Title

Techno-economic and carbon dioxide emission assessment of carbon black production

Authors

Rosner, Fabian
Bhagde, Trisha
Slaughter, Daniel S
et al.

Publication Date

2024

DOI

10.1016/j.jclepro.2023.140224

Journal of Cleaner Production 436 (2024) 140224

Contents lists available at ScienceDirect

Journal of Cleaner Production

journal homepage: www.elsevier.com/locate/jclepro

Techno-economic and carbon dioxide emission assessment of carbon black production

Fabian Rosner [a,b,*], Trisha Bhagde [c], Daniel S. Slaughter [d], Vassilia Zorba [c,e], Jennifer Stokes-Draut [a]

[a] *Energy Technologies Area, Lawrence Berkeley National Laboratory, CA, 94720, USA*
[b] *Renewable Energy and Chemical Technologies Lab, Department of Civil and Environmental Engineering, University of California, Los Angeles, Los Angeles, CA, 90095, USA*
[c] *Laser Technologies Group, Lawrence Berkeley National Laboratory, Berkeley, CA, 94720, USA*
[d] *Chemical Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA, 94720, USA*
[e] *Department of Mechanical Engineering, University of California at Berkeley, Berkeley, CA, 94720, USA*

ARTICLE INFO

Handling Editor: Panos Seferlis

Keywords:
Carbon black
Techno-economics
CO2 emissions
Efficiency
Tail gas utilization
Hydrogen

ABSTRACT

The over 15 million metric tonnes of carbon black produced annually emit carbon dioxide in the range of 29–79 million metric tonnes each year. With the renaissance of carbon black in many new renewable energy applications as well as the growing transportation sector, where carbon black is used as a rubber reinforcement agent in car tires, the carbon black market is expected to grow by 66% over the next 9 years. As such, it is important to better understand energy intensity and carbon dioxide emissions of carbon black production. In this work, the furnace black process is studied in detail using process models to provide insights into mass and energy balances, economics, and potential pathways for lowering the environmental impact of carbon black production. Current state-of-the-art carbon black facilities typically flare the tail gas of the carbon black reactor. While low in heating value, this tail gas contains considerable amounts of energy and flaring this tail gas leads to low overall efficiency (39.6%). The efficiency of the furnace black process can be improved if the tail gas is used to produce electricity. However, the high capital investment cost and increased operating costs make it difficult to operate electricity generation from the tail gas economically. Steam co-generation (together with electricity generation) on the other hand is shown to substantially improve energy efficiency as well as economics, provided that steam users are nearby. Steam co-generation can be achieved via back-pressure steam turbines so that the low-pressure exhaust steam (~2 bar/120 °C) can be used locally for heating or drying purposes. Furthermore, the potential of utilizing hydrogen to reduce carbon dioxide emissions is investigated. Using hydrogen as fuel for the carbon black reactor instead of natural gas is shown to reduce the carbon dioxide footprint by 19%. However, current prices of hydrogen lead to a steep increase in the levelized cost of carbon black (47%).

1. Introduction

Carbon black (CB) is a large-scale commodity with a market size of 19.3 billion USD, or approximately 15 million metric tonnes, in 2023 that is expected to grow by over 66% in the next 9 years (Precedence Research, 2023; ChemAnalyst, 2023a). Carbon black is often used as an umbrella term for a group of industrial products including furnace, thermal, channel, and acetylene blacks. The various types of blacks consist of elemental carbon in the form of aggregates. These aggregates are produced by coalescing fine carbon particles which are comprised of graphite-like carbon layer stacks – obtained from the partial combustion or pyrolysis of hydrocarbon feedstocks (Wang et al., 2003). Based on the production process, different grades of carbon black are obtained. A wide range of these grades can now be produced with the modern oil-furnace process (Wang et al., 2003) which accounts for over 95% of the global carbon black production (Wang et al., 2003; European Commission, 2007).

Carbon black differentiates itself from other forms of carbon – such as, coke, graphite, and charcoal – due to the formation of aggregates with complex configurations, quasi-graphitic structures, and its small size, ranging from tens to a few hundred nanometers. Unlike bulk carbon, such as diamond, graphite, coke and charcoal, carbon black is

---

* Corresponding author. Energy Technologies Area, Lawrence Berkeley National Laboratory, CA, 94720, USA.
E-mail address: fabianrosner@ucla.edu (F. Rosner).

https://doi.org/10.1016/j.jclepro.2023.140224
Received 31 August 2023; Received in revised form 28 November 2023; Accepted 14 December 2023

formed via homogeneous nucleation of atomic carbon or free radicals and ions in the vapor phase, initiated by the partial oxidation of hydrocarbons. This formation mechanism makes it possible to reach high carbon purities which distinguishes it from soot, an impure byproduct of hydrocarbon combustion (Wang et al., 2003). The purity range of rubber-grade furnace black normally ranges from 97.3 to 99.3% with hydrogen (0.2–0.8%), oxygen (0.2–1.5%), nitrogen (0.1–0.3%), sulfur (0.2–1.2%), and ashes (0.1–1.0%) being the major contaminants (Wang et al., 2003). Hydrogen and oxygen mostly form functional groups on the surface and edges of the graphitic layers. Hydrogen and oxygen impurities are introduced with the feedstock and/or air (Wang et al., 2003). Sulfur impurities are commonly found in the interior, inaccessibly bound in the particle, and originate from thiophenes, mercaptans and sulfides present in aromatic feedstocks; nitrogen impurities have their source in the feedstock which often contains nitrogen heterocycles; and ash formation is mostly related to the quench water quality (Wang et al., 2003).

The main use of carbon black currently is as rubber reinforcement agent for car tires, which accounts for about 65% of its use (European Commission, 2007). Other applications include the manufacturing of plastics, mechanical rubber, inks, paints, coatings, paper and UV-light absorbents (European Commission, 2007). The car tire sector is the strongest driver for the demand increase of carbon black, largely due to a growing mobility sector in Asia (Precedence Research, 2023). Additionally, the growing demand for plastics as well as battery and fuel cell electrodes is expected to increase the demand for carbon black in the coming years (Precedence Research, 2023).

Different grades of carbon black are needed for each application. In rubber reinforcement applications, typically produced by the furnace black process, the surface energy of the carbon black has a larger impact upon the mechanical stability than the purity of the carbon black (Denka, 2023). In applications where high electrical conductivities are needed, e.g. lithium batteries, acetylene black is often used because of its higher purity (>99.8%), high graphitization and small amounts of surface hydrogen and oxygen groups (Denka, 2023).

While with the introduction of zoned axial flow reactors, high-temperature bag filters and vacuum cleanup systems not much has changed in the production of carbon black since the 1970s (Wang et al., 2003), the study of the physical properties of carbon black and its synthesis mechanism is an active area of research, especially with new applications of carbon black arising in the context of renewable energy technologies and batteries (Khodabakhshi et al., 2020). Most academic literature on carbon black focuses on understanding either synthesis routes to better control particle formation to tune its properties (Skillas et al., 2005; Naseri and Thomson, 2019; Ono et al., 2014); or post-production treatment methods to alter the particle structure (Lee et al., 2021; Lee and Roh, 2020) or surface chemistry (Ma et al., 2018; Diby et al., 2022) to modify particle characteristics. Alternative production pathways of carbon black are also being explored e.g. via spent tire pyrolysis (Nunes et al., 2022; Costa et al., 2022) or methane pyrolysis with hydrogen co-production (Fulcheri et al., 2023; Msheik et al., 2022).

Few studies focus on process design, resource and energy efficiency, greenhouse gas emissions or economics of industrial carbon black production. Dhulipalli (1990) studied mass and energy balances of the oil furnace black process and developed an empirical oil furnace reactor model based on experimental correlations that relate operating conditions, such as temperature, air-to-gas-ratio and residence time, to carbon black properties, such as surface area and structure, as well as yield. Based on this model, a range of operating conditions (varying air, natural gas, and oil feed rates) were simulated, which showed that residence time, air-to-gas ratio and concentration of alkali metals have a great impact upon carbon black properties and yield. More recently, Abdallas Chikri and Wetzels (Abdallas Chikri and Wetzels, 2020) established mass and energy balances for the Cabot plant in the Netherlands and studied options for decarbonizing the facility. In their study, three decarbonization options are considered: 1) electrification by using plasma technology, 2) carbon capture and storage, and 3) feedstock substitution. The authors conclude that all these options come with downsides. Plasma technology is immature and faces challenges meeting product requirements. Carbon capture and storage is mature; however, sulfur present in current feedstocks could increase costs for gas treatment. And lastly, substituting the primary feedstock with biogenic methane faces economic barriers due to low yields while substituting the secondary natural gas fuel can only partially decarbonize the process.

Mergenthaler et al. (2017) studied the exergy destruction in a carbon black plant and analyzed the exergoeconomic performance by quantifying the cost of exergy destruction. The analysis showed that the tail gas combustion is the leading cause for exergy destruction in a carbon black plant followed by the steam generation (boiling heat exchanger) and carbon black reactor. Yet, steam generation was the main cost factor for exergy destruction. Considering process limitations or avoidable/unavoidable exergy destruction, replacing the water quenches with heat recovery steam generators was identified as the most practical improvement. Kozman et al. (2007) conducted an energy audit of a carbon black plant and concluded that a combined heat and power (CHP) unit could prove useful for supplying the plant with electricity and steam for air pre-heating and oil-preheating. Savings in electricity and natural gas cost were estimated to offset investment costs within 3.5 years. However, given that their proposed CHP unit uses carbon black oil as fuel, which needs to be paid for, rather than the reactor's tail gas, which is essentially free, as well as considering the small size of 5.7 MW_{el}, this seems to be an overly optimistic estimate. Details needed to verify their estimate were not provided in the paper.

The tail gas of the carbon black reactor would be a better feedstock for a CHP unit since this would reduce the feedstock cost to essentially zero. Producing steam and sometimes electricity from the low heating value tail gas is a common practice in Europe (European Commission, 2007). However, this is only a feasible option if users for steam and/or electricity are available. In the United States, the tail gas is commonly flared (European Commission, 2007). This difference in tail gas treatment practices appears to be motivated by higher energy prices in Europe (European Commission, 2007). Tail gas recycling to the reactor as fuel has been proposed but not commercialized (European Commission, 2007). Our analysis indicates the low heating value of the tail gas makes it difficult to maintain the reactor temperature.

Considering today's climate change concerns, converting the partial oxidation products from the reactor to carbon dioxide in a flare without extracting its useful energy and ultimately increasing the carbon dioxide footprint of industrial activities is questionable. Carbon dioxide emission factors for carbon black production in literature range from 1.90 to 5.25 kg of carbon dioxide per kg of carbon black (kg_{CO2} per kg_{CB}) (Abdallas Chikri and Wetzels, 2020; EFDB; Last and Schmick, 2011; Boulamanti and Moya; Engineered Carbon, 2019). These estimates represent a large variety of plant configurations, feedstock compositions and product types. Cumulatively, these result in annual carbon dioxide emissions in the range of 29–79 million metric tonnes globally. For comparison, the International Energy Agency (IEA) estimates global primary chemicals production (ethylene, propylene, benzene, toluene, mixed xylenes, ammonia and methanol) emitted 935 million metric tonnes of greenhouse gases in 2022 (IEA, 2023). The Netherlands Environmental Assessment Agency explored various high-level concepts for the decarbonization of the carbon black industry including electrification, renewable drop-in fuels and carbon capture. However, the report points out that these all options come with technological uncertainties and economic penalties (Abdallas Chikri and Wetzels, 2020).

Besides concerns related to the carbon dioxide intensity of carbon black production, carbon black production gives rise to other air pollutants. Incomplete combustion creates carbon monoxide emissions as well as volatile organic compounds, the oxidation of feedstock sulfur and nitrogen gives rise to SO_x and NO_x, and incomplete product recovery leads to particulate matter emissions (slip through carbon) (European Commission, 2007). Releasing carbon black into the environment is a concern as it causes respiratory problems, such as asthma and lung cancer, as well as cardiovascular dysfunctions in humans and animals (Niranjan and Thakur, 2017). With the introduction of high-performance bag filters and vacuum clean up systems, great progress has been made in reducing slip through carbon emission over the past decades (Wang et al., 2003).

Given expected growth in the carbon black market and the need for carbon black for many new renewable energy applications, it is critical to understand the environmental implications of carbon black production and explore options of how to improve resource utilization and reduce the greenhouse gas footprint of carbon black production. In this work, the first publicly-available comprehensive cost and carbon dioxide emission analysis of the furnace black production process is presented based on rigorous process modeling. New insights into plant performance as well as balance-of-plant components are provided. These insights enable us to estimate carbon dioxide emissions by source and establish economic performance. Moreover, the techno-economic performance and carbon dioxide emission profile of various tail gas utilization scenarios are evaluated as well as the value of renewable hydrogen as secondary feedstock in the furnace black process.

2. Methodology

The technical performance of a hypothetical furnace black production facility located in the United States is evaluated using the ProSim software package. This section provides an overview of the design basis used to develop the process simulations as well as the framework for the economic analysis.

2.1. Design basis

2.1.1. Feedstock

The feedstock used for carbon black production impacts both the purity of the carbon product and the carbon yield. The highest yield can be achieved with aromatic hydrocarbons consisting of 3–4 rings (European Commission, 2007). Thus, tar oils or petrochemical oils from refineries are excellent feedstocks. They typically consist of 10–15% of monocyclic aromatics, 50–60% of bicyclic aromatics, 25–35% of tricyclic aromatics, and 5–10% of tetracyclic aromatics (European Commission, 2007). An indication of the aromaticity of the feedstock is the atomic C/H ratio. Values between 0.6 and 1.1 are typically considered favorable (Dhulipalli, 1990). With highly aromatic feedstocks, carbon yields of up to 65% are possible (Wang et al., 2003); however, values around 55% are more typical (Abdallas Chikri and Wetzels, 2020).

In this study, the feedstock composition is based upon Dow Chemical's Carbon Black Feedstock which is a complex mixture of C12 and higher components including naphthalene, methyl-indenes, anthracene, fluorene and other polyaromatic components (Dow Chemical Company). A typical composition can be found in Table 1.

For simplification all biphenyl compounds have been merged into biphenyl and all asphaltenes and other polycyclics are represented by pyrene. The sulfur content is assumed to be 400 ppm (Dow Chemical Company). The lower heating value (LHV) of the fuel is 38.5 MJ per kg, which is comparable to heavy fuel oil. Due to the high viscosity of the feedstock oil, 24 cSt at 60 °C (Dow Chemical Company), it is typically stored at temperatures between 70 and 120 °C (Donnet et al., 1993). A temperature of 90 °C is assumed. The storage tank is heated by steam and excess hot feedstock return. To keep the tank homogenous, the feedstock is recirculated and agitated via jet mixing. The recirculation rate is based upon a tank volume turnover rate of 0.09 h^{-1} considering a 30-day storage (Körting Hannover, 2023). Jet mixers typically operate around 20 bar (Sintemar, 2023) which also falls into the pressure range of typical atomizers in the carbon black furnace (6–40 bar) (Donnet et al., 1993).

Table 1
Feedstock composition.

Compound	wt.-%
Naphthalene	10.0
Methylnaphthalene	20.0
Biphenyl	10.0
Fluorene	5.0
Anthracene	5.0
Pyrene	50.0
H_2S	400 ppm

2.1.2. Carbon black reactor

Modern carbon black reactors can operate at capacities of up to 5 metric tonnes per hour (European Commission, 2007; JiangXi, 2014), though throughput depends on the grade of carbon black produced. While it would be technically possible to build even larger reactors, this is not viable as individual production runs of a particular grade of carbon black would become too short to be economical (Donnet et al., 1993). It is assumed that the reactor units have a production capacity of 4.4 metric tonnes per hour with four production trains operating in parallel resulting in an annual production capacity of 154,500 metric tonnes. The reactor uses natural gas as secondary feedstock/fuel which is burned in the excess of air in the reactor's combustion zone. In the subsequent pyrolysis zone, the primary feedstock is injected and decomposed into carbon black while the remaining oxygen from the combustion zone reacts with the primary feedstock producing additional heat for the endothermic decomposition reactions. The carbon black yield in this work is assumed to be 55%, which is in the typical range of 40–65% (Wang et al., 2003; Abdallas Chikri and Wetzels, 2020; Boulamanti and Moya). Side reactions can lead to the formation of tar and other side-products which need to be disposed of; however, waste generation from the furnace black process is small (European Commission, 2007). Reaction temperatures in the pyrolysis zone range from 1200 to 1900 °C, which is hot enough to support the Boudouard reaction and gas phase reactions such as the water gas shift reaction and reforming reactions. The reactor temperature in this work is assumed to be 1588 °C, based on a natural gas consumption of 14.0 kmol per metric tonne of carbon black product (typical range: 13.2–17.9 $kmol_{NG}$ per $tonne_{CB}$) (European Commission, 2007) and an air consumption factor of 52% (typical range: 30–80%) (Donnet et al., 1993). The heat loss is assumed to be 2%-LHV_{NG} (Donnet et al., 1993). In the last section of the reactor, the reaction is quenched via liquid water injection, which brings the gas temperature down to 790 °C. Common reactor outlet temperatures range from 500 to 900 °C (European Commission, 2007). Some of the remaining heat from the reactor tail gas is recuperated by preheating the primary feedstock to 225 °C (European Commission, 2007), and combustion air to 600 °C (European Commission, 2007; Donnet et al., 1993). The air is supplied at a pressure of 1.5 bar (Donnet et al., 1993), close to the reactor's operating pressure (EUROTECNICA, 2023); however, for feedstock atomization a boost compressor is used to provide 122.5 kg of air per metric tonne of feedstock at a pressure of 8 bar (Donnet et al., 1993). After heat recuperation, a second water quench is employed to reduce the gas temperature down to 232 °C where the carbon can be separated from the gas in a baghouse (European Commission, 2007; Donnet et al., 1993). The simulated tail gas composition from the reactor is: moisture 41.0 mol.-% (typical range: 29.6–50.0), nitrogen 37.4 mol.-% (typical range: 32.7–46.2), hydrogen 8.8 mol.-% (typical range: 6.6–14.0), carbon monoxide 7.4 mol.-% (typical range: 6.1–11.7), and carbon dioxide 2.9 mol.-% (typical range: 1.5–3.9), which is in good agreement with values reported in literature (European Commission, 2007). The lower heating value is with 42 kJ per mol within the common range of 40–85 kJ per mol (European Commission, 2007). A simplified flowsheet including the carbon black production unit with reactor is shown in Fig. 1. The accompanying state-point stream data are provided in the Appendix, Table A1. A tabular comparison of input and output data with literature is provided in Table A2. Additionally, a short thermodynamic description of reactor model is provided together with

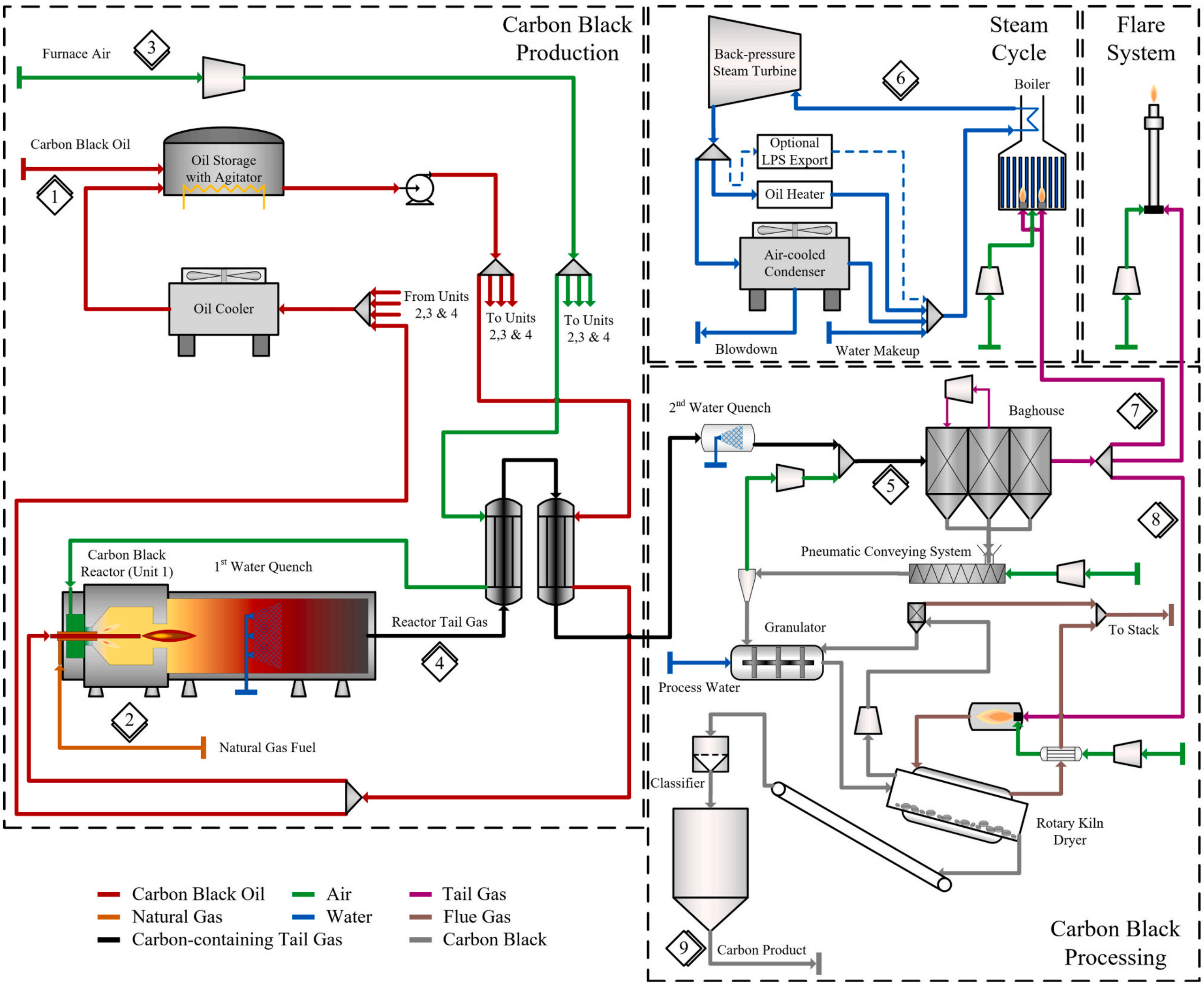

Fig. 1. Simplified flowsheet of the furnace black process. The flowsheet is a representation of scenarios: CB-Elect$_{CB}$ and CB-Elect$_{CB}$ + Steam$_{Sell}$. Corresponding state-point stream data at selected locations, as indicated by the numbers, are presented in the appendix, Table A1.

Table A2.

2.1.3. Carbon black processing

The carbon black is entrained in the reactor's tail gas stream and recovered in a baghouse. Modern filter materials allow these separators to operate at temperatures up to ~260 °C. Temperatures in the excess of 200 °C are necessary to prevent water condensation in the filters (European Commission, 2007). The baghouse uses a pulse-jet cleaning system that used 0.2% of the filtered gas at 6 bar (Turner et al., 1998). After the baghouse, the carbon black is transported to the granulator using a pneumatic conveying system. The air-to-carbon weight ratio is 2.5 with a pressure drop of 6 inches of water (Bhatia). The granulator uses a mixture of 50 wt.-% water and 50 wt.-% carbon black to produce agglomerates. Additionally, 1 wt.-% of molasses are added (Lawrence, 1973), represented by polyvinyl alcohol. The carbon black is then dried in an indirect rotary kiln dryer where the carbon black is heated to 200 °C using the tail gas as fuel (European Commission, 2007; Donnet et al., 1993). The design of the carbon black processing unit is based upon industrial designs (EUROTECNICA, 2023; Idreco, 2023) and shown in Fig. 1

2.1.4. Other plant areas

In the base case scenario, the tail gas from the reactor that is not used in the carbon black drying process is burned in a stack. Other plant areas that are not shown on the flowsheet are the vacuum cleanup system, the water system, the product packaging system and other miscellaneous electricity uses such as lights, control room and other staff facilities. The vacuum cleanup system moves 5.85 kg$_{Air}$ per kg$_{CB}$ (Schwartz et al., 1974) at a standard vacuum pressure of −0.24 barg (Brøndum A/S, 2023). Since the data source was from 1970, the vacuum system with the highest air flow is selected assuming that emission controls today are more stringent than in the 1970s. Water quality is a critical part in carbon black processing, for the quenches as well as for the granulator. The water is assumed to be drinking water quality (European Commission, 2007) from municipal water works which is further treated onsite via ultrafiltration and ion exchange (Conklin).

For some scenarios, a steam cycle for the generation of electricity and steam for export is included. In these scenarios, each of the production trains has its individual boiler (Mergenthaler et al., 2017) with economizer, evaporator and superheater. The boiler produces steam at 85 bar and 540 °C. The steam turbine is a single pressure turbine with an air-cooled condenser. In scenarios with electricity generation only for the plant (self-sufficient) or with steam export, the turbine is a back-pressure turbine with an exhaust pressure of 2 bar. This allows for efficient heat rejection in the air-cooled condenser as well as for sufficiently high temperature steam that can be used for many industrial drying and heating applications as well as for the regeneration of many carbon capture sorbents. For scenarios with the goal to maximize electricity generation, the turbine exhaust pressure is 0.25 bar.

2.2. Economics

The base year for the economic analysis is 2023. For the economic analysis the levelized cost of carbon black (LCCB) is compared for the different scenarios assuming an operating period of 30 years and an initial capital expenditure period of 2.5 years (capital cost expenditure 10%, 35%, 25%, 20%, 10% per half year). The financing structure follows the energy system analysis guidelines of the U.S. Department of Energy (U.S. Department, 2019) which results in a capital charge factor of 0.0765. Using the capital charge factor and Equation (1), the LCCB can be estimated.

$$LCCB = \frac{(CCF)(TOC) + OC_{\text{fix}} + (CF)(OC_{\text{var}})}{(CF)(CBPY)} \tag{1}$$

The *LCCB* denotes the initial-year carbon black production expenses, calculated via various parameters encompassing the capital charge factor (*CCF*), the total overnight capital expenditure of the facility (*TOC*), both fixed and variable annual operational costs (OC_{fix} and OC_{var}), the operational utilization of the plant/capacity factor (CF), and the yearly carbon black output at maximum capacity (*CBPY*). The TOC comprises the total plant cost (TPC), pre-production expenditures, inventory expenses, financial costs, land expenses, and other ownership costs (for details, refer to (U.S. Department, 2019)).

Fixed operational costs include taxes and insurance at a rate of 2% of the TPC, coupled with operational labor costs. The labor force for the studied carbon black facility is assumed to be 5 adept operators remunerated at a rate of $40.85 per hour, and 21 shift employees compensated with $30.00 per hour. Operating labor is estimated based on Cabot's Franklin Louisiana plant (CABOT, 2023). For scenarios with steam cycle, an additional skilled worker and an additional shift worker are employed. The labor overheads are projected to constitute 30% of the operational expenses, with an additional 25% for indirect expenditures. Within the maintenance expenses, labor outlays comprise 35% of the overall maintenance costs, while administrative and auxiliary labor costs constitute 25% of the cumulative operational and maintenance labor expenses (U.S. Department, 2019).

Variable operational costs, such as maintenance expenditures, are contingent upon plant availability/capacity factor. Other variable expenditures include feedstock, fuel, electricity (depending on scenario), water, water treatment chemicals, molasses, and waste disposal. Additionally, any byproduct revenue such as electricity and steam are dependent upon plant availability. An overview of the consumable costs and byproduct sales prices within the carbon black facility is provided in Table 2. All expenditures are adjusted to the year 2023 using an annual escalation of 3%.

The cost of hydrogen is estimated based on current PEM electrolyzer technology whereby carbon-emission-free electricity is purchased via a power purchase agreement. The cost of steam is estimated based on the referenced natural gas price. It is assumed that steam needs to provide a cost advantage of 15% over natural gas heating, on an energy content basis to be attractive to regional customers. All scenarios are based on today's US regulations regarding carbon dioxide emissions and no carbon dioxide emission tax is assumed.

2.3. Study scenarios

Table 3 provides an overview of the study scenarios. Tail gas in the table below refers to excess tail gas that is not used as fuel in the rotary kiln dryer.

Table 2
Cost summary of consumables and byproducts.

Consumables Price	Value	Unit	Cost Year	Ref.
Carbon Black Oil	469	$/tonne	2023	Zauba (2023)
Natural Gas	13.40	$/MWh	2023	U.S. Energy Information Administration (2023a)
Hydrogen	8.00	$/kg	2023	[a]
Electricity	76.20	$/MWh	2023	U.S. Energy Information Administration (2023b)
Raw Water	0.89	$/m^3	2016	Bunch et al. (2017)
Water Treatment Chemicals	0.61	$/m$^3_{\text{Raw Water}}$	2015	DuPont (2023)
Molasses	3.20	$/kg	2022	ChemAnalyst (2023b)
Liquid Waste Discharge	1.27	$/m^3	2016	Bunch et al. (2017)
Byproduct Sales Price	**Value**	**Unit**	**Cost Year**	**Ref.**
Electricity	51.36	$/MWh	2023	Niedens (2023)
Steam	7.10	$/kg	2023	[b]

[a] Calculated based on current PEM electrolyzer and electricity cost.
[b] Calculated based on energy content of NG and current NG cost with 15% discount.

Table 3
Study scenarios.

Scenario Identifier	Description
CB-Flare	Base case scenario where all the tail gas is flared
CB-Elect$_{CB}$	Scenario where a portion of the tail gas is used to raise steam for a back-pressure steam turbine to cover the plant's own electricity demand
CB-Elect$_{CB}$ + *Steam$_{Sell}$*	Scenario where a portion of the tail gas is used to raise steam for a back-pressure steam turbine to cover the plant's own electricity demand and the low-pressure turbine exhaust steam is sold to neighboring consumers
CB-Elect$_{Max}$	Scenario where all the tail gas is used to raise steam for a condensing steam turbine that is optimized for maximum electricity production to cover the plant's own electricity demand and sell excess electricity (no low-pressure steam available)
CB-Elect$_{Sell}$ + *Steam$_{Sell}$*	Scenario where all the tail gas is used to raise steam for a back-pressure steam turbine to cover the plant's own electricity demand, sell excess electricity and the low-pressure turbine exhaust steam is sold to neighboring consumers
CB-Hydrogen	Scenario similar to the CB-Flare case except that hydrogen is used instead of natural gas as secondary feedstock/fuel

3. Results and discussion

3.1. Plant technical performance

The plant capacity for all study scenarios is 154,500 metric tonnes per year based on four trains with an hourly production capacity of 4.4 metric tonnes. This plant size and configuration is typical for new large-scale carbon black plants such as in Jining, Shandong Province, China (JiangXi, 2014). A 90% capacity factor is assumed to account for downtime due to maintenance, making the actual annual production 139,100 metric tonnes of carbon black per year. This corresponds to a primary feedstock consumption of 252,400 metric tonnes of carbon black oil per year at the actual production capacity. Additionally, 439,500 MWh_{LHV} of natural gas per year is used in the carbon black reactors as fuel. The cold gas efficiency of the reactors is 78.5%; however, considerable amounts of energy-containing byproducts such as H_2 and CO leave the reactor as well. Ultimately, only 40.7% of the feedstock's energy content is carried over to the carbon black product (natural gas fuel scenarios). In the *CB-Hydrogen* scenario, where the same air consumption factor as in the natural case is used, the cold gas efficiency and product energy content are slightly improved to 79.6% and 41.5%, due to the higher adiabatic flame temperature of hydrogen, leading to a reduced fuel energy input (439,500 MWh_{LHV} per year in the case of natural gas vs. 376,300 MWh_{LHV} per year in the case of hydrogen).

In the *CB-Flare* scenario where no electricity is co-generated, electricity on the order of 52,500 MWh per year needs to be purchased from utilities. Defining a meaningful efficiency metric for this analysis is difficult since various forms of energy, chemical energy and electrical energy, are used. For simplicity an overall efficiency is used that treats all forms of energy input into the carbon black plant as equal, resulting in an overall efficiency of the *CB-Flare* scenario of 39.6%. However, one could argue that in order to produce the required amount of electricity, primary energy resources at a higher rate are consumed. In the United States, about 2.83 units of primary energy are used to produce 1 unit of electricity (Lawrence Livermore National Laboratory, 2022), which would decrease the efficiency to 38.5%.

In the $CB\text{-}Elect_{CB}$ scenario, where electricity is co-generated on site from the tail gas to cover the plant's electric load, the overall efficiency is 40.3%. The actual electricity consumption of the $CB\text{-}Elect_{CB}$ scenario is in fact higher than the electric load of the *CB-Flare* scenario (59,400 and 52,500 MWh per year, respectively). Nevertheless, utilizing the previously unused tail gas to produce electricity significantly improves its performance. A summary of the balance-of-plant electric load is provided for the $CB\text{-}Elect_{CB}$ scenario in the appendix, Table A3.

A further efficiency improvement can be achieved if the steam leaving the turbine (at 2 bar) is exported to serve heat loads at nearby off-site consumers. When this option is available, the overall efficiency increases to 46.2% in the $CB\text{-}Elect_{CB} + Steam_{Sell}$ scenario. Even higher efficiencies can be obtained when fully utilizing the tail gas; either by maximizing electricity production for export ($CB\text{-}Elect_{Max}$ scenario with 47.9%) or by selling electricity and steam ($CB\text{-}Elect_{Sell} + Steam_{Sell}$ scenario with 72.4%). Particularly, steam export substantially boosts the overall plant efficiency.

The *CB-Hydrogen* scenario is similar to the *CB-Flare* scenario except that hydrogen is used as fuel rather than natural gas. The impact of switching from natural gas to hydrogen leads to an efficiency of 40.5%, an improvement of 0.9%-points over the *CB-Flare* scenario. This efficiency increase is driven primarily by a lower demand for heat (higher adiabatic flame temperature/higher energy release per oxidant) and a lower electricity demand (less combustion air needed and tail gas with a higher heating value).

Direct carbon dioxide emissions from the plant are 467,100 metric tonnes per year for the natural gas scenarios and 377,300 metric tonnes per year for the hydrogen scenario. In the base case scenario (*CB-Flare*), additional emissions from the use of electricity add another 20,300 metric tonnes per year (based on U.S. average grid emission factor of 386 kg_{CO2} per MWh (U.S. Energy Information Administration, 2021)), leading to specific CO_2 emissions of 3.50 kg_{CO2} per kg_{CB}. Other upstream emissions associated with feedstock or fuel production are not included in this analysis. Using hydrogen as fuel can reduce the specific carbon dioxide emissions down to 2.85 kg_{CO2} per kg_{CB} (not accounting for indirect emissions associated with its production). Producing electricity on site from the tail gas reduces the carbon dioxide emission factor to 3.36 kg_{CO2} per kg_{CB} in the $CB\text{-}Elect_{CB}$ scenario, and 3.04 kg_{CO2} per kg_{CB} in the $CB\text{-}Elect_{CB} + Steam_{Sell}$ scenario, assuming that steam heating offsets emissions from natural gas-based heating applications (natural gas heating is assumed to be 85% efficient). In the $CB\text{-}Elect_{Max}$ scenario where electricity is exported, 92,000 metric tonnes of carbon dioxide emissions are offset per year leading to an effective carbon dioxide emission factor of 2.70 kg_{CO2} per kg_{CB} (based on U.S. average grid emission factor of 386 kg_{CO2} per MWh (U.S. Energy Information Administration, 2021)). However, as the grid becomes cleaner and the value of the offset decreases, the effective carbon dioxide emission factor will increase in the future. Considering electricity and steam export ($CB\text{-}Elect_{Sell} + Steam_{Sell}$), the emission factor of carbon black production can be reduced to 1.45 kg_{CO2} per kg_{CB}. Yet, it needs to be mentioned again that this value will increase in a cleaner energy future; nevertheless, the $CB\text{-}Elect_{Sell} + Steam_{Sell}$ is the most desirable scenario from a sustainability perspective as it utilizes resources most efficiently. Comparing the furnace black process to other carbon black production processes, as reported in literature, shows that these emission values are significantly lower than carbon dioxide emissions of the thermal black process which are reported at 5.25 kg_{CO2} per kg_{CB} (EFDB). Acetylene black on the other hand has a lower emission value with 0.78 kg_{CO2} per kg_{CB} (EFDB); however, it's production cost is substantially higher due to high feedstock costs.

The water consumption of the plant ranges from 6.5 to 7.0 kg_{Water} per kg_{CB}, which is lower than values reported by manufacturers (10.3 kg_{Water} per kg_{CB}) (Engineered Carbon, 2019). Our analysis only accounts for process related water consumption and the difference is likely attributed to auxiliary water consumption by the plant personnel (e.g., restrooms, cleaning, indoor uses). The results are summarized in Table 4.

3.2. Plant economic performance

The total plant cost of the base case (*CB-Flare*) is \$183.1M. Oil storage, carbon black production, and carbon black processing account for 7%, 23% and 29% of the costs, respectively. The remaining plant costs are attributed to the flare system, water supply system and auxiliary plant equipment such as instrumentation, controls, electrical, piping, buildings and site improvements. A detailed breakdown of these cost factors can be found in the appendix, Table A4. Considering preproduction costs (\$24.6M), inventory capital (\$43.6M) and other owner costs, such as land, financing, etc., (\$33.3M), the total overnight capital cost is \$284.6M. In the case of the *CB-Hydrogen* scenario, the total plant cost is reduced to \$178.3M due to lower combustion air demand and water quenching needs. However, the high fuel cost of hydrogen makes preproduction costs and startup costs increase resulting in an overnight capital cost of \$286.6M. In the case of co-generation of electricity and steam, the steam cycle capital expenditures push the overnight capital cost over \$329.3M in the case of the $CB\text{-}Elect_{CB}$ and $CB\text{-}Elect_{CB} + Steam_{Sell}$ scenarios, and over \$400M in the cases of the $CB\text{-}Elect_{Max}$ and $CB\text{-}Elect_{Sell} + Steam_{Sell}$ scenarios. More details can be found in the appendix, Table A4.

Fixed operating costs are relatively similar between the cases and range from \$17.0M to \$19.4M per year. Cost increases in operating labor are observed for the scenarios with steam cycle due to increased staffing. Maintenance labor costs are highly correlated with the total plant cost leading to higher maintenance labor costs for plants with additional equipment. Moreover, higher plant costs also lead to higher property tax and insurance costs.

Variable operating costs are dominated by the cost of the carbon black oil feedstock (\$118.4M per year for all scenarios). In the cases with natural gas as fuel, an additional \$5.9M per year is spent on fuel. Replacing natural gas fuel with renewable hydrogen is currently very expensive and will increase annual fuel costs to \$90.3M. In the flare cases, *CB-Flare* and *CB-Hydrogen*, annual electricity costs account for \$4.0M and \$3.8M, respectively. More details on the variable operating costs including maintenance materials, raw water, water treatment, liquid discharge and molasses can be found in the appendix, Table A4.

Lastly, the byproduct revenue is considered. No byproduct revenue is included in the $CB\text{-}Elect_{CB}$ scenario as the generated electricity only covers the plant's own electricity consumption. In the $CB\text{-}Elect_{CB} + Steam_{Sell}$ scenario \$2.1M per year is generated from selling steam. In the $CB\text{-}Elect_{Max}$ scenario the revenue is increased to \$12.2M per year from the sales of electricity to the grid. In the $CB\text{-}Elect_{Sell} + Steam_{Sell}$ scenario a total of \$18.6M is generated, \$9.2M from electricity and \$9.4M from steam. To understand the tradeoff between increased capital and operating expenditures and generated revenue, the LCCB is analyzed. In the *CB-Flare* scenario, the LCCB is \$1296 per metric tonne. Capital-related expenditures account for \$156 per metric tonne, fixed operating expenditures for \$149 per metric tonne and variable operating expenses

Table 4
Mass and energy balances from simulations.

Plant Design Capacity	Unit	CB-Flare	CB-Elect$_{CB}$	CB-Elect$_{CB}$ +Steam$_{Sell}$	CB-Elect$_{Max}$	CB-Elect$_{Sell}$ +Steam$_{Sell}$	CB-Hydrogen
CB Production Capacity	metric tonnes/year	154,500	154,500	154,500	154,500	154,500	154,500
Plant Capacity Factor	%	90	90	90	90	90	90
Actual CB Production	metric tonnes/year	139,100	139,100	139,100	139,100	139,100	139,100
Consumables at 90% Capacity Factor							
Carbon Black Oil	metric tonnes/year	252,400	252,400	252,400	252,400	252,400	252,400
Natural Gas	metric tonnes/year	33,500	33,500	33,500	33,500	33,500	0
Hydrogen	metric tonnes/year	0	0	0	0	0	11,300
Electricity	MWh$_{Elect}$/year	52,500	0	0	(238,400)	(178,600)	50,100
Raw Water	metric tonnes/year	960,100	961,800	961,800	967,600	967,700	898,300
Steam	metric tonnes/year	0	0	(298,200)	0	(1,329,000)	0
Energy Consumption at 90% Capacity Factor							
Carbon Black Oil	MWh$_{LHV}$/year	2,700,200	2,700,200	2,700,200	2,700,200	2,700,200	2,700,200
Natural Gas	MWh$_{LHV}$/year	439,500	439,500	439,500	439,500	439,500	0
Hydrogen	MWh$_{LHV}$/year	0	0	0	0	0	376,300
Electricity	MWh$_{Elect}$/year	52,500	0	0	(238,400)	(178,600)	50,100
Steam	MWh$_{Therm}$/year	0	0	(185,900)	0	(828,500)	0
Carbon Black	MWh$_{LHV}$/year	(1,265,500)	(1,265,500)	(1,265,500)	(1,265,500)	(1,265,500)	(1,265,500)
Efficiency Metrics							
Overall Efficiency	%	39.6%	40.3%	46.2%	47.9%	72.4%	40.5%
GHG Emission Metrics							
Direct CO2 Emissions	metric tonnes/year	467,100	467,100	467,100	467,100	467,100	377,300
CO_2 Emissions form Grid	metric tonnes/year	20,280	0	0	(92,000)	(68,900)	19,300
CO_2 Emissions from Heat	metric tonnes/year	0	0	(44,200)	0	(197,200)	0
Specific CO_2 Emissions	kg$_{CO2}$/kg$_{CB}$	3.50	3.36	3.04	2.70	1.45	2.85

for $991 per metric tonne of which the feedstock cost accounts for $852 per metric tonne. In the *CB-Elect$_{CB}$* scenario, the cost of carbon black increases to $1313 per metric tonne. By producing electricity on site, electricity purchases are reduced by an equivalent of $29 per metric tonne. However, capital expenses and operating expenses increase by $25 and $21, respectively, leading to an overall increase in cost of carbon black. Additional income from selling steam (*CB-Elect$_{CB}$ + Steam$_{Sell}$* scenario), approximately $15 per metric tonne of carbon black, does not suffice to make this system integration more profitable than the *CB-Flare* scenario. More promising is the *CB-Elect$_{Max}$* scenario which generates revenue at an equivalent of $88 per metric tonne of carbon black. In this case, the revenue can offset investment and operating cost leading to an LCCB of $1291 per metric tonne. An even more attractive option is the *CB-Elect$_{Sell}$ + Steam$_{Sell}$* scenario where the system is not optimized for electricity generation but allows for combined electricity and steam production in a back pressure turbine. Here the combined revenue is $134 per metric tonne of carbon black which reduces the LCCB down to $1240 per metric tonne.

Using hydrogen as carbon free fuel instead of natural gas substantially increases the cost of carbon black. At current renewable hydrogen prices, switching from natural gas to hydrogen leads to fuel costs of $650 per metric tonne of carbon black versus $42 per metric tonne in the case of natural gas. As a result, the LCCB increases to $1901 per metric tonne. Even with current tax incentives in the United States of up to $3 per kg of hydrogen, which would reduce the cost of hydrogen to $5 per kg, the LCCB would exceed $1655 per metric tonne. A hydrogen price of $0.61 per kg is necessary to breakeven with the *CB-Flare* scenario assuming that the use of hydrogen has no adverse impact upon product quality and yield. The results are illustrated in Fig. 2, and detailed breakdowns of the LCCB are presented in the appendix, Table A5.

Additionally, a sensitivity study of the impact of commodity price fluctuations is presented in Fig. 3 to further investigate the relative significance of market uncertainties around the carbon black oil feedstock, natural gas, electricity, and renewable hydrogen. The results show that carbon black production is highly sensitive to the carbon black oil feedstock and moderately sensitive to natural gas and electricity prices. While in general lower prices are more favorable in order to reduce the LCCB, in cases with electricity co-generation for export, lower electricity prices are counter-productive and increase the LCCB. Thus, in a future with cheap renewable electricity, it will be even more challenging to recuperate investment costs associated with the co-generation of electricity from the reactor's tail gas. The fuel cost sensitivity for the *CB-Hydrogen* case is significantly higher than for the other cases, due to the comparatively high cost of hydrogen (on an energy basis), and as previously mentioned a significant cost reduction of hydrogen needs to be achieved in order to make this case economically attractive.

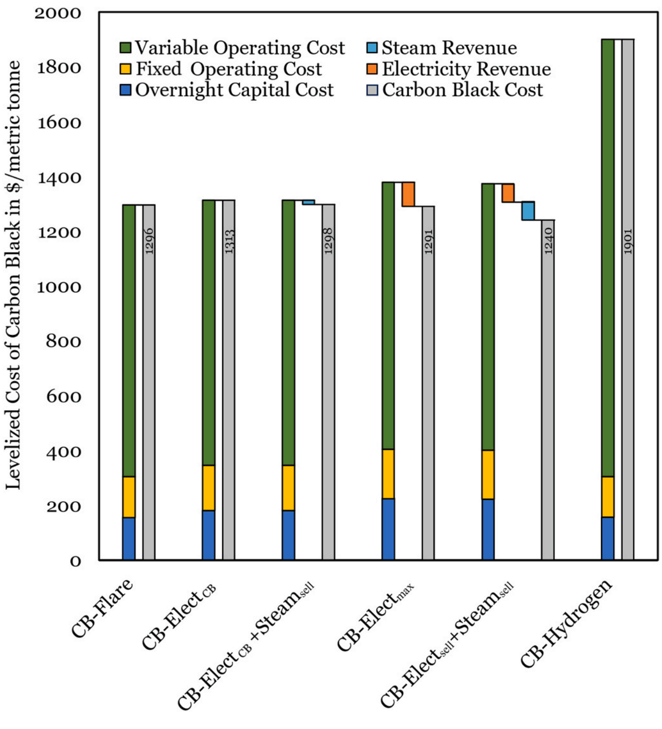

Fig. 2. Levelized cost of carbon black.

4. Conclusion

A detailed process model of a carbon black plant has been developed

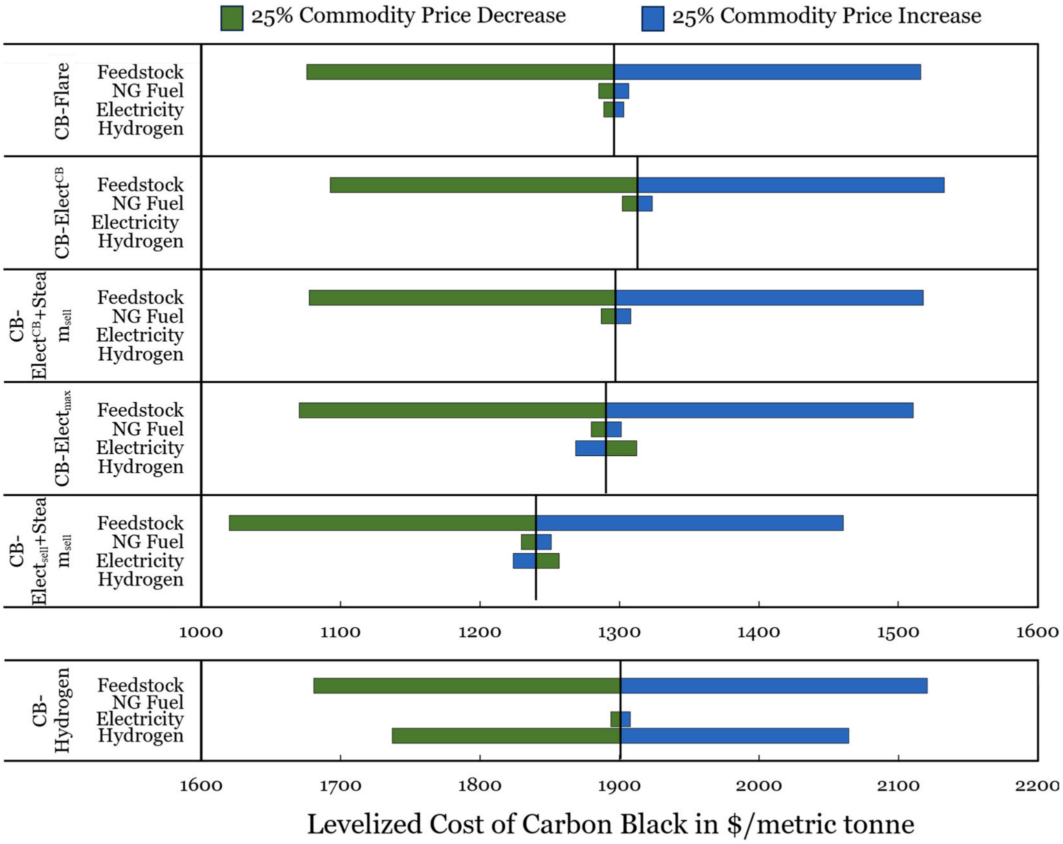

Fig. 3. Sensitivity analysis of the cost of carbon black.

to estimate mass and energy balances. The performance of a state-of-the-art carbon black plant with tail gas flare has been compared to various tail gas utilization options and their thermodynamic and carbon dioxide footprint have been compared. Moreover, an economic model that provides insights into cost driving factors of carbon black production has been presented and was used to identify economically viable tail gas utilization scenarios and to evaluate a scenario in which hydrogen is used as fuel for the carbon black reactor instead of natural gas.

The analysis shows that the energy efficiency in the conventional plant configuration with tail gas flare is low (39.6%) leading to specific carbon dioxide emissions of 3.50 kg_{CO2} per kg_{CB}. Utilizing the tail gas to produce electricity is shown to increase efficiency and reduce the carbon dioxide footprint. While the on-site carbon dioxide emissions do not change by co-generating electricity in a carbon black plant, carbon dioxide emission from the electrical grid can be offset. Similarly, steam generation is shown to greatly benefit plant efficiency and carbon dioxide footprint. Moreover, by replacing natural gas with hydrogen as fuel, a carbon dioxide emission reduction of 19% is possible.

The economic analysis shows that utilizing the tail gas economically is challenging. Generating electricity to supply the plant's electric load is uneconomical even if the low pressure (2 bar) steam leaving the turbine is sold to nearby customers. Maximizing electricity generation by utilizing all the available tail gas is marginally economical, leading to a 0.4% reduction in levelized cost of carbon black. Considering that carbon black plants produce several grades of carbon blacks with varying operating conditions, varying water needs for agglomeration, and varying drying temperatures, it remains to be seen whether this economic advantage would be realized in real-world plant operation. Additionally, uncertainties about varying feedstock composition and reactor performance add further uncertainties to the economic analysis and long-term profitability of the studied utilization scenarios which do not consider such variations. Significantly higher cost savings are seen when electricity and steam are co-generated while utilizing all of the available tail gas, which simultaneously increases the efficiency to 72.4%. This scenario represents the most attractive option from a climate and economic perspective. Using hydrogen to reduce carbon dioxide emissions is not an economical solution unless the cost of renewable hydrogen falls below the U.S. Department of Energy's target of $1 per kg. The break-even cost of hydrogen for carbon black production in the furnace black process is $0.61 per kg.

Using current production processes, such as the furnace black process, for carbon black production will continue to be carbon dioxide intensive and lead to large quantities of carbon dioxide emitted into the atmosphere. Co-generation of electricity and steam is shown to be most effective in reducing the carbon dioxide footprint, however, the furnace black process also gives rise to other pollutants such as CO (incomplete combustion), SO_x (oxidation of feedstock sulfur), NO_x and other nitrogen compounds (oxidation of feedstock nitrogen and thermal NO_x), volatile organic compounds (incomplete combustion) as well as particulate matter (slip through carbon). More information on emission intensity of these pollutants can be found in (European Commission, 2007). In the long run new more sustainable carbon black production processes will be needed. Ideally, these processes will use biogenic carbon resources or carbon dioxide as a feedstock, e.g., plasma- or laser-based processes that support the homogeneous gas phase condensation at low temperatures.

CRediT authorship contribution statement

Fabian Rosner: Conceptualization, Formal analysis, Investigation, Methodology, Software, Visualization, Writing – original draft, Writing – review & editing. **Trisha Bhagde:** Conceptualization, Writing – review & editing. **Daniel S. Slaughter:** Conceptualization, Writing – review & editing. **Vassilia Zorba:** Conceptualization, Funding acquisition, Writing – review & editing. **Jennifer Stokes-Draut:** Conceptualization, Supervision, Writing – review & editing.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

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

Acknowledgements

The authors gratefully acknowledge support from the Laboratory-Directed Research and Development (LDRD) program at Lawrence Berkeley National Laboratory (LBNL) provided by the Director, Office of Science, of the US Department of Energy under Contract Number DE-AC02-05CH11231. The views and opinions of the authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, expressed or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. The US Government retains, and the publisher, by accepting the article for publication, acknowledges, that the US Government retains a non-exclusive, paid-up, irrevocable, world-wide license to publish or reproduce the published form of this manuscript, or allow others to do so, for US Government purposes.

Nomenclature

CB	Carbon Black
CBPY	Annual CB Production
CCF	Capital Charge Factor
CF	Capacity Factor
CHP	Combined Heat and Power
fix	Fixed Annual Costs
IEA	International Energy Agency
LCCB	Levelized Cost of Carbon Black
LHV	Lower Heating Value
LPS	Low Pressure Steam
NG	Natural Gas
OC	Operating Costs
PEM	Proton Exchange Membrane
TOC	Total Overnight Capital
TPC	Total Plant Cost
var	Variable Annual Costs

Appendix

Table A1
State Point Stream Data for Scenarios: CB-Elect$_{CB}$ and CB-Elect$_{CB}$ + Steam$_{Sell}$

Stream Number	Unit	1	2	3	4	5	6	7	8	9
Pressure	bar	1.0	4.0	1.0	1.3	1.1	85.0	1.0	1.0	1.0
Temperature	°C	15.0	15.0	15.0	789.5	231.0	540.0	231.9	231.9	200.0
Molar Vapor Fraction	–	0.00	1.00	1.00	0.86	0.89	1.00	1.00	1.00	0.00
Mass Flow Rate	kg/h	32,000	4,250	133,420	55,817	75,786	37,809	14,245	7,855	4,408
Molar flow rate	kmol/h	188.8	246.1	4632.3	2706.4	3584.6	2098.7	641.8	353.9	367.0
Composition	mole-basis									
Nitrogen	–	–	0.0160	0.7785	0.3335	0.3357	–	0.3744	0.3744	–
Oxygen	–	–	Trace	0.2073	Trace	0.0224	–	0.0249	0.0249	–
Water	–	–	Trace	0.0102	0.3055	0.3679	1.0000	0.4103	0.4103	–
Carbon Dioxide	–	–	0.0100	0.0040	0.0336	0.0258	–	0.0287	0.0287	–
Carbon Monoxide	–	–	–	–	0.0879	0.0664	–	0.0740	0.0740	–
Hydrogen	–	–	–	–	0.1039	0.0785	–	0.0875	0.0875	–
Methane	–	–	0.9309	–	Trace	Trace	–	Trace	Trace	–
Ethane	–	–	0.0320	–	–	–	–	–	–	–
Propane	–	–	0.0110	–	–	–	–	–	–	–
Hydrogen Sulfide	–	0.0020	Trace	–	Trace	Trace	–	Trace	Trace	–
Sulfur Dioxide	–	–	–	–	Trace	Trace	–	Trace	Trace	–
Carbon Black Oil	–	0.9980	–	–	–	–	–	–	–	–
Carbon Black	–	–	–	–	0.1356	0.1034	–	–	–	1.0000
Total	–	1	0.9999	1	1	1	1	1	1	1

Table A2
Comparison of Input and Output Data with Literature

Variable	Type*	This work	Literature	Reference
Carbon Black Yield	Input	55 wt.-%	40-65 wt.-%	(Wang et al., 2003; Abdallas Chikri and Wetzels, 2020; Boulamanti and Moya)
Natural Gas Fuel Flow	Input	14.0 $kmol_{NG}/tonne_{CB}$	13.2–17.9 $kmol_{NG}/tonne_{CB}$	European Commission (2007)
Air Consumption Factor	Input	52 mol.-%	30–80 mol.-%	Donnet et al. (1993)
Reactor Heat Loss	Input	2 %-LHV_{NG}	1–2 %-LHV_{NG}	Donnet et al. (1993)
Air Preheat Temperature	Input	225 °C	150–250 °C	European Commission (2007)
Fuel Preheat Temperature	Input	600 °C	400–800 °C	(European Commission, 2007; Donnet et al., 1993)
Reactor Temperature	Output	1588 °C	1200–1900 °C	European Commission (2007)
Quench Water Flow Rate	Input	5 m^3/t_{CB}	No Data	N/A
Reactor Outlet Temperature	Output	790 °C	500–900 °C	European Commission (2007)
Heat Recuperation Outlet Temperature	Output	540 °C	at least 400	Donnet et al. (1993)
Baghouse Inlet Temperature	Output	231 °C	200–280 °C	(European Commission, 2007; Donnet et al., 1993)
Tail gas composition: H2O	Output	41.0 mol.-%	29.6–50.0 mol.-%	European Commission (2007)
Tail gas composition: H2	Output	8.8 mol.-%	6.6–14.0 mol.-%	European Commission (2007)
Tail gas composition: CO	Output	7.4 mol.-%	6.1–11.7 mol.-%	European Commission (2007)
Tail gas composition: CO2	Output	2.9 mol.-%	1.5–3.9 mol.-%	European Commission (2007)
Tail gas LHV	Output	42 kJ/mol	40–85 kJ/mol	European Commission (2007)

*Input values are values used as setpoints in the process models based on the presented literature data in order to obtain the output values presented here. These values are in good agreement with literature data (also presented in Table A2 for ease of comparison).

Thermodynamic reactor model description. The carbon black reactor is a reactor network model where in the first reactor (representing the pyrolysis zone) the carbon black oil is decomposed via pyrolysis to its elemental components using the carbon yield specified in Table A2. Subsequently, an equilibrium reactor is used to establish the gas composition. Here the combustion air (from Table A2), fuel (NG from Table A2), unconverted carbon black feedstock oil and the non-carbon elements from the pyrolysis are equilibrated based upon the minimization of the Gibbs free energy. Quench water is added to the equilibrium reactor to reach an outlet temperature of 1300 °C since the gas phase reactions, such as reforming, only proceed at appreciable rates above this critical temperature (Alves et al., 2021). Therefore, the following introduction of water solely results in the quenching of the gas mixture.

Table A3
Balance-of-Plant Electricity Generation and Consumption: CB-$Elect_{CB}$

Electricity Generation at Full Load Operation	Value	Unit
Steam Turbine	7532	kW_{Elect}
Auxiliary Load at Full Load Operation	Value	Unit
Steam Cycle Auxiliaries	160	kW_{Elect}
Process Water Pumping	106	kW_{Elect}
Oil Storage and Pumping	1594	kW_{Elect}
Carbon Black Reactor System	2264	kW_{Elect}
Baghouse	119	kW_{Elect}
Boiler System	769	kW_{Elect}
Flare System	193	kW_{Elect}
Carbon Black Transport	223	kW_{Elect}
Carbon Black Dryer	49	kW_{Elect}
Vacuum Cleanup	803	kW_{Elect}
Packaging	499	kW_{Elect}
Miscellaneous	753	kW_{Elect}
Total	7532	kW_{Elect}

Table A4
Capital Expenditures and Annual Operating Costs

Item	Unit	CB-Flare	CB-$Elect_{CB}$	CB-$Elect_{CB}$ +$Steam_{Sell}$	CB-$Elect_{Max}$	CB-$Elect_{Sell}$ +$Steam_{Sell}$	CB-Hydrogen
Overnight Capital Cost	$	**284,557,000**	**329,304,000**	**329,304,000**	**409,247,000**	**403,806,000**	**286,586,000**
Preproduction Costs	$	24,566,000	26,174,000	26,174,000	27,949,000	27,831,000	32,246,000
Inventory Cost	$	43,567,000	43,750,000	43,750,000	44,081,000	44,059,000	43,534,000
Other Owner Costs	$	33,311,000	39,771,000	39,771,000	51,476,000	50,679,000	32,466,000
Total Plant Cost	$	183,113,000	219,609,000	219,609,000	285,740,000	281,237,000	178,339,000
Oil Storage	$	*13,142,000*	*13,142,000*	*13,142,000*	*13,142,000*	*13,142,000*	*13,142,000*
CB Production	$	*41,848,000*	*41,848,000*	*41,848,000*	*41,848,000*	*41,848,000*	*40,051,000*
CB Processing	$	*53,551,000*	*53,551,000*	*53,551,000*	*53,551,000*	*53,551,000*	*52,546,000*
Steam Cycle	$	*0*	*22,475,000*	*22,475,000*	*63,197,000*	*60,423,000*	*0*
Flare System	$	*2,663,000*	*2,663,000*	*2,663,000*	*2,663,000*	*2,663,000*	*2,574,000*
Water Supply	$	*1,565,000*	*1,566,000*	*1,566,000*	*1,571,000*	*1,571,000*	*1,516,000*

(continued on next page)

Table A4 (*continued*)

Item	Unit	CB-Flare	CB-Elect$_{CB}$	CB-Elect$_{CB}$ +Steam$_{Sell}$	CB-Elect$_{Max}$	CB-Elect$_{Sell}$ +Steam$_{Sell}$	CB-Hydrogen
Inst., Elect., Pipe., etc.	$	*70,344,000*	*84,365,000*	*84,365,000*	*109,769,000*	*108,039,000*	*68,510,000*
Fix Operating Cost	$/a	**20,700,000**	**23,088,000**	**23,088,000**	**25,133,000**	**24,998,000**	**20,552,000**
Labor Cost	$/a	17,038,000	18,696,000	18,696,000	19,418,000	19,374,000	16,985,000
Operating Labor	$/a	*11,884,000*	*12,893,000*	*12,893,000*	*12,893,000*	*12,893,000*	*11,884,000*
Maintenance Labor	$/a	*1,747,000*	*2,064,000*	*2,064,000*	*2,642,000*	*2,606,000*	*1,704,000*
Adm. & Sup. Labor	$/a	*3,408,000*	*3,739,000*	*3,739,000*	*3,884,000*	*3,875,000*	*3,397,000*
Property Tax & Insurance	$/a	3,662,000	4,392,000	4,392,000	5,715,000	5,625,000	3,567,000
Variable Operating Cost	$/a	**137,756,000**	**134,288,000**	**134,288,000**	**135,272,000**	**135,213,000**	**221,838,000**
Maintenance Materials Cost	$/a	2,919,000	3,449,000	3,449,000	4,416,000	4,356,000	2,848,000
Liquid Discharge	$/a	153,000	155,000	155,000	163,000	163,000	143,000
Feedstock & Energy Cost	$/a	134,684,000	130,683,000	130,683,000	130,694,000	130,694,000	218,846,000
Carbon Black Oil	$/a	*118,420,000*	*118,420,000*	*118,420,000*	*118,420,000*	*118,420,000*	*118,420,000*
Natural Gas	$/a	*5,886,000*	*5,886,000*	*5,886,000*	*5,886,000*	*5,886,000*	*0*
Hydrogen	$/a	*0*	*0*	*0*	*0*	*0*	*90,349,000*
Electricity	$/a	*4,003,000*	*0*	*0*	*0*	*0*	*3,818,000*
Raw Water	$/a	*1,054,000*	*1,056,000*	*1,056,000*	*1,063,000*	*1,063,000*	*986,000*
Water Treatment Chem.	$/a	*738,000*	*739,000*	*739,000*	*743,000*	*744,000*	*690,000*
Molasses	$/a	*4,583,000*	*4,583,000*	*4,583,000*	*4,583,000*	*4,583,000*	*4,583,000*
Byproduct Revenue	$/a	**0**	**0**	**2,116,000**	**12,244,000**	**18,602,000**	**0**
Electricity	$/a	0	0	0	12,244,000	9,172,000	0
Steam	$/a	0	0	2,116,000	0	9,431,000	0

Table A5
Breakdown of the Levelized Cost of Carbon Black

Item	Unit	CB-Flare	CB-Elect$_{CB}$	CB-Elect$_{CB}$ +Steam$_{Sell}$	CB-Elect$_{Max}$	CB-Elect$_{Sell}$ +Steam$_{Sell}$	CB-Hydrogen
Overnight Capital Cost	$/t	**156**	**181**	**181**	**225**	**222**	**158**
Preproduction Costs	$/t	14	14	14	15	15	18
Inventory Cost	$/t	24	24	24	24	24	24
Other Owner Costs	$/t	18	22	22	28	28	18
Total Plant Cost	$/t	101	121	121	157	155	98
Oil Storage	$/t	*7*	*7*	*7*	*7*	*7*	*7*
CB Production	$/t	*23*	*23*	*23*	*23*	*23*	*22*
CB Processing	$/t	*29*	*29*	*29*	*29*	*29*	*29*
Steam Cycle	$/t	*0*	*12*	*12*	*35*	*33*	*0*
Flare System	$/t	*1*	*1*	*1*	*1*	*1*	*1*
Water Supply	$/t	*1*	*1*	*1*	*1*	*1*	*1*
Inst., Elect., Pipe., etc.	$/t	*39*	*46*	*46*	*60*	*59*	*38*
Fix Operating Cost	$/t	**149**	**166**	**166**	**181**	**180**	**148**
Labor Cost	$/t	123	134	134	140	139	122
Operating Labor	$/t	*85*	*93*	*93*	*93*	*93*	*85*
Maintenance Labor	$/t	*13*	*15*	*15*	*19*	*19*	*12*
Adm. & Sup. Labor	$/t	*25*	*27*	*27*	*28*	*28*	*24*
Property Tax & Insurance	$/t	26	32	32	41	40	26
Variable Operating Cost	$/t	**991**	**966**	**966**	**973**	**972**	**1,595**
Maintenance Materials Cost	$/t	21	25	25	32	31	20
Liquid Discharge	$/t	1	1	1	1	1	1
Feedstock & Energy Cost	$/t	969	940	940	940	940	1,574
Carbon Black Oil	$/t	*852*	*852*	*852*	*852*	*852*	*852*
Natural Gas	$/t	*42*	*42*	*42*	*42*	*42*	*0*
Hydrogen	$/t	*0*	*0*	*0*	*0*	*0*	*650*
Electricity	$/t	*29*	*0*	*0*	*0*	*0*	*27*
Raw Water	$/t	*8*	*8*	*8*	*8*	*8*	*7*
Water Treatment Chem.	$/t	*5*	*5*	*5*	*5*	*5*	*5*
Molasses	$/t	*33*	*33*	*33*	*33*	*33*	*33*
Byproduct Revenue	$/t	**0**	**0**	**15**	**88**	**134**	**0**
Electricity	$/t	0	0	0	88	66	0
Steam	$/t	0	0	15	0	68	0
Levelized Cost of CB	**$/t**	**1,296**	**1,313**	**1,298**	**1,291**	**1,240**	**1,901**

References

Abdallas Chikri, Y., Wetzels, W., 2020. Decarbonization Options for the Dutch Carbon Black Industry. PBL Netherlands Environ Assess Agency, TNO.

Alves, L., Pereira, V., Lagarteira, T., Mendes, A., 2021. Catalytic methane decomposition to boost the energy transition: scientific and technological advancements. Renew. Sustain. Energy Rev. 137 https://doi.org/10.1016/j.rser.2020.110465.

Bhatia A. Pneumatic Conveying Systems, CED Engineering, Course No: M05-010 n.d.

Boulamanti A, Moya JA. Energy efficiency and GHG emissions: Prospective scenarios for the Chemical and Petrochemical Industry, Science for Policy report: EUR 28471 EN 2017:1–237. https://doi.org/10.2760/20486.

Brøndum A/S, V., 2023. Insight into the technical aspects of vacuum cleaners. https://broendum.com/en/insight-into-the-technical-aspects-of-vacuum-cleaners/.

Bunch, S., Cort, K., Jhonson, E., Elliott, D., Stoughton, K.M., 2017. Water and Wastewater Annual Price Escalation Rates for Selected Cities across the United States. US Dep Energy.

CABOT, 2023. Frankiln Louisiana plant information. https://www.cabotcorp.com/company/worldwide-locations/north-america/usa-louisiana-franklin#:~:text=Today%2Capproximately130employeesproduce,priority in everything we do.

ChemAnalyst, 2023a. Carbon black market analysis: decode the future of carbon black. https://www.chemanalyst.com/industry-report/carbon-black-market-440.

ChemAnalyst, 2023b. Polyvinyl alcohol price trend and forecast. https://www.chemanalyst.com/Pricing-data/polyvinyl-alcohol-1108#:~:text=InIndia%2CpricesofPolyvinyl,Ex-Mumbai in March 2022.

Conklin HL. Water Requirements of the Carbon-Black Industry, GEOLOGICAL SURVEY WATER-SUPPLY PAPER 1330-B 1956.

Costa, S.M.R., Fowler, D., Carreira, G.A., Portugal, I., Silva, C.M., 2022. Production and upgrading of recovered carbon black from the pyrolysis of end-of-life tires. Materials 15. https://doi.org/10.3390/ma15062030.

Denka, 2023. Product information denka black. https://www.denka.co.jp/eng/product/detail_00025/.

Dhulipalli, S.B., 1990. Modelling of Oil Furnace Black Manufacturing Process Using Aspen. Thesis Ohio Univ.

Diby, I.C.P., Atheba, P.G., Kaliaguine, S., 2022. Controlled air oxidation for surface functionalization of pyrolytic carbon black. Ind. Eng. Chem. Res. 61, 13805–13815. https://doi.org/10.1021/acs.iecr.2c01092.

Donnet, J.-B., Bansal, R.C., Wang, M.-J., 1993. Carbon Black: Science and Technology. Marcel Dekker, Inc, 0-8247-8975-X.

Dow Chemical Company. MSDS Product Data Sheet Dow Chemical Company: Carbon Black Feedstock. Form No 778-01901 n.d.

DuPont, 2023. Water application value engine, 1.82, 824.

EFDB, 2023. Emission Factor Database: Carbon Black.

Engineered Carbon, Orion, 2019. Paving Our Path Forward to a Sustainable Future - 2018 Sustainability Report.

European Commission, 2007. Best Available Techniques for the Manufacture of Large, vol. I. Inorganic Chemicals - Solids and Others Industry.

Fulcheri, L., Rohani, V.J., Wyse, E., Hardman, N., Dames, E., 2023. An energy-efficient plasma methane pyrolysis process for high yields of carbon black and hydrogen. Int. J. Hydrogen Energy 48, 2920–2928. https://doi.org/10.1016/j.ijhydene.2022.10.144.

Idreco, 2023. Indirect rotary dryers. https://www.idreco.com/indirect-rotary-dryers/.

IEA, 2023. Tracking Chemicals. https://www.iea.org/energy-system/industry/chemicals#tracking.

JiangXi, Tyrepress, 2014. Black Cat Inaugurates a Further Carbon Black Plant. https://www.tyrepress.com/2014/03/jiangxi-black-cat-inaugurates-a-further-carbon-black-plant/.

Khodabakhshi, S., Fulvio, P.F., Andreoli, E., 2020. Carbon black reborn: structure and chemistry for renewable energy harnessing. Carbon N Y 162, 604–649. https://doi.org/10.1016/j.carbon.2020.02.058.

Körting Hannover, A.G., 2023. Tank Mixing Systems with Liquid Jet Mixing Nozzles. 130-Mixing Nozzles-EN-171024.

Kozman, T.A., Da Costa, J., Lee, J., 2007. Combined heat and power system for a carbon black manufacturer: system selection and specification. Cogener. Distrib. Gener. J. 22, 6–22. https://doi.org/10.1080/15453660709509128.

Last, G.V., Schmick, M.T., 2011. Identification and Selection of Major Carbon Dioxide Stream Compositions. PNNL, 20493.

Lawrence, K.M., 1973. United States patent: WET-PELLETING of carbon black. Appl Number 346, 831.

Lawrence Livermore National Laboratory, 2022. Energy Flow Charts: Estimated U.S Energy Consumption in 2021.

Lee, S.M., Roh, J.S., 2020. Pore development process according to burn-off of activated carbon black with CO2 gas. Fullerenes, Nanotub. Carbon Nanostruct. 28, 808–814. https://doi.org/10.1080/1536383X.2020.1763316.

Lee, S.M., Lee, S.H., Roh, J.S., 2021. Analysis of activation process of carbon black based on structural parameters obtained by XRD analysis. Crystals 11, 1–11. https://doi.org/10.3390/cryst11020153.

Ma, T., Cao, Y., Chen, H., 2018. Synthesis and characterization of cationic carbon black pigment with quaternary ammonium groups and its dyeing properties for wool fabrics. Colloids Surfaces A Physicochem Eng Asp 549, 43–49. https://doi.org/10.1016/j.colsurfa.2018.04.005.

Mergenthaler, P., Schinkel, A.P., Tsatsaronis, G., 2017. Application of exergoeconomic, exergoenvironmental, and advanced exergy analyses to Carbon Black production. Energy 137, 898–907. https://doi.org/10.1016/j.energy.2017.03.107.

Msheik, M., Rodat, S., Abanades, S., 2022. Experimental comparison of solar methane pyrolysis in gas-phase and molten-tin bubbling tubular reactors. Energy 260. https://doi.org/10.1016/j.energy.2022.124943.

Naseri, A., Thomson, M.J., 2019. Development of a numerical model to simulate carbon black synthesis and predict the aggregate structure in flow reactors. Combust. Flame 207, 314–326. https://doi.org/10.1016/j.combustflame.2019.06.001.

Niedens, L.U.S., 2023. Electricity Prices Expected to Drop. Investopedia. https://www.investopedia.com/electricity-prices-may-fall-7229665.

Niranjan, R., Thakur, A.K., 2017. The toxicological mechanisms of environmental soot (black carbon) and carbon black: focus on Oxidative stress and inflammatory pathways. Front. Immunol. 8, 1–20. https://doi.org/10.3389/fimmu.2017.00763.

Nunes, L.J.R., Guimarães, L., Oliveira, M., Kille, P., Ferreira, N.G.C., 2022. Thermochemical conversion processes as a path for sustainability of the tire industry: carbon black recovery potential in a circular economy approach. Cleanroom Technol. 4, 653–668. https://doi.org/10.3390/cleantechnol4030040.

Ono, K., Watanabe, A., Dewa, K., Matsukawa, Y., Saito, Y., Matsushita, Y., et al., 2014. Detailed kinetic analysis of the impact of nucleation behavior and particle size distribution on the configurations of carbon black. J. Nanoparticle Res. 16 https://doi.org/10.1007/s11051-014-2519-7.

Precedence Research, 2023. Carbon black market - global industry analysis. Report Code 2785.

Schwartz, W.A., Higgins, F.B., Lee, J.A., Newirth, R., Pervier, J.W., 1974. Engineering and Cost Study of Air Pollution Control for the Petrochemical Industry Volume 1: Carbon Balck Manufacture by the Furnace Process.

Sintemar, 2023. JET MIXER P43. https://www.sintemar.com/en/products/jet-mixer-p43.

Skillas, G., Becker, C., Mühlenweg, H., Behnisch, J., 2005. Simulation of particulates in a carbon black reactor. J. Nanoparticle Res. 7, 15–27. https://doi.org/10.1007/s11051-004-5746-5.

Turner, J.H., McKenna, J.D., Vatavuk, W.M., 1998. Particulate Matter Controls: Baghouses and Filters. EPA Air Pollut Control Cost Man.

U.S. Department, 2019. Of Energy/NETL. Quality Guidelines for Energy System Studies; Cost Estimation Methodology for NETL Assessments of Power Plant Performance. NETL-PUB, 22580.

U.S. Energy Information Administration, 2021. How Much Carbon Dioxide Is Produced Per Kilowatthour of U.S. Electricity Generation? https://www.eia.gov/tools/faqs/faq.php?id=74&t=11.

U.S. Energy Information Administration, 2023a. United States Industrial Natural Gas Prices. https://www.eia.gov/dnav/ng/NG_PRI_SUM_A_EPG0_PIN_DMCF_M.htm.

U.S. Energy Information Administration, 2023b. Average price of electricity to ultimate customers by end-use sector, table 5.6.A. https://www.eia.gov/electricity/monthly/epm_table_grapher.php?t=epmt_5_6_a.

Wang, M.-J., Gray, C.A., Reznek, S.A., Mahmud, K., Kutsovsky, Y., 2003. Kirk-Othmer Encyclopedia of Chemical Technology: Carbon Black. https://doi.org/10.1002/0471238961.0301180204011414.a01.pub2.

www.eurotecnica.it. EUROTECNICA 2023. https://www.eurotecnica.it/en/•-et-blackTM-carbon-process.html.

Zauba, 2023. Import export data of India: U.S. Carbon black oil. https://www.zauba.com/import-carbon+black+oil/hs-code-27079900/p-1-hs-code.html.