

Carbon-calcium composite conversion of calcium carbide-acetylene system: On the imperative roles of carbon capture and solid waste recycling[☆]

Hongxia Wang^a, Wanyi Xu^a, Maimoona Sharif^a, Xiaomei Wu^a, Guangxu Cheng^a, Xiaomi Cui^b, Zaoxiao Zhang^{a,*}

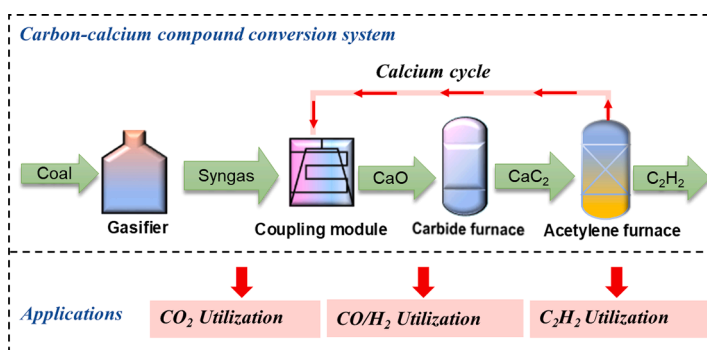
^a State Key Laboratory of Multiphase Flow in Engineering, School of Chemical Engineering and Technology, Xi'an Jiaotong University, No. 28 Xianning West Road, Xi'an 710049, PR China

^b Yang Quan Coal Industry Co., Ltd, Taiyuan 030000, Shanxi, PR China

HIGHLIGHTS

- A novel carbon-calcium compound conversion system is proposed.
- Improved system realizes carbon capture and utilization and solid waste recycling.
- The proposed calcium looping process has a relatively higher exergy efficiency of 48.97%.
- Direct carbon footprint of calcium looping system decreased substantially.
- Calcium looping system obtained the largest reduction in raw material input.

GRAPHICAL ABSTRACT



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ABSTRACT

As an important national basic industry in China, the production of calcium carbide faced with huge pressure on energy conservation and emission reduction because of the CO₂ emission and solid waste carbide slag. Therefore, it is necessary to realize the recycling of carbon and calcium in the production process of calcium carbide. A novel system of carbon-calcium compound conversion for calcium carbide-acetylene production was proposed in this work, which combines two-stage carbon capture and calcium carbide waste slag reuse processes to achieve CO₂ enrichment and calcium cycle. Based on the simulation data, the proposed system was comprehensively evaluated by material conversion, exergy and exergoeconomic analyses. It was found that the improved process performed better with an effective C, H, Ca atomic conversion rate for carbide furnace of 85.41% and CO₂ capture efficiency of 90.35%, compared with the referenced process of 64.51% and 0, respectively. The exergoeconomic analysis results suggested that more focus should be put on carbide furnace, acetylene reactor, re-carbonization furnace, gasifier and calciner since they are the top five of capital investments and exergy destruction. Besides, the carbide furnace, acetylene reactor, re-carbonization furnace and gasifier have relatively lower exergoeconomic factor (f_k) values of 1.00%, 0.93%, 2.27% and 3.07%, respectively, indicating that exergy destruction costs of these components can be decreased with the improvement of system thermodynamic and

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* Corresponding author.

E-mail address: zhangzx@xjtu.edu.cn (Z. Zhang).

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equipment performance. Furthermore, the calcium looping process formed based on the improved oxy-thermal method (OTM) process, using the captured CO₂ to mineralize carbide slag to form another calcification cycle for the production of calcium carbide-acetylene, has a higher exergy efficiency of 48.97% than the referenced process of 47.85%, and also achieves the lowest carbon emissions and the obvious reduction in CaO input. Results revealed that the proposed calcium looping system with high-efficiency, low-carbon and clean for calcium carbide-acetylene production, could be a promising process for carbon emission reduction in practical applications.

Nomenclature

Abbreviation

AR	Acetylene reactor
C	Calcliner
CEPCI	Chemical engineering plant cost index
CF	Carbide furnace
COOL	Cooler
G	Gasifier
H	Heater
HEX	Heat exchanger
RF	Re-carbonization furnace
SEP	Separator
SPECO	Specific exergy cost

Symbols

c	Specific exergy cost, \$/GJ
\dot{C}	Exergy cost rate, \$/h
\dot{E}_x	Exergy rate, kW
E_{xm}	Mole exergy, kW
e_x	Specific exergy, kJ/mol
f_k	Exergoeconomic factor
ΔG_f^0	Standard generating Gibbs function
h_i	Specific enthalpy, kJ/mol
i_r	Interest rate
m	Mass, kg
n	Operating years
r_k	Relative exergy cost difference
s_i	Specific entropy, kJ/(mol K)
Y	Ratio

y_k	Exergy destruction ratio
y_k^*	Relative exergy destruction ratio
Z	Cost of component, \$
\dot{Z}_k	Cost rate of component, \$/h

Greek letters

τ	Annual plant operating hours, h
γ	Maintenance factor
ϕ	Mole flux, mol/s
η_k	Exergy efficiency

Superscripts and subscripts

CI	Capital investment
ch	Chemical
D	Exergy destruction
$frac$	Fraction
F	Fuel
i	i -th component
in	Inlet
j	j -th component
k	k -th component
m	Raw material
OM	Operating and maintenance
out	Outlet
p	Target product
P	Product
ph	Physics
q	Thermal energy
tot	Total
0	Ambient environment or base year

1. Introduction

China's abundant coal resources are the raw materials for the production of many important chemicals, such as calcium carbide-acetylene industry [1,2]. Currently, China is the largest producer and consumer of calcium carbide in the world, and the actual output of calcium carbide reached 28.88 million tons in 2020 [3,4]. As one of the important basic chemical raw materials, calcium carbide is widely used in acetylene gas production, organic synthesis, oxyacetylene welding, etc. [5–7]. It is easy for CaC₂ to react with water to generate acetylene, which is an indispensable raw material for coal chemical industry [8]. Therefore, as the core part of acetylene production, coal-to-calcium carbide is worthy of in-depth study [9].

At present, calcium carbide production includes electro-thermal method (ETM) and oxy-thermal method (OTM). Electro-thermal method (ETM) originated early, and calcium carbide is formed by the reaction of calcium oxide and coke at a high temperature about 2000 °C produced by electric arc [10,11]. Generally, the power consumption of producing 1 ton of pure calcium carbide is about 3500 kWh [9]. Therefore, the ETM consumes a huge amount of electricity, which basically relies on coal power, and the conversion efficiency of coal

power is about 40% [12,13]. In conclusion, high energy consumption, high pollution and low efficiency restrict the development of ETM, which demonstrates that the process needs to be improved [14]. Some scholars turn to oxy-thermal method (OTM) as an alternative, which directly uses the heat from combustion of coal for calcium carbide production, avoiding the energy loss of electric arc discharge [15]. OTM uses little electricity because part of the coke is burned to provide heat for the reaction. The rest of the coke reacts with quicklime to produce calcium carbide and a large amount of tail gas. In general, the purity of CO in tail gas produced by calcium carbide process reaches as high as 90% through OTM [1]. Direct discharge or burning of this high purity tail gas will cause waste and environmental pollution, and it can be used as raw material for chemical products. Liu et al. [16] proposed a fixed-bed oxy-thermal calcium carbide production process using oxygen as gasification agent. Guo et al. [17] analyzed the thermodynamics of the low rank coal-based oxy-thermal calcium carbide-acetylene system and the results showed that a large amount of carbon consumption and energy discharge of off-gas played dominant role in CaC₂ production. Regretfully, it is still in the experimental stage under the current limited technical conditions [16,18]. The main drawbacks of the OTM are high consumption of oxygen and coke, large amount of CO/H₂-rich gas, and ineffectively utilized solid waste [19]. Whereas the OTM as a potential new technical approach has attracted extensive research attention.

Obviously, the calcium carbide production process needs to consume a large amount of coal resources to provide energy, which will also lead to serious pollution. It needs further investigation whether OTM can overcome these defects and behave better in energy-saving and environmental protection. Detailed data for the assessment of OTM are insufficient at present stage. For example, Huo et al. [9] (2021) and Mi et al. [1] (2014) etc. have done exergy analysis on a calcium carbide system, but they do not give the exergy efficiency of the system in the end. Huo et al. [20], Zhang et al. [21], and Ma et al. [19] also analyzed the calcium carbide industry, but only evaluated and analyzed the system from individual aspects such as life cycle assessment, energy analysis or exergy analysis. However, there is a lack of design improvement of calcium carbide process and systematic and comprehensive analysis of the whole process. To improve the energy utilization efficiency and explore the energy saving potential, researchers did a lot of work on the energy and exergy balance study of the system, meanwhile some energy evaluation indicators were proposed [22–24]. Mi et al. [1] assessed the energy use and carbon footprint for OTM and ETM calcium carbide manufacturing processes and proposed three system indexes of multi-product comprehensive energy consumption, exergy consumption and carbon emission, results showed that OTM had significantly better environmental performance. Huo et al. [9] made a techno-economic analysis on the low rank coal to CaC_2 process. Ma et al. [19] analyzed the energy and exergy flow of a new calcium carbide production process and the comprehensive energy consumption and exergy consumption were 10.22 kWh/kg- CaC_2 and 9.15 kWh/kg- CaC_2 , respectively. Zhang et al. [21] made a life cycle assessment of the calcium carbide-acetylene production process. These literatures analyze calcium carbide system only from a few aspects, and comprehensive and systematic evaluation is required. Therefore, it is aimed at establishing a comprehensive evaluation system from the aspects of material conversion, energy utilization, economy and carbon reduction capacity.

To develop an energy efficient, low-carbon and environmentally friendly calcium carbide manufacturing technique, three cases of oxy-thermal calcium carbide-acetylene process systems were proposed and a comparison of their performance are comprehensively discussed in this work. Firstly, the differences in the process flow composition of three kinds of coal-carbide-acetylene process systems were compared. Then, the indexes of material conversion of the three processes are analyzed to reveal the atomic conversion, CO_2 capture rate, carbon emission. Moreover, the exergy analysis of the three processes was done, and the exergy efficiency of each process was compared. Exergoeconomic analysis was made for the optimal process and the starting point for energy saving and consumption reduction was revealed through the cost analysis of each key component. Finally, a carbon emission reduction system has been established based on improved process which coupling two-stage carbon and calcium recycling to realize CO_2 capture and solid waste resource utilization. The results of this work are helpful to improve the assessment of calcium carbide-acetylene evaluation system and give meaningful suggestions for carbon emission reduction and sustainable calcium recycling, leading to the further clean production development of the existing oxy-thermal process.

2. System description and assumptions

The current development of calcium carbide production by OTM is not mature enough for industrial application, and researchers put a lot of effort to improve it. In the early stage, the equipment and process research on OTM of calcium carbide were mainly carried out by Liu's team in China [16,25–27]. Here, the OTM calcium carbide process adopted by Ge et al. [25] (which is referred to as the referenced process later) was compared with the process proposed in this paper, and the schematic diagram of the referenced OTM process is shown in Fig. 1. Case 1 is the basic process of OTM research and it reflects the basic operation units of the OTM calcium carbide production process, and mainly includes four modules: coal pyrolysis, calcination (preparation of raw material CaO), calcium carbide furnace and acetylene generator.

Fig. 2 is the schematic diagram of the improved calcium carbide-acetylene system proposed in this paper based on the referenced process (Case 1), which consists of four main submodules, including gasifier, coupling module of re-carbonization furnace and calciner, carbide furnace and acetylene furnace. In this system, about 30 wt% of the coal is used to provide energy through steam gasification, and the other part of coal participates in the reaction of calcium carbide formation. At the same time, the system coupled with the re-carbonization and calcination module, which not only recycled carbide slag generated by the system to achieve calcium circulation, but also captured part of the CO_2 in the process, and the calcium carbide products are further co-produced with the downstream product acetylene. The entire system focuses on the efficient, clean, and high-value conversion of coal.

The detailed working principle of this improved system can be summarized as follows. Part of the coal (point 1) enters the gasifier through the preheater (Heater 2) and water (point 16) through heat exchange as a steam gasification agent (point 17) to cause coal gasification reaction. The syngas (point 5) and a small amount of preheated quicklime CaO (point 3) enter the re-carbonization furnace. The CO_2 in the syngas is absorbed by calcium and converted into CaCO_3 , and then the syngas with high heating value (mainly CO , H_2 , point 7) is separated and sent to the calcium carbide furnace. The CaCO_3 (point 8) is decomposed into CaO and CO_2 in the calciner, and CaO (point 11) is separated from the gas (point 10) by a separator. A part of CaO (point 12) is then fed into the calcium carbide furnace for standby through the separator, and the rest (point 13) is returned to the re-carbonization furnace for recycling. The gas (point 10) is separated by the separator to CO_2 (point 14) and high-temperature steam (point 15). The steam is used as the raw material (point 18) of the acetylene reactor after heat exchange. Coal (point 21) and quicklime CaO (point 12) undergo calcium carbide formation reaction under the action of high-calorific value gas (point 7) (Eq. (3)), and the generated calcium carbide (point 27) is sent to the acetylene reactor (Eq. (4)), and the remaining products (point 24) are separated by the separator to separate the tail gas (point 26) and by-products (point 25) such as CaCO_3 and Ca(OH)_2 . The product in the acetylene generator is separated from the acetylene (point 30) and calcium carbide slag (point 29) through a separator, and the calcium carbide slag (point 29) and the by-products (CaCO_3 and Ca(OH)_2 , point 25)

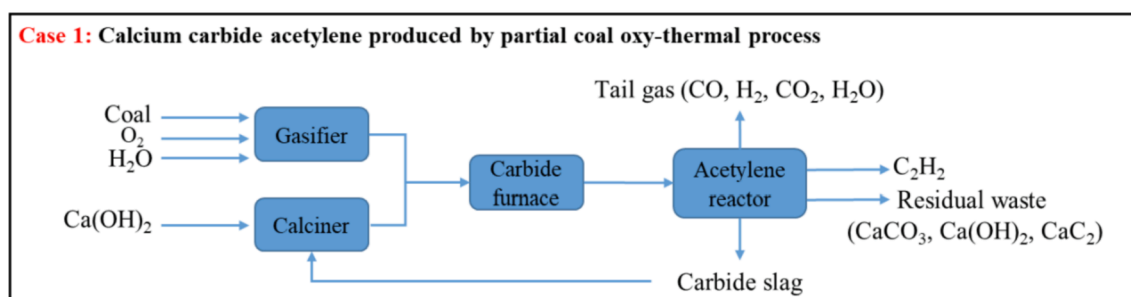


Fig. 1. Schematic diagram of the referenced OTM process [25].

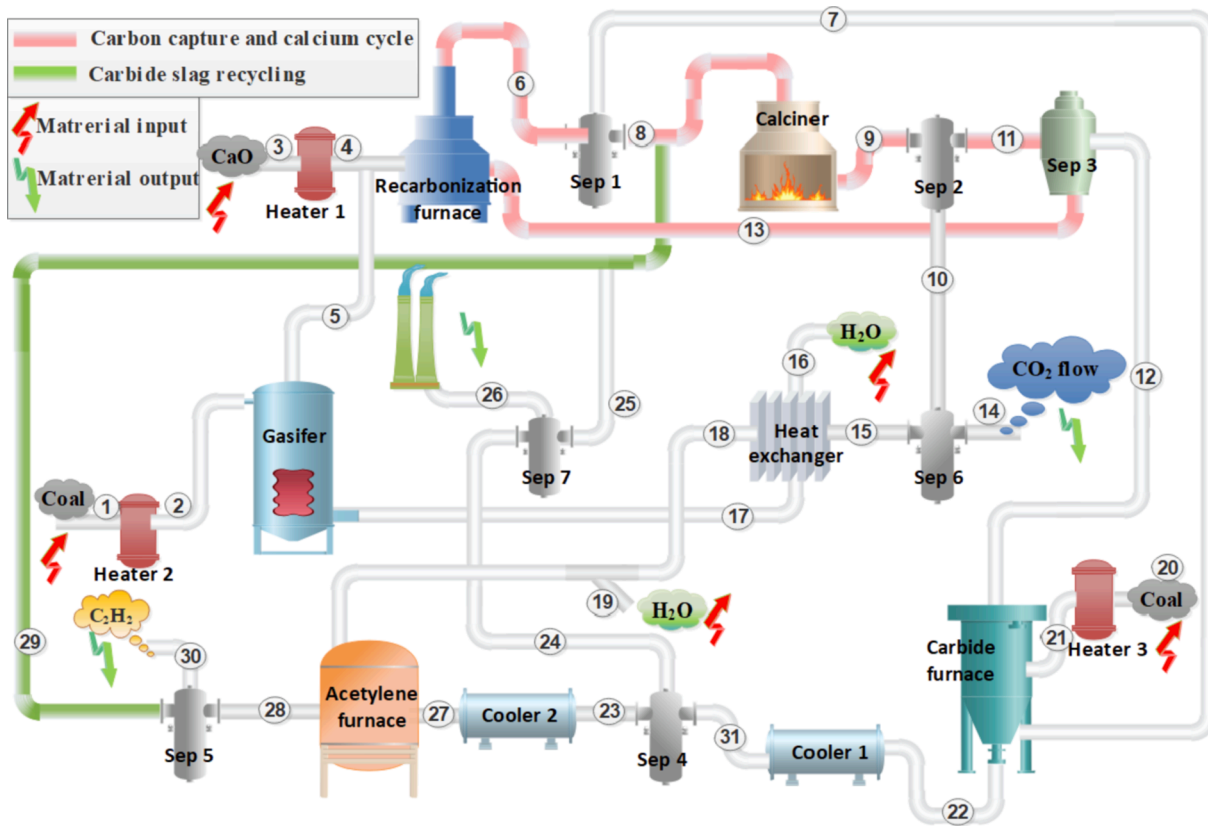


Fig. 2. Schematic diagram of an improved coal to calcium carbide-acetylene system.

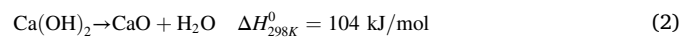
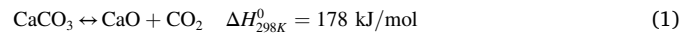
of the calcium carbide furnace are sent to the calciner to continue high-temperature calcination (Eqs. (1)-(2)), then the generated CaO is used for calcium recycling.

Some basic assumptions are considered to simplify the modeling and analysis:

- (1) The system is in a steady-state operation and thermodynamic equilibrium.
- (2) Kinetic and potential energy changes are omitted.
- (3) Pressure losses and heat losses in all pipelines are neglected.

- (4) The coal involved in this paper is coke with a purity of 100%.

Calcination decomposition:



Calcium carbide reaction:

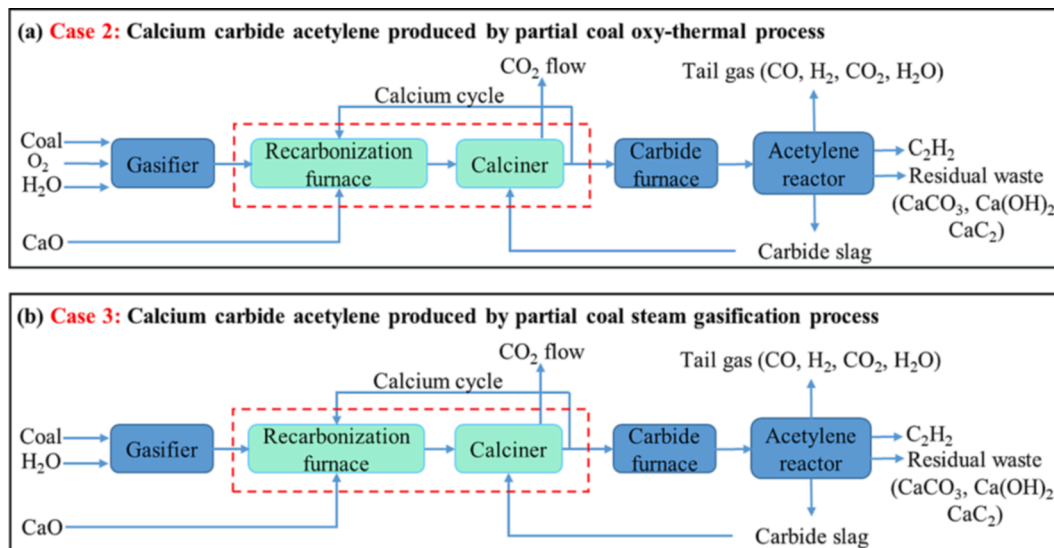
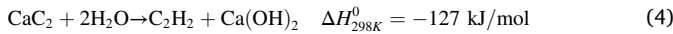


Fig. 3. Schematic diagram of two cases of improved coal-based calcium carbide-acetylene process: (a) calcium carbide-acetylene produced by partial coal oxy-thermal process; (b) calcium carbide-acetylene produced by partial coal steam gasification process.

Acetylene reaction:



Based on the improved system shown in Fig. 2, two process cases as shown in Fig. 3 were established, which mainly includes five modules: coal pyrolysis, re-carbonization, calcination, calcium carbide furnace and acetylene generator. The process of Case 2 (Fig. 3a) is exactly the same as that of Case 3 (Fig. 3b), except that the gasification agent of the two coal pyrolysis modules is different (Case 2 is oxygen and water vapor, the same as the referenced system, and Case 3 is water vapor). Compared with Case 1, Case 2 and Case 3 add a calcium recycling module coupled re-carbonization and calcination. It is worth noting that this coupled module can not only capture the CO₂ generated in the upstream, but also recycle the calcium carbide waste slag generated in the downstream.

3. Methodology

The entire process is modeled and simulated using Aspen Plus V10.0 software, and the correlated equations for the exergoeconomic evaluation are solved by the MATLAB. For the process model established in Aspen, the process components and the corresponding state equations are specified from the database. The process flow sheet is constructed by selecting appropriate unit operation blocks and connecting materials.

3.1. Material conversion

For the evaluation of material conversion in polygeneration systems, the conversion rate of raw materials and the yield of main products are usually used to describe the utilization of raw materials. In order to describe the utilization or conversion rate of a certain element in a substance, Trost proposed the concept of atom economy, which refers to how many reactant atoms are converted into target products [28]. After that, the concept of atomic economy was widely used in chemical production systems. Even if the yield of chemical products reaches 100%, the atom economy of the process may be very low. Therefore, Patel et. al believe that the atom economy is only one way to evaluate the chemical process, and the process should be evaluated in conjunction with energy consumption, pollutant emissions and product prices [29].

The material conversion process of coal-based co-production system is actually the process of distribution, migration and utilization of carbon, hydrogen, oxygen and other elements in coal. In addition to the material conversion characteristics of the poly-generation system, researchers often pay attention to its energy utilization. Therefore, some basic evaluation indicators have been established for the co-production system of coal-based carbon-calcium compound conversion to calcium carbide and acetylene, which preliminarily reveals the material conversion characteristics of the system.

The effective atomic yield of carbide furnace module is defined as the ratio of the total mass of carbon, hydrogen and calcium in the target products to the total mass of carbon, hydrogen and calcium in the raw material when the raw material is converted into the target products CaC₂, H₂ and CO by chemical reaction, as expressed in Eq. (5)

$$Y = \frac{\sum_i (m_{p,i}^C + m_{p,i}^H + m_{p,i}^{Ca})}{\sum_j (m_{m,j}^C + m_{m,j}^H + m_{m,j}^{Ca})} \quad (5)$$

where $m_{m,j}^C$, $m_{m,j}^H$, $m_{m,j}^{Ca}$ are the masses of C, H, Ca elements in raw material j , and $m_{p,i}^C$, $m_{p,i}^H$, $m_{p,i}^{Ca}$ are the masses of C, H, Ca elements in the target product i , respectively.

The CO₂ capture rate of the re-carbonization module is expressed as

$$Y_{\text{CO}_2 \text{ capture}} = \frac{m_{\text{frac.in}} - m_{\text{frac.out}}}{m_{\text{frac.in}}} \quad (6)$$

where $m_{\text{frac.in}}$ is the mass of CO₂ entering the re-carbonization module,

$m_{\text{frac.out}}$ is the mass of CO₂ flowing out of the re-carbonization module.

The CO₂ reduction (which represents the amount of CO₂ emission reduction achieved due to the carbon capture module in the improved process) and CO₂ emissions per unit of C₂H₂ product are respectively expressed as

$$Y_{\text{CO}_2 \text{ reduction}} = \frac{m_{\text{CO}_2 \text{ reduction,tot}}}{m_{\text{C}_2\text{H}_2 \text{,tot}}} \quad (7)$$

$$Y_{\text{CO}_2 \text{ emission}} = \frac{m_{\text{CO}_2 \text{,tot}}}{m_{\text{C}_2\text{H}_2 \text{,tot}}} \quad (8)$$

where $m_{\text{CO}_2 \text{ reduction,tot}}$ is the mass of CO₂ enriched by the entire system, $m_{\text{CO}_2 \text{,tot}}$ is the mass of CO₂ emitted by the entire system, $m_{\text{C}_2\text{H}_2 \text{,tot}}$ is the mass of the final target product C₂H₂ of the system.

3.2. Exergy modeling

The usefulness of energy depends entirely on the convertibility of this energy form. The part of energy that can theoretically be converted into useful work in any form of energy under the ambient conditions is known as the exergy or effective energy. That is, exergy can be used to characterize the quality or grade of energy [30]. Relative to the complete equilibrium state, the exergy possessed by the system is the sum of physical exergy and chemical exergy, which are as Eqs. (9)-(11):

$$\dot{E}_x = \dot{E}_{x,ph} + \dot{E}_{x,ch} \quad (9)$$

$$\dot{E}_{x,ch} = \sum_{i=1}^k \phi_i x_i e_{x_i}^{ch} + RT_0 \sum_{i=1}^k \phi_i x_i \ln x_i \quad (10)$$

$$\dot{E}_{x,ph} = \sum_{i=1}^k [\phi_i (h_i - h_0) - \phi_i T_0 (s_i - s_0)] \quad (11)$$

where $e_{x_i}^{ch}$ is the standard chemical exergy of a pure component i , h_i and s_i are the specific enthalpy and specific entropy of component i , h_0 and s_0 are the specific enthalpy and specific entropy of component i in the environmental state, respectively. ϕ_i is mole flux and x_i is mole fraction. The standard chemical exergy of gas can be found in reference [31]. The specific enthalpy and entropy can be obtained from the result dataset of Aspen. For some compounds of which standard chemical exergy cannot be found in the literature, the generation reaction system can be used to obtain the standard chemical exergy of the substance [31]. Assuming that the compound $A_a B_b C_c$ is generated from the elements or stable elemental substances A, B and C, and its formation reaction is carried out under p_n , T_n , the standard chemical exergy per mole of compound can be obtained from the exergy balance equation:

$$(E_{x,m,A_a B_b C_c})_n = n_a (E_{x,m,A})_n + n_b (E_{x,m,B})_n + n_c (E_{x,m,C})_n + (\Delta G_f^0)_{A_a B_b C_c} \quad (12)$$

where $(\Delta G_f^0)_{A_a B_b C_c}$ is the standard generating Gibbs function of compound $A_a B_b C_c$, which can be directly founded in the data book [31]. n_a , n_b , n_c are the number of atoms of each element in chemical formula $A_a B_b C_c$.

The exergy destruction $\dot{E}_{x,D,k}$ within the component during the operation is calculated at the component level, which is the difference between exergy of fuel and exergy of product, as described by Eq. (13).

$$\dot{E}_{x,D,k} = \dot{E}_{x,F,k} - \dot{E}_{x,P,k} \quad (13)$$

The exergy destruction ratio y_k and relative exergy destruction ratio y_k^* of each component are defined by Eqs. (14) and (15) [32].

$$y_k = \frac{\dot{E}_{x,D,k}}{\dot{E}_{x,F,k}} \quad (14)$$

$$y_k^* = \frac{\dot{E}_{x,D,k}}{\sum \dot{E}_{x,D,k}} \quad (15)$$

The exergy efficiency for k -th component can be expressed by Eq. (16).

$$\eta_{ex,k} = \frac{\dot{E}_{xP,k}}{\dot{E}_{xF,k}} = 1 - \frac{\dot{E}_{xD,k}}{\dot{E}_{xF,k}} \quad (16)$$

Table 1 summarizes the definitions of exergetic fuel and exergetic product of each component and lists the exergy destruction equation and exergy efficiency expression of each component.

3.3. Exergoeconomic modeling

Exergoeconomic analysis is an effective method that combines exergy and economic analysis to evaluate the cost of exergy. Its main purpose is to calculate the unit exergy cost of the product flow by revealing the cost formation process. Based on the energy and economic analysis principles of the system components, the exergoeconomic analysis can comprehensively analyze the costs associated with each exergy flow and thermal system component. In this paper, the specific exergy cost (SPECO) method is used because it provides a general, systematic and definite approach for developing exergy efficiency of thermal systems and their components [33].

The cost balance equation for k -th system component can be expressed as [34]

$$\sum \dot{C}_{out,k} + \dot{C}_{w,k} = \sum \dot{C}_{in,k} + \dot{C}_{q,k} + \dot{Z}_k \quad (17)$$

where the terms $\sum \dot{C}_{in,k}$ and $\sum \dot{C}_{out,k}$ are the incoming and outgoing cost rate of k -th component, $\dot{C}_{w,k}$ and $\dot{C}_{q,k}$ are the cost rate associated with the output power and the input thermal energy of k -th component. Meanwhile the cost rate \dot{C} in the above equation can be written as

$$\dot{C} = c\dot{E} \quad (18)$$

where c is the specific exergy cost for each stream. The term \dot{Z}_k is the total cost rate associated with the capital investment \dot{Z}_k^{CI} , operation and maintenance costs \dot{Z}_k^{OM} for the k -th component, given by

$$\dot{Z}_k = \dot{Z}_k^{CI} + \dot{Z}_k^{OM} \quad (19)$$

$$\dot{Z}_k^{CI} = \left(\frac{CRF}{\tau}\right) \cdot Z_k \quad (20)$$

where τ is annual plant operation hours, CRF is capital recovery factor, as expressed in Eq. (21)

$$CRF = \frac{i_r(1 + i_r)^n}{(1 + i_r)^n - 1} \quad (21)$$

The \dot{Z}_k^{OM} is given by Eq. (22)[23], in which γ is maintenance factor.

$$\dot{Z}_k^{OM} = \left(\frac{\gamma}{\tau}\right) \cdot Z_k \quad (22)$$

Z_k is the cost equation for each component, which is summarized in Appendix A (Table A1). Among them, cost per unit exergy (c_{in}), 130, 0.093, 0.78, 30, 1100 and 2200 are all constants, which can be obtained directly from references [22,23], while heat power (\dot{Q}_{core}), heat transfer area (A_{HEX}), mass flow rate (\dot{m}_k) and electrical power (\dot{W}_{sep}) need to be read from ASPEN and substituted into the cost equations in turn to calculate the Z_k of the corresponding component. It is worth noting that the cost of each component must be based on the same referenced year. Therefore, the Chemical Engineering Plant Cost Index (CEPCI) is used to aggregate the cost data of all components to 2020. The detailed

Table 1

The exergetic fuel, exergetic product, exergy destruction and exergy efficiency of each component of the improved system.

Component	Exergetic fuel $\dot{E}_{xP,k}$	Exergetic product $\dot{E}_{xP,k}$	Exergy destruction $\dot{E}_{xD,k}$	Exergy efficiency $\eta_{ex,k}$
Gasifier	$\dot{E}_2 + \dot{E}_{17}$	\dot{E}_5	$\dot{E}_2 + \dot{E}_{17} - \dot{E}_5$	$\dot{E}_5 / (\dot{E}_2 + \dot{E}_{17})$
Re-carbonization furnace	$\dot{E}_4 + \dot{E}_5 + \dot{E}_{13}$	\dot{E}_6	$\dot{E}_4 + \dot{E}_5 + \dot{E}_{13} - \dot{E}_6$	$\dot{E}_6 / (\dot{E}_4 + \dot{E}_5 + \dot{E}_{13})$
Calciner	$\dot{E}_8 + \dot{E}_{25} + \dot{E}_{29}$	\dot{E}_9	$\dot{E}_8 + \dot{E}_{25} + \dot{E}_{29} - \dot{E}_9$	$\dot{E}_9 / (\dot{E}_8 + \dot{E}_{25} + \dot{E}_{29})$
Carbide furnace	$\dot{E}_7 + \dot{E}_{12} + \dot{E}_{21}$	\dot{E}_{22}	$\dot{E}_7 + \dot{E}_{12} + \dot{E}_{21} - \dot{E}_{22}$	$\dot{E}_{22} / (\dot{E}_7 + \dot{E}_{12} + \dot{E}_{21})$
Acetylene reactor	$\dot{E}_{18} + \dot{E}_{19} + \dot{E}_{27}$	\dot{E}_{28}	$\dot{E}_{18} + \dot{E}_{19} + \dot{E}_{27} - \dot{E}_{28}$	$\dot{E}_{28} / (\dot{E}_{18} + \dot{E}_{19} + \dot{E}_{27})$
Heat exchanger	$\dot{E}_{17} - \dot{E}_{16}$	$\dot{E}_{15} - \dot{E}_{18}$	$\dot{E}_{17} - \dot{E}_{16} - (\dot{E}_{15} - \dot{E}_{18})$	$(\dot{E}_{15} - \dot{E}_{18}) / (\dot{E}_{17} - \dot{E}_{16})$
Separator 1	\dot{W}_{sep1}	$\dot{E}_7 + \dot{E}_8 - \dot{E}_6$	$\dot{E}_6 + \dot{W}_{sep1} - (\dot{E}_7 + \dot{E}_8)$	$(\dot{E}_7 + \dot{E}_8 - \dot{E}_6) / \dot{W}_{sep1}$
Separator 2	\dot{W}_{sep2}	$\dot{E}_{11} + \dot{E}_{10} - \dot{E}_9$	$\dot{W}_{sep2} - (\dot{E}_{11} + \dot{E}_{10} - \dot{E}_9)$	$(\dot{E}_{11} + \dot{E}_{10} - \dot{E}_9) / \dot{W}_{sep2}$
Separator 4	\dot{W}_{sep4}	$\dot{E}_{23} + \dot{E}_{24} - \dot{E}_{31}$	$\dot{W}_{sep4} - (\dot{E}_{23} + \dot{E}_{24} - \dot{E}_{31})$	$(\dot{E}_{23} + \dot{E}_{24} - \dot{E}_{31}) / \dot{W}_{sep4}$
Separator 5	\dot{W}_{sep5}	$\dot{E}_{30} + \dot{E}_{29} - \dot{E}_{28}$	$\dot{W}_{sep5} - (\dot{E}_{30} + \dot{E}_{29} - \dot{E}_{28})$	$(\dot{E}_{30} + \dot{E}_{29} - \dot{E}_{28}) / \dot{W}_{sep5}$
Separator 6	\dot{W}_{sep6}	$\dot{E}_{15} + \dot{E}_{14} - \dot{E}_{10}$	$\dot{W}_{sep6} - (\dot{E}_{15} + \dot{E}_{14} - \dot{E}_{10})$	$(\dot{E}_{15} + \dot{E}_{14} - \dot{E}_{10}) / \dot{W}_{sep6}$
Separator 7	\dot{W}_{sep7}	$\dot{E}_{26} + \dot{E}_{25} - \dot{E}_{24}$	$\dot{W}_{sep7} - (\dot{E}_{26} + \dot{E}_{25} - \dot{E}_{24})$	$(\dot{E}_{26} + \dot{E}_{25} - \dot{E}_{24}) / \dot{W}_{sep7}$
Heater 1	$\dot{Q}_{Heater1}$	$\dot{E}_4 - \dot{E}_3$	$\dot{Q}_{Heater1} - (\dot{E}_4 - \dot{E}_3)$	$(\dot{E}_4 - \dot{E}_3) / \dot{Q}_{Heater1}$
Heater 2	$\dot{Q}_{Heater2}$	$\dot{E}_2 - \dot{E}_1$	$\dot{Q}_{Heater1} - (\dot{E}_2 - \dot{E}_1)$	$(\dot{E}_2 - \dot{E}_1) / \dot{Q}_{Heater2}$
Heater 3	\dot{Q}_{Heate3}	$\dot{E}_{21} - \dot{E}_{20}$	$\dot{Q}_{Heater1} - (\dot{E}_{21} - \dot{E}_{20})$	$(\dot{E}_{21} - \dot{E}_{20}) / \dot{Q}_{Heate3}$
Cooler 1	\dot{Q}_{cool1}	$\dot{E}_{22} - \dot{E}_{31}$	$\dot{Q}_{cool1} - (\dot{E}_{22} - \dot{E}_{31})$	$(\dot{E}_{22} - \dot{E}_{31}) / \dot{Q}_{cool1}$
Cooler 2	\dot{Q}_{cool2}	$\dot{E}_{23} - \dot{E}_{27}$	$\dot{Q}_{cool} - (\dot{E}_{23} - \dot{E}_{27})$	$(\dot{E}_{23} - \dot{E}_{27}) / \dot{Q}_{cool}$

conversion formula of component cost in different years is shown in Eq. (23)[23].

$$\dot{Z}_k = \dot{Z}_k^0 \times \frac{CEPCI(\text{of the present year})}{CEPCI^0(\text{of the reference year})} \quad (23)$$

Appendix A (Table A2) lists the cost balance equations and required auxiliary equations of the components, which are based on the Fuel-Product-Loss principle of the SPECO method. Meanwhile, it also stipulates the appropriate boundary conditions for all imported streams. For example, the costs of imported materials such as coal, water and quicklime are listed in Table 2, including the values of some important design and operating parameters used in the model.

Moreover, several evaluation parameters are employed to assess the exergoeconomic behavior of a system, as listed in Table 3. r_k describes the relative cost difference between the exergetic fuel and exergetic product of the component, f_k denotes the contribution of capital investment on the total investment of components.

4. Model validation

The model verification is implemented at the component level in this paper. In order to verify the proposed coal-based calcium carbide-acetylene model, the gasification gas composition of the three aforementioned models was compared. Fig. 4 shows the comparison of the syngas composition produced by the gasifier in the three models. It can be seen that the main components of gasification syngas (CO, H₂, CO₂) account for more than 80% in all the three cases, which is consistent with the actual situation of coal gasification process. Among them, the main components of Cases 1 and 2 account for 88.05% and 85.53%, and the relative error is 2.8% which indicates that the model is reasonable. The total proportions of high calorific value gases (CO, H₂) in Case 1 (60.70%) and Case 2 (58.36%) are basically the same, and the Case 3 (79.25%) is slightly higher than Cases 1 and 2. It is because the use of steam as gasification agent in Case 3 will generate higher calorific value gas H₂. Besides, the fluid state equations of three cases and the selection and operation parameters of the other main reaction modules such as carbide furnace and acetylene furnace are consistent. For example, the selection of carbide furnaces in Case 1, Case 2 and Case 3 are all RGibbs, and the reaction conditions of the carbide furnace are both 1927 °C and 101.325 kPa. Similarly, the selection of acetylene reactors in three cases is also the same, which is RGibbs, the reaction temperature is 40 °C, and the pressure is 101.325 kPa. Consequently, the modeling and simulation results in this paper are basically reliable.

5. Results and discussion

5.1. Material conversion analysis

In this section, some evaluation indexes related to material conversion are calculated for the three cases, including the C, H, Ca effective atom yield of calcium carbide furnace module ($Y_{C|H|Ca}$), CO₂ capture rate ($Y_{CO_2\text{capture}}$), and CO₂ reduction ($Y_{CO_2\text{reduction}/C_2H_2}$), CO₂ emissions ($Y_{CO_2\text{emission}/C_2H_2}$). Table 4 lists the calculation results of each index. It can

Table 2

Values of some important parameters used in the model of the proposed system [22,23].

Parameter	Value
Operation year (n)	20
Annual plant operating hours (τ)	8000
The interest rate (i_r)	0.12
Maintenance factor (γ)	0.06
Coal cost (\$/GJ)	1.5
Quicklime cost (\$/GJ)	0.006944
Water cost (\$/GJ)	0.1222

Table 3

Exergoeconomic evaluation parameters.

Items	Functions
Average costs per unit exergy of fuel	$c_{F,k} = \dot{C}_{F,k}/\dot{E}_{F,k}$
Average costs per unit exergy of product	$c_{P,k} = \dot{C}_{P,k}/\dot{E}_{P,k}$
Cost rate of exergy destruction	$\dot{C}_{D,k} = c_{F,k} \cdot \dot{E}_{D,k}$
Relative cost difference	$r_k = (c_{P,k} - c_{F,k})/c_{F,k} = \frac{\dot{C}_{D,k} + \dot{Z}_k}{c_{F,k} \dot{E}_{P,k}}$
Exergoeconomic factor	$f_k = \dot{Z}_k / (\dot{Z}_k + \dot{C}_{D,k})$

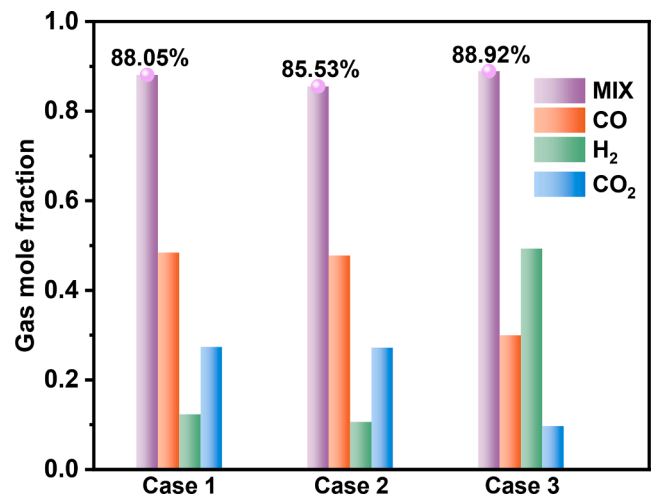


Fig. 4. Comparison of main components of gasification syngas in three cases.

Table 4

Comparison of material conversion and energy utilization index values in three cases.

Index	Case 1	Case 2	Case 3
$Y_{C H Ca}$	64.51%	81.75%	85.41% max
$Y_{CO_2\text{capture rate}}$	—	92.62% max	90.35%
$Y_{CO_2\text{reduction}/C_2H_2} / t \text{ CO}_2 \cdot (t^{-1} C_2H_2)$	—	2.06	2.81 max
$Y_{CO_2\text{emission}/C_2H_2} / t \text{ CO}_2 \cdot (t^{-1} C_2H_2)$	2.25	2.90×10^{-3}	5.26×10^{-5} min

be seen that Case 3 shows the highest C, H and Ca effective atom conversion rate of 85.41%. As the Case 2 and Case 3 systems combine re-carbonization and calcination coupled calcium recycling processes, these two systems can capture part of the CO₂ generated in the upstream, and the carbon capture rate is above 90%. Due to the characteristics of the coupled calcium cycle process of Case 2 and Case 3, these two cases can capture CO₂ of 2.06 and 2.81 t CO₂·(t⁻¹ C₂H₂) respectively, for further CO₂ utilization to create possible economic benefits. The CO₂ emissions per unit acetylene product of Case 2 and Case 3 are low, which is owing to the excellent carbon capture performance of these two cases.

5.2. Exergy analysis

Based on the thermodynamic properties and gas composition of each stream in Appendix A (Table A3), the exergy at each point of Case 3 can be calculated according to the stream numbers as shown in Fig. 2. The exergy performance of each component and the overall system, including exergy efficiency and exergy destruction, can be obtained by the exergy balance equation. The results are summarized in Table 5.

Case 3 finally reached the target of annual output of 170000 tons of calcium carbide, and the further production of acetylene can reach an output of 50000 tons/year. It can be seen that the overall exergy flow destruction of Case 3 is 117501.73 kW. The exergy destructions of the

Table 5
The exergy results of the proposed coupling system (Case 3).

Component	$\dot{E}_{x_{f,k}}$ (kW)	$\dot{E}_{x_{p,k}}$ (kW)	$\dot{E}_{x_{d,k}}$ (kW)	η_k (%)	y_k (%)	y_k^* (%)
Component level results						
Gasifier	31321.22	18715.27	12605.95	59.75	40.25	11.03
Re-carbonization furnace	26693.66	17043.66	9650	63.85	36.15	8.44
Calciner	21291.84	18292	3000	85.91	14.09	2.63
Carbide furnace	107440.53	53524.54	53915.99	49.28	50.18	47.18
Acetylene reactor	56494.3	36362.37	20131.93	64.36	35.64	17.62
Heat exchanger	1060.4734	637.33	423.1434	60.10	39.90	0.37
Separator 1	13151.92	12548.13	603.79	95.41	4.59	0.53
Separator 2	9406.95	7971.85	1435.1	84.74	15.26	1.26
Separator 4	46151	44495.59	1655.41	96.41	3.59	1.45
Separator 5	29874.73	28549.5	1325.23	95.56	4.44	1.16
Separator 6	1741.21	1615.86	125.35	92.80	7.20	0.11
Separator 7	19090.19	18238.19	852	95.54	4.46	0.75
Heater 1	639.761	297.19	342.571	46.45	53.55	0.30
Heater 2	1098.22	586.87	511.35	53.44	46.56	0.45
Heater 3	2112.95	1088.5	1024.45	51.52	48.48	0.90
Cooler 1	21327.5	16915	4412.5	79.31	20.69	3.86
Cooler 2	4802.31	2534	2268.31	52.77	47.23	1.98
System level results						
	212046.73	94545	117501.73	44.59		

Table A1

The cost equations and CEPCI from the base years of components in the proposed system [22,23].

Component	Cost equation
Gasifier	$Z_G = c_{in} \times \dot{Q}_{core}$
Re-carbonization furnace	$Z_{RF} = c_{in} \times \dot{Q}_{core}$
Calciner	$Z_C = c_{in} \times \dot{Q}_{core}$
Carbide furnace	$Z_{CF} = c_{in} \times \dot{Q}_{core}$
Acetylene reactor	$Z_{AR} = c_{in} \times \dot{Q}_{core}$
Heat exchanger	$Z_{HEX} = 130 \times \left(\frac{A_{HEX}}{0.093}\right)^{0.78}$
Heater 1	$Z_{H1} = 30 \times \dot{m}_k$
Heater 2	$Z_{H2} = 30 \times \dot{m}_k$
Heater 3	$Z_{H3} = 30 \times \dot{m}_k$
Cooler 1	$Z_{COOL1} = 30 \times \dot{m}_k$
Cooler 2	$Z_{COOL2} = 30 \times \dot{m}_k$
Separator 1	$Z_{SEP1} = 1100 \times \dot{W}_{sep1}$
Separator 2	$Z_{SEP2} = 2200 \times \dot{W}_{sep2}$
Separator 4	$Z_{SEP4} = 1100 \times \dot{W}_{sep4}$
Separator 5	$Z_{SEP5} = 1100 \times \dot{W}_{sep5}$
Separator 6	$Z_{SEP6} = 2200 \times \dot{W}_{sep6}$
Separator 7	$Z_{SEP7} = 1100 \times \dot{W}_{sep7}$

Notes: $CEPCI^{2020}=612.36$ [40] $CEPCI^0=468.2$ [32,23] $c_{in} = 283\$/kW_{th}$.

carbide furnace, acetylene reactor, gasifier and re-carbonization furnace are 53915.99 kW, 20131.93 kW, 12605.95 kW, and 9650 kW, which account for 47.18%, 17.62%, 11.03%, and 8.44% of the total exergy destruction, respectively.

Since these components are the key energy-consuming modules in the system, it is recommended that these units should be optimized during design and analysis. As shown in Table 5, the exergy destruction of the carbide furnace is 53915.99 kW, which is 4.28 times and 2.68 times that of the gasifier and acetylene reactor, respectively. This is mainly because the operating temperature of the carbide furnace (1927 °C) is far outweigh than gasifier (700 °C) and acetylene reactor (40 °C), leading to a larger heat loss occurs in the carbide furnace.

For the heat exchange device such as Heat exchanger, Heater 1, Heater 2, Heater 3, Cooler 1 and Cooler 2, the relative exergy destruction of Cooler 1 is comparatively large, which is 3.86%. That is mainly because of the extremely large temperature difference between the inlet and the outlet fluids. For example, the inlet and outlet temperatures of Cooler 1 are 1927 °C and 800 °C, with a temperature difference up to 1127 °C. Large temperature differences result in the exergy loss during

Table A2

Cost balance and auxiliary equations for the components of the proposed system.

Component	Exergetic cost rate balance equation	Auxiliary equation
Gasifier	$\dot{C}_5 = \dot{C}_2 + \dot{C}_{17} + \dot{Z}_{gas}$	$\dot{C}_2 = \dot{C}_1$
Re-carbonization furnace	$\dot{C}_6 = \dot{C}_4 + \dot{C}_5 + \dot{C}_{13} + \dot{Z}_{rf}$	nil
Calciner	$\dot{C}_8 = \dot{C}_8 + \dot{C}_{29} + \dot{C}_{25} + \dot{Z}_{cal}$	nil
Carbide furnace	$\dot{C}_{22} = \dot{C}_7 + \dot{C}_{12} + \dot{C}_{21} + \dot{Z}_{cf}$	nil
Acetylene reactor	$\dot{C}_{28} = \dot{C}_{18} + \dot{C}_{19} + \dot{C}_{27} + \dot{Z}_{ag}$	nil
Heat exchanger	$\dot{C}_{26} + \dot{C}_{18} = \dot{C}_{16} + \dot{C}_{15} + \dot{Z}_{Hex}$	$\dot{C}_{26} = \dot{C}_{16} = 0$
Separator 1	$\dot{C}_7 + \dot{C}_8 = \dot{C}_6 + \dot{C}_{w,sep1} + \dot{Z}_{sep1}$	$\dot{C}_7 = \dot{C}_8$
Separator 2	$\dot{C}_{11} + \dot{C}_{10} = \dot{C}_8 + \dot{C}_{w,sep2} + \dot{Z}_{sep2}$	$\dot{C}_{11} = \dot{C}_{10}$
Separator 3	$\dot{C}_{12} + \dot{C}_{13} = \dot{C}_{11} + \dot{C}_{w,sep3} + \dot{Z}_{sep3}$	$\dot{C}_{12} = \dot{C}_{13}$
Separator 4	$\dot{C}_{23} + \dot{C}_{24} = \dot{C}_{31} + \dot{C}_{w,sep4} + \dot{Z}_{sep4}$	$\dot{C}_{23} = \dot{C}_{24}$
Separator 5	$\dot{C}_{30} + \dot{C}_{29} = \dot{C}_{28} + \dot{C}_{w,sep5} + \dot{Z}_{sep5}$	$\dot{C}_{30} = \dot{C}_{29}$
Separator 6	$\dot{C}_{15} + \dot{C}_{14} = \dot{C}_{10} + \dot{C}_{w,sep6} + \dot{Z}_{sep6}$	$\dot{C}_{15} = \dot{C}_{14}$
Separator 7	$\dot{C}_{26} + \dot{C}_{25} = \dot{C}_{24} + \dot{C}_{w,sep7} + \dot{Z}_{sep7}$	$\dot{C}_{26} = \dot{C}_{25}$
Heater 1	$\dot{C}_4 = \dot{C}_3 + \dot{C}_{q1} + \dot{Z}_{Hea1}$	$\dot{C}_3/\dot{E}_3 = \dot{C}_4/\dot{E}_4 = 0.025$
Heater 2	$\dot{C}_2 = \dot{C}_1 + \dot{C}_{q2} + \dot{Z}_{Hea2}$	$\dot{C}_1/\dot{E}_1 = \dot{C}_2/\dot{E}_2 = 5.4$
Heater 3	$\dot{C}_{21} = \dot{C}_{20} + \dot{C}_{q3} + \dot{Z}_{Hea3}$	$\dot{C}_{20}/\dot{E}_{20} = \dot{C}_{21}/\dot{E}_{21} = 5.4$
Cooler 1	$\dot{C}_{31} = \dot{C}_{22} + \dot{Z}_{Cooler1}$	$\dot{C}_{22}/\dot{E}_{22} = \dot{C}_{31}/\dot{E}_{31}$
Cooler 2	$\dot{C}_{27} = \dot{C}_{23} + \dot{Z}_{Cooler2}$	$\dot{C}_{23}/\dot{E}_{23} = \dot{C}_{27}/\dot{E}_{27}$

fluid passes through the Cooler 1, which is the source of exergy destruction for this component.

In addition, an exergy diagram of the improved system Case 3 is depicted in Fig. 5, where the black blocks represent module components, the red blocks represent heaters, the blue blocks represent cooler and heat exchanger, and the yellow lines represent the exergy flow of the stream. In the improved system Case 3, the exergy flow starts mainly from the coal fuel source with $\dot{E}_{x,coal}=29584$ kW, then sequentially enters into gasifier, re-carbonization furnace, calciner and carbide furnace and so on. In each component block, the exergy of fuel and product and the corresponding exergy destruction can be visually obtained through the Sankey diagram. For example, the exergy of fuel flows into gasifier is No. 2 and 17 streams, which is 31321 kW in total. The corresponding

Table A3
Thermodynamic properties and costs of exergy streams for the calcium carbide acetylene system (Case 3).

State	P (bar)	T (°C)	m (kg/h)	h (kJ/kg)	s (kJ/(kg·K))	\dot{E}_{ph} (kW)	\dot{E}_{ch} (kW)	\dot{E} (kW)	Cost	
									\dot{C} (\$/h)	c (\$/GJ)
1	1	25	3600.00	0.00	0.0000	0	29583.88	29583.88	159008.62	19.3494
2	1	700	3600.00	1098.22	1.7151	586.87	29583.88	30170.75	159313.60	19.0094
3	1	25	4037.57	-11325.24	-1.8888	0	2208.1	2208.1	51.05	0.0832
4	1	650	4037.57	-10754.81	-0.8643	297.19	2208.1	2505.29	228.71	0.3287
5	1	700	11382.60	-4693.76	4.4943	2161.62	16553.65	18715.27	161913.95	31.1452
6	1	650	23612.80	-9777.55	-0.2829	2986.46	14057.2	17043.66	187477.98	39.5995
7	1	650	1660.45	2604.45	10.6949	994.35	23805.66	24800.01	160180.89	23.2521
8	1	650	21952.40	-10714.14	-1.1721	2067.36	2724.42	4791.78	30953.93	23.2553
9	1	900	59421.60	-9420.24	0.4742	8746.23	10545.61	19291.84	126434.69	23.5936
10	1	900	19498.00	-8642.44	1.4657	3662.17	1340.5	5002.67	23694.51	17.0509
11	1	900	39923.60	-9800.10	-0.0950	5126.74	17134.28	22261.02	105359.05	17.0384
12	1	900	31731.00	-9615.47	0.0443	4134.09	13260.76	17394.85	80143.05	16.5862
13	1	900	8192.54	-10515.18	-0.6347	992.64	4480.46	5473.1	25216.00	16.5861
14	1	900	15842.00	-7966.33	1.5296	2371.73	2013.75	4385.48	16549.05	13.5850
15	1	900	3654.75	-11573.27	0.3515	1537.18	484.98	2022.16	7630.21	13.5839
16	1	25	7782.60	-15972.08	-9.3240	-0.0034	90	89.9966	39.59	1.5838
17	1	102	7782.60	-15545.16	-8.0748	117.75	1032.72	1150.47	2441.86	7.6410
18	1	500	3654.75	-12482.36	-0.5921	899.85	484.98	1384.83	5227.97	13.5906
19	1	25	4143.51	-15972.08	-9.3240	-0.00179	47.92	47.91821	21.12	1.5867
20	1	25	7807.15	0.00	0.0000	0	64157.17	64157.17	342845.67	19.2378
21	1	650	7807.15	974.314	1.5844	1088.5	64157.17	65245.67	343432.44	18.9493
22	1	1927	41198.60	-3755.15	1.8857	23543.27	29981.27	53524.54	583998.38	39.2791
23	1	800	18489.40	16.87	1.7955	2536.25	55059.70	57595.94	831427.12	51.9679
24	1	800	22709.20	-10207.4	-0.3873	4092.48	19417.16	23509.64	339491.63	51.9859
25	1	800	21430.48	-11226.9	-1.2972	2607.77	1071.21	3678.99	37781.73	36.9705
26	1	800	1278.33	6885.86	14.8667	1484.71	28178.65	29663.36	304700.56	36.9790
27	1	40	18489.25	-918.17	0.3145	1.85	55059.7	55061.55	831427.12	54.3599
28	1	40	26287.52	-6385.05	-1.8260	1.47	36360.9	36362.37	836775.21	82.8436
29	1	40	16036.23	-13290.78	-3.9065	1.97	4412.9	4414.87	57466.06	46.8593
30	1	40	10251.29	4417.68	1.4286	-0.5	60497.5	60497.5	787615.78	46.8687
31	1	800	41198.59	-5618.86	0.5923	6628.73	29981.27	36610	583998.38	57.4268

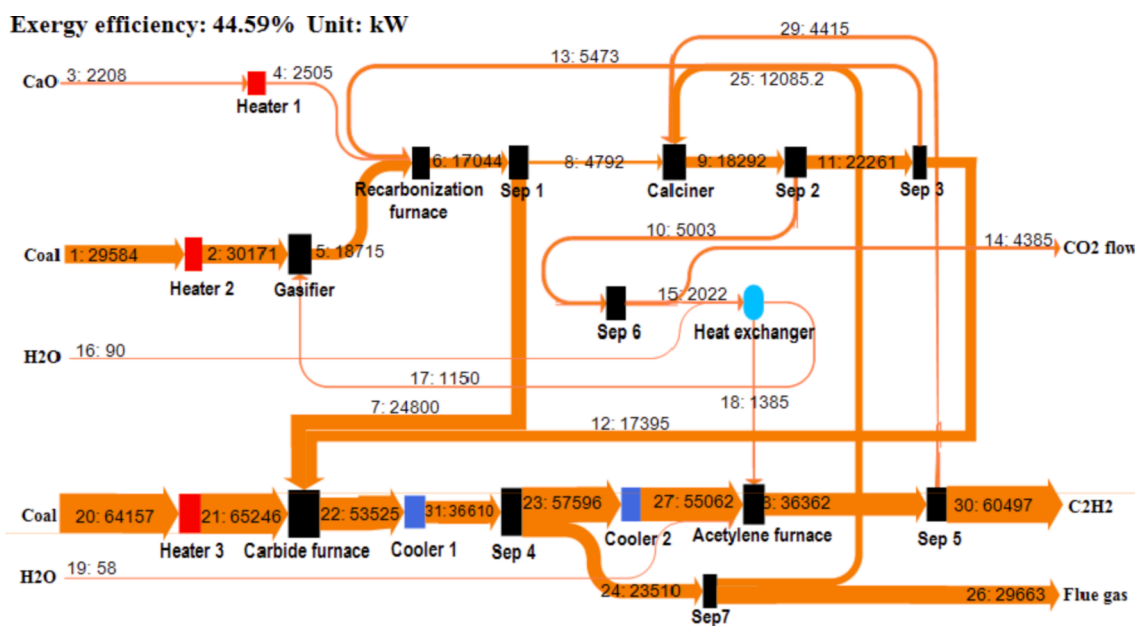


Fig. 5. Sankey diagram to show the exergy flow through the improved system (Case 3).

exergy of product is No. 5 stream, which is 18715 kW. As a result, the exergy destruction of the gasifier is calculated to be 12606 kW. For the heat exchanger component, the fuel exergy is defined as the difference between the exergy of inlet stream 16 and the outlet stream 17, which is calculated to be 1060 kW. Similarly, the exergy of product is 637 kW, which is the exergy difference between No. 15 and 18 streams. Accordingly, the exergy destruction of the heat exchanger is 423 kW.

In the same way, the exergy flow diagrams of Case 1 and Case 2

processes have been drawn, as shown in Figs. 6 and 7 in the Appendix. In summary, we draw the yield and conversion indexes of the three cases in radar chart Fig. 8. Wherein the indexes of chart more outward represented that the process was better, so it can be seen that the process performance order of the three cases were Case 3 > Case 2 > Case 1. And Case 3 used steam as gasifier to avoid using air separation unit compared with Case 2, and since it was previously known that the Case 3 gasification module produces more high thermal value gases, and Case 3 is

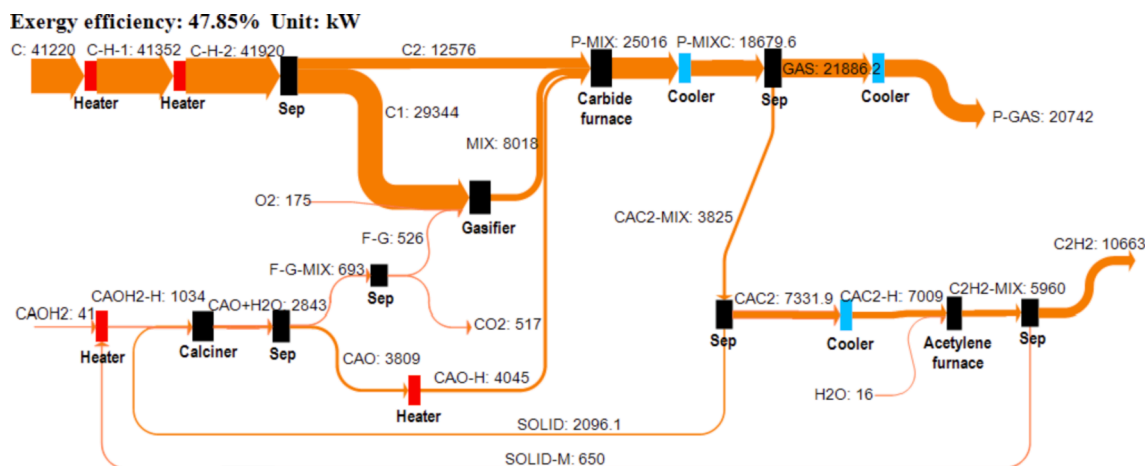


Fig. 6. Sankey diagram to show the exergy flow through the referenced system (Case 1).

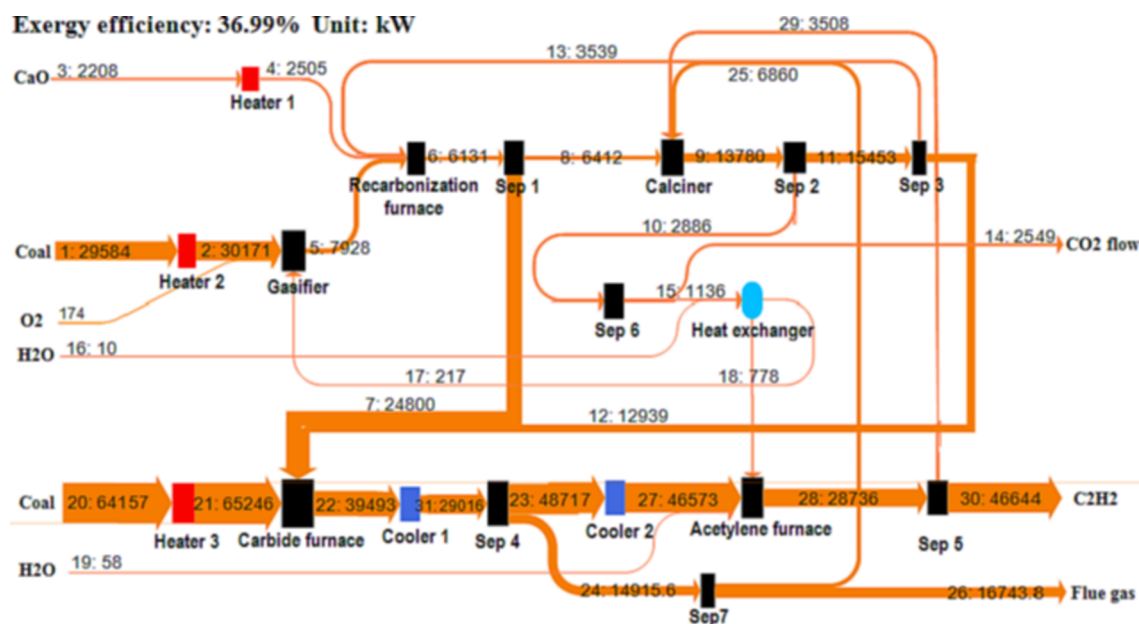


Fig. 7. Sankey diagram to show the exergy flow through the proposed improved system (Case 2).

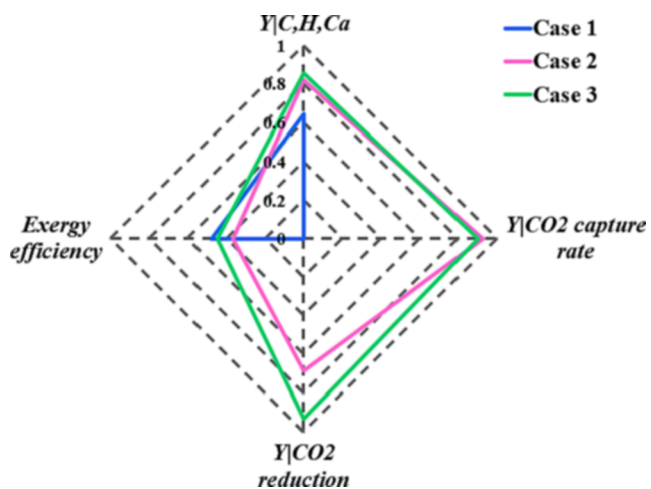


Fig. 8. Radar diagram of process performance comparison of three cases.

considered to be a relatively superior process. Therefore, in the next section, an exergoeconomic economic analysis is further conducted on the improved OTM system (Case 3) process.

5.3. Exergoeconomic analysis

Appendix (Table A3) also depicts the system cost associated with the exergies of the fluid streams in the basic design case for the improved carbon-calcium compound conversion system according to the stream numbers shown in Fig. 1.

Appendix (Table A4) presents the main results of the exergoeconomic analysis for the improved system (Case 3). Nowadays, in some research work, $\dot{C}_{D,k} + \dot{Z}_k$ is used to evaluate the importance of the system components in terms of the exergoeconomic aspects, and a large $\dot{C}_{D,k} + \dot{Z}_k$ value means that this component is more important [35,36]. The exergoeconomic factor f_k is an important index used to identify the major cost resource (capital investment, operation and maintenance cost or exergy destruction cost), which is defined as the ratio of the non-exergy-related cost rate to the total cost rate [34]. A low value of f_k for a major component suggests that cost savings in the entire system can

Table A4
The exergoeconomic analysis results of the improved system (Case 3).

Components	Average cost of per unit exergy of fuel $c_{F,k}$ (\$/GJ)	Average cost of per unit exergy of product $c_{P,k}$ (\$/GJ)	Cost rate of exergy destruction $\dot{C}_{D,k}$ (\$/h)	Cost rate of capital investment \dot{Z}_k (\$/h)	Sum cost rate of exergy destruction and capital investment $\dot{C}_{D,k} + \dot{Z}_k$ (\$/h)	Relative cost difference r_k (%)	Exergoeconomic factor f_k (%)
Gasifier	18.5919	31.15	65102.23	158.4929	65260.72	67.52	0.2429
Re-carbonization furnace	25.2678	39.60	67731.86	119.3122	67851.17	56.72	0.1758
Calciner	21.3380	24.88	17781.70	232.9726	18014.67	16.62	1.2932
Carbide furnace	19.5599	39.28	292941.62	241.9973	293183.62	100.81	0.0825
Acetylene reactor	53.3157	56.28	298152.33	99.0006	298251.33	55.38	0.0332
Heat exchanger	8.1550	13.57	958.54	0.0263	958.56	66.39	0.0027
Separator 1	0.0771	1.05	12.94	4.5504	17.49	6.50	26.0197
Separator 2	0.0771	1.18	30.75	6.5605	37.31	21.84	17.5830
Separator 4	0.0771	47.49	35.47	2.8026	38.27	4.01	7.3224
Separator 5	0.0771	1.05	28.40	10.4174	38.81	6.34	26.8392
Separator 6	0.0771	1.08	2.69	1.2143	3.90	11.26	31.1337
Separator 7	0.0771	0.59	18.26	3.7506	22.01	5.63	17.0427
Heater 1	0.0771	2.15	7.34	0.0011	7.34	115.29	0.0145
Heater 2	0.0771	1.87	10.96	0.0010	10.96	87.14	0.0087
Heater 3	0.0771	1.94	21.95	0.0021	21.95	94.12	0.0094
Cooler 1	0.0771	0.0000008	94.55	0.0037	94.55	26.09	0.0039
Cooler 2	0.0771	0.0000118	48.60	0.0083	48.61	89.53	0.0171

be obtained by improving the component efficiency (reducing the exergy destruction). For example, improve the performance of equipment through proper technical retrofit to reduce losses. On the other hand, if a major component has a high value of f_k , it means that the investment cost of this component is high, and it is necessary to reduce the investment cost to improve the economy [23].

From Appendix (Table A4), it is worth mentioning that the carbide furnace, acetylene reactor, re-carbonization furnace, gasifier and calciner have the top five high values of $\dot{C}_{D,k} + \dot{Z}_k$ in the overall system, which means that these components are the most important modules. Moreover, the f_k values of these components are 0.08%, 0.03%, 0.18%, 0.24% and 1.29%, respectively (as shown in Fig. 9), most of these f_k values are relatively small, indicating that $\dot{C}_{D,k}$ are dominant among the exergy destruction costs and the capital investment costs of these components, which can be decreased at the expense of their capital investment. In addition, the f_k values of the separators components are relatively high over the system, but the $\dot{C}_{D,k}$ and \dot{Z}_k values are much lower than the key components such as gasifier, calcium carbide, acetylene reactor, etc., suggesting that both the small values $\dot{C}_{D,k}$ and \dot{Z}_k are more dominant. Moreover, the heat exchanger, heater and cooler have a very small f_k value, which indicates that these components have a large exergy destruction cost. Therefore, the exergy destruction cost can be reduced by improving the exergy efficiency of these components, so as to achieve the purpose of cost saving.

The relative cost difference r_k is another parameter to evaluate the

exergoeconomic performance of components. A small r_k value indicates that the cost of capital investment and operating and cost of exergy destruction contribute less to the increase of specific cost of the exergetic product. Therefore, the components with the greater relative cost difference should be paid more attention. For instance, the f_k and r_k of carbide furnace are 0.08% and 100.81% (as shown in Fig. 9), revealing that the relatively high cost rate of exergy destruction dominates the r_k , which confirms that the reduction in the exergy destruction cost is significant.

5.4. Process carbon emission reduction optimization

The improved OTM system (Case 3) enriches the CO₂ produced by the process. If these flue gases can be further converted into chemicals, it will not only reduce carbon emissions, but also improve the added value of the system [37].

Therefore, the carbide slag produced by the Case 3 system is used to absorb the enriched CO₂ and convert it into CaCO₃ to enter the calcination module for calcium recycling, as shown in Fig. 10, this is the so-called CO₂ mineral storage, also known as CO₂ mineralization [38,39]. In summary, we refer to this new Case 4 as the calcium looping process, which has been improved layer by layer to achieve two-stage cyclic capture of CO₂ and the resource utilization of the solid waste carbide slag. To note that, this process not only uses the CO₂ produced by the system, but also the minerals produced can be further recycled for the production of calcium carbide-acetylene, which is an energy conversion

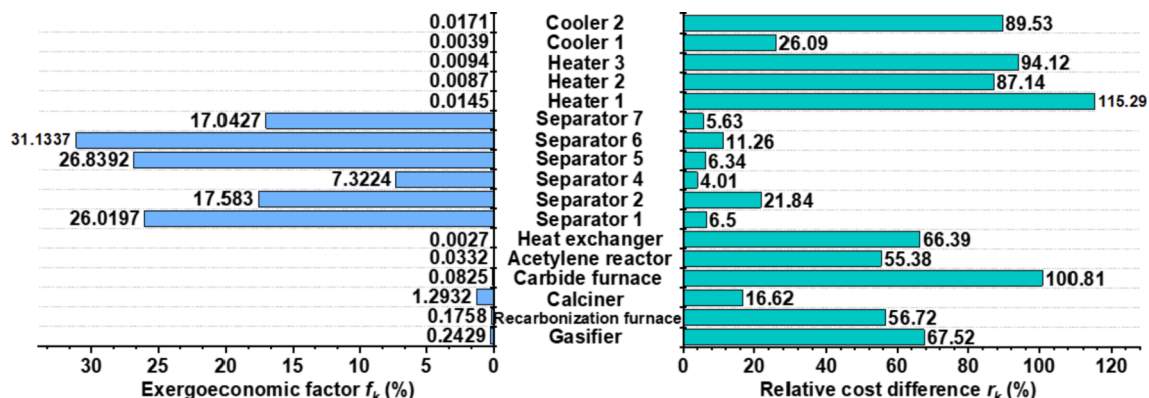


Fig. 9. Exergoeconomic factor and relative cost difference of the components for the improved system (Case 3).

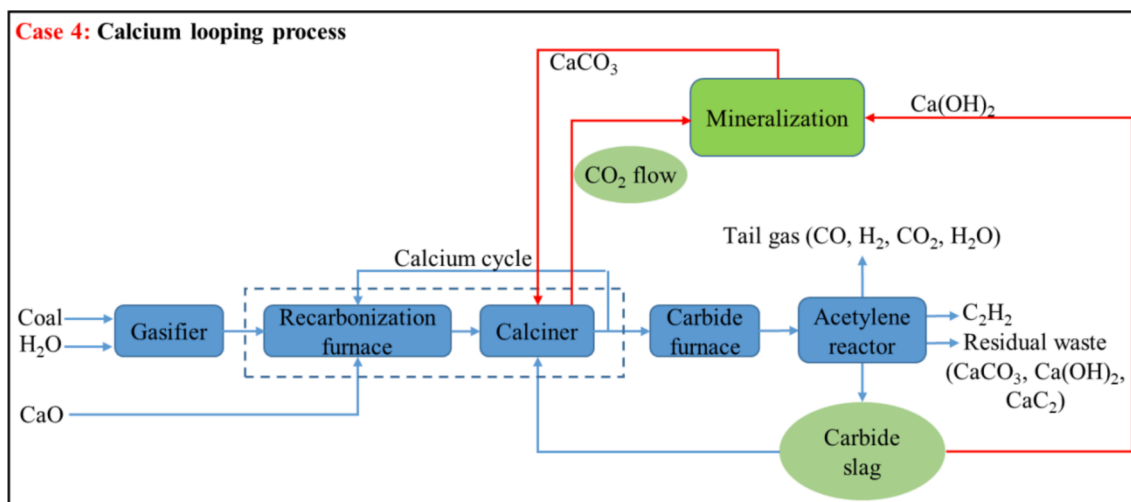
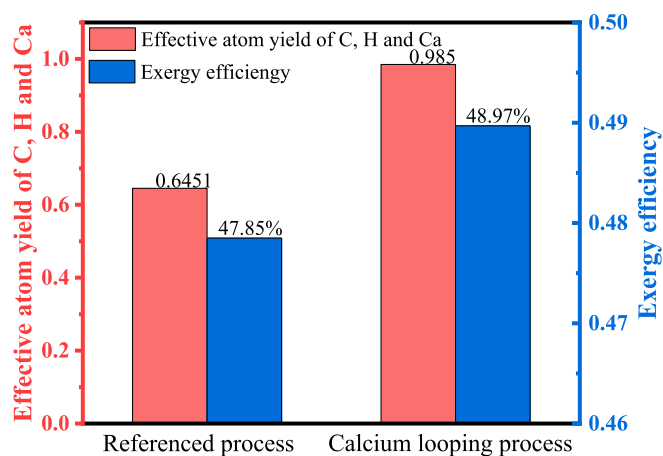


Fig. 10. Schematic diagram of the calcium looping process (Case 4).

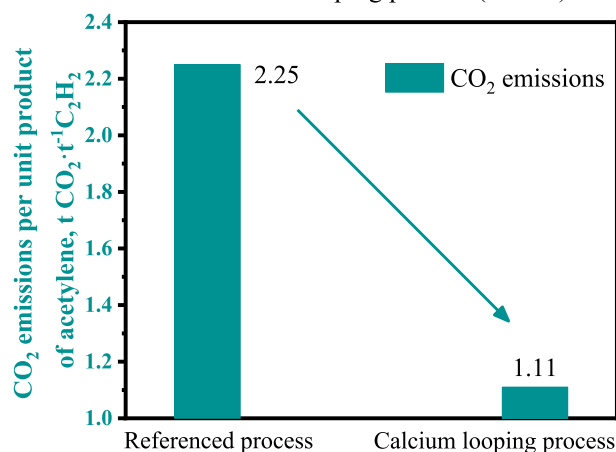
technology for energy conservation and emission reduction.

In order to investigate the performance of this calcium looping process, the performances of the referenced OTM process (Case 1) and

the calcium looping process (Case 4) were compared. Fig. 11(a) displays the effective atom yield and exergy efficiency of these two systems. Compared with the referenced OTM system (Case 1), the calcium



(a) Comparison of effective atomic yield and exergy efficiency of referenced OTM process and calcium looping process (Case 4)



(b) Comparison of CO₂ emissions between referenced OTM process (Case 1) and calcium looping process (Case 4)

Fig. 11. Performance comparison of referenced OTM process (Case 1) and calcium looping process (Case 4).

looping process has the better effective atom yield and exergy efficiency. Moreover, calcium looping process improves the exergy efficiency of Case 3, and the exergy efficiency of Case 4 reaches 48.97%. From Fig. 11 (b), the calcium looping process has lower CO₂ emission than the referenced process.

Further, the direct equivalent carbon footprint and the carbon footprint in the form of CO₂ among the referenced OTM system (Case 1) and calcium looping system (Case 4) were compared, as shown in Fig. 12. Among them, the CO₂ emission of the Case 4 is lower than the referenced OTM process (Case 1). Fig. 12 also shows the emission reduction of carbide slag (CS) in the system for per ton of target product acetylene produced, and the reduction in the input of CaO raw materials for per ton of carbide slag recycled. Finally, Case 4 achieves the lowest carbon emissions and the significant reduction in CaO input. Therefore, the improved calcium looping process (Case 4) can not only improve the efficiency of the system and reduce carbon emissions, but also convert waste gases into high value-added products, which is indeed a clean and efficient potential production process.

6. Conclusions

In summary, a novel carbon-calcium compound conversion process of calcium carbide-acetylene production is proposed, which has satisfactory effect of carbon capture and calcium carbide waste slag reuse. Then, the material conversion, exergy, exergoeconomic and carbon emission analyses are conducted to comprehensively compare the proposed system with the referenced process. From the evaluations and discussions, the conclusions are drawn below:

- (1) Compared with the referenced calcium carbide-acetylene production system (Case 1), the proposed improved novel carbon-calcium compound conversion processes (Case 2 and Case 3) can capture the upstream CO₂ and utilize the downstream carbide waste slag, and the CO₂ capture efficiencies reach up to 92.62% and 90.35%, respectively.
- (2) The proposed process especially Case 3 performed better with C, H, Ca effective atom yield 85.41% and CO₂ capture efficiency 90.35%, compared with the referenced process (Case 1) of 64.51% and 0, respectively. Case 4 is a further improved process based on Case 3 process, which shows better performance, such as with the highest effective atom yield 98.5% etc.
- (3) Exergoeconomic analysis indicated that the carbide furnace, acetylene reactor, recarbonization furnace, gasifier and calciner are the most important components of the improved system due to the fact that these are the top five high values of sum cost rate ($\dot{C}_{D,k} + \dot{Z}_k$). Besides, the carbide furnace, acetylene reactor, recarbonization furnace and gasifier have relatively lower f_k values of 0.08%, 0.03%, 0.18% and 0.24%, respectively, showing that efforts should be made to improve system thermodynamic and equipment performance and reduce exergy destruction.
- (4) The improved calcium looping process has a higher exergy efficiency of 48.97% than the referenced process of 47.85%. Besides, calcium looping process achieves the lowest carbon emissions and the significant reduction in CaO input. In the end, it is believed that the calcium looping process is a powerful process to better realize the high efficiency, energy conservation and two-stage emission reduction of the calcium carbide production process.

CRedit authorship contribution statement

Hongxia Wang: Methodology, Software, Validation, Formal analysis, Investigation, Data curation, Writing – original draft. **Wanyi Xu:** Methodology, Investigation. **Maimoona Sharif:** Investigation. **Xiaomei Wu:** Investigation. **Guangxu Cheng:** Investigation, Supervision.

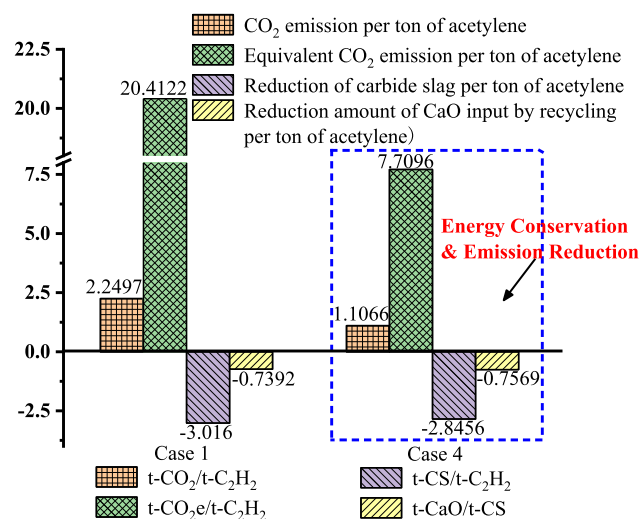


Fig. 12. Comparison of system direct equivalent carbon footprint and CaO input reduction of referenced OTM system (Case 1) and calcium looping system (Case 4).

Xiaomi Cui: Investigation. **Zaoxiao Zhang:** Conceptualization, Validation, Writing – review & editing, Supervision, Funding acquisition.

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.

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Appendix A

Thermodynamic properties and costs of exergy streams for the system of coal-based carbon-calcium composite conversion to calcium carbide and acetylene are listed in Table A3.

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