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RESEARCH

Research on Carbon Emission of Solar Grade Polysilicon Produced by Metallurgical Route Using Digital Simulation Technology

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Abstract
Under the enormous pressure of carbon reduction, we need to have a clear understanding of the environmental impact of the energy-intensive and high-emission polysilicon industry. With the rapid development of technology, we now have the ability to monitor the inflow and outflow of materials in enterprises, so as to obtain the life cycle inventory required for environmental impact assessment. And solve the problems of large data collection workload and long working cycle encountered in conventional life cycle assessment. By combining digital simulation technology and life cycle assessment, we analyze carbon dioxide (CO_2) emission in each production process of 1 kg solar grade polysilicon (SoG-Si) by metallurgical route (MR) in detail. We not only analyze four typical production processes of MR, namely slag refining, hydrometallurgy, directional solidification and electron beam refining. The production process of metallurgical grade silicon is also analyzed. It is obtained that the production of 1 kg SoG-Si by MR will produce 69.77 kg CO_2. The contribution analysis shows that the CO_2 produced by electron beam refining, metallurgical silicon smelting, secondary directional solidification and primary directional solidification is more significant, reaching 38.47%, 20.88%, 15.84% and 14.50%, respectively. The sensitivity analysis shows that the sensitivity of electric power in the process of electron beam refining, secondary directional solidification, primary directional solidification and metallurgical silicon smelting is significant, reaching 38.47%, 15.77%, 14.45% and 13.81%, respectively. In addition, according to the analysis results, the improvement suggestions to reduce CO_2 emission are given.

Keywords Carbon emission · Solar grade polysilicon · Metallurgical route · Digital simulation · Life cycle assessment

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Abbreviations

DS	Digital simulation
IEA	International Energy Agency
ISR	Improved Siemens route
LCA	Life cycle assessment
LCI	Life cycle inventory
MG-Si	Metallurgical grade silicon
MR	Metallurgical route
PV	Photovoltaic
SoG-Si	Solar grade polysilicon

1 Introduction

China has a vast territory and a large population. In the post-COVID-19 era, China has a huge energy demand for economic recovery. In 2021, China's electricity demand increased by 10%, which is equivalent to the total demand of the whole Africa. However, coal plays a leading role in China's energy structure, so China's per capita carbon dioxide (CO_2) emissions have exceeded the average level of developed economies [1]. Under the background of "carbon peaking, carbon neutrality" and energy security, China urgently needs to make a low-carbon energy transformation.

Photovoltaic (PV) power generation has received much attention and strong support from governments around the world due to its current and expected power equalization cost lower than fossil energy or other renewable energy [2, 3], and its carbon footprint is much lower than that of fossil fuel power generation technology [4], and its environmental friendliness. China's PV industry has developed rapidly with the strong support of the government, and currently accounts for more than 80% of all solar panel manufacturing stages (such as polysilicon, ingots, wafers, cells and modules). China has become the world's largest manufacturer of solar PV industry and has begun to lead the global photovoltaic industry [5].

At present, the mainstream PV cell in the market is crystalline silicon cell, which accounts for more than 95% of the global market [6, 7]. Although PV generation is regarded as an environment-friendly energy source by the public, and has little environmental impact during operation, from the perspective of the entire life cycle, its environmental impact is mainly concentrated in the production and manufacturing stage [8], especially the production process of solar grade polysilicon (SoG-Si), the core material of PV solar panels, will produce a lot of environmental loading [9–15]. No matter which crystal type is used in the solar cell, its raw material is high-purity polysilicon with purity of 6N or higher [16], so it is of great significance to study the carbon emission of polysilicon production.

As an internationally recognized environmental impact assessment method, life cycle assessment (LCA) has been widely used in environmental impact studies of all walks of life. It can systematically, objectively and quantitatively analyze the direct and indirect environmental impacts of the system [17, 18]. In recent years, with the rapid development of PV industry and the gradual improvement of people's awareness of sustainable development and environmental protection, many researchers have applied LCA to examining PV power generation's impact on environment. So far, such research cases using LCA have been conducted towards the PV systems in China [19–21], Europe [22], Singapore [23] and other countries [24]. Meanwhile, some researchers have also carefully studied using LCA the recycling process of end-of-life PV modules [25–30]. Although some researchers have conducted researches on the environmental impact of polysilicon, these researches are not detailed enough in terms of carbon emission [31–34]. In addition, compared with other studies on the environmental impact of polysilicon, this paper also conducted a detailed analysis of the environmental impact of the production process of metallurgical grade silicon (MG-Si, precursor material). In today's increasingly strict carbon emission, it is of great significance to conduct a detailed study on the carbon emission of polysilicon, a high-carbon emission industry.

With the rapid development of PV industry, it is expected that the installed PV capacity of the world will reach terawatt level in the next five years [35], and the demand for SoG-Si will also increase. At present, the production of SoG-Si is almost completely produced by the improved Siemens route (ISR). Although it has a large output and high purity, it has high energy consumption per unit product and serious carbon emission. In contrast, the metallurgical route (MR) has lower energy consumption per unit product and smaller carbon emission. Although MR has encountered some bottlenecks in impurity removal, with more and more researches on impurity removal in metallurgical silicon [36–41], and under the huge pressure of emission reduction, we believe that MR will have great potential for development with its obvious environmental advantages.

In addition, with China's efforts to promote the establishment of carbon emission baseline in all industries and the development of carbon trading market, more and more enterprises need a carbon emission monitoring system that can be quickly generated to suit their own enterprises. With the rapid development of sensor, internet of things and other technologies, it is now entirely possible to track and monitor the energy consumption, material consumption and waste production volume of each production process at the enterprise level, obtain the life cycle inventory (LCI) required by environmental impact assessment, and solve the problems of large data collection workload and long working cycle encountered in conventional LCA. So we should find a new breakthrough in the field of digital simulation (DS) to solve the pain points of conventional LCA.

In recent years, the rapid development of information technology has driven the transformation of manufacturing to intelligent manufacturing. As a particularly effective research tool, DS has received the attention of scientists because of its efficiency, speed and low cost. The development of aviation, aerospace and atomic energy technologies in the 1940s and 1950s drove the progress of simulation technology. The sudden advancement of computer technology in the 1960s provided advanced simulation tools and accelerated the development of simulation technology. Currently, many researchers have explored and studied DS in chemical [42, 43], agricultural [44–46], medical [47–50], smart cities [51, 52], and more widely in manufacturing [53–56]. For example, Yang et al. explored the solid structure, dissolution behavior, thermodynamic properties, and nucleation kinetics of malonamide using DS [57]. Du et al. developed a three-dimensional computational fluid dynamics full-loop model with multiphase distribution to investigate the fluidization behavior and chemical looping gasification performance of a circulating fluidized bed using DS. The simulation results matched well with the experimental results and verified the validity of the simulation model [58]. Pilta et al. combined digital twin technology with machine learning and applied it to bearing anomaly detection and crack size identification. The experimental results showed that the average accuracy of bearing failure mode recognition and crack size recognition were 99.5% and 99.6%, respectively [59]. Liu et al. proposed a digital twin-driven shop floor adaptive scheduling method. The method achieves real-time monitoring of the scheduling environment, accurately captures abnormal events in the production process, and combines with the scheduling algorithm, which can well solve the dynamic events in the actual production process [60].

By reading others' studies on DS, there are some studies on the whole factory, but they mainly focus on the operation monitoring and shop floor scheduling of the factory, and no one has yet applied DS to the environmental impact of the factory. This study combines DS technology and LCA technology to provide a detailed analysis of the carbon footprint of a polysilicon factory in China, providing data and technical support for enterprises to choose a more low-carbon production mode and implement carbon emission regulation. In addition, as far as the author knows, this is one of the most detailed studies on the carbon footprint of SoG-Si production by MR.

2 Methods

In this study, the carbon emissions of SoG-Si produced by metallurgical process were analyzed in detail using a combination of DS technology and LCA. DS&LCA used Plant Simulation software to model the production process of SoG-Si by MR and build a DS model, and then the model was simulated to obtain the environmental impact of each production process.

2.1 Objectives and Scope

The main objective of this study is to quantitatively analyze the CO_2 emission of each production process of SoG-Si by MR. In this study, the production of 1 kg SoG-Si by MR was used as the functional unit.

This study covers as many processes as possible for the production of SoG-Si by MR, which is divided into the MG-Si production stage and the SoG-Si production stage. The research scope of the MG-Si production stage includes nine processes, including silica washing and drying, batching, metallurgical silicon smelting, silicon ladle transport, out of furnace refining, casting, cooling demoulding, fracture, weighing and packaging. The research scope of the production stage of SoG-Si includes five processes: slag refining, hydrometallurgy, primary directional solidification, electron beam refining and secondary directional solidification. The system boundary is shown in Fig. 1.

2.2 Software and Databases

The software used is Plant Simulation v14.0. CLCD v0.8 databases, Ecoinvent v3.1 databases, and ELCD v3.0 databases serve as databases for background data. CLCD is the most complete LCA database in China, representing the

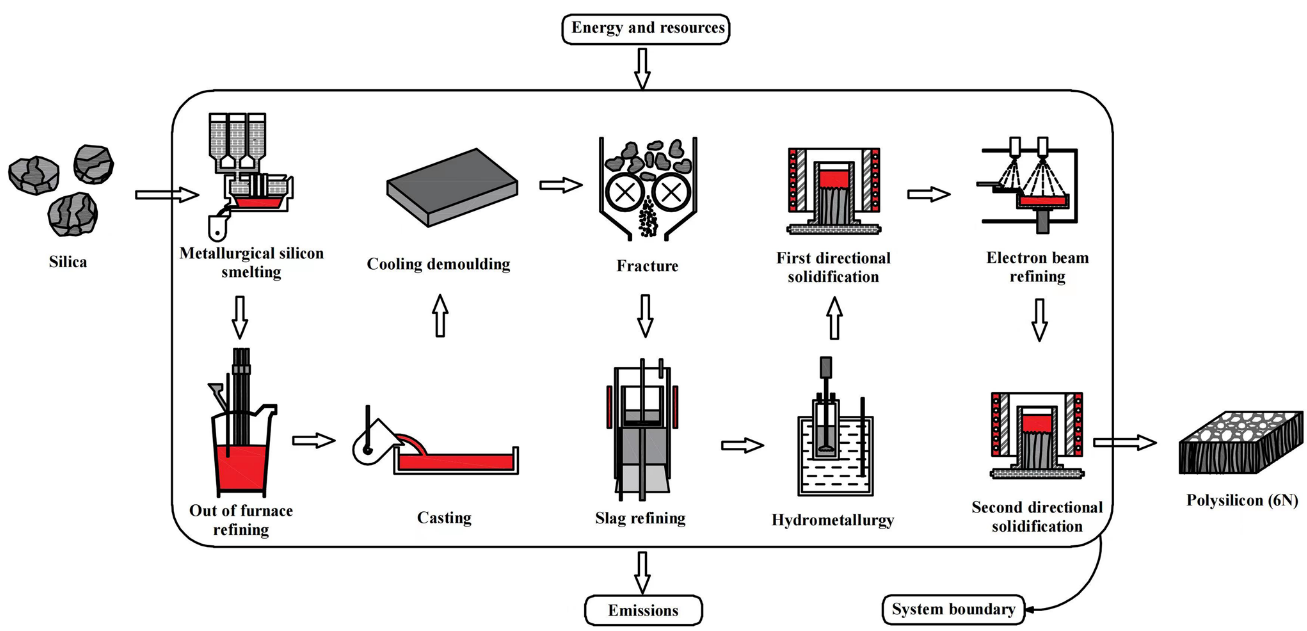

Fig. 1 LCA boundary of the SoG-Si production by MR

average level of the Chinese market. The role of the Ecoinvent v3.1 database and the ELCD v3.0 database was to make up for a very small portion of the missing data in the CLCD v0.8 database.

2.3 Computational Logic

In order to obtain the total CO_2 emission data and the emission data of each production process, we split and sorted the collected date, so as to obtain the data of energy consumption, material inflow and outflow and pollutant emission in each production process. Based on these data and the carbon emission factors given by the Intergovernmental Panel on Climate Change, we can calculate the CO_2 emissions of a certain material and a certain production process, from which we can calculate the total CO_2 emissions.

2.4 Digital Simulation Modeling

According to the collected data, we use the software to establish a DS model for the production of SoG-Si by MR. Mass balance, element balance and energy balance are used as the basis for simulation, so as to obtain the inflow and outflow data of materials in each production process. Then the environmental impact of each production process of the DS model is quantified. The DS model in this study is divided into two parts, as shown in Figs. 2 and 3. Figure 2 is the simulation process of the MG-Si production process, and Fig. 3 is the simulation process of the SoG-Si production process.

2.5 Data Sources and Assumptions

The data used for DS modeling are all from the field survey of relevant enterprises. They are the actual production data of relevant enterprises with high quality. These enterprises are typical representatives in this field, representing the mainstream level of China's production of SoG-Si using MR at that time.

LCI data is the collection and collation of energy and material inflow and outflow and environmental emission data within the entire research scope of the target product, which is the basis of LCA. The LCI of energy consumption, material inflow and outflow, and pollutant emission in each production process of SoG-Si produced by MR is shown in Table 1.

In this study, the loss of workshop infrastructure, wear and tear of production equipment, transportation of intermediate products, personnel flow and other data that have little impact on the evaluation results are ignored and excluded from the scope of this study. In addition, due to the high concentration ratio of polysilicon industry in China, the environmental impact caused by transportation between industrial silicon factories and polysilicon factories doesn't consider in this paper.

3 Results and Discussion

3.1 Contribution Analysis

Through the simulation of Plant Simulation software and the life cycle assessment based on the material inflow and

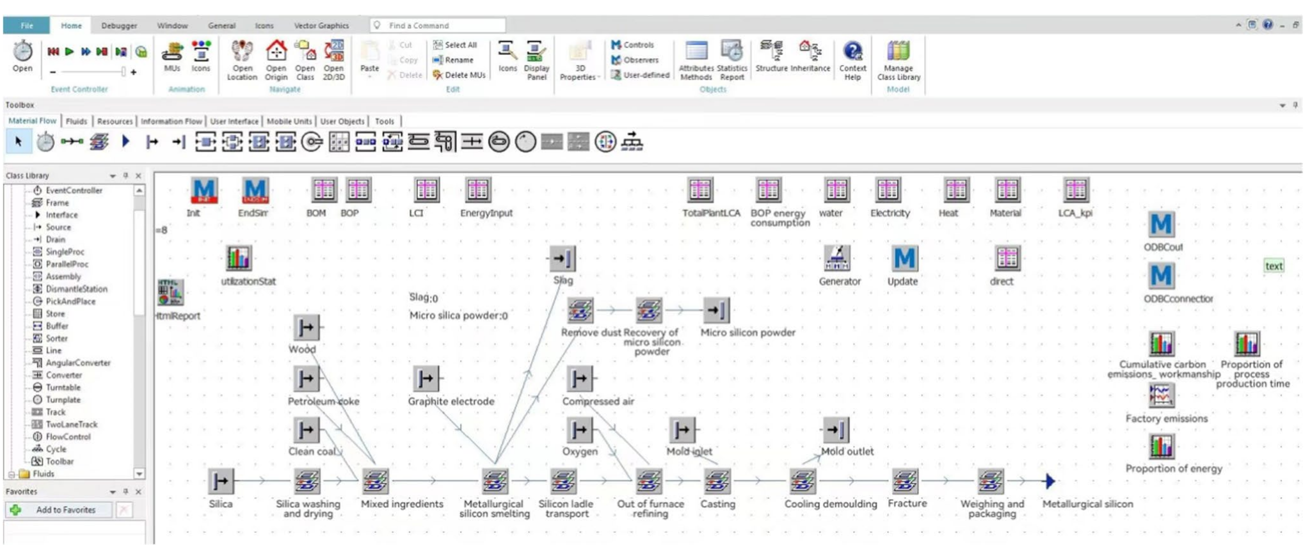

Fig. 2 Simulation process of MG-Si

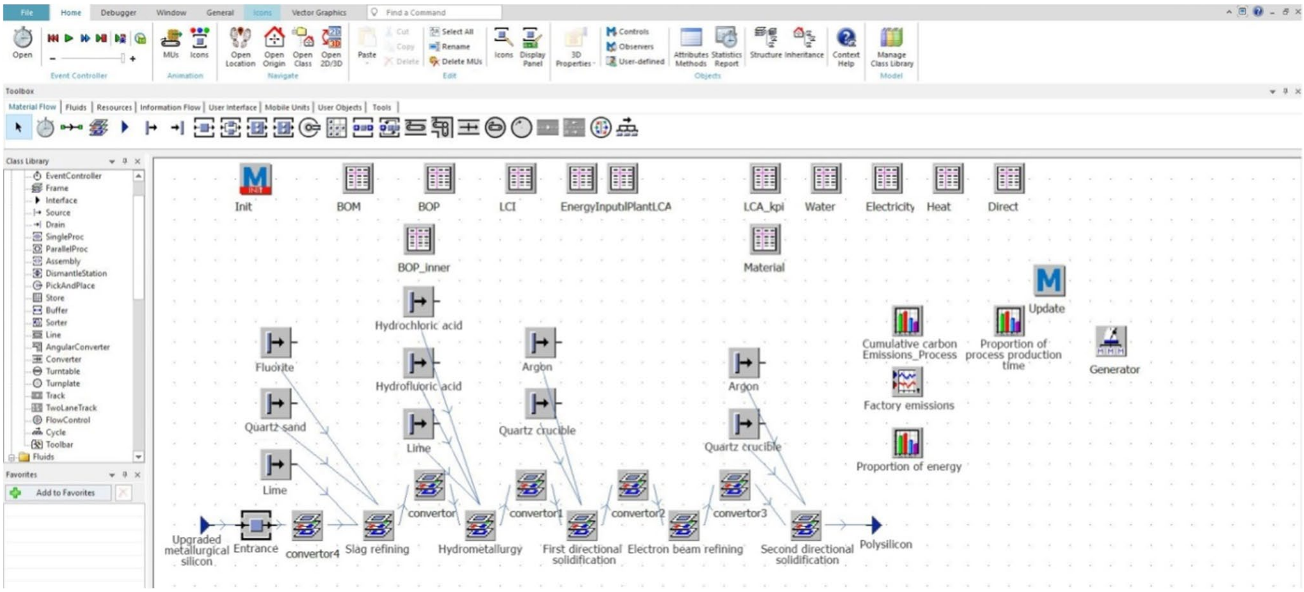

Fig. 3 Simulation process of SoG-Si

outflow data obtained from the simulation, it is concluded that the production of 1 kg SoG-Si by MR will produce 69.77 kg CO_2, among which the emission of CO_2 in the electron beam refining process is the highest, reaching 26.84 kg. The second is the CO_2 emitted in the metallurgical silicon smelting process, which reaches 14.57 kg, accounting for 20.88%; the next is the CO_2 emitted in the secondary directional solidification process, which reaches 11.05 kg, accounting for 15.84%; the last is the CO_2 emitted in the primary directional solidification process, reaching 10.12 kg, accounting for 14.50%. These four processes account for 89.69% of the total CO_2 emissions. The CO_2 emissions of each production process are shown in Fig. 4.

The main reason of CO_2 emission in the three production processes of electron beam refining, primary directional solidification and secondary directional solidification is the massive use of electric power. The main reason of CO_2 emission in the production process of metallurgical silicon is the massive use of electric power and the direct emission of CO_2. In the production site of metallurgical silicon, silica and carbonaceous reducing agents are constantly added, and this process is not carried out in a closed furnace, so it will directly emit a lot of waste gas.

3.2 Sensitivity Analysis

Sensitivity refers to the ratio of the rate of change of the target indicator to the rate of change of the process inventory data, that is, the contribution rate of each input or output in the LCI to the target indicator. If the sensitivity of inventory data is large, that is the focus of improvement. Materials or material process with high sensitivity (> 2.00%) are shown in Fig. 5.

As can be seen from the figure, the highest sensitivity is the power consumption in the electron beam refining process, which reaches 38.47%. Then the electricity consumption in secondary directional solidification process, primary directional solidification process and metallurgical silicon smelting process is 15.77%, 14.45% and 13.81%, respectively. Then, the direct emission of CO_2 in the process of metallurgical silicon production and the power consumption in the process of silica washing and drying, which are 6.74% and 4.19% respectively.

It can be seen that in the whole production process, the sensitivity of electricity is the largest, accounting for 91.06%. The electricity in this study comes from the power grid, because coal plays a dominant role in China's energy structure [61, 62], so electricity is the focus of improvement. In addition, the direct emission of CO_2 in the process of metallurgical silicon production is also very high, accounting for 6.74%, which is also the focus of improvement. According to the carbon emission data of each production process and material obtained from contribution analysis and sensitivity analysis, the carbon flow diagram of SoG-Si produced by MR is shown in Fig. 6.

3.3 Improvement Analysis

In terms of the entire production process of polysilicon, the use of electricity generates the most CO_2 emissions.

Table 1 The LCI of SoG-Si production process by MR

Process	Flows of each process step	Value
Metallurgical grade silicon manufacturing stage		
1	Silica washing and drying	
	Inputs	
	Silica	3.085 kg
	Electricity	3.159 kWh
	Industrial tap water	0.451 kg
	Outputs	
	Silica (after drying)	3.085 kg
	Waste water	4.151 kg
2	Mixed ingredients	
	Inputs	
	Silica (after drying)	3.085 kg
	Wood	1.090 kg
	Petroleum coke	0.560 kg
	Clean coal	0.968 kg
	Outputs	
	Finished ingredients	5.699 kg
3	Metallurgical silicon smelting	
	Inputs	
	Finished ingredients	5.669 kg
	Electricity	10.408 kWh
	Cooling water	12.514 kg
	Graphite electrode	0.167 kg
	Outputs	
	Discharged silicon	1.239 kg
	Slag	0.462 kg
	CO2	4.448 kg
	Nitrogen oxide	0.166 kg
Process	Flows of each process step	**Value**
	Sulfur dioxide	0.665 kg
	Carbon monoxide	0.079 kg
	Hydrogen chloride	0.001 kg
	Particulate matter	0.077 kg
4	Silicon ladle transport	
	No inputs and outputs	
5	Out of furnace refining	
	Inputs	
	Discharged silicon	1.239 kg
	Compressed air (1000 kPa gauge)	0.0004 m^3
	Oxygen	0.003 m^3
	Electricity	0.005 kWh
	Outputs	
	Refined silicon	1.239 kg
	Slag	0.124 kg
6	Casting	
	Inputs	
	Refined silicon	1.239 kg
	Outputs	
	Silicon ingot with mold	1.239 kg
7	Cooling demoulding	
	Inputs	

Table 1 (continued)

Process	Flows of each process step	Value
	Silicon ingot with mold	1.239 kg
	Outputs	
	Silicon ingot	1.239 kg
8	Fracture	
	Inputs	
	Silicon ingot	1.239 kg
	Electricity	0.929 kWh
	Outputs	
	Unpacked metallurgical silicon	1.239 kg
9	Weighing and packaging	
	Inputs	
	Unpacked metallurgical silicon	1.239 kg
	Electricity	0.149 kWh
	Outputs	
	Packaged metallurgical silicon	1.239 kg
Polysilicon manufacturing stage		
10	Slag refining	
	Inputs	
	Metallurgical grade silicon	1.239 kg
	Electricity	0.800 kWh
	Lime	0.033 kg
	Quartz sand	0.041 kg
	Fluorite	0.008 kg
	Outputs	
	Refined polysilicon	1.155 kg
	Slag	0.166 kg
11	Hydrometallurgy	
	Inputs	
	Refined silicon	1.155 kg
	Electricity	1.400 kWh
	Hydrochloric acid	0.360 kg
	Hydrofluoric acid	0.150 kg
	Lime	0.350 kg
	Fresh water	12.550 kg
	Outputs	
	Polysilicon (3.5N)	1.109 kg
	CaF_2	0.164 kg
	Liquid waste	13.294 kg
12	First directional solidification	
	Inputs	
	Polysilicon (3.5N)	1.109 kg
	Electricity	10.880 kWh
	Argon	0.001 kg
	Quartz crucible	0.210 kg
	Silicon nitride	0.001 kg
	Circulating water	4.200 kg
	Outputs	
	Polysilicon (4.5N)	1.098 kg
	Waste crucible	0.197 kg
13	Electron beam refining	
	Inputs	

Table 1 (continued)

Process	Flows of each process step	Value
	Polysilicon (4.5N)	1.098 kg
	Electricity	29.000 kWh
	Outputs	
	Polysilicon (5.5N)	1.010 kg
14	Second directional solidification	
	Inputs	
	Polysilicon (5.5N)	1.010 kg
	Electricity	11.880 kWh
	Argon	0.001 kg
	Quartz crucible	0.180 kg
	Silicon nitride	0.001 kg
	Circulating water	4.200 kg
	Outputs	
	Polysilicon (6N)	1.000 kg
	Waste crucible	0.197 kg

Therefore, cleaner power sources such as hydropower, wind power and solar power should be selected, which will greatly reduce the carbon emissions in the process of SoG-Si production by MR. Studies by Mendez and Fan et al. also support this view [33, 34]. Fortunately, China has begun to vigorously promote the adjustment of energy structure, and certain results have been achieved. According to the data released by the National Energy Administration of China, by the end of 2021, the total installed capacity of photovoltaic power generation connected to the grid in China has reached 306 million kW, ranking first in the world for seven consecutive years. In addition, with the smooth operation of Baihetan Hydropower Station and the continuous expansion of offshore wind power projects, the proportion of clean energy in China's energy structure is steadily increasing. It is believed that the environmental impact of power generation in the future will be less and less, thus promoting the reduction of the environmental impact of the polysilicon industry.

It should be noted that in addition to electricity in the production process of polysilicon, the direct emission of CO_2 in the production process of metallurgical silicon is also a lot, this is because of the CO_2 produced by the carbon reducing agent after oxidation, so we should look for more low-carbon and renewable reducing agent to reduce silica, so as to reduce the production of CO_2, in addition, the installation of electric furnace flue gas purification device, Improve the capture of CO_2, reduce CO_2 emissions. Furthermore, the use of more scientific and reasonable electric furnace structure, more efficient smelting of metallurgical silicon, reduce power consumption.

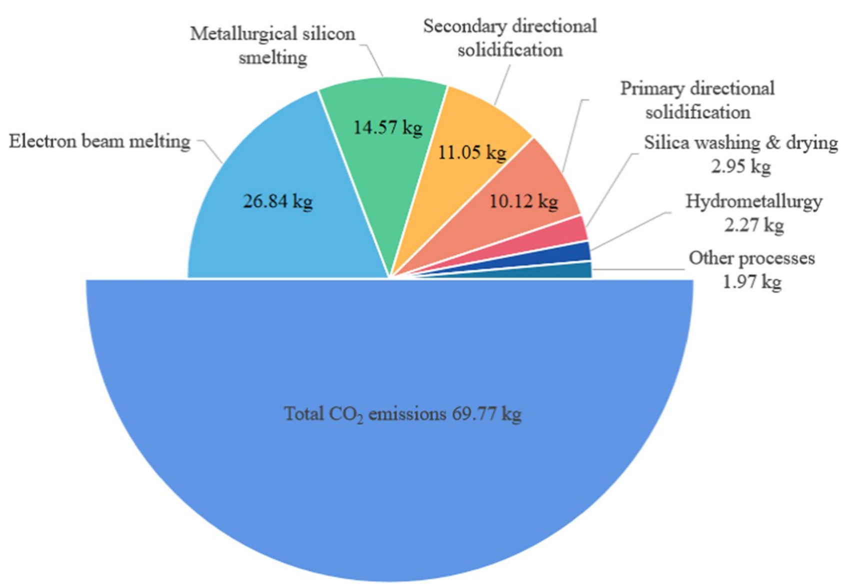

Fig. 4 The CO2 emission proportion of each production process

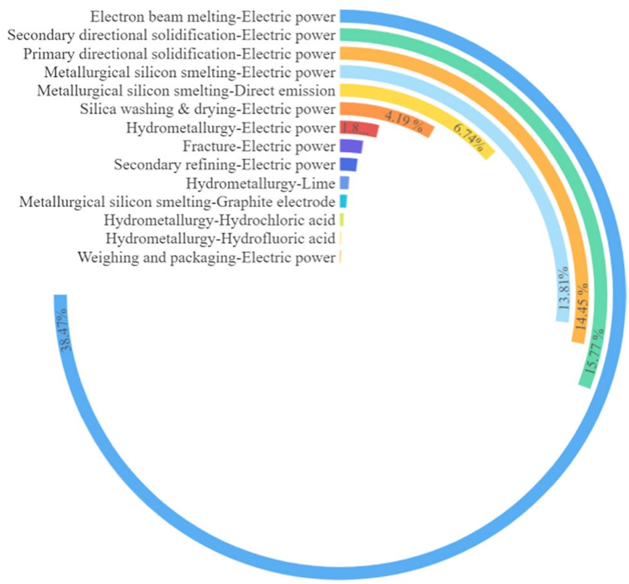

Fig. 5 Material or materials process with high sensitivity

In the future, when the factory needs to upgrade due to energy saving and carbon reduction or technological update, the existing DS model can be modified to build a new DS model, and the accumulated historical operation data can be used to simulate the newly constructed DS model, and the corresponding environmental impact assessment can be obtained. And according to the simulation results to guide the real physical factory upgrade.

3.4 Comparison with Improved Siemens Route

According to the author's previous research, the ISR produces 113.30 kg CO_2 per 1 kg of SoG-Si, while the MR produces 69.77 kg CO_2 per 1 kg of SoG-Si, which is relatively lower, only 61.58% of the ISR, which has obvious environmental advantages. Although the purity of SoG-Si produced by the MR is not as high as that produced by the ISR, we believe that the MR has great development potential in the future, rather than a simple technical supplement, under the huge promotion of carbon reduction and further in-depth research of the MR impurity removal technology.

4 Conclusions

This research analyzed the CO_2 emission of SoG-Si produced by MR through the combination of DS technology and LCA, elaborated the environmental advantages of SoG-Si produced by MR, and provided reference and data support for the clean production of polysilicon. In addition, this study will promote enterprises and regulatory authorities to implement carbon emission regulation of factories, and provide data support for enterprises' energy conservation, carbon reduction and environmental protection. The main conclusions are as follows:

(1) According to the calculation, 69.77 kg CO_2 will be produced for every 1 kg of SoG-Si.

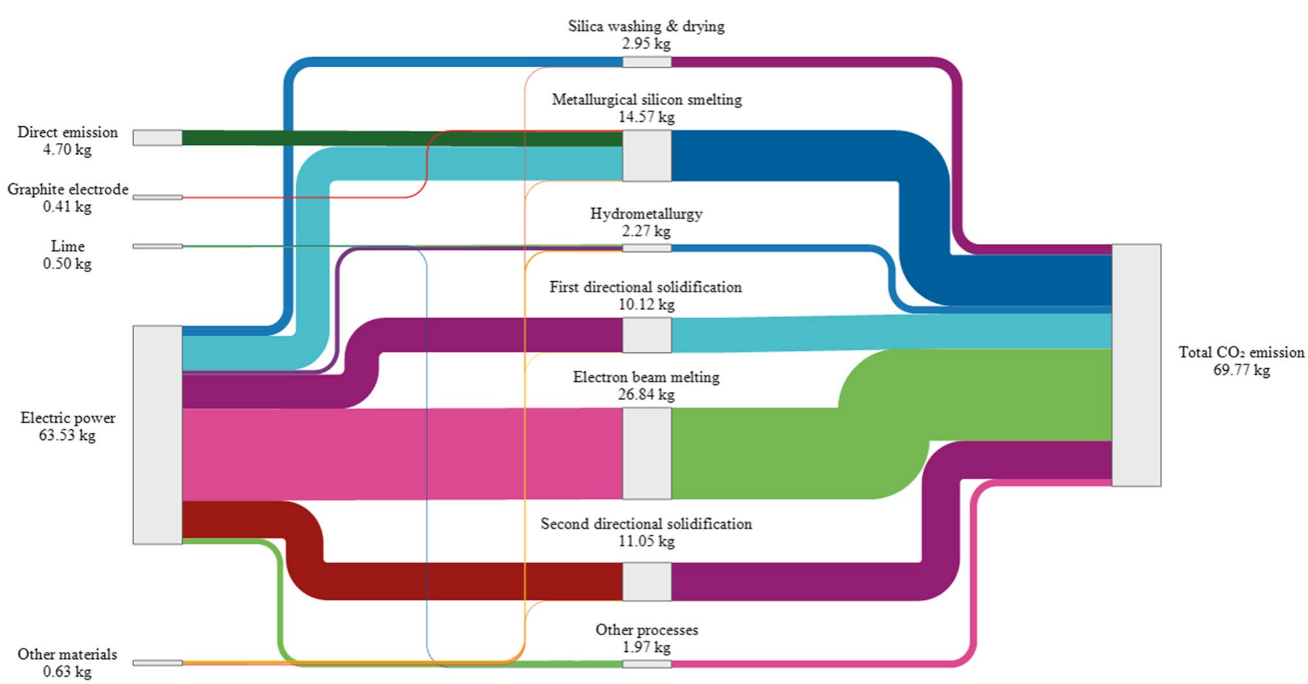

Fig. 6 Carbon flow diagram of 1 kg SoG-Si produced by MR

(2) The emission of CO_2 in the process of electron beam refining is the largest, reaching 26.84 kg, accounting for 38.47%, followed by the emission of CO_2 in the process of metallurgical silicon smelting, reaching 14.57 kg, accounting for 20.88%, followed by the emission of CO_2 in the process of secondary directional solidification and primary directional solidification, 11.05 kg and 10.12 kg, accounting for 15.84% and 14.50%, respectively.
(3) In the production process of metallurgical silicon, more low-carbon and renewable reducing agents should be used to reduce silica and installed with electric furnace flue gas purification device, so as to reduce the production of CO_2 and improve the capture of CO_2, so as to reduce CO_2 emissions. Furthermore, the use of more scientific and reasonable electric furnace structure, so as to more efficient smelting of metallurgical silicon, reduce power consumption and environmental emissions.
(4) The use of electricity generates the largest CO_2 emissions, accounting for 91.06%. Since coal accounts for the largest proportion in China's energy structure, and the power structure plays a very important role in carbon emissions, clean energy should be used as much as possible in the production process to reduce CO_2 emissions.
(5) DS technology combined with LCA will greatly promote enterprises and regulatory authorities to implement carbon emission supervision of factories.

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Author Contributions Shengqiang Yang: Conceptualization, Methodology, Validation, Formal analysis, Writing – original draft, Data curation. Zhiqiang Yu: Writing – review & editing, Project administration, Fund acquisition. Wenhui Ma: Supervision, Guidance. Lin Ma: Investigation, Writing – review & editing. Chaochun Li: Software, Modeling. Ling Fu: Software, Calculation. Ming Li: Software, Calculation. Zewen Zhao: Investigation, Date collection. Yuchen Yang: Investigation, Data analysis.

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Data Availability All data generated or analyzed in this study are included in this published article.

Declarations

Ethical Approval The results/data/figures in this paper have not been published elsewhere and have not been considered by other publishers.

Consent to Participate All authors have agreed to participate in this research work.

Consent for Publication All authors agree to publish the manuscript in its current form.

Competing Interests The authors declare no competing interests.

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