demand for needle coke and graphite ore in the baseline scenario, as well as the boundaries of the 95% confidence interval (two standard deviations) for each of them. The figure shows a growing relative uncertainty with time, but also a higher uncertainty for needle coke than graphite ore because of a higher demand but also fewer data in the description of the processes. Similar figures for the other scenarios are present in the annexe 6.3. The uncertainty is also shown as with error bars in Figure 19. Table 17 presents the same results as table 16 but with the range of uncertainty (95% confidence).



(a)

(b)

Figure 19: Demand with error bars, corresponding to 95% interval, for (a) graphite ore and (b) needle coke in the six scenarios in 2030 and 2050

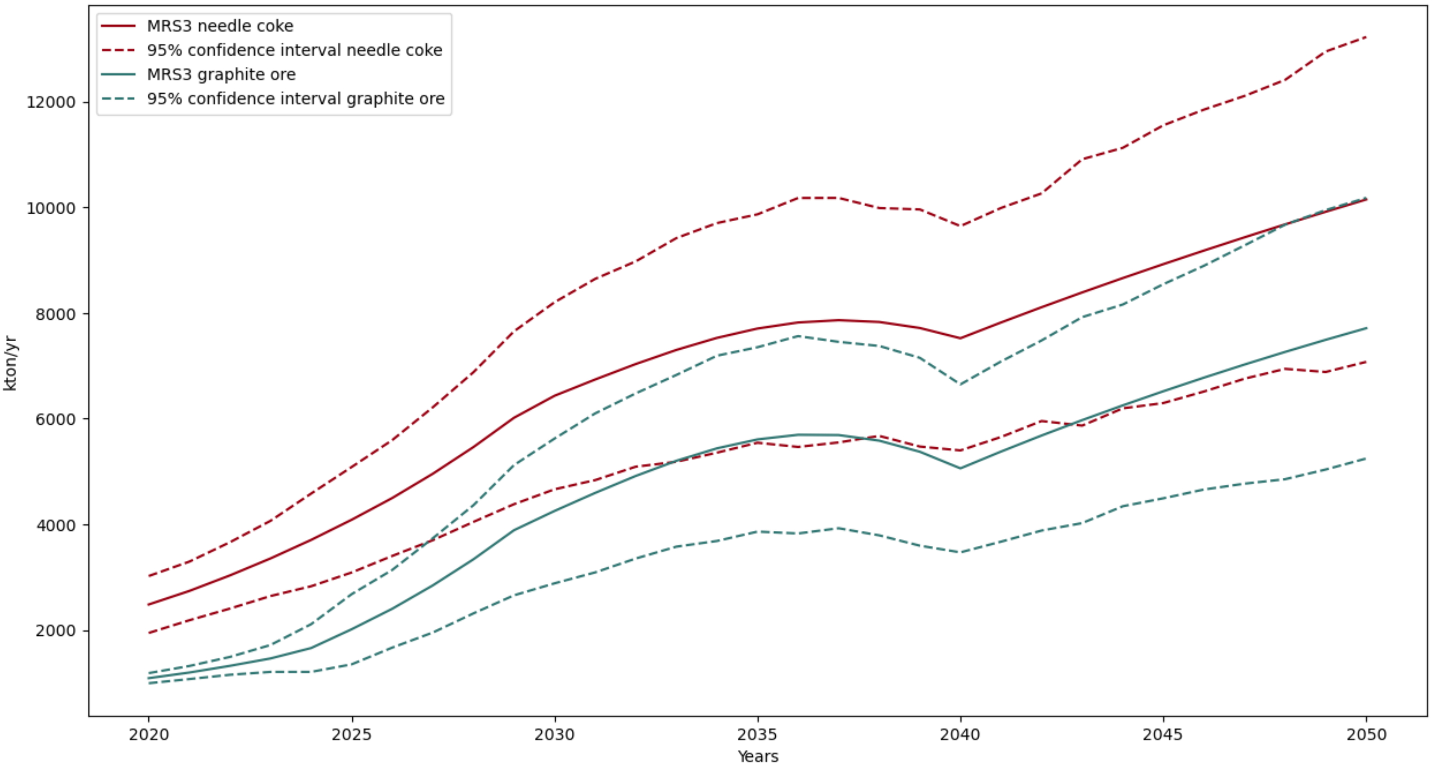


Figure 20: Demand for raw materials in the baseline scenario, with 95% confidence interval

3.3 Supply of graphite ore

The reserves of graphite are unevenly distributed around the globe, as shown in the table 9 showing the main producers of graphite. Turkey, China and Brazil have the largest graphite reserves with respectively 28%, 23% and 22% of the global reserves. However, the reserves in the different countries are of very different nature. Turkey has the largest reserves, but there are mostly composed of amorphous graphite, China's reserves contain both amorphous and flake graphite, whereas Brazil only produces flake graphite. The production is also concentrated in very few countries, China alone produced 79% of the world's natural graphite in 2021 and a similar share for the production of flake graphite only. Brazil is the second producer of natural graphite but produces only 6.8% of the total graphite, 8.4% if considering only flake graphite [101]. Several other countries are expanding their production, such as Mozambique, which opened the largest graphite mine in the world in 2017 [94].

Country	Production 2021	Reserves (kt)
China	820 000	73 000 000
Brazil	68 000	70 000 000
Mozambique	30 000	25 000 000
Russia	27 000	-
Madagascar	22 000	26 000 000
Ukraine	17 000	-
Norway	13 000	600 000
North Korea	8 700	2 000 000
Canada	8 600	-
India	6 500	8 000 000
Vietnam	5 400	-
Sri Lanka	4 300	1 500 000
Mexico	3 500	3 100 000
Turkey	2 700	90 000 000
Austria	500	-
Germany	300	-
Tanzania	150	18 000 000
Uzbekistan	110	7 600 000

Table 9: Main graphite producing countries

The US geological survey also contains a database with the locations of different graphite mines, tonnage, and the grade of graphite ore. The map 21 shows the geographic distribution of graphite production around the globe, highlighting the importance of China. The USGS dataset is, unfortunately, missing several important mines and does not reflect the entire span of graphite production. For example, the largest mine in the world, operated by Syrah in Mozambique, does not figure in the dataset because it opened too recently, in 2019, whereas the latest USGS report on mines dates from 2017. Very few Chinese mines are present in the dataset, clearly reflecting gaps in the data. It is therefore important to remember that the mines on map 21 are just a geographical indication of some production sites but do not represent the whole set of graphite mines. On the other hand, the countries' production is extracted from the most recent USGS report from 2022 and includes every producing country.

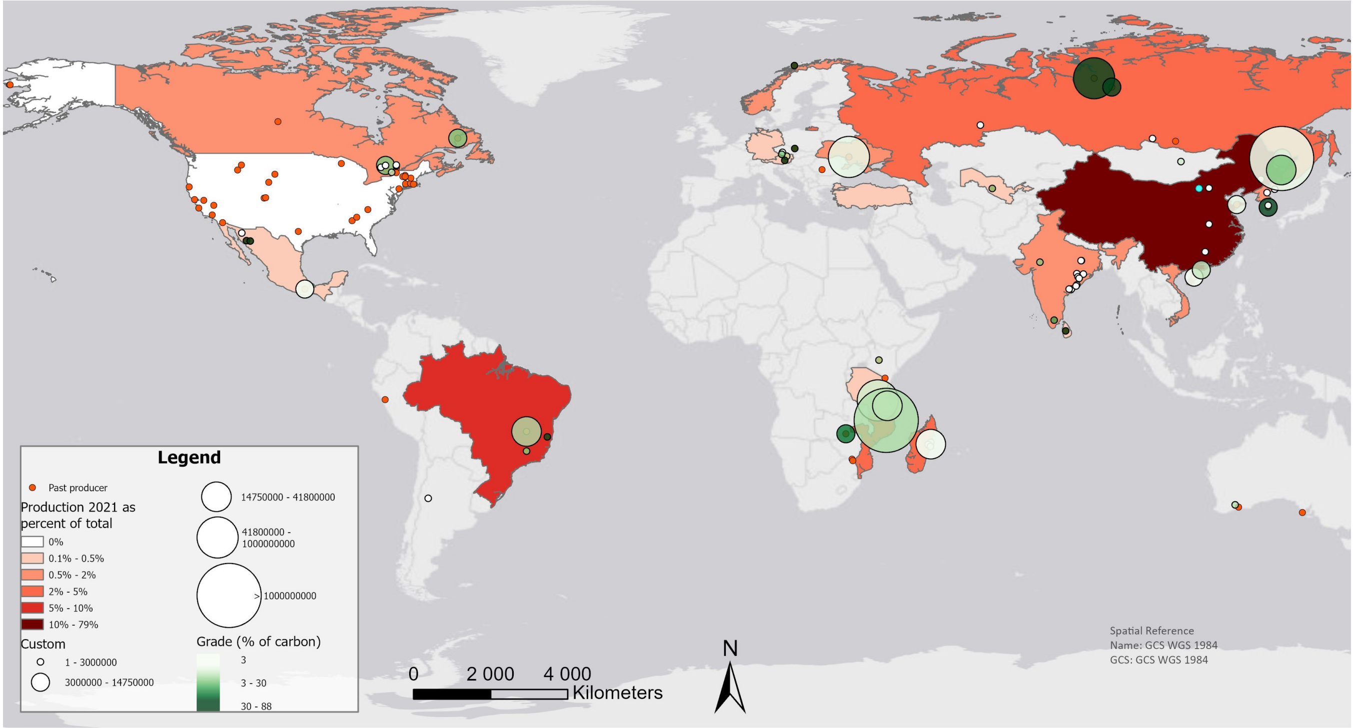


Figure 21: Map of the graphite production and reserves. The main producing countries are shown and colored with their share in the global production. The main graphite mines are displayed showing their reserves of graphite and the grade of the graphite ore [101][100]

To update the dataset with recent graphite mining projects and lacking mines, the dataset from the USGS was updated with new mines and their reserves, such as the Syrah mine in Mozambique and several important Chinese mines.

No scenarios were established for the natural graphite supply due to the lack of public information on current and future mining projects, especially in China, the leading producing country.

For graphite ore, it can also be relevant to look into cumulated resource use to study the depletion of the resource. Figure 22 shows the cumulated use of the resource and the global reserves established by the USGS in 2022 [100]. It is important to keep in mind that reserves are a dynamic concept and keep evolving based on resource depletion but also on new geological studies. Therefore the figure 22 does not show that natural graphite ore will necessary be depleted in 2043 for the scenario MRS4-NG but is an indicator of potential stress on the resource.

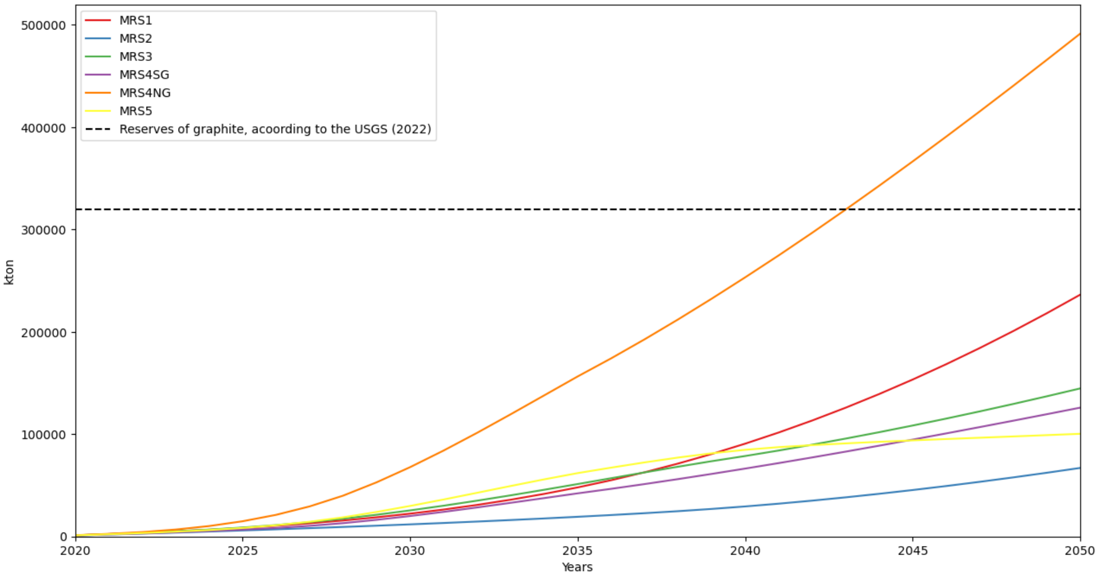


Figure 22: Cumulated demand for graphite ore in the 6 scenarios

3.4 Supply of needle coke

3.4.1 Current petroleum system

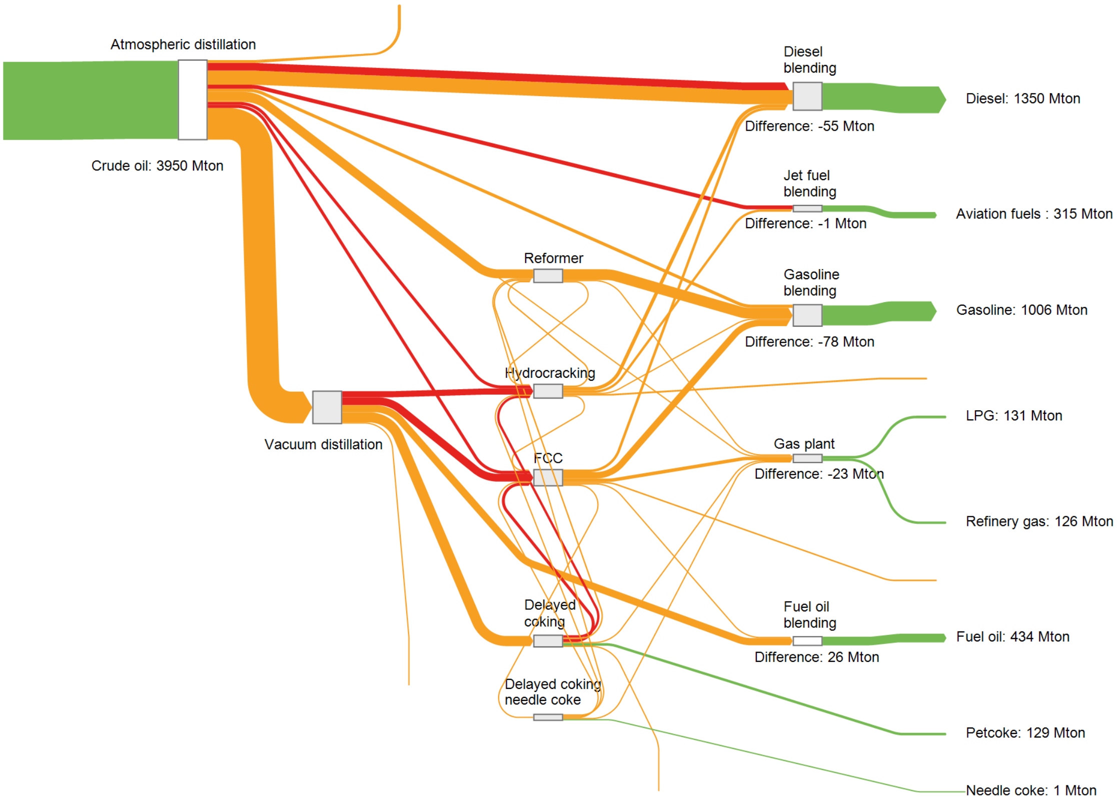


Figure 23: Sankey of the petroleum production in 2017, after adjustments to minimize the mass balances in the blending processes. The flows in green are quantified directly from statistics, and the flows in orange and red are calculated from transfer coefficients based on the crude oil input. The flows in red are those whose shares to each target process are unknown and were calibrated.

The petroleum production system was first quantified for 2017, based on statistics from the OECD and calibrated to minimize mass balance errors, as shown in figure 23. The approach is not perfect as there remain mass baølance inconsistencies after calibration of the system. These inconsistencies can be explained by several factor. There might be stocks in the system, as it is calibrated on the data from one year only (2017), which might lead to discrependencies between the inflows and outflows of the system. The system has also been simplified, and some processes have been excluded, which might lead to underestimating losses or the yield or certain products. Finally, the processes have been described thanks to literature, but the yields used are oil dependent, and might not correspond to the global average oil used in the study.

3.4.2 Scenarios

To provide a range for the amount of needle coke that can be supplied in the future, the current system of petroleum refineries was scaled depending on the scenario. The IEA offers crude oil production forecasts for 2030 and 2050. For each scenario, two variants are given, one corresponding to a linear scale-up of the current system and a second one when optimizing the system for needle coke production. The second variant gives the higher end of the needle coke production, based on different yields in the FCC and delayed coking processes, as well as heavier crudes. In figure 24, the petroleum refinery system is shown for the year 2050 in the net zero scenarios. Assuming similar yields than in the current refining system, the production of needle coke would reach 3600 ktons.

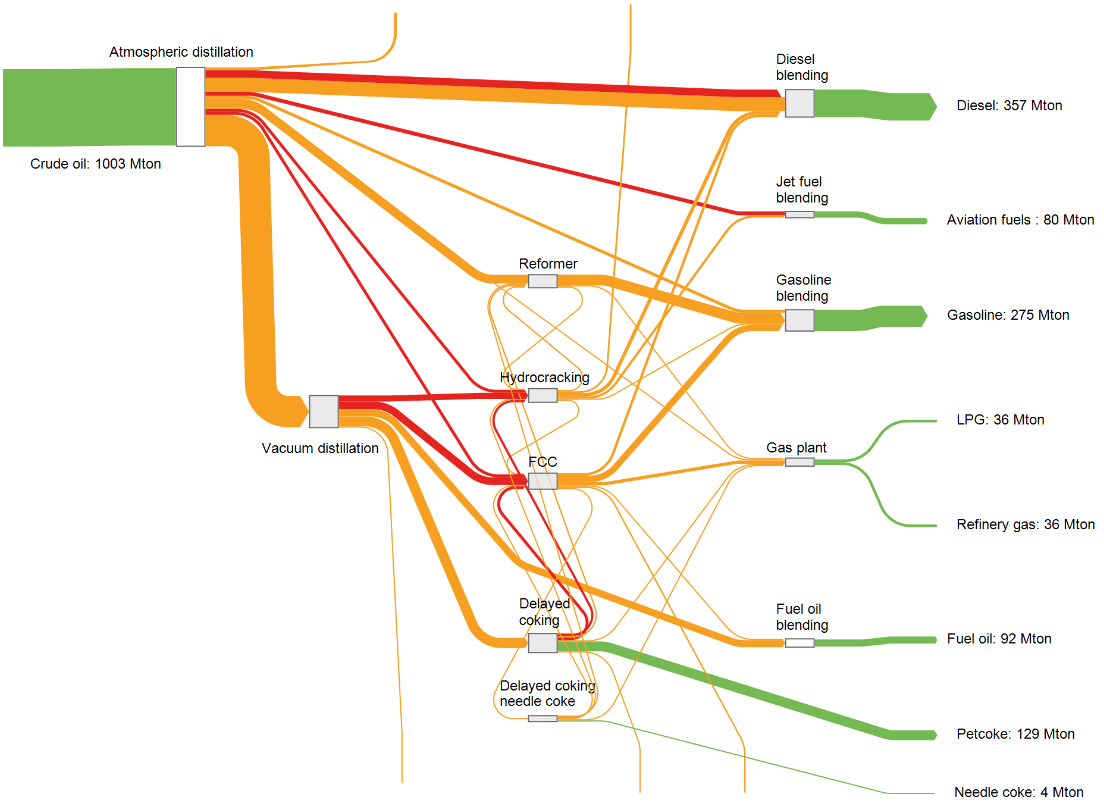
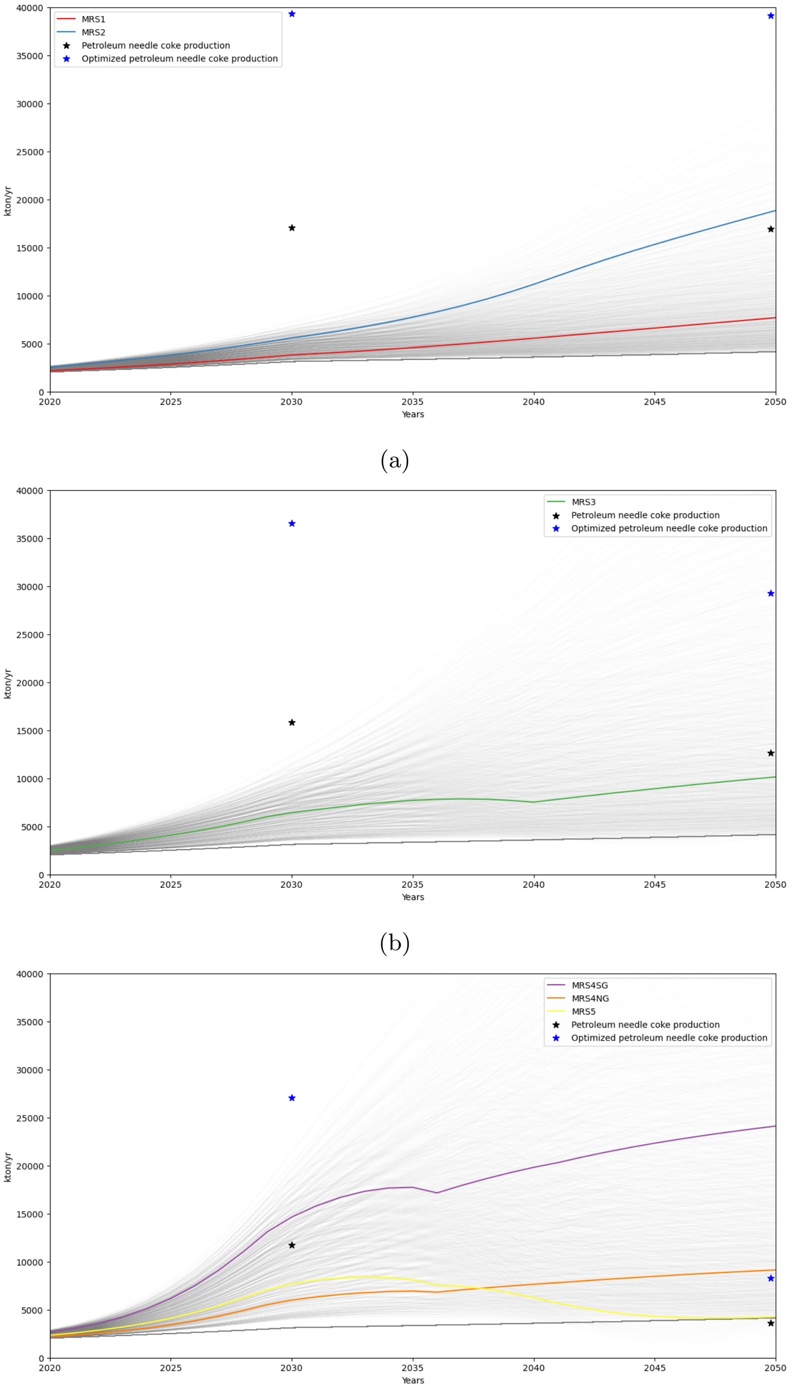


Figure 24: Sankey of the petroleum production in 2050, for the net zero production and assuming no optimization of needle coke production. This corresponds to the configuration with the lowest crude oil output.

Doing so for all three scenarios, with the optimized and non-optimized refining system to get a full range of the needle coke output, the predicted maximum supply can be compared with the demand for needle coke in the different scenarios.



(a)

(b)

(c)

Figure 25: Needle coke demand and supply for (a) STEP scenarios, (b) SD scenarios, (c) Net Zero scenarios. The maximum supply of needle coke in the current and optimized petroleum system is shown by stars for the years 2030 and 2050.

Figure 25 displays the demand scenarios for the 3 EV penetration scenarios: STEP, SD and Net Zero, as well as the maximum supply of needle coke associated with each scenario, both for the optimized and non-optimized petroleum refining system. The figure shows that the supply of needle coke is primarily a concern for scenarios with fast EV penetration. In this case, sobriety and recycling are necessary to keep the demand lower than the potential supply. Out of the six demonstration scenarios, only two MRS4-SG and MRS4-NG show a potential mismatch between the supply and demand of needle coke. In these scenarios, rapid EV penetration drives essential growth in the demand for needle coke, all the while causing the rapid decrease in the demand for diesel and gasoline and, therefore, the supply of their byproduct, needle coke. However, with no changes in the petroleum system to optimize the output of needle coke, even the scenario MRS5, with high recycling and sobriety, shows a higher demand than the maximum supply of needle coke. The bar chart in figure 26 shows the extent of the supply, both optimized and not, in the six scenarios. The values for the demand and supply in all six scenarios are summarized in table 18.

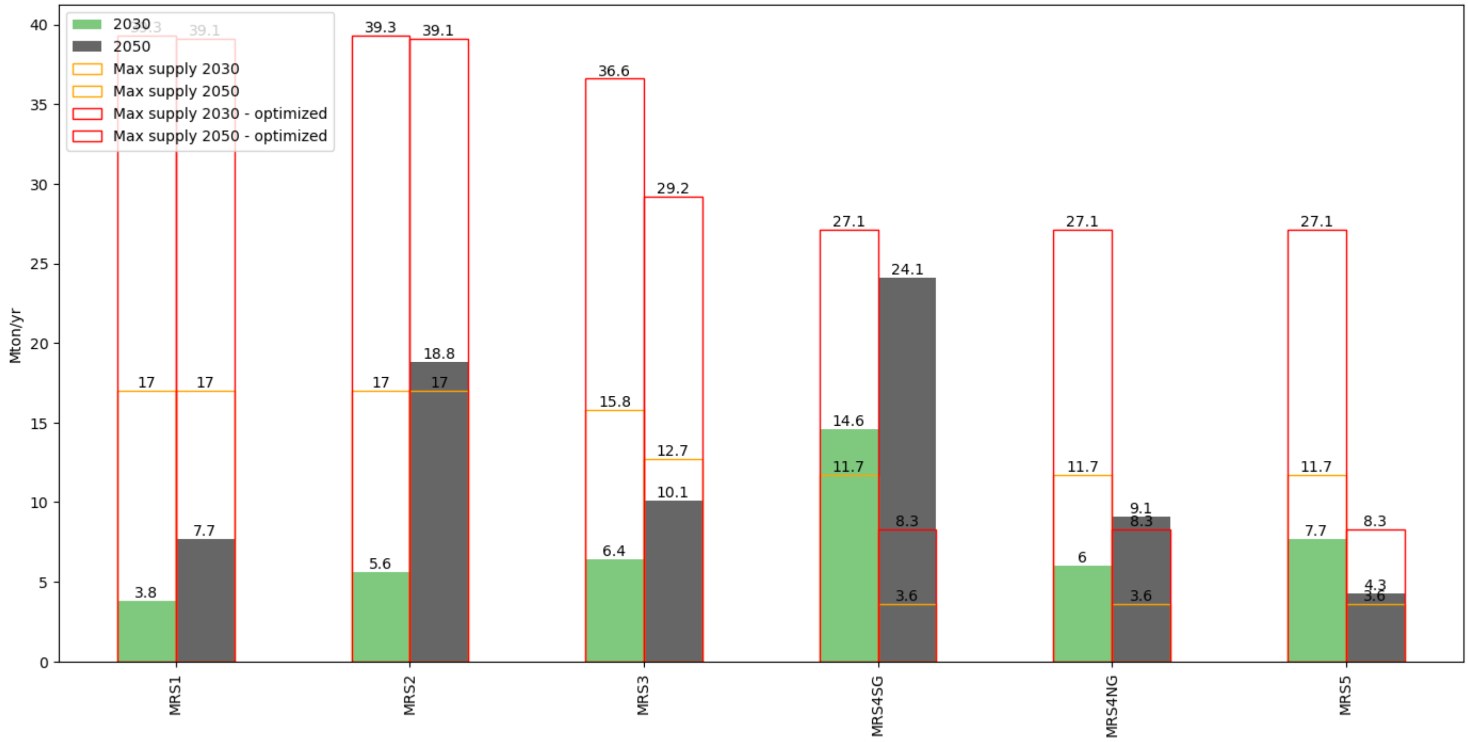


Figure 26: Needle coke demand and supply for the six scenarios

4 Discussion

4.1 Robustness of the model

4.1.1 Impact of assumptions

The demand model is highly dependent on the MATILDA model, and the robustness directly derives from this model. It is, however, essential to note that the primary goal of developing such a parametric model is acknowledging that we do not try to predict the future but rather to provide a range of possibilities to policymakers depending on the technological, economic and societal changes. This way, anyone can build their scenario using the scenario-building tool online to visualise the direct consequences that some changes could have on the battery value chain.

The supply model is based on several strong assumptions that can impact the robustness of the results. In particular, the supply of needle coke is subject to great precaution. Petroleum refineries are highly flexible, and which process is used at what time is highly dependent on economic tendencies and physical constraints. The quality of crude oil, for example, is predominant in determining the yields of petroleum products at each process. Some flexibility was introduced in the petroleum model to consider potential changes to maximise the needle coke output. It would, however, be tough to determine what the system could look like in the following decades. It is also important to remember that some processes from petroleum refineries have been overlooked. It is believed that these processes do not significantly influence the overall dynamics ruling the refineries, but the results lose accuracy because of this choice. The simplified model developed does not replace detailed refinery models such as PRELIM, which was partly used to understand the refining system [1]. However, this simplified model is adapted to analyse the consequences of different crude oil scenarios and allows for tweaking the yields to model the result of refining changes. It is essential to highlight that the goal of this study is not to accurately predict the output of needle coke from refineries in the following years, as it is neither the main scope nor crucial to understanding the graphite supply. The goal is instead to estimate the range of products for this material, which is essential to the graphite value chain, also recognise shortcomings in these calculations and what could increase or lower the production of petroleum needle coke.

Today, graphite is produced from needle coke as a precursor. However, not all needle coke used for making graphite is a petroleum byproduct. Petroleum needle coke accounts for around 80% of the graphite precursors, the other 20% consisting mainly of coal-derived needle coke [105]. The choice was made to model only the primary precursor, i.e. petroleum coke. This assumption might lead to underestimating the maximum production of needle coke. However, it was assumed for calculating that number that all FCC decant oil (the primary feedstock for needle coke production) was used for producing needle coke. In contrast, today, a large share of this product is used as a heavy fuel in the shipping industry [104].

4.1.2 Uncertainty analysis

An uncertainty analysis was conducted to understand the consequences on the robustness of the model of the added layer to MATILDA, ie, the processes in the graphite value chain. This analysis estimates the possible range of results once the set of parameters to the parametric model has been chosen. Therefore, The goal is to analyse the range of results within a given scenario, not between scenarios.

The figures 20, 33, 34, 35, 36, 37 show the demand for raw materials with the 95% confidence interval corresponding to two standard deviations on each side of the mean for each parameter. These figures show that there exists an important range of uncertainty regarding the demand for raw resources, especially in the later years of the model. This is due to the approach chosen for assigning uncertainties to each parameter, where the uncertainty is time-dependent. The further the year from the source for the parameter to the year the model is run for, the higher the uncertainty. This approach allows us to take into account the evolution of processes in the future, as the efficiency of the graphite chain is unlikely to remain the same in a 30 years time range.

Table 17 also summarizes the raw material demand at the horizons 2030 and 2050 with their associated uncertainty. These ranges do not disqualify the results of the supply and demand comparison. For scenarios where the supply and demand are very close, such as MRS2 and MRS5 with the non-optimized max supply or MRS4NG with the optimized max supply (see table 18), the uncertainty is large enough for the demand to swing from one side to the other of the supply figures. The uncertainty results are, therefore, a reminder that the numbers should not be taken for granted but as an indication of what scenarios might see supply constraints. When the supply is within the uncertainty range of the demand, then it can be expected that prices for needle coke will rise importantly because of supply constraints and bottlenecks in the value chain.

The uncertainty analysis was only conducted on the demand model, but it would be important to have a range of uncertainty on the supply model also, knowing the range of maximum needle coke that can be supplied (and graphite ore if a supply model for natural graphite is developed).

4.1.3 Limitations on data availability

The efficiency data for each graphite production process are primarily obtained from life cycle inventories (LCIs) dealing with natural or synthetic graphite production. However, many of these LCIs have incomplete data regarding specific processes. Although extensive documentation is available for the critical processes for each route, such as graphitisation for synthetic graphite and beneficiation and purification for natural graphite, research on operations specific to certain industries is lacking. The table 10 summarises which processes are included in the papers dealing with graphite production, highlighting that the LIB-specific steps (coating and spheronisation) are widely ignored in the literature.

Study	Notter [74]	Gao [38]	Engels [30]	Majong [67]	Rui [82]	Dunn [26]	Dai [22]	Surotseva [93]
Type of graphite	Natural	Natural	Natural	Natural	Both	Synthetic	Synthetic	Synthetic
Calcination (SG)	NA	NA	NA	NA	No	No	No	Yes
Baking (SG)	NA	NA	NA	NA	No	No	No	Yes
Graphitization (SG)	NA	NA	NA	NA	Yes	Yes	Yes	Yes
Beneficiation (NG)	Yes	Yes	Yes	Yes	Yes	NA	NA	NA
Purification (NG)	Yes	Yes	Yes	Yes	Yes	NA	NA	NA
Spheronization (both)	No	No	Yes	No	Yes	No	No	No
Coating (both)	No	No	Yes	No	Yes	No	No	No

Table 10: Summary of processes included in graphite studies

Concerning the spheronization of natural graphite, this is illustrated by the yield of spherical graphite from purified graphite, which varies from 40% to 84.6% for natural graphite [30][82][93]. In several studies, this process is just mentioned and not quantified because of a lack of measurements. The variatiation and lack of data can be explained by the fact that the process is particular to each manufacturer. The description of the spheronisation process for synthetic graphite is even less thorough. It is mentioned by Surotseva et al. and Majong et al. but never quantified [93][67].

The baking of the precursor specific to EAF electrode graphite is rarely described. Different studies describe the baking process with ratios of coke and pitch, but most of these studies are outdated and not necessarily descriptive of the current electrode sector [92]. Moreover, graphite manufacturers explained that the process was specific to EAF electrodes and not used for making battery anode material. Still, Surotseva et al. includes the baking process even though their study is about batteries [93].

Finally, the coating process is highly uncertain. The process is optional in manufacturing battery anode material, but most manufacturers mention it in their value chain. However, none of the papers used for this study quantifies this process, especially the share of coal tar pitch compared to the graphite, except for Engels et al. [30].

Table 10 summarises the critical processes in the different graphite studies. Many studies overlook the BAM-specific steps and instead focus on the well-documented processes, which can be detrimental to fully understanding the battery value chain and accurately evaluating its environmental impacts. The spheronisation process is crucial because it generates a high amount of waste or byproduct (fines), drastically raising the necessary raw material. The coating process requires coal tar pitch and is therefore responsible for high emissions due to coal production. This comparison highlights the importance of including all relevant processes in graphite studies and the need for more manufacturer data and measurements to measure the impact of graphite production and LIB manufacturing accurately.

4.2 Supply constraints for natural graphite

In 2021, the global natural graphite production was estimated to reach 1000 ktons [100]. All scenarios see a drastic increase in the demand for graphite ore as shown in table 16, from 1286 to 14810 ktons in 2030 and from 1312 to 25673 ktons in 2050 for the six selected scenarios. Looking at the annual production of graphite required to meet the electrification of the transportation sector is interesting to think of the changes in terms of infrastructure. It is also relevant to look at the cumulated resource use in figure 22 to investigate the depletion of graphite ore. Only one scenario, the MRS4-NG, exceeds the total graphite ore reserves in 2043. All other scenarios remain far below this boundary. Furthermore, it can be expected that new graphite deposits are discovered in the future, raising the global graphite reserves. It can therefore be assumed that the reserves of graphite are not the main limitation to the production of natural graphite ore.

The supply-side study aims to estimate how much graphite could be produced. However, estimating such a figure is complex, considering most of the production is located in China, and information about Chinese mines is usually not disclosed to the public. Consequently, it is essential to understand natural graphite production's current and future limitations. These limitations include geopolitical considerations, environmental impacts and infrastructure development time.

4.2.1 Geopolitic and economic considerations

The map 21 shows China's predominant role in natural graphite production, with 79% of the global production located there. This concentration of production raises concern in Western industries, which have planned massive electrification of their means of transportation, but produce little to no graphite.

China has among the largest reserves of graphite and has shown its capacity to rapidly expand its production in the last years, and could potentially continue to provide most of the world's graphite in the next years and decades. Western countries try, however, to diversify their supply, relying more on Eastern African countries and Brazil. The dependence on China for strategic resources in the ecological transition is considered to be an important problem in these countries [21][101]. Mozambique and Madagascar, in particular, have attractive reserves and have seen recent ambitious natural graphite projects open. The most striking example is the opening of the world's largest graphite mine in Mozambique by the Australian company Syrah [94]. However, the lack of infrastructure in these countries is an important obstacle to the development of ambitious graphite projects that could supply enough battery anode material and diversify the geographical origin of graphite. Another major limitation is the lack of significant investments in natural graphite projects. With the current price of graphite, most of the new important projects could struggle economically. If the price doesn't increase much because of a rising graphite demand, most projects will not be viable [35]

Recent changes in the natural graphite value chain have shown that price is the main driver of graphite demand and is more important even than quality. The anode price only makes for 10% of the battery, and the cathode materials are more critical when it comes to the performance of LIBs. The quality requirements for natural graphite have already been reduced to lower prices, as graphite battery anode material used to be graphitised after the coating step. Battery manufacturers have noticed that a carbonisation step, with lower temperatures and less energy-intensive, is enough to reach a satisfying grade of the material and sufficient performance of the anode. This example illustrates how flexible the natural graphite value chain can be. If the prices were to rise further because of supply constraints, it is expected that the battery sector would lower the requirements for graphite in the anode [35].

4.2.2 Environmental impact and regulations

One of the main issues with developing new natural graphite mines and installations is regulations and, consequently, development time.

Concerning the environmental impact, mining tailing is usually released in water bodies, which is associated with pollution at a local level. This pollution is regulated and is one of the reasons for the slow development time of graphite mines in Europe. Potential constraints in natural graphite supply are most likely due to inadequate infrastructure. There is a chance that the current infrastructure, which includes everything from graphite mining operations to beneficiation and purifying facilities, may find it challenging to keep up with the rapid adoption of legislation aimed at decarbonizing the transportation sector. Natural graphite facilities typically take 8 to 10 years to construct. However, the European Union (EU) has set a goal to outlaw electric vehicles within ten years by 2033 [33][11]. In Scandinavia, it is estimated that opening a new mine takes 15 to 20 years, from the exploration phase until production can start [10]. This extended timeline may favour the establishment of synthetic graphite infrastructure over developing new natural graphite mines. Moreover, it may benefit countries with lower environmental, social, and governance (ESG) concerns and existing production capabilities, thereby decreasing the supply security of the European battery value chain. As a response, the EU enacted the European Critical Raw Materials Act, with fixed goals for the share of imported mined, processed and recycled material. The goal of this act is also to reduce the dependence of the supply of a single third country, such as China in the case of Graphite [32].

In Norway and Sweden, mines often also face protests due to the local population of reindeer. Sami people fight to protect their land and the reindeer population. An agreement has to be found between the mining company and the Sami population. If no deal is found, the state can also deem the project of national interest to bypass the agreement process. These projects are highly controversial and mediatized, highlighting that the local population does not easily accept the environmental impacts of mining and that relying on a sharp increase of natural resource mining to ensure the transition of the transportation sector might not be a sustainable solution [10][70]. These local Scandinavian examples illustrate potential issues with the social acceptance of graphite mining by local communities, which is a rising issue in Europe but could also become a larger issue in other parts of the world.

4.2.3 Graphite fines overproduction

Another issue related to natural graphite production for battery anode material is the production of graphite fines or its overproduction. A crucial step in the processing of graphite fines is the spheronisation process, where grains are milled and shaped to a specific size and circular shape to improve the performance of the anode in the battery. This process presents the lowest yield of the entire natural graphite value chain, around 45% [30]. The yield varies depending on the intended grain size of the BAM, ranging from 60% for 23μm grains to as low as 35% for 10μm grains [35]. However, the remaining share of the graphite is not lost (only a small share is) but is a byproduct: graphite fines.

Graphite fines are a high-quality graphite product with a graphite content of around 94-95% carbon and small particle size, smaller than $10\mu m$. Graphite fines are traditionally used by the pencil and recarburising industry; the share of natural graphite in the latter is increasing. However, these sectors can not absorb the growing production of graphite fines, and new uses have to be found to avoid the waste of this byproduct.

In the model, the conservative assumption was made that all sectors using natural graphite can use graphite fines (except for the battery one). This assumption is optimistic, as specific uses require large graphite flakes, such as refractories. Even with such an approach, the scenarios show an overproduction of graphite fines compared to the NG demand of all non-battery sectors in the following years. Table 11 shows that all scenarios present overproduction of graphite fines at some point. Scenario MRS5 is the only scenario where the demand for NG from other sectors exceeds the production of graphite fines again in the future, thanks to systematic recycling.

Scenario	First year (last year)
MRS1	2025
MRS2	2038
MRS3	2024
MRS4-NG	2022
MRS4-SG	2027
MRS5	2025 (2042)

Table 11: First year (and last year) with overproduction of graphite fines in the different scenarios

This overproduction of a valuable byproduct calls for new uses in order to avoid important amounts of waste production. New uses for the resource are already emerging, with the example of artificial flakes made from graphite fines. These flakes are the result of the compressing of graphite fines and can replace natural flakes in certain applications. The share of natural graphite for certain applications which tolerate both natural and synthetic graphite could also raise to reuse this resource. However, these possible evolutions will unlikely provide effective solutions for reusing the growing amount of graphite fines, especially in scenarios with high consumption of natural BAM.

The most promising solution might be to establish processes that allow for making anode material out of the graphite fine, as the use of graphite from the battery sector is expected to become several times the uses from non-battery sectors. Abrego-Martinez et al. developed a process to agglomerate fines together using binders before carbonising and coating them. The obtained material shows similar performances to commercial graphite anode material and could be an interesting way of reducing waste and, consequently, the environmental impact of anode manufacturing [3].

4.3 Supply constraints for needle coke

As shown in Figure 25 and Table 18, the supply of needle coke could be constrained in scenarios with fast EV penetration. The decarbonisation of the petroleum sector reduces the dependence on crude oil and subsequently impacts needle coke production. This section is dedicated to understanding factors that could increase or decrease the supply of needle coke presented in the results.

4.3.1 Limitations in the needle coke value chain

First, it is crucial to remember that most petroleum coke is not used to make graphite. Only needle coke is, and it makes up a very small portion of the total output of petroleum coke. Due to its low contaminant content, low coefficient of thermal expansion (CTE), and high aromaticity, needle coke is a particularly unique product that differs significantly from other varieties of coke. While most refineries have a delayed coking plant to upgrade the heavier fractions of the crude oil, only a few businesses globally have one dedicated to needle coke production [80][20].

The two industrial feedstocks for needle coke production are Fluid catalytic cracking decant oils (FCCDO) or coal tar pitches. Needle coke is mainly made from petroleum, with FCCDO representing about 80 % of needle coke feedstock [104]. If the model might underestimate the supply of coke, it is also important to note that the figure obtained with the supply model assumes that all FCC decant oil is used for needle coke production even though a large share of this feedstock might not be suitable. The requirements for needle coke feedstocks are summarized in table 12. The electrical resistivity, coke hardness, sulphur content, and nitrogen content of a graphite electrode, in addition to CTE, can all impact how well it performs in batteries [16].

Parameter	**Value**
Aromatic carbon, wt% of total carbon	75 min.
sulfur content, wt%	0.5 max.
Nitrogen content, wppm	700-1000 max.
Quinoline Insolubles (QI), wt%	0.1 max.

Table 12: Feedstock characteristics for producing needle coke, from Cais et al. [16]

Another important point to make is that the delayed coking unit for needle coke is very different from traditional delayed coking and requires important adaptations in the refinery. The coking process usually lasts more than 32 hours, followed by an extended post-treatment step of an extra 6 hours, which is required to produce higher-strength coke and further reduce the volatile matter in the produced coke as summarized in table 13[16]. Increasing refinery production capacity takes at least 2 years, limiting the flexibility of needle coke production [97]. This further limits how much needle coke can be produced from the available FCC decant oil.

Parameter	**Fuel coke**	**Anode coke**	**Needle coke**
Temperature °C	488-498	496-510	504-510
Pressure, psig (kg/cm²g)	15 (1.05)	18-60 (1.3-4.2)	60-120 (4.2-8.4)
Recycle, LV%	0-5	0-50	60-150
Coking time, hours	9-18	24	32-36

Table 13: Comparison of typical delayed coking parameters for different coke types, from Cais et al. [16]

4.3.2 Sulfur content

The FCC is a refinery unit used to upgrade the heavier fractions of the distillation units into gasoline and diesel, but is also valuable for producing needle coke because it concentrates aromatics, producing high-quality needle coke feedstock (the decant oil) [20]. On the other hand, the sulfur present in the feedstock is usually concentrated in the heavier fractions of the FCC products, which are used for producing needle coke. Needle coke producers tend to maximise the yield of decanted oils (DO) in the fluid catalytic cracking (FCC) units, to produce large amounts of this highly aromatic product [104].

High sulfur content in needle coke leads to sulfur puffing during graphitisation. Puffing refers to the release of sulfur during the graphitisation stage when the temperature of the graphite precursor reaches 1300 to 1700°C. This sulfur release impacts the structure of the graphite and decreases, in particular, its electrical and thermal conductivity. Puffing usually occurs when the concentration of sulfur in the needle coke is higher than 0.8 wt% [14]. Sulfur puffing has been studied extensively as it affects the structure of the graphite and leads to a higher coefficient of thermal expansion (CTE), an issue in the electrode industry, where graphite is subject to high temperatures. Sulfur puffing is also an issue for the battery industry because it affects the electrical properties of the graphite material, such as electric conductivity [14][103]. To avoid the sulfur puffing phenomenon, needle coke producers usually favour a conservative approach, limiting their feedstock to 0.5% sulfur content [44].

Competition with other sectors

The sulfur content is also a constraint for other sectors using petroleum, especially the transport sector. The levels of sulfur for most transportation fuels are highly regulated. As an example, the maximum allowed content of sulfur in gasoline varies from 10 ppm (0.001%) in Europe to 500 ppm (0.05%) in southeast Asia [91]. These stringent limitations result from health and environmental concerns regarding sulfur emissions. The emissions of sulfur oxides are responsible for respiratory problems and asthma among the exposed populations; sulfur oxides also cause acid rains which are harmful to sensitive ecosystems [77][86].

The maritime sector was historically the sulfur-consuming sector, as the limitations of sulfur content on heavy fuels used by ships were much less stringent than for road fuels. However, the limits on the sulfur content of maritime fuels have been drastically reduced in the last years, both in Emission Control Areas (European and American costs) and on open seas, as shown in figure 27. This decrease directly impacts the supply of low-sulfur feedstock for needle coke production as the competition for sweet products rises significantly. In particular, the primary needle coke feedstock, FCC decant oil, is also prized by the maritime sector for use as fuel.

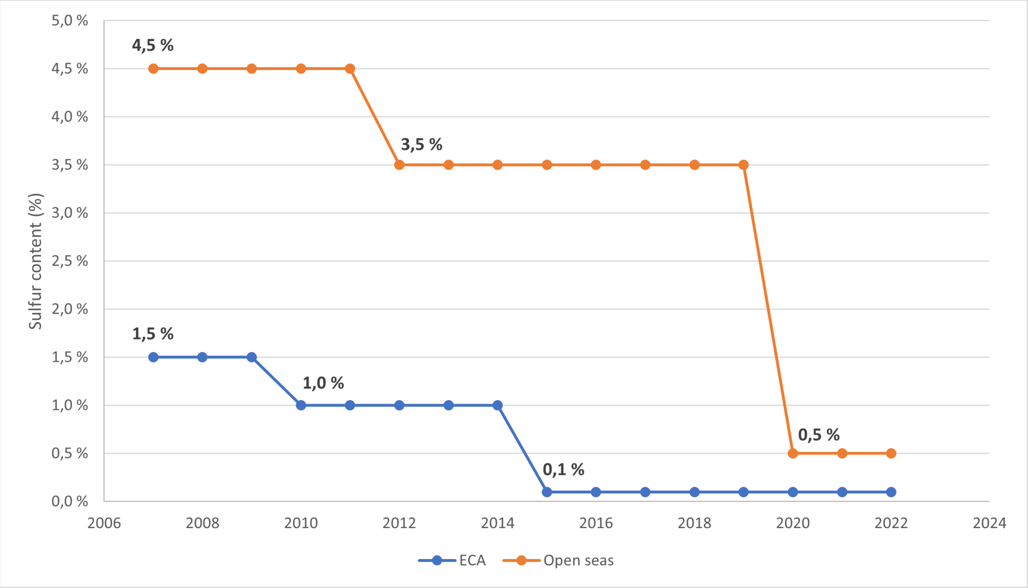


Figure 27: Sulfur limit for maritime fuels [52]

Treatment of sulfur content in the feedstock

Because low-sulfur petroleum products, particularly decant oil, are more and more desirable, it is essential to investigate methods to remove sulfur. The most widespread way to remove sulfur in petroleum products is hydrotreating or hydrodesulfurisation. This method cracks the product using hydrogen to remove the sulfur from the petroleum product, thus producing H2S. Because it uses hydrogen and requires high-temperature heating, this process is relatively energy-intensive and expensive [20][91]. Moreover, most of the hydrogen used in refineries is obtained through methane reforming and not from renewable sources. This method is responsible for consequent CO2 emissions.

Finally, hydrotreating is only efficient for removing non-heterocyclic sulfur compounds, the yellow and green categories in figure 28. Sulfur contained in aromatic rings is not affected by this method. According to John Clark, the share of heterocyclic sulfur compounds in needle coke feedstock can reach up to 80%, meaning that hydrotreatment is particularly limited to desulfurising them [20].

Hydrotreatment is, however, a solution for feedstocks with an appropriate sulfur content regarding the 0.5% limit and is currently used to reach the required sulfur content for needle coke production. Extensive hydrotreatment also negatively impacts the coke yield. Needle coke manufacturers, therefore, must find a balance between the coke yield and the sulfur content of the product, playing on using different fractions of the decant oil and hydrotreating them [2]. Tanabe et al. also shows that severe desulfurisation of Decant Oil can negatively impact the CTE of the resulting coke, implying that the levels of sulfur in the feedstock can only be partially decreased [96].

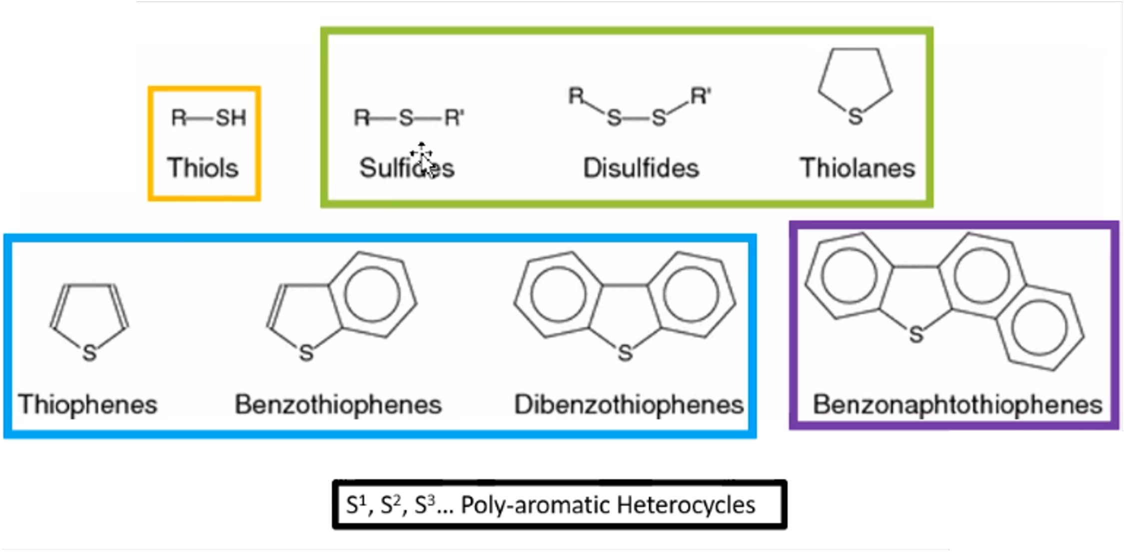


Figure 28: Sulfur compounds

The hydrocracking process can also remove sulfur from petroleum products. Hydrocracking is the second process, with FCC, capable of upgrading products with high boiling points into products with low boiling points. Hydrocracking can remove heterocyclic sulfur because it cracks the aromatics present in the feedstock. However, whereas the goal of hydrotreating is to remove impurities, the role of hydrocracking is to obtain more valuable products; removing sulfur is an unintended effect of this process [20].

Treatment of sulfur during graphitisation

When the coke used for graphitisation presents a high sulfur level, inhibitors can reduce the extent of the puffing. Oxide inhibitors are a common type of inhibitor used for lowering sulfur puffing. Iron III oxide, for example, shows significant results when used to reduce the puffing of the coke during graphitisation. The extent of puffing can also be influenced by grain size in the coke, the conditions of coke calcination, and graphitisation. Modifying the calcination and graphitisation heating pattern allows to control gas evaporation, thus influencing sulfur puffing. The synthetic graphite manufacturer, therefore, also has a role in graphite puffing, which is not only dependent on the feedstock [36].

To summarise, sulfur is highly undesirable in the production of needle coke. Crude oil production is shifting to heavier and more sour crude oils. The average global API of crude oil has risen from 31.3 to 32.8, whereas the sulfur content has increased from 1.13% to 1.27% [91]. Heavier oils have higher yields of heavy products, such as petroleum coke. But a higher sulfur content is detrimental to the graphite quality due to sulfur puffing during the graphitisation phase. Needle coke producers, therefore, favour feedstocks with less than 0,5% sulfur. Refineries have different processes that remove sulfur from petroleum to produce low-sulfur decant oil from sour crude oil. However, these processes also have their limitations. Both methods are expensive because they require hydrogen, which also has a high carbon footprint when produced from gas reforming. Hydrotreatment is common in refineries but cannot remove all the types of sulfur in the oil. Hydrocracking can remove these types of sulfur, but it is a stringent process used for upgrading heavy fractions into lighter ones. It is also important to remember that refineries focus on producing gasoline and diesel and that reducing the sulfur content in needle coke feedstocks is far from being a priority for them. Last, there exist inhibitors to reduce sulfur puffing during graphitisation.

Because of feedstock quality and competition with other sectors, it is very optimistic to assume that all FCC decant oil is used to produce petroleum needle coke, as assumed in the supply model. However, to raise the production of needle coke and decrease the prices due to competition, other precursors than FCC decant oil can produce synthetic graphite.

4.3.3 Alternative carbon precursors

First, there already exist other precursors than petroleum needle coke. As explained precedently, coal tar pitch is also used to produce needle coke. Coal needle coke is highly aromatic, one of the main characteristics of a graphite precursor. However, the presence of nitrogen impurities, the carcinogenic potential and the energy intensity of the processes explain why petroleum needle coke is more popular than its coal counterpart. Finally, the availability of coal tar pitch is limited [104]. Another option could be waxy oil, a byproduct of the Fischer Tropsch process in the production of GTL and CTL. waxy oil lacks aromaticity, but it can develop later during the coking process. waxy oil presents several significant advantages, such as low levels of contaminants (sulfur and nitrogen), lower greenouse gases emissions than petroleum and coal coke and no carcinogenic potential. However, waxy oil is not yet used in producing needle coke because of its low aromaticity and limited availability [105].

In the case of supply constraints, graphite manufacturers could also opt for lower qualities of petroleum coke, even if it would have consequences on the performance of batteries. These performance losses are acceptable in the case of cheaper and smaller vehicles which would not require batteries with as high of a density and capacity. Shifting to lower qualities of petroleum coke would drastically reduce the prices for raw materials, as needle coke is usually 20 to 40 times more expensive than other types of petroleum coke [20]. Usually, the product value of coke is much lower than the price of the crude oil needed to make it [69]. There are essential savings in reducing the quality requirements for the graphite precursor, but the impact on the battery's performance and safety must not be neglected.

Other types of carbon can also be used to replace graphite as an anode material in batteries. Hard carbon, for example, which designates non-graphitizable carbon, is becoming an industrial alternative to graphite. Hard carbon is especially popular for non-lithium batteries but is also gaining popularity for LIBs.

Finally, extensive research has been done to convert bio carbons into biographite to reduce the dependency of graphite production on hydrocarbons. Usually, these carbons are not graphitizable due to their physical properties, but they can become biographite using specific processes. These feedstocks, mainly from cellulose or lignin from trees, could heavily reduce the dependence of the LIB sector on fossil fuels. The most promising feedstock might be lignin from trees, as presented by Stora Enso [62]. Several lab-scale experiences have been conducted to produce battery anode material from bio sources. Banek et al. successfully converted lignocellulosic feedstocks to high-quality biographite through carbonization and graphitization. The resulting biographite demonstrated excellent performance in lithium-ion cells, although the scalability of the method was limited due to the use of a high-intensity laser [6]. Zhao et al. produced battery-grade biographite from glucose through carbonization and graphitization. The biographite exhibited high quality and performed well in lithium-ion cells [114]. Gomez-Martin converted medium-density fiberboard into battery-grade biographite by impregnating it with iron chloride and subjecting it to high-temperature treatment. The biographite obtained showed high quality and reasonable performance in lithium-ion cells [43]. Sagues et al. successfully developed a simple process to convert several biomaterials into high-performance anode material [84]. These lab-scale experiences demonstrate the feasibility of producing anode material from different biocarbon, but the reproducibility of the process at an industrial scale is yet to be proven. Compared with petroleum-based graphite, the cost of these methods might significantly limit their development at a larger scale.

4.4 Challenges with the recycling of graphite

Currently, the demand for graphite from sectors other than lithium-ion batteries (LIBs) is significant, and the EV sector does not yet have a dominant role in graphite demand. Figure 13 illustrates this trend. However, a large portion of this graphite is not recoverable, and recycling currently plays a limited role in securing the supply of battery anode material (BAM). Graphite used in electrodes for electric arc furnaces is melted into the iron and cannot be recovered. Graphite in refractories is mixed with clays, magnesia and other refractory material, making recycling complex [50]. Graphite used in lubricants, pencils, and brake linings is also consumed during use. As a result, graphite from LIB anodes offers the highest potential for recycling.

Recycling plays a crucial role in enhancing the circularity of the graphite industry and alleviating pressure on synthetic and natural graphite supply chains. Graphite recycling also helps reduce environmental pressures associated with graphite production by lowering emissions and mitigating other environmental and health impacts related to raw material extraction. Furthermore, graphite recycling is essential for securing the supply of BAM, particularly in regions with high battery usage but low graphite production, such as Europe.

Given the projected growth of electric vehicles and graphite demand, significant amounts of graphite are expected to exit the use phase in the following decades. As shown in figure 17 and the sensitivity analysis in figure 14, the development of recycling technologies only has a significant impact in the later decades of the model once the amount of graphite in EOL batteries is sufficient to provide second-life graphite. In the scenario, MRS5, where direct recycling is assumed, the very effective recycling combined with a lower demand thanks to sobriety allows for a nearly circular graphite value chain. This scenario is also the only one where both fast electrification of the transport sector and sufficient needle coke supply happen simultaneously. This is mainly thanks to efficient and systematic recycling of graphite in batteries.

However, several technological challenges need to be overcome for recycling to fulfil these critical roles. Graphite recycling faces a significant challenge due to the degradation of the graphitic structure during its use in batteries. Although graphite is highly stable, it undergoes various ageing mechanisms that complicate the recycling process. The primary factors contributing to this challenge include the disordering of the graphite structure during use, the intercalation and deintercalation of lithium atoms within the graphite material, and the formation of a solid electrolyte interphase (SEI) [71][11]. These mechanisms introduce complexities and affect the quality and performance of recycled graphite, making the recycling process more intricate. Due to graphite degradation during battery use, only a maximum of 10% recycled graphite can be incorporated into new battery anodes without compromising performance, according to Vianode [87]. This is not a hard limit but recycled graphite is today of too low quality, and using high amounts of it in the graphite mix has significant consequences on the battery's performance. This limitation hinders the role of recycling in replacing natural and synthetic graphite. Therefore, it is crucial to understand graphite ageing mechanisms better and improve the characterization of high-quality battery anode materials. There are no indicators to evaluate graphite quality specifically for use in LIBs aside from testing battery performance.

In the three selected scenarios that include graphite recycling, the mentioned 10% limit of recycled graphite is reached in only a few years. The first year where this limit is exceeded is 2034 in scenarios MRS4-G and MRS4-SG and 2021 in scenario MRS5. Acknowledging that scenario MRS is the only one where both fast electrification and low raw resource demand are reached simultaneously, it is crucial to better understand the ageing mechanisms of graphite. This would allowto improve its recycling to retrieve battery-grade graphite from spent batteries and rise the share of recycled graphite that can be used without compromising battery performance.

A significant challenge for graphite recycling is not primarily technical but regulatory: tracing graphite anodes. Tracing graphite source, grade, and origin in LIBs is essential for recycling manufacturers to determine its performance in anodes. The battery anode's performance can be adjusted based on the client's requirements, particularly regarding the natural-to-synthetic graphite ratio. Knowing the composition of recycled graphite allows for the adjustment of anode material accordingly. Digital product passports (DPPs) serve as unique identifiers for a product's life cycle and are gaining popularity. The European Commission promotes DPPs as a means to enable circularity in products, including batteries. DPPs could be highly valuable for graphite recycling, facilitating the adaptation of recycling processes to suit each unique product, based on the source and composition of the batter yanode [24]. Following new rules for batteries, all batteries with a capacity larger than 2kWh will be required to have a DPP in the European Union, which could greatly help the recycling of graphite material [8].

4.5 Alternative battery chemistries

In section 4.3.3, the role of different precursors in synthetic graphite production has been discussed to reduce the pressure on needle coke supply. Different battery chemistries, less dependent on graphite than Lithium Ion batteries, could also decrease the pressure on the graphite supply.

The most promising alternative today seems to be Sodium-ion batteries (SIB). Sodium is much more abundant than lithium, and its price is also more than 30 times lower than lithium's [88]. Today, SIBs are not preferred to LIBs for transportation means because of lower capacities, limited rate and cycling performance, a low energy density and Na deposition leading to safety issues [110]. However, extensive research in the last years to solve these issues have been conducted, and SIBs could partially replace LIBs, at least for specific applications.

Graphite is the predominant anode material for LIB anodes, particularly because of its capacity to intercalate lithium ions. However, it does not intercalate sodium ions and is therefore irrelevant for Sodium-Ion Batteries [88]. Instead, other carbon anodes are preferred, mainly hard carbons, which show the best performance in terms of capacity and reversibility, and the development of electrolytes favouring this material [109]. Conversion alloy materials are promising anode materials for SIBs [78][61]. The development of SIBs could also allow for easier use of biocarbon because these batteries do not require an anode material with a crystalline structure like graphite [87].

The capacity of sodium is three times lower than that of lithium, and sodium-ion batteries are mostly expected to replace LIBs for stationary applications [88]. However, would the prices of LIBs rise too fast, it can also be expected to find SIBs in the transportation sector, especially for lighter, smaller vehicles. SIBs are just one example of chemistry that could replace LIBs, and their development has grown much faster in the last few years than expected, mainly because of lithium supply constraints. Supply constraints for lithium and the development of chemistry alternatives have consequences on the demand for graphite, and it, therefore, seems to be tightly linked to the supply of lithium [87]. LIBs made of graphite anodes still seem to be the main choice for high-performance batteries. Still, the evolution of prices could lead to vehicle manufacturers constantly trying to find a balance between performance and costs and favour different chemistries depending on the vehicle category.

4.6 Future work

The main limitation of this study is the lack of quantitative analysis of the future supply of natural graphite. As explained, the lack of data regarding existing and future mines is a concern when planning the supply of this crucial material. Further work on the topic is necessary to evaluate the possibility of graphite ore developments regionally and assess the potential of the different countries around the globe to raise their production of graphite ore but also their refining capacities to produce BAM out of it. Understanding the future supply and considering regional sources for it is a crucial step to understanding and planning the decarbonisation of the future supply.

On the synthetic side, it is essential to investigate the supply of low-sulfur petroleum further and better understand how the supply of needle coke depends on the crude oil quality and how it could evolve. Some extensive models exist at a refinery scale [1]. However, there is still a lack of research on the global refining system, its products and potential evolutions due to environmental policies and transitions to reduce hydrocarbon uses.

To simplify the modelling and because the other graphite users were not included in the system definition, the recycling to and from other graphite sectors was overlooked. Some studies have modelled the entire graphite cycle in specific regions, including all industries [112]. There is a gap in extensive research on global graphite flows with scenarios to plan future use and cross-sectoral recycling opportunities. This study's modelling approach for recycling was only dependent on the availability of scrap graphite and EOL batteries. Other than the recycling technology itself, the physical limitations of graphite recycling have been overlooked, such as the degradation of graphite during use. Exploring the ageing of graphite and implementing the limits on using recycled graphite in a dynamic model would allow us to understand the bottlenecks in graphite recycling and the need for infrastructure.

Finally, the impact of the penetration of alternative chemistries on the demand for batteries is still not fully understood. A major improvement would be implementing lithium-free chemistries to the model to explore scenarios where these technologies would become significant in the transition of the transport sector and understanding the coupling between two crucial batteries for the energy transition, lithium and graphite.

5 Conclusion

This thesis used Material Flow Analysis to quantify the graphite cycle for different scenarios and understand this system's supply of critical resources. The MATILDA model was used to quantify the demand from the battery sector in the different scenarios, whereas other graphite uses were quantified thanks to ECGA outlooks. A parametric model was developed and published to allow for multiple scenario choices based on the various parameters from the MATILDA model and the share of natural and synthetic graphite in batteries. On the other side, the maximum supply of needle coke was quantified for the different EV penetration scenarios using a simplified model of the petroleum refining system. The current situation was studied for natural graphite, as well as limitations and opportunities for expanding the extraction and refining of graphite ore.

The results show that a fast electrification of the transportation sector has drastic consequences on the demand for graphite. Both the natural and the synthetic value chains are constrained. Regarding synthetic graphite, phasing out petroleum could lead to supply shortages in the long term, especially in ambitious scenarios in terms of climate goals. The supply of needle coke to the synthetic graphite value chain could be further constrained by rising levels of sulfur in crude oil and increased competition for low-sulfur petroleum products. However, the availability of alternative carbon precursors, other petroleum cokes, hard carbon or biocarbon could ensure the supply for synthetic graphite production.

Regarding natural graphite, the short-term issues are more concerning because of the length of procedures to expand graphite mining and refining infrastructure. The long development time of natural graphite production could hinder the projects in East Africa, which aim at reducing the dependence of Western industries on the Chinese production of graphite. However, the environmental impacts of graphite mining on local populations should not be overlooked, and the decarbonisation of the transport sector must not lead to a problem shifting. Another rising issue with natural graphite production for battery anodes is the overproduction of graphite fines. This valuable byproduct could rapidly become waste if no new uses are found to value it.

The only way to achieve large-scale electrification while ensuring the supply of raw resources is to rely heavily on recycling. Today, significant economic, structural, and technical barriers prevent recycled graphite from being reused in batteries. Nowadays, using a high share of recycled graphite in battery anodes has measurable consequences on the battery performance, and it is not yet possible to retrieve used graphite to a similar grade to primary graphite. This study highlights the need for further research on graphite recycling to understand the ageing mechanisms during the use phase of batteries.

However, even systematic and efficient graphite recycling is insufficient to decrease resource utilisation effectively. The study shows the importance of societal and habit changes, especially in the long term. Reducing vehicle ownership and the size of vehicles are crucial and effective means to decrease the need for critical materials. These steps are also essential to allow for the penetration of less performant battery chemistries, which could help diversify the demand for critical materials, among which figures graphite.

The penetration of alternative battery chemistries, such as SIBs, might add to the growth of the battery sector. Considering the penetration of LIBs is mainly constrained by the supply of critical materials, lithium in particular, SIBs could expand the production of batteries rather than replace LIBs. It is also important to note that the need for graphite in batteries is tightly linked to the demand for lithium. Graphite is crucial for its capacity to intercalate lithium ions but is not required in other battery chemistries, such as SIBs. The production of graphite could therefore be constrained by the supply of lithium, known for its criticality, rather than its own supply.

The overall message of this study is to highlight that replacing thermal vehicles with electric ones to maintain the same level of affluence has drastic consequences on critical material demand. Electric vehicles, because they have significantly lower emissions when using decarbonised electricity, are highly beneficial for climate change mitigation but lead to impact shifting due to their dependency on critical materials such as graphite. Climate change is unfortunately not the only challenge, and the planetary boundaries call for a more profound societal change, accepting to travel less, and with other means, should they be public transport, cycling or walking.

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6 Appendices

6.1 MFA calculations

Material flow analysis uses several calculation methods to quantify flows within a system:

- **Transfer coefficient**: There exist a relationship between two flows. Given flows A and B, there exist a coefficient x such as:
$$A = x \cdot B \tag{3}$$
- **Mass balance**: At every process, the sum of inflows is equal to the sum of outflows and stock change.
$$\sum Inflows = \sum Outflows + Stockchange \tag{4}$$
- **Concentration**: When a system is defined for several layers, some flows will have a concentration between the layers. In this case study, we have a dry matter layer and a graphite (or carbon) layer. Given a flow A with a concentration c in graphite, we have the following equation:
$$A_{Gr} = c \cdot A_{DM} \tag{5}$$

To calculate all flows within a system , there also needs to be a certain amounts of inputs, ie flows which value is given directly from a parameter or a set of parameters and not calculated from other flows.

The mathematical modelling behind MFA principles is therefore fairly simple. The difficulty of calculating MFA resides in establishing a mathematical model of the system, ie writing down all the equations in the system to make it solvable (number of equations = number of unknowns). From there, each flow can be expressed only in function of the parameters, this is called the analytical solution. Conducting such an analysis is an effective method for humans to comprehend a system and subsequently perform further analysis, a sensitivity analysis for example. However, when it comes to program MFA, this mathematical approach is complex to put in place, writing down every equation in the mathematical model can be complex and long, and also makes it hard when changes are required in the system. There is therefore a need to develop a more systemic method for quantifying flows in MFA.

The model presented here is inspired by the more organic way of performing MFA analysis, first starting from the initial flows, the inputs (those who are calculated directly from parameters) and then calculating flows connected to them by one of the equations above (mass balance or transfer coefficient), and so on until every flow is quantified. To do so and mimic this 'natural' way of calculating, I have decided to implement a recursive code

The input to the model is an excel sheet with its parameters, the parameters can be of 4 different types:

- **Rates**: These parameters define a transfer coefficient between two flows.
- **Concentrations**: These parameters define the concentration of a flow on the graphite layer.

- **Input**: These parameters directly give the value of a parameter, on a given layer.
- **Mass balance**: These parameters indicate that a certain parameter has to be calculated from mass balance at a certain process, it could be assumed that all processes must be balanced, but in certain cases it is not desirable. As an example, for some MFAs one wants to study the imbalances at certain processes due to the use of different data sources.

All the parameters are defined as following:

- **Transfer type**: What the type of the parameter is (from the previous list)
- **Source process**: Source of the target flow
- **Source flow**: Input flow for the calculations
- **Source unit**: Unit of the source flow
- **Target process**: Target of the target flow
- **Target flow**: Output flow for the calculations
- **Target unit**: Unit of the target flow
- **Description**: Description of the parameter
- **layer**: The layer the parameter applies to
- **value**: The value of the parameter

Each parameter also has a distribution (usually normal), a minimum, a maximum and pedigree coefficients for the uncertainty analysis, as described in the section

The model is a Python-based object-oriented code, which only requires the previously mentioned sheet as input. From there, the model will automatically quantify the flows in the given system, given the fact that enough parameters are given as input. The code comprises 3 different classes, the Process, the Flow and the MFA System. The code and data are available on GitHub at the following address: `https://github.com/mfa-indecol/graphite-cycle.git`.

6.2 Pedigree coefficient explanation

Indicator	***Definition***	***Score: 1***	***Score: 2***	***Score: 3***	***Score: 4***
Reliability	Focus on the data source: documentation of data generation, e.g., assessment of sampling method, verification methods, and reviewing processes.	Methodology of data generation well documented and consistent, peer-reviewed data.	Methodology of data generation is described but not fully transparent; no verification.	Methodology not comprehensively described, but principle of data generation is clear; no verification.	Methodology of data generation unknown, no documentation available.
Completeness	Composition of the date of all relevant mass flows. Possible over- or underestimation is assessed.	Value includes all relevant processes/flows in question.	Value includes quantitatively main processes/flows in question.	Value includes partial important processes/flows, certainty of data gaps.	Only fragmented data available; important processes/mass flows are missing.
Temporal correlation	Congruence of the available date and the ideal date with respect to time reference.	Value relates to the right time period.	Deviation of value 1 to 5 years.	Deviation of value 5 to 10 years.	Deviation more than 10 years.
Geographical correlation	Congruence of the available date and the ideal date with respect to geographical reference.	Value relates to the studied region.	Value relates to similar socioeconomical region (GDP, consumption pattern).	Socioeconomically slightly different region.	Socioeconomically very different region.
Other correlation	Congruence of the available date and the ideal date with respect to technology, product, etc.	Value relates to the same product, the same technology, etc.	Values relate to similar technology, product, etc.	Values deviate from technology/product of interest, but rough correlations can be established based on experience or data.	Values deviate strongly from technology/product of interest, with correlations being vague and speculative.

Table 14: Definition of the data quality indicators in the pedigree matrix, from Laner et al [59]

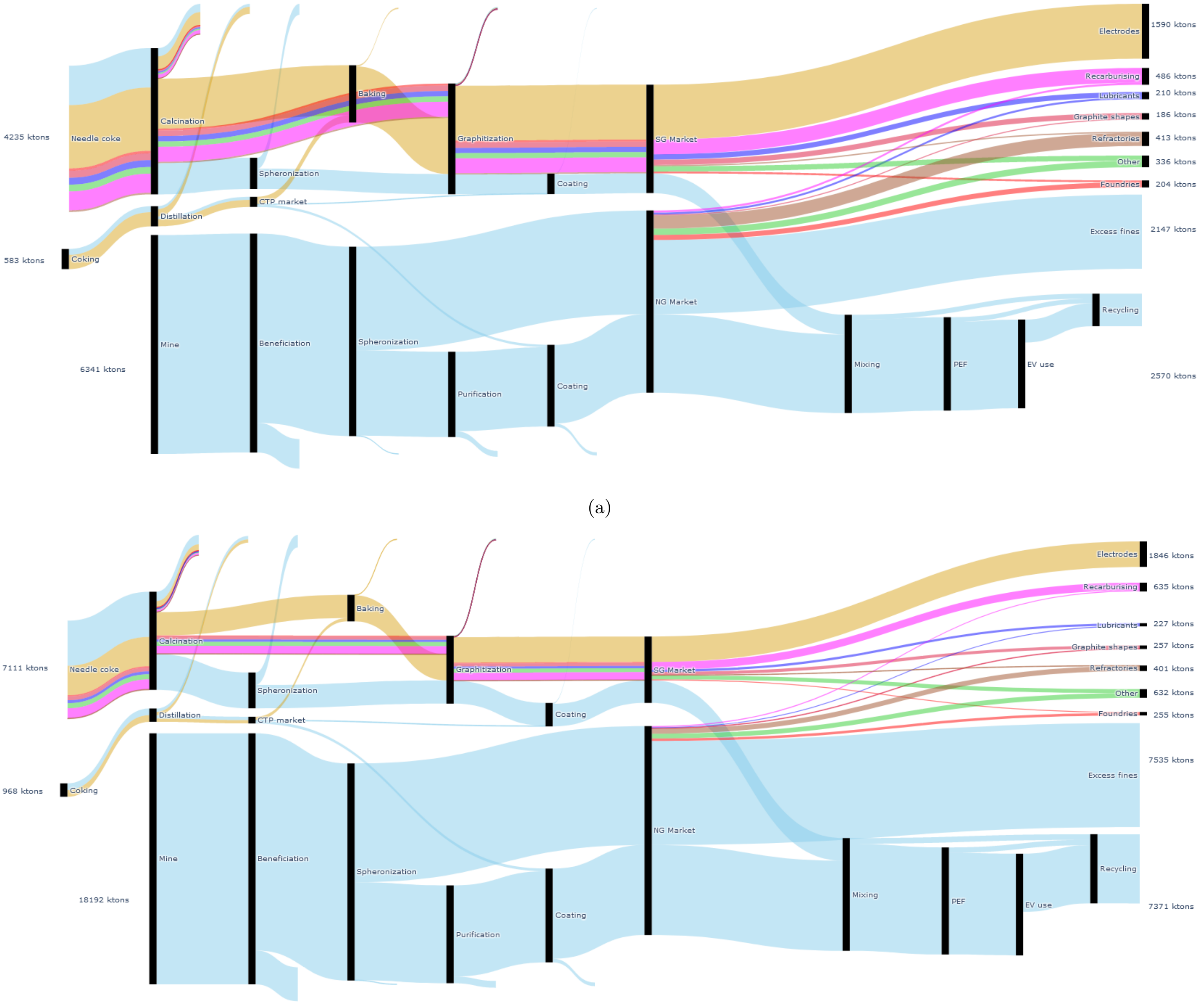
Parameter	Value	Std 2020	Reliability	Completeness	Temp corr.	Geo corr.	Other corr.	Source
TC coal tar	0,04	22 %	1	1	4	3	1	[92]
TC coal tar pitch	0,5	10 %	2	1	3	1	2	[54]
TC beneficiation	0,87	2 %	1	1	1	1	1	[64][30]
TC spheronization (NG)	0,45	2 %	1	1	1	1	1	[30]
TC purification	0,93	2 %	1	1	1	1	1	[30]
TC coating (NG)	0,99	2 %	1	1	1	1	1	[30]
TC calcination	0,74	8 %	2	2	1	2	1	[93]
TC spheronization (SG)	0,65	8 %	2	2	1	2	1	[93]
TC baking	1,23	3 %	1	1	2	1	1	[54][42][93]
TC graphitization	0,98	23 %	3	2	3	3	2	[13]
TC coating (SG)	0,99	2 %	1	1	1	1	1	[30]
TC mixing	0,95	7 %	2	1	1	1	1	Assumption
TC PEF	0,95	7 %	2	1	1	1	1	Assumption
TC assembly	1	7 %	2	1	1	1	1	Assumption
TC EV prod	1	7 %	2	1	1	1	1	Assumption
Share pitch coating (NG)	0,05	2 %	1	1	1	1	1	[30]
Share pitch coating (SG)	0,05	2 %	1	1	1	1	1	[30]
Share pitch baking	0,19	22 %	3	1	3	1	1	[95]
Share fines	1,22	2 %	1	1	1	1	1	[30]
C Coal	0,6	10 %	2	1	3	1	2	[54]
C Coal Tar	0,6	10 %	2	1	3	1	2	[54]
C Coal Tar Pitch	0,6	10 %	2	1	3	1	2	[54]
C NG Ore	0,09	7 %	1	1	3	1	1	[101]
C NG	0,95	2 %	1	1	1	1	1	[30]
C Spheronized NG	0,95	2 %	1	1	1	1	1	[30]
C Graphite fines	0,95	2 %	1	1	1	1	1	[30]
C Purified NG	0,99	2 %	1	1	1	1	1	[30]
C Coated NG	0,99	2 %	1	1	1	1	1	[30]
C Green Coke	0,93	8 %	2	2	1	2	1	[93]
C Calcined Coke	0,99	8 %	2	2	1	2	1	[93]
C Spheronized coke	0,99	8 %	2	2	1	2	1	[93]
C SG	0,99	2 %	1	1	1	1	1	[30]
C Coated SG	0,99	2 %	1	1	1	1	1	[30]
C BAM	0,99	2 %	1	1	1	1	1	[30]
C Electrodes	0,99	2 %	1	1	1	1	1	[30]
C Batteries	0,99	2 %	1	1	1	1	1	[30]
C EV	0,99	2 %	1	1	1	1	1	[30]

Table 15: Parameters for the demand model and their score for the different quality indicators

6.3 Scenario results

6.3.1 Sankey diagrams

6.3.2 Sankeys

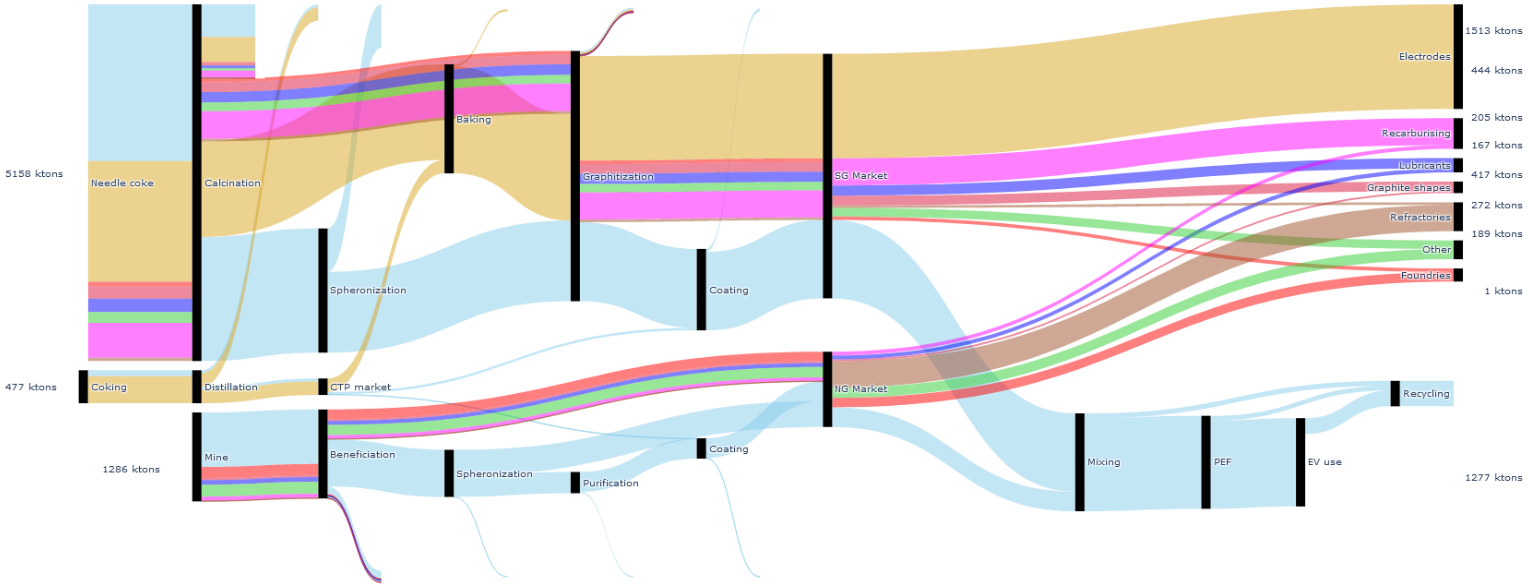


(a)

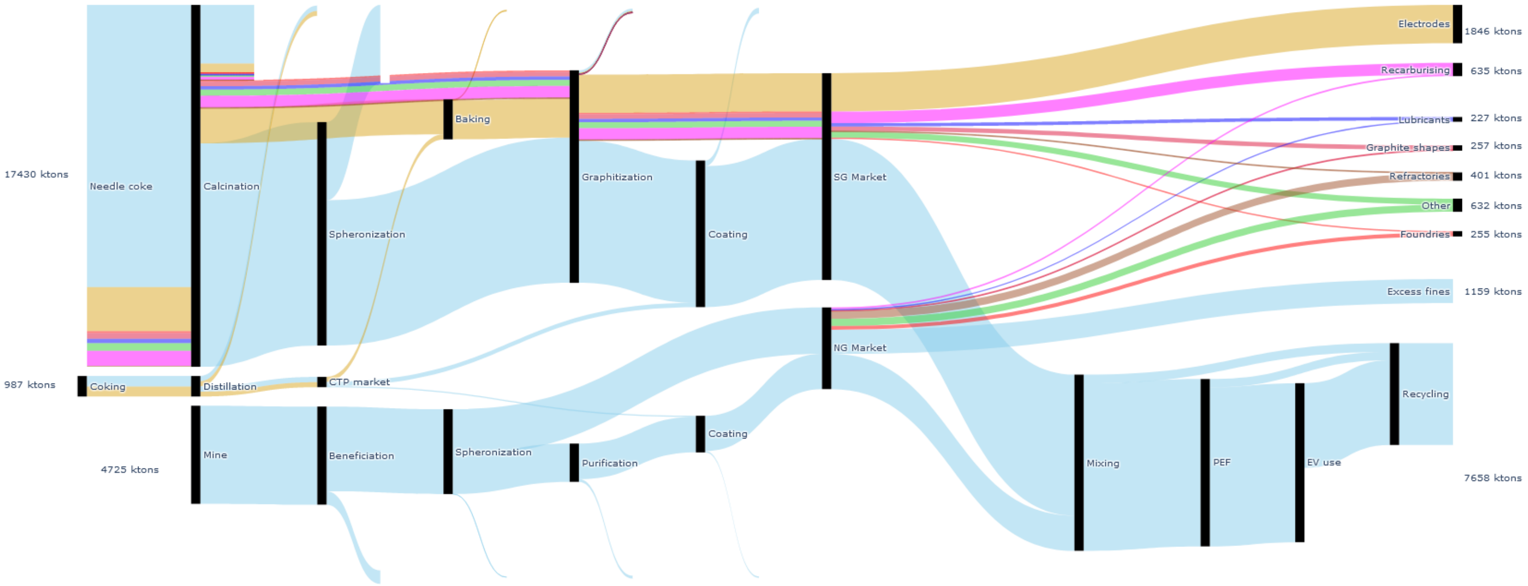
(b)

(The Sankey diagrams have different scales)

Figure 29: Sankey of the graphite value chain for Scenario MRS1 (a) in 2030 and (b) in 2050 on the graphite layer in kton



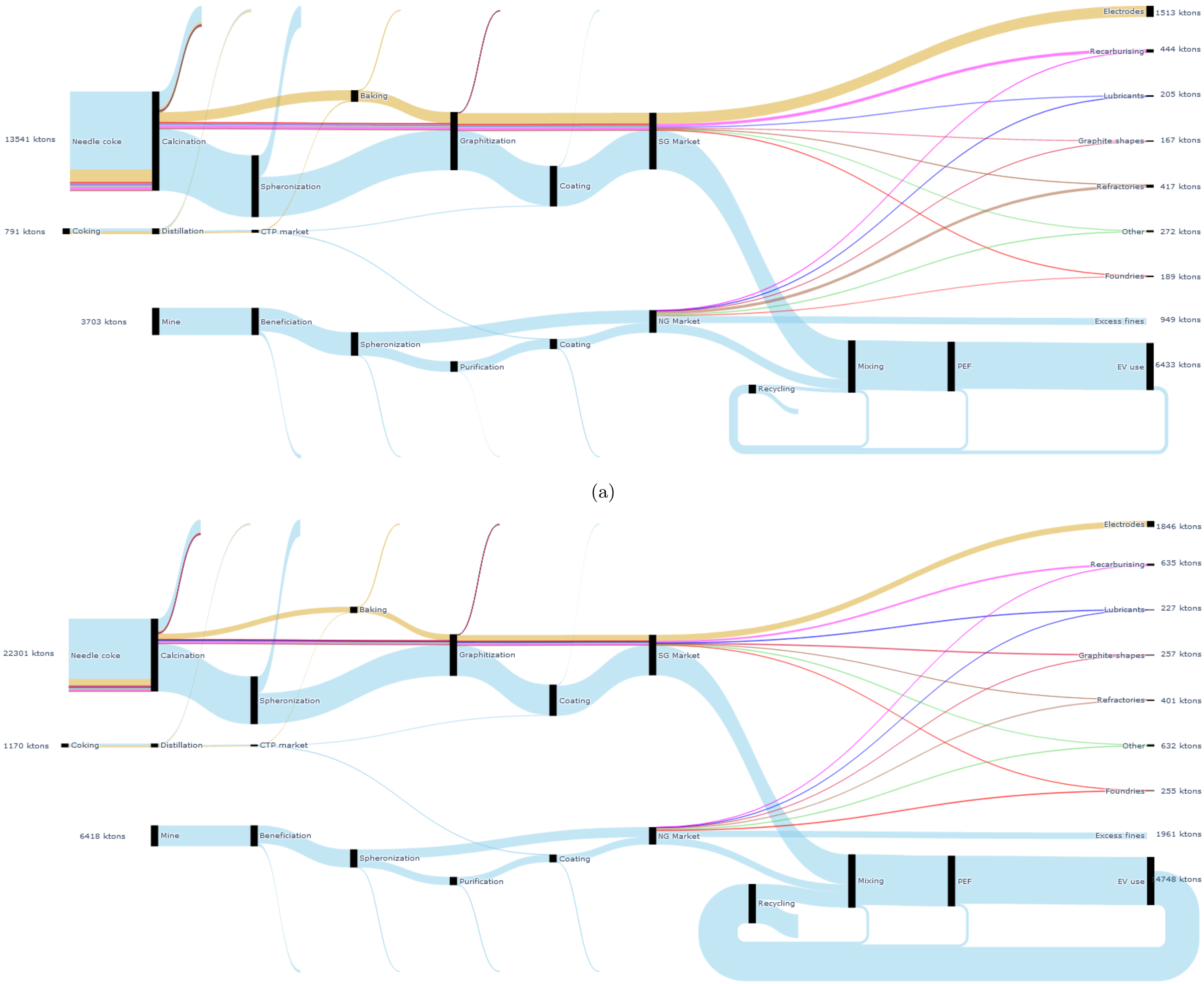
(a)



(b)

(The Sankey diagrams have different scales)

Figure 30: Sankey of the graphite value chain for Scenario MRS2 (a) in 2030 and (b) in 2050 on the graphite layer in kton

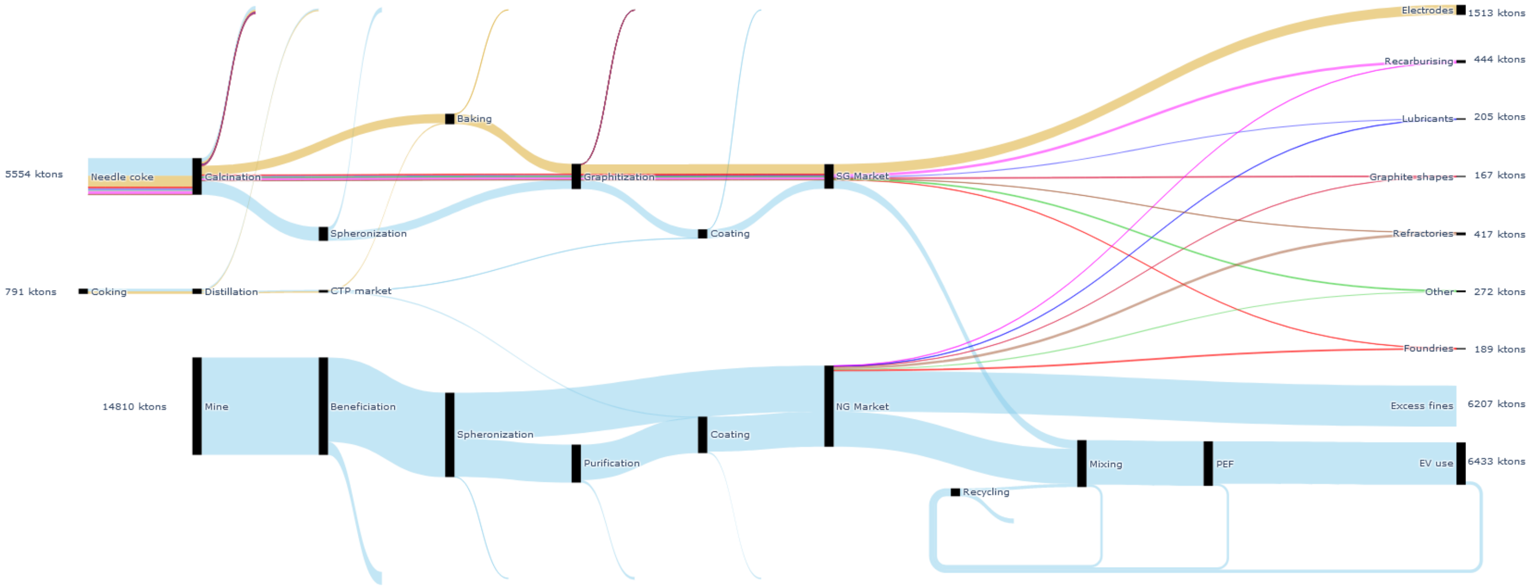


(a)

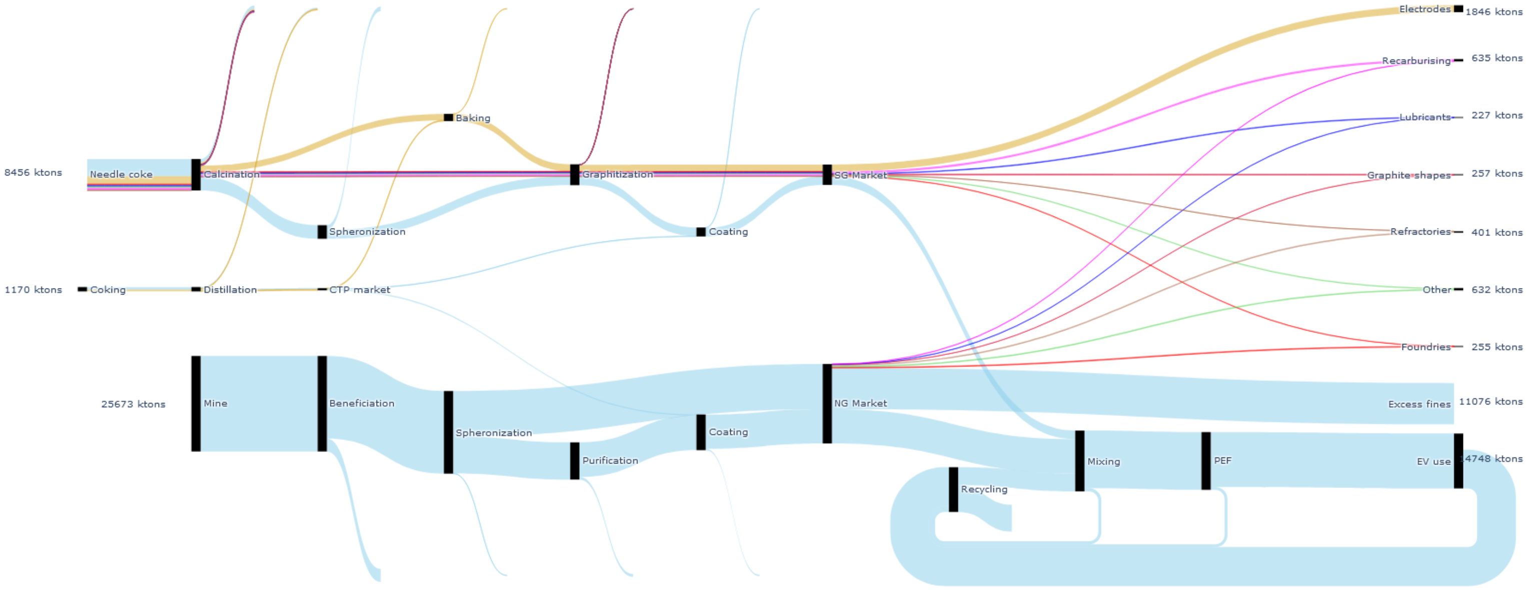
(b)

(The Sankey diagrams have different scales)

Figure 31: Sankey of the graphite value chain for Scenario MRS4-NG (a) in 2030 and (b) in 2050 on the graphite layer in kton



(a)



(b)

(The Sankey diagrams have different scales)

Figure 32: Sankey of the graphite value chain for Scenario MRS4-NG (a) in 2030 and (b) in 2050 on the graphite layer in kton

6.3.3 Summary scenario results

	Needle coke (ktons/yr)		Graphite Ore (ktons/yr)	
Scenario \Year	2030	2050	2030	2050
MRS1	3817	7687	3556	18192
MRS2	5576	18843	1286	4725
MRS3	6433	10146	4254	7711
MRS4-NG	6004	9141	14810	25673
MRS4-SG	14639	24109	3703	6418
MRS5	7688	4265	5868	1312

Table 16: Demand for graphite ore and needle coke in the six scenarios in 2030 and 2050

6.3.4 Uncertainty

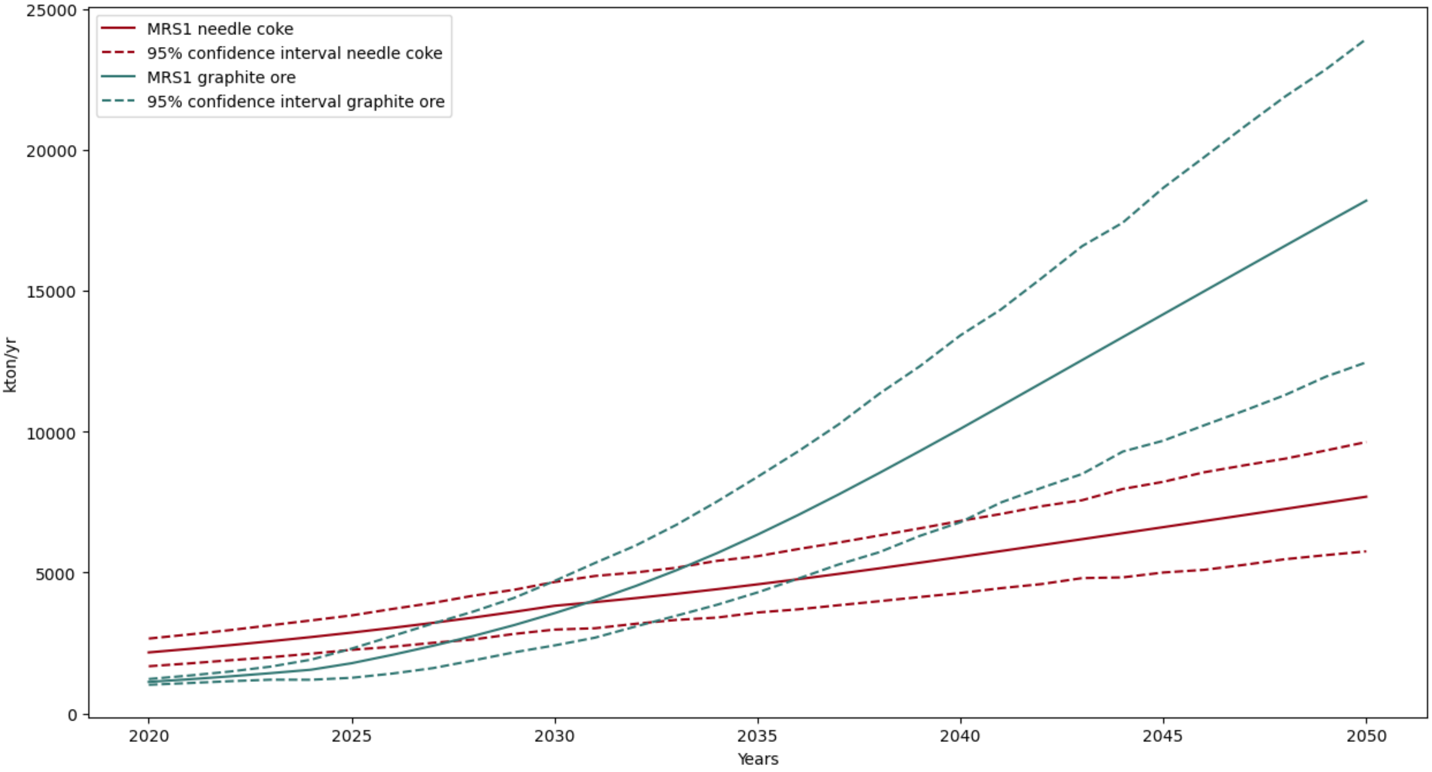


Figure 33: Demand for raw materials in the scenario MRS1, with 95% confidence interval

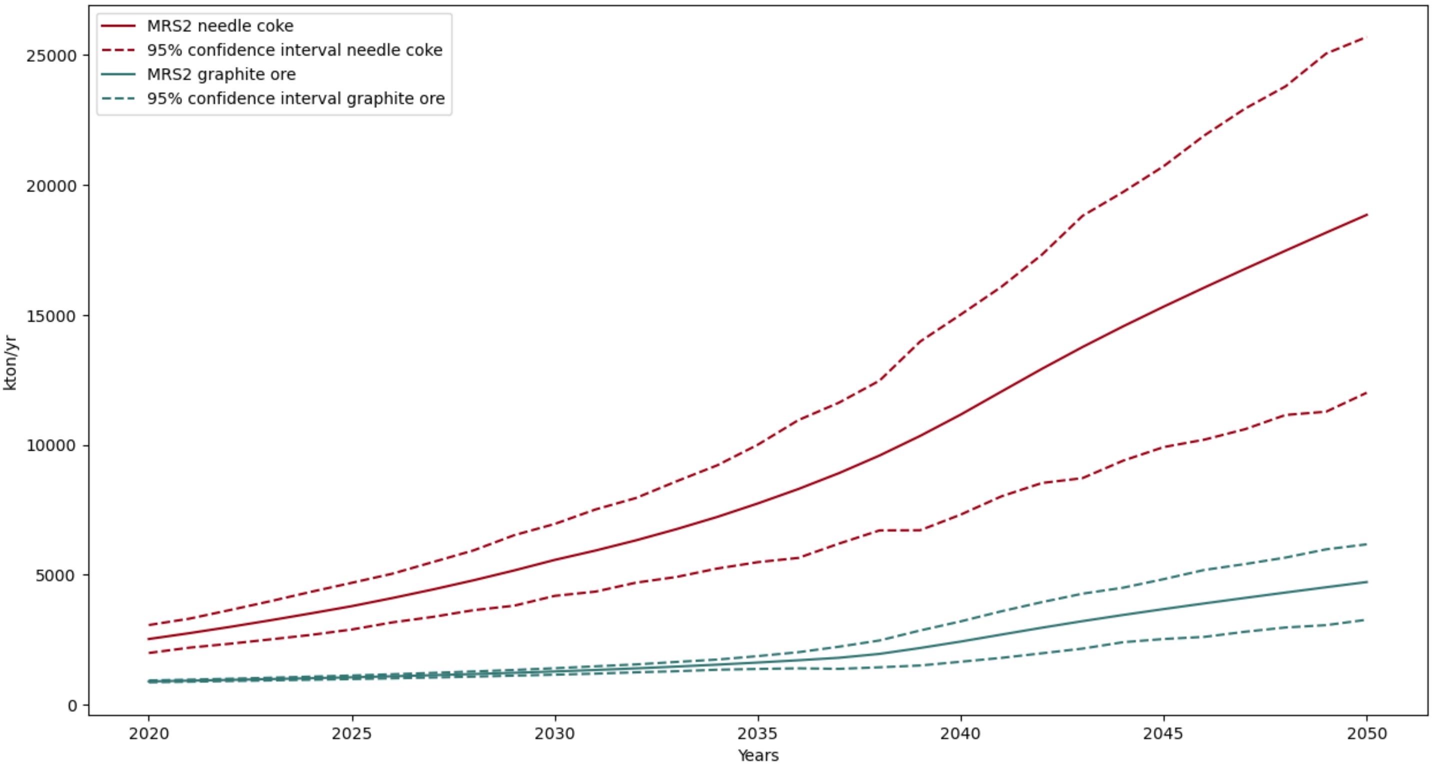


Figure 34: Demand for raw materials in the scenario MRS2, with 95% confidence interval

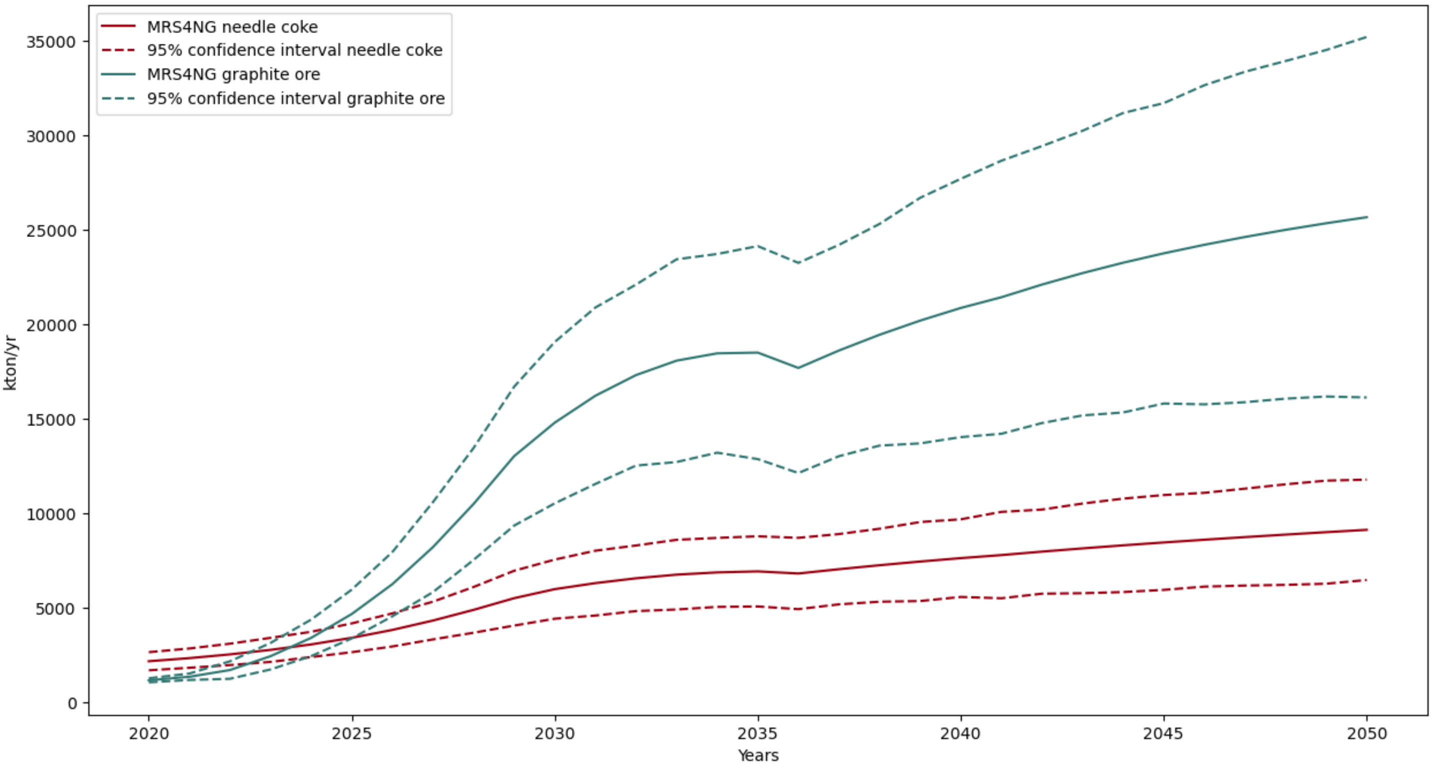


Figure 35: Demand for raw materials in the scenario MRS4-NG, with 95% confidence interval

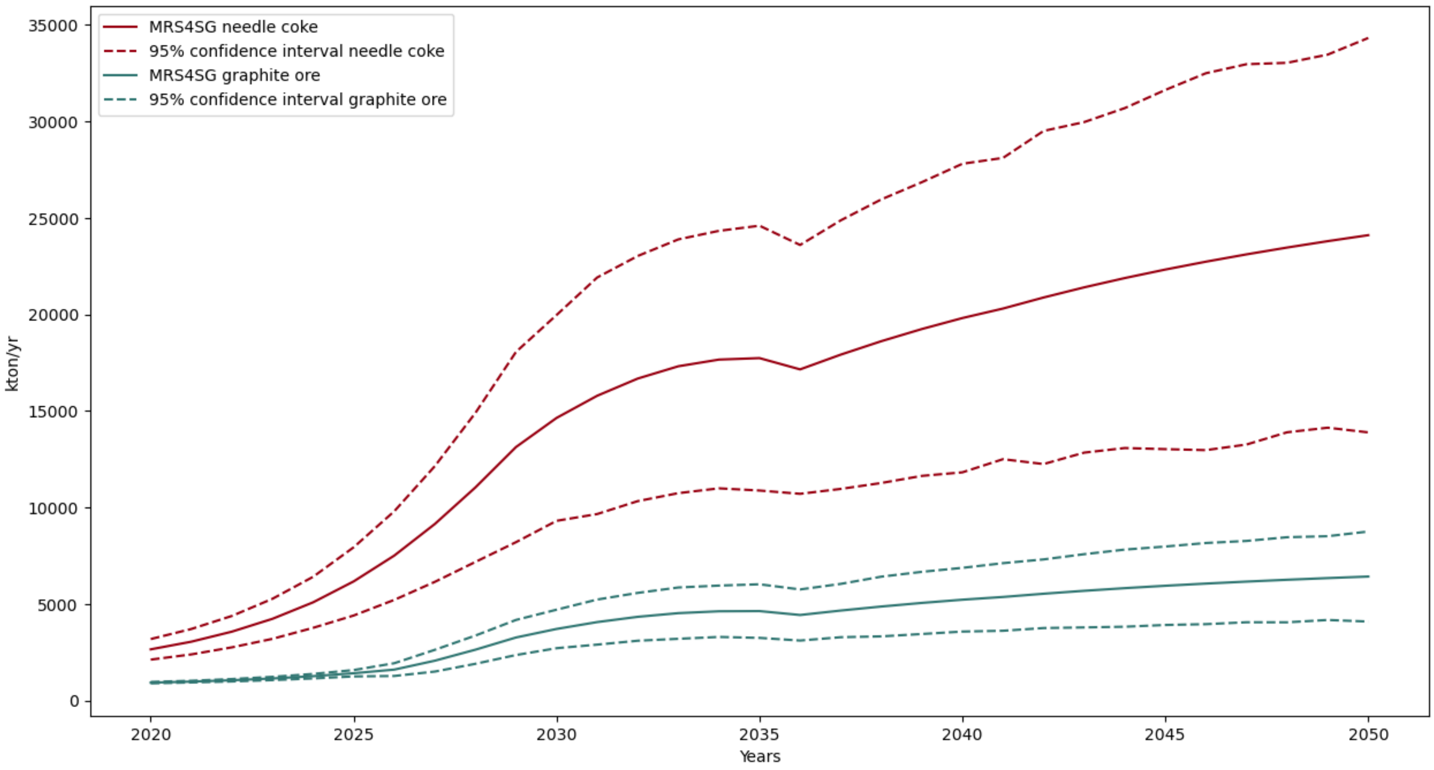


Figure 36: Demand for raw materials in the scenario MRS4-SG, with 95% confidence interval

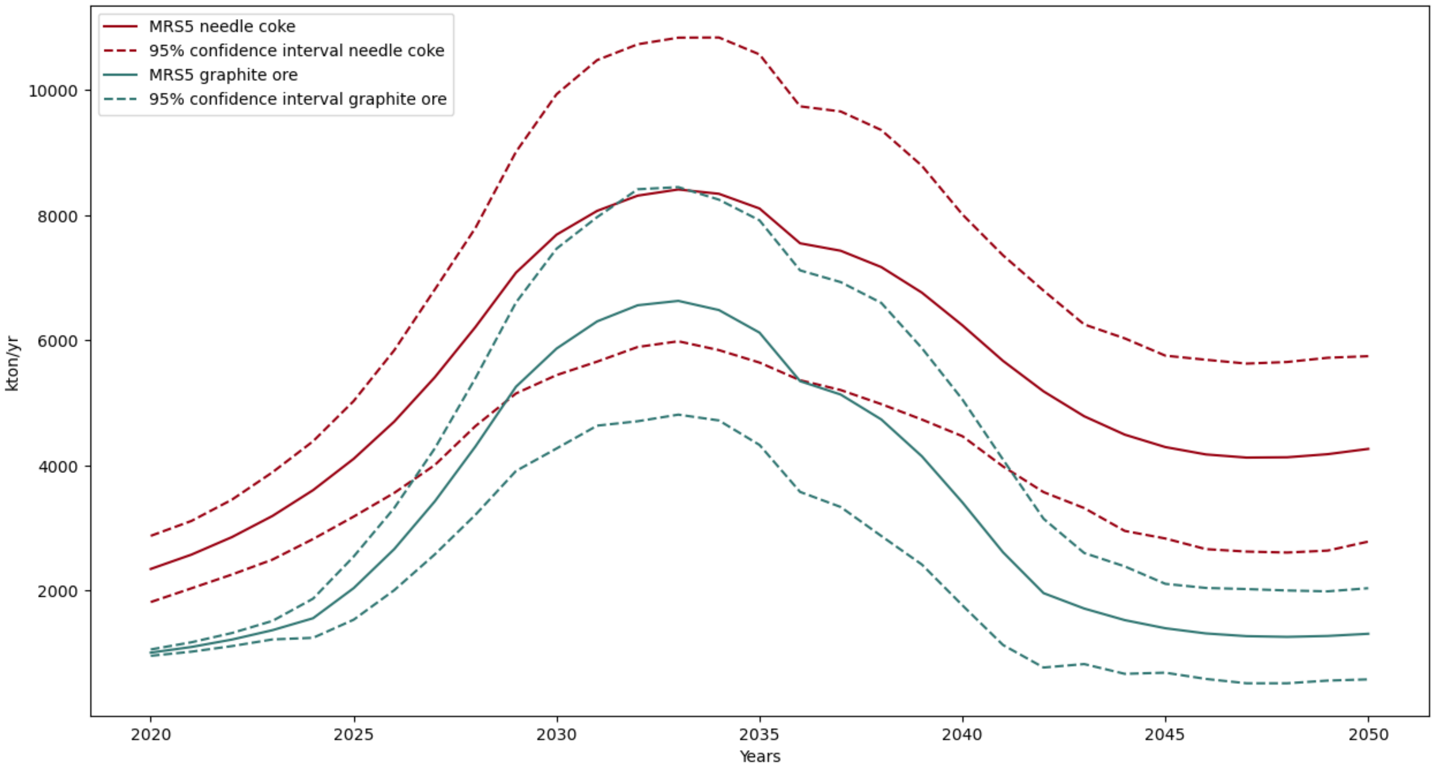


Figure 37: Demand for raw materials in the scenario MRS5, with 95% confidence interval

	Needle coke (ktons/yr)		Graphite Ore (ktons/yr)	
Scenario \Year	2030	2050	2030	2050
MRS1	3817 ± 844	7687 ± 1940	3556 ± 1144	18192 ± 5736
MRS2	5576 ± 1383	18843 ± 6840	1286 ± 125	4725 ± 1450
MRS3	6433 ± 1770	10146 ± 3073	4254 ± 998	7711 ± 2465
MRS4-NG	6004 ± 1563	9141 ± 2654	14810 ± 4267	25673 ± 9531
MRS4-SG	14639 ± 1770	24109 ± 10220	3703 ± 998	6418 ± 2333
MRS5	7688 ± 2244	4265 ± 1481	5868 ± 1596	1312 ± 728

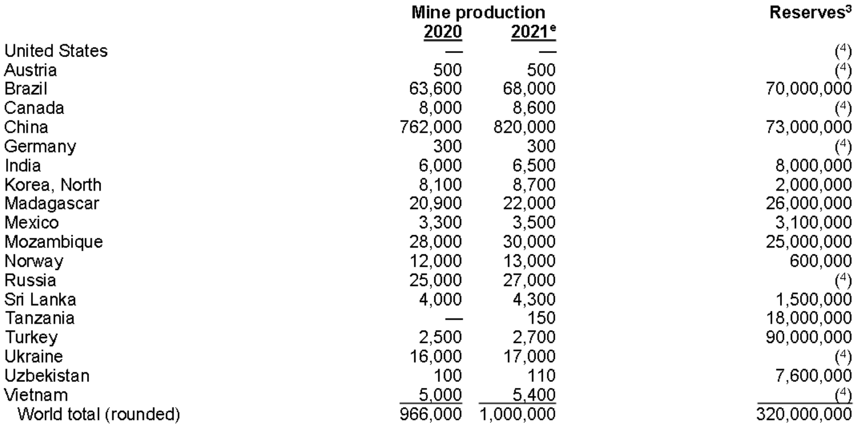
Table 17: Demand for graphite ore and needle coke in the six scenarios in 2030 and 2050, with 95% confidence interval

6.3.5 Supply of coke

	Demand (ktons/yr)		Max supply (ktons/yr)		Max supply - optimized (ktons/yr)	
Scenario \Year	2030	2050	2030	2050	2030	2050
MRS1	4235	7111	17039	16953	39320	39123
MRS2	5158	17430	17039	16953	39320	39123
MRS3	5950	9385	15840	12672	36554	29243
MRS4-NG	5554	8456	11730	3596	27070	8299
MRS4-SG	13451	22301	11730	3596	27070	8299
MRS5	7111	3945	11730	3596	27070	8299

Table 18: Demand and supply for needle coke in the six scenarios in 2030 and 2050

6.4 Natural graphite production



	Mine production		Reserves[3]
	2020	2021[e]	
United States	—	—	(4)
Austria	500	500	(4)
Brazil	63,600	68,000	70,000,000
Canada	8,000	8,600	(4)
China	762,000	820,000	73,000,000
Germany	300	300	(4)
India	6,000	6,500	8,000,000
Korea, North	8,100	8,700	2,000,000
Madagascar	20,900	22,000	26,000,000
Mexico	3,300	3,500	3,100,000
Mozambique	28,000	30,000	25,000,000
Norway	12,000	13,000	600,000
Russia	25,000	27,000	(4)
Sri Lanka	4,000	4,300	1,500,000
Tanzania	—	150	18,000,000
Turkey	2,500	2,700	90,000,000
Ukraine	16,000	17,000	(4)
Uzbekistan	100	110	7,600,000
Vietnam	5,000	5,400	(4)
World total (rounded)	966,000	1,000,000	320,000,000

Table 19: Production and reserves of graphite [100]

NTNU

Norwegian University of
Science and Technology