Contents lists available at ScienceDirect

Applied Energy

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

Towards net-zero emission cement and power production using Molten Carbonate Fuel Cells

Daya R. Nhuchhen^{*}, Song P. Sit, David B. Layzell

Canadian Energy Systems Analysis Research (CESAR) Initiative, University of Calgary, Calgary, AB, Canada

HIGHLIGHTS

• Design and model for a low emission cement and power production system.

- Uses molten carbonate fuel cells in fuel-flexible design that includes plastics.
- Achieves 92% reduction in process and energy emissions from cement production.
- Simultaneously produces grid power with a carbon intensity of 52 kgCO₂/MWh.
- Specific primary energy consumption for CO₂ avoided is only 1.5 to 5.9 GJ/tCO₂.

ARTICLE INFO

Keywords: Cement plant emissions Molten Carbonate Fuel Cell Carbon capture Power co-generation HDPE disposition ASPEN plus modeling

ABSTRACT

Achieving net-zero greenhouse gas emissions in cement production requires major reductions in both process and energy emissions. This study proposes an integrated low emission cement and power production (LECAPP) system that incorporates external reforming molten carbonate fuel cells to capture the CO_2 emissions from a natural gas-fired cement plant. The system uses either natural gas or high-density polyethylene to generate the hydrogen demanded by the fuel cells while producing both low-carbon electricity (1,201 kWh/t clinker with a carbon intensity of 52 kgCO₂/MWh, of which 1,000 kWh/t clinker is available for export) and a CO_2 stream for sequestration. The carbon intensity assigned to clinker production (57 kgCO₂/t clinker) is a 92% reduction from a clinker plant without carbon management. When plastics are used to generate hydrogen for the fuel cells, 144 kg plastics/t clinker would be diverted from landfills. Compared to other carbon capture methods, the LECAPP system performs better and its overall specific primary energy consumption is estimated to be in the range of 1.52–5.94 gigajoules per tCO₂ avoided. The LECAPP system offers promise as a viable technology in the transition to net zero-emission energy systems.

1. Introduction

At least 73 nations have committed to net-zero greenhouse gas (GHG) emissions by 2050 [1], creating a major challenge for the cement industry. Switching fuel supply to zero-emission sources would only address 25% [2] to 40% [3] of GHG emissions associated with cement-making since the majority of the CO_2 emissions are process-based, coming from the limestone feedstock.

Efforts to reduce both process and energy emissions are limited to developing new kinds of cement, replacing cement/concrete with other construction materials or incorporating carbon capture and storage (CCS) into the plants making the clinker that accounts for 70+% of most

types of cement [4,5]. Carbon capture technologies include amine scrubbing [6], calcium looping [7], chilled ammonia [8], electrochemical separation [9], metal oxide sorbents [10] and oxy-combustion [8].

Molten carbonate fuel cells (MCFC) have recently been identified as another powerful technology for capturing CO_2 [11] from the flue gas produced by coal or natural gas-fired power plants. They have the advantage of also generating low carbon, base load electricity [12], and high-grade waste heat [13] that could be used to produce more power using steam turbines or organic Rankine cycles.

Models incorporating MCFCs into natural gas-fired, gas turbine power plants have assessed how current density, CO₂ and fuel utilization

* Corresponding author. *E-mail address:* daya.nhuchhen@ucalgary.ca (D.R. Nhuchhen).

https://doi.org/10.1016/j.apenergy.2021.118001

Received 2 January 2021; Received in revised form 27 August 2021; Accepted 2 October 2021 Available online 21 October 2021

0306-2619/© 2021 The Authors. Published by Elsevier Ltd. This is an open access article under the CC BY license (http://creativecommons.org/licenses/by/4.0/).









Fig. 1. Schematic process flow diagram of the LECAPP system incorporated with MCFC as an integrated CO2 capture and power cogeneration system.

factors, and CO₂ concentration at the cathode inlet impacted the net electricity generation efficiency [14,15]. Others [16,17] have examined the use of MCFC with coal-fired power plants. The cost of CO₂ capture from coal or natural gas-fired power plant using MCFCs is estimated to range from \$25 to \$110/tCO₂ avoided [18,19], values competitive with amine technologies depending on the price obtained for the additional low carbon electricity.

The above-mentioned studies assumed that natural gas (NG) is being reformed to hydrogen in the anode of MCFCs. Other studies have considered external reforming of carbon-based fuels to syngas (containing H_2) which is then supplied to the MCFC to generate power [20–22] and concentrate CO₂ [23,24].

To date, two studies and one patent [25] have considered the use of MCFCs to decarbonize clinker production. While Spinelli et al. [26] provide a detailed process simulation, De Silvestri et al. [27] present with the results of an experimental study on the MCFC integrated calcium looping system in a cement plant. It should be noted that both Spinelli's and De Silvestri's designs only achieved a 70% reduction, less than that needed to reach net-zero targets.

The present study describes an integrated low emission cement and power production (LECAPP) system that incorporates external reforming MCFCs to capture the CO_2 emissions from an NG-fired cement plant. It contributes to a new body of knowledge in three ways:

First, instead of using internal reforming of NG to make hydrogen at the anode of the MCFC [25,26], this study uses external reformation of solid or gaseous fuels to generate hydrogen-rich syngas for the MCFC. This approach allows the LECAPP system to be fuel-flexible, creating opportunities for using negative-value, waste-derived solid alternative fuels, such as plastics. One previous study [21] integrated plasma arc gasification of waste-derived fuels with an MCFC to generate electricity, but their analysis did not include the CO₂ capture of its flue gas.

Second, this study presents a new MCFC model using generalized cell reaction, which facilitates assessing cell performance as a function of the syngas composition generated from the gasification of solid fuels or the reforming of gaseous fuels. This overcomes the limitation of previous models of Gibbs free energy change and Nernst voltage loss factor [14,15,28], which are developed for ideal cell reaction of the MCFC with 100% fuel utilization factor [29].

Finally, the LECAPP system described here provides detailed material and energy flows that are necessary to achieve a 90+% reduction in both process and energy emissions of clinker-making.

2. Methods

A process model of the LECAPP system (Fig. 1) was developed in ASPEN Plus software (Version 10) and used to simulate the performance of molten carbonate fuel cells (MCFCs) in the capture of CO_2 emissions from the flue gas of an NG-fueled clinker production plant. The LECAPP system incorporated the external-reforming of gaseous, liquid or solid wastes (e.g. high-density polyethylene, HDPE) to provide syngas containing hydrogen as a fuel to the MCFCs.

2.1. LECAPP system

The LECAPP system includes four subsystems: Syngas generator (SG) to produce syngas using a steam methane reformer for natural gas (Case 1: NG-based SG) or a steam gasifier for plastic wastes (HDPE, Case 2: HDPE-based SG); Molten Carbonate Fuel Cells (MCFCs) to concentrate the CO₂ and cogenerate power; Steam Turbines (ST) to recover power from high-temperature gas streams; and a CO₂ Purification Unit (CPU) with multi-stage compression, inter-stage cooling and gas/liquid separation to produce a liquid CO₂ stream. The major operating conditions of each LECAPP subsystem are shown in Fig. S1 in Supplementary (S) Information. The detailed ASPEN Plus process modeling diagrams are shown in Figs. S2 (Case 1) and S3 (Case 2).

Heat integration with the cement plant was also carried out by using the CO_2 lean stream in the LECAPP system as shown in Fig. 1, which would supply thermal energy to preheat the raw materials (16.2 GJ/hr) and the air streams (Streams 11 & 14 to 75 °C and Stream 17 to 125 °C).

The following sections describe each subsystem of the LECAPP system in greater detail.

Syngas Generator (SG). The SG was designed as an equilibrium reactor that produced the syngas containing H_2 needed to operate the MCFCs. An equilibrium reactor model was used for the SG to predict the composition of syngas, tar and unconverted carbon (C). It included 49



$m_{1}H_{2} + m_{2}CH_{4} + m_{3}CO + m_{4}CO_{2}$ $+ m_{5}H_{2}O + \sum others$ $m_{1}O_{2} + n_{2}CO_{2} + \sum others$ $m_{0}O_{2,t} + m_{1}O_{2} + n_{2}CO_{2} + \sum others$ $m_{0}O_{2,t} + m_{1}O_{2} + n_{2}CO_{2} + \sum others$ $m_{1}O_{2} + n_{2}CO_{2} + \sum others$

Fig. 2. Molten carbonate fuel cell showing: A) generalized cell reactions; B) overall mole flows balance.

chemical species (**Table S1**) and the Gibbs free energy minimization method was deployed to determine the equilibrium syngas compositions at 800 $^{\circ}$ C and a steam-to-carbon (S/C) molar ratio of 2.

To reform NG in the steam methane reformer (Case 1) or to gasify HDPE in the steam gasifier (Case 2), steam at 400 °C was produced by feeding water at 1.3 bar and 25 °C to a steam generator. The quantity of NG needed to be reformed or the HDPE to be gasified was estimated from the amount of H₂ in the syngas from the SG, which was needed to operate the MCFCs. Thermal energy demand for reforming reaction in the steam methane reformer or gasification reaction in the steam gasifier was provided by Furnace 1 that burned NG with 15% excess air supply (air-NG molar ratio of 11).

The syngas produced from the SG was cleaned and cooled to 650 °C before being fed to the anode inlet of the MCFCs. To remove and limit solid carbon or inert ash residues entering the MCFCs [30], a solid–gas separator such as an efficient cyclone or a ceramic filter was placed after the SG. Similarly, a liquid–gas separator was used after the syngas cooler to remove heavy condensable compounds. The syngas at 650 °C after the cleaning and cooling, also defined as the light syngas, consists mainly of H₂, CO, CO₂, H₂O, and traces amount of other gases including CH₄. The light syngas was fed into the anode inlet of the MCFCs. The unused chemicals at the anode outlet of the MCFCs, and the heavy hydrocarbons and unconverted carbon (shown in Figs. S2A and S3A) sepfvre burned in an oxy-boiler to produce the steam necessary for the SG.

Molten Carbonate Fuel Cells (MCFCs). In this study, an MCFC subsystem was fueled at the anode with light syngas produced from the

SG (Fig. 1). A mixture of flue gases and air was supplied to the cathode inlet of the MCFCs. There were three sources of flue gases, namely the flue gas from the clinker-making plant (Stream 1), the flue gas (Stream 12) from Furnace 1, and the flue gas (Stream 15) from Furnace 2. To provide enough oxygen at the cathode, the hot air (335 °C) from the clinker-making plant (Stream 16) and a stream of ambient air preheated to 125 °C (Stream 17) were also mixed with all the flue gases. While the amount of hot air from the clinker-making plant was kept constant, the amount of preheated ambient air supplied (Stream 17) was varied to ensure enough was oxygen available at the cathode inlet of the MCFCs. To preheat the temperature of the mixed gas stream 2' to 650 °C, Furnace 2 provided necessary thermal energy by burning NG with 15% excess air supply (air-fuel molar ratio of 11).

To estimate cell voltage and electrical current in the MCFC design, the necessary ideal overall cell reaction of the MCFC fueled by pure H_2 can be written as:

$$H_2 + CO_2 + 0.5O_2 \to H_2O + CO_2 \tag{1}$$

This shows that 1 mol of H_2 supplied at the anode inlet captures 1 mol of CO_2 from the cathode inlet, thereby releasing a pair of electrons flowing from the anode to the cathode as shown in Fig. 2A. This 100% fuel and oxygen utilization in MCFCs is, however, not possible because it results in an extreme (infinite) cell voltage loss [31]. Therefore, a generalized overall cell reaction representing anodic and cathodic cell reactions of the MCFC fueled by the light syngas at less than 100% fuel utilization can be written as:

(2)

```
m_1H_2 + m_2CH_4 + m_3CO + m_4CO_2 + m_5H_2O + n_1O_2 + n_2CO_2 \rightarrow m_1H_2 + m_2CH_4 + m_3CO + m_4CO_2 + m_5H_2O + n_1O_2 + n_2CO_2 \rightarrow m_1H_2 + m_2CH_4 + m_3CO + m_4CO_2 + m_5H_2O + n_1O_2 + n_2CO_2 \rightarrow m_1H_2 + m_2CH_4 + m_3CO + m_4CO_2 + m_5H_2O + n_1O_2 + n_2CO_2 \rightarrow m_1H_2 + m_2CH_4 + m_3CO + m_4CO_2 + m_5H_2O + n_1O_2 + n_2CO_2 \rightarrow m_1H_2 + m_2CH_4 + m_3CO + m_4CO_2 + m_5H_2O + n_1O_2 + n_2CO_2 \rightarrow m_1H_2 + m_2CH_4 + m_3CO + m_4CO_2 + m_5H_2O + n_1O_2 + n_2CO_2 \rightarrow m_1H_2 + m_2CH_4 + m_3CO + m_4CO_2 + m_5H_2O + n_1O_2 + n_2CO_2 \rightarrow m_1H_2 + m_2CH_4 + m_3CO + m_4CO_2 + m_5H_2O + m_1O_2 + n_2CO_2 \rightarrow m_1H_2 + m_2CH_4 + m_3CO + m_4CO_2 + m_5H_2O + m_1O_2 + m_2CO_2 \rightarrow m_1H_2 + m_2CH_4 + m_3CO + m_4CO_2 + m_2H_2O + m_2O_2 \rightarrow m_1H_2 + m_2CH_4 + m_3CO_2 + m_2H_2O + m_2O_2 \rightarrow m_1H_2 + m_2CH_4 + m_3CO_2 + m_2H_2O_2 \rightarrow m_2H_2O
```

where *m* and *m* represent the molar flow rates of gas species (mole/s) at the anode inlet and outlet respectively, and *n* and *n* represent the molar flow rates of gas species (mole/s) at the cathode inlet and outlet, respectively. The subscripts represent the gas species: 1 for H₂, 2 for CH₄, 3 for CO, 4 for CO₂ and 5 for H₂O for *m* and *m* at the anode and 1 for O₂ and 2 for CO₂ for *n* and *n* at the cathode of each MCFC. It was assumed here (Fig. 2B) that other chemical species than these 5 in the mixture of flue gas and the light syngas did not engage in any reactions when they flowed through the cells. However, one should note that other chemical species such as sulfur or mercury released from the solid or gaseous fuels may degrade the effectiveness of electrode and electrolyte of the fuel cell, thereby lowering cell voltage and cell life. Therefore, the contaminations and other gases should not exceed the limit as suggested by the manufacturer [17,29].

Steam Turbine (ST). The steam turbine (ST) cycle analyzed here consists of a single condensing steam turbine. At the turbine inlet, steam pressure of 130 bar [14], 176 bar [32] and 180 bar [33] has been reported in the literature. Although the temperature of steam at the turbine inlet was reported to be up to 565 °C [14], this study set the steam temperature at 540 °C at the turbine inlet to ensure material safety [33] and the evaporator pressure of 180 bar. The condenser was set at about 0.06 bar (saturation temperature of about 35 °C) and modeled to produce a liquid water stream at its exit. Other details and arrangements of the heat exchangers in the ST cycle are shown in Fig. S1C.

 CO_2 Purification Unit (CPU). The CO_2 rich stream from the waste heat recovery power cycle was cooled down to 28 °C in a cooler (refer to Fig. S2C for the LECAPP system with NG-based SG (Case 1) and Fig. S3C for the LECAPP system with HDPE-based SG (Case 2)). The cooled gas stream was first sent to a gas–liquid separator and then to the multistage compressors system at a compression ratio of 2.5 of each stage. The compressed gas stream from each stage was also cooled down to 28 °C again by an inter-stage cooler. After the 5th stage, the highpressure CO_2 stream was cold enough to liquify. Fig. S1E depicts the CPU in greater detail including a cooling tower to cool and reuse the cooling water needed in the inter-stage coolers. More details of process flow diagrams are available in Figs. S2C and S3C.

2.2. Key assumptions

Process simulation of the LECAPP system integrated into a clinkermaking plant, as shown in Fig. 1, was carried out in the ASPEN Plus simulation software (Version 10). The process simulation included the following assumptions:

- The source of the clinker flue gas and its gas composition is from a 4,200 tonne (t)/day clinker production plant fueled with natural gas. More details on the clinker production plant are provided elsewhere [2].
- A wide range of current density 700–2,000 Ampere/m² has been adopted in different studies [14,23,32,34–36]. This study has used a cell current density of 1,500 Ampere/m².
- The molar ratio of the total CO_2 at the cathode inlet to the CO_2 transfer from cathode to anode, defined here as the CO_2 utilization factor (U_{CO_2}), is 0.90.
- The molar ratio of H₂/CO₂ $\left(\frac{m_1}{m_{CO_2,t}}=1\right)$ of unity was maintained (refer to Fig. 2B).
- The fraction of oxygen in the flue gas stream at the outlet of the cathode is 0.05.
- Pressure drops in devices handling gases and liquid are 0.01 bar and 0.05 bar, respectively. The pressure drop in the solid and tar separators are 0.03 bar each.

- The MCFCs are maintained at 650 °C with negligible heat losses.
- Natural gas is assumed to be 100% methane.
- The elemental composition of HDPE is: C (86.1%); H (13.0%); N (0.0%); S (0.0%); Cl (0.0%); O (0.9%) and negligible ash content on dry weight basis; and its proximate analysis (dry weight basis) is 0.28% fixed carbon and 99.7% volatile matter [37].
- Preprocessed HDPE ready to be used is assumed available on site for gasification.
- Steam reforming and gasification reactions are assumed to reach equilibrium at the operating conditions.
- The lower heating value (LHV on a dry basis) of NG and HDPE [37] are 50.16 MJ/kg and 43.3 MJ/kg, respectively.
- The logarithmic mean temperature difference for the heat exchanger is 10 $^\circ\mathrm{C}.$
- Isentropic efficiencies of pump, compressor and turbine are 85%, 80%, and 85%, respectively.
- Mechanical efficiency for the turbine, pump, and compressor is 95% each.
- DC to AC voltage conversion in the fuel cell is 95%.
- The electricity demand for the air separation unit is 200 kWh/tO₂ [38].
- \bullet GHG emissions other than CO_2 are neglected in the emissions analysis.

2.3. MCFC model

To design the MCFC subsystem, key parameters such as fuel cell power, ideal cell efficiency (η_{ideal}) and voltage efficiency ($\eta_{voltage}$) can be estimated by using the Gibbs free energy change $\Delta G^o(T)$, enthalpy change ($\Delta H^o(T)$), entropy change ($\Delta S^o(T)$) and reversible cell voltage ($V^o(T)$) of the cell reaction [39]. The ideal cell efficiency is the ratio of the Gibbs free energy change to the enthalpy change. The voltage efficiency is the ratio of the actual cell voltage (V_{cell}) over the reversible cell voltage ($V^o(T)$) of the fuel cell operated at a temperature T (Kelvin). In the following sections, a review of existing MCFC models and a new proposed MCFC model are presented.

In the literature, the anode of the MCFC is often modeled as an equilibrium reactor where a water–gas shift reaction occurs to produce more hydrogen for the fuel cell [28,29]. This indicates that the overall Gibbs free energy change and the cell voltage are a function of the gas composition of the fuel source at the anode inlet. However, existing studies [14,15,28] adopted a temperature-dependent (Kelvin) model of the Gibbs free energy change which was derived only for the hydrogen oxidation reaction. The temperature-dependent model to estimate the reversible cell voltage and the model containing the gas composition of the ideal cell reaction to estimate Nernst voltage loss factor were mainly used in the existing study [29] as shown below.

$$\Delta G^o(T) = 242000 - 45.8T \tag{3a}$$

$$V(T,P) = \frac{\Delta G^{o}(T)}{2F} - \frac{RT}{2F} \ln \left(\frac{P^{a}_{H_{2}O} \times P^{a}_{CO_{2}}}{P^{a}_{H_{2}} \times P^{c}_{O_{2}} \otimes Y^{c}_{CO_{2}}} \right)$$
(3b)

The terms F and R are the Faraday constant (96,485 C per mole of electron transfer) and universal gas constant (8.314 J/mole/K), respectively. The Nernst voltage loss factor uses the partial pressure of gases involved in the standard hydrogen oxidation reaction with a 100% fuel utilization factor as shown in Eq. (1). As the MCFC system incorporates more gases than just hydrogen, as shown in Eq. (2), this study has presented a new model using the enthalpy change and entropy change of the generalized cell reaction as:

$$\Delta G^{o}(T) = \Delta H^{o}(T) - T\Delta S^{o}(T).$$
(4a)

$$\Delta H^{o}(T) = \Delta H^{o}(298) + (\dot{m_{5}} - m_{5}) \times I(C_{p})_{H_{2}O}^{T} + (\dot{m_{1}} - m_{1}) \times I(C_{p})_{H_{2}}^{T} + (\dot{m_{2}} - m_{2}) \times I(C_{p})_{CH_{4}}^{T} + (\dot{m_{3}} - m_{3}) \times I(C_{p})_{CO}^{T} + (\dot{n_{1}} - n_{1}) \times I(C_{p})_{O_{2}}^{T}.$$
(4b)

$$\Delta S^{o}(T) = \Delta S^{o}(298) + (m_{5}^{'} - m_{5}) \times I\left(\frac{C_{p}}{T}\right)_{H_{2}O}^{T} + (m_{4}^{'} - m_{4} + n_{2}^{'} - n_{2}) \times I\left(\frac{C_{p}}{T}\right)_{CO_{2}}^{T} + (m_{1}^{'} - m_{1}) \times I\left(\frac{C_{p}}{T}\right)_{H_{2}}^{T} + (m_{2}^{'} - m_{2}) \times I\left(\frac{C_{p}}{T}\right)_{CH_{4}}^{T} + (m_{3}^{'} - m_{3}) \times I\left(\frac{C_{p}}{T}\right)_{CO}^{T} + (n_{1}^{'} - n_{1}) \times I\left(\frac{C_{p}}{T}\right)_{O_{2}}^{T}.$$
(4c)

where $\Delta H^o(298)$ and $\Delta S^o(298)$ are the enthalpy and entropy changes, respectively of the generalized cell reaction at the reference temperature condition (298 K). $I(C_p)_s^T$ and $I(\frac{C_p}{T})_s^T$ are the results of the integration of the specific heat capacity (C_p) and $\frac{C_p}{T}$ of gas species (s), respectively. The specific heat capacity of gas (J/mole/K) a function of temperature (T) can be expressed [40] as:

$$C_p(T) = A + BT + CT^2 + DT^3$$
(4d)

The constant terms A, B, C and D are presented in **Table S2**. A summary of the derivation of enthalpy change and entropy change is presented in **Appendix A**.

Using the Gibbs free change, the Nernst cell voltage (V(T, P)) can be estimated using reversible cell voltage $(V^o(T))$ and Nernst cell voltage loss (V_{loss}) .

$$V(T,P) = V^{o}(T) - V_{loss}$$
(5a)

electron leakage through the electrolyte and other contaminations. They are known as activation, ohmic, and concentration polarization losses. While the activation polarization losses occur mainly to overcome the activation energy of the electrochemical reaction on the catalytic surfaces, the ohmic polarization losses are due to the flow of current. The concentration polarization loss, on the other hand, is due to the mass transport limitations of the reactants [41]. Therefore, the actual cell voltage was estimated as:

$$V_{cell} = V(T, P) - (R_a + R_c + R_{ohmic})i_{cell}$$
(6a)

where R_a and R_c are the internal cell resistances due to concentration and activation polarizations at the anode and cathode of the MCFC, respectively. R_{ohmic} is the ohmic cell resistance that results in an ohmic polarization loss. These cell resistances can be determined [35] as:

$$R_{ohmic} = 5.0 \times 10^{-5} \exp\left(3,016\left(\frac{1}{T} - \frac{1}{923}\right)\right)$$
(6b)

$$R_a = 22.7 \times 10^{-10} \exp\left(\frac{53,500}{RT}\right) \times p_{H_2}^{a^{-0.42}} \times p_{H_2o}^{a^{-0.17}} \times p_{CO_2}^{a^{-1.00}}$$
(6c)

$$R_c = 7.5 \times 10^{-10} \exp\left(\frac{77,229}{RT}\right) \times p_{O_2}^{c} \stackrel{-0.43}{\longrightarrow} \times p_{CO_2}^{c} \stackrel{-0.09}{\longrightarrow}$$
(6d)

$$V_{loss} = \frac{RT}{2m_{CO_2}^{t}F} ln \left(\frac{\left(y_{H_2}^{a,e} \frac{p^{a,e}}{P^o} \right)^{m_1} \times \left(y_{CH_4}^{a,e} \frac{p^{a,e}}{P^o} \right)^{m_2} \times \left(y_{CO_2}^{a,e} \frac{p^{a,e}}{P^o} \right)^{m_3} \times \left(y_{CO_2}^{a,e} \frac{p^{a,e}}{P^o} \right)^{m_4} \times \left(y_{H_2O}^{a,e} \frac{p^{a,e}}{P^o} \right)^{m_5} \times \left(y_{CO_2}^{c,e} \frac{p^{e,e}}{P^o} \right)^{m_5} \times \left(y_{CO_2}^{c,e} \frac{p^{e,e}}{P^o} \right)^{m_5} \times \left(y_{CO_2}^{a,e} \frac{p^{a,e}}{P^o} \right)^{m_5} \times \left(y_{CO_2}^{a,e} \frac{p^{a$$

$$V^{o}(T) = \frac{|\Delta G^{o}(T)|}{2m_{CO,t}F}$$
(5c)

where the superscripts 'a', 'c', 'e', and 'i' represent the anode, cathode, exit, and inlet of the fuel cell, respectively. The term P^o refers to the standard atmospheric pressure condition. More details are provided in **Section S5.**

To validate the generalized MCFC model, results of both Eq. (4a) and Eq. (5a) were compared with the existing models Eqs. (3a) and (3b). The results of the validation are summarized in **Appendix B**. The results show that the new model developed here predicts the Nernst voltage loss factor more accurately because it incorporates the changes in concentration of gases resulted from the excess fuel supply at the anode or oxygen supply at the cathode of the MCFC.

In addition to the Nernst voltage loss, there are also losses due to

where p_s is the average partial pressure at anode and cathode of a gas species ('s') with respect to the reference pressure. *T* is the average cell temperature in Kelvin and i_{cell} is the current density of the fuel cell in (Ampere/m²). Validation of the model predicted actual cell voltage with the experimental result published by Milewski et al. [42] is provided in **Appendix B**. The results confirm that the new MCFC model has a better prediction accuracy than the existing model.

2.4. Calculations

MCFC: The DC efficiency of a fuel cell can be calculated as:

$$\eta_{MCFC,DC} = \eta_{ideal} \times \eta_{voltage} \tag{7a}$$

The AC efficiency of the fuel cell can be expressed as follows where η_{dc-ac} is the DC to AC conversion efficiency:

$$\eta_{MCFC,AC} = \eta_{dc-ac} \times \eta_{ideal} \times \eta_{voltage}$$
(7b)



Fig. 3. Energy (E) and CO_2 (e) flows in the clinker-making plant and power plant in the reference (ref) and LECAPP (after) scenarios. [$e_{fuel,LECAPP}$ is the carbon emissions from the intrinsic fuel demand in the LECAPP system]

The AC power from the fuel cell (MCFC) can be calculated as:

$$P_{MCFC} = \eta_{dc-ac} \times \eta_{ideal} \times \eta_{voltage} \times |\Delta H^o(T)|$$
(7c)

The MCFC power production (P_{MCFC}) can also be determined with the help of actual cell voltage and the Faradaic current generation of the fuel cell, which is also summarized in **Section S5**.

Similarly, a fuel cell can also be characterized by using the amount of fuel and oxygen utilized during its operation. The fuel utilization factor (U_f) is defined as the ratio of the fuel consumed by the fuel cell to the fuel supplied at the anode inlet (refer to Fig. 2B) and can be expressed as:

$$U_{f} = \frac{LHV_{CH_{4}} \times \left(m_{CH_{4}} - \dot{m_{CH_{4}}}\right) + LHV_{CO} \times \left(m_{CO} - \dot{m_{CO}}\right) + LHV_{H_{2}} \times \left(m_{H_{2}} - \dot{m_{H_{2}}}\right)}{LHV_{CH_{4}} \times m_{CH_{4}} + LHV_{CO} \times m_{CO} + LHV_{H_{2}} \times m_{H_{2}}}$$
(7d)

where LHV_{CH4} , LHV_{CO} and LHV_{H_2} are respectively the lower heating value of methane (803 MJ/kmole), carbon monoxide (283 MJ/kmole) and hydrogen (242 MJ/kmole) [43]. Depending upon the DC or AC power demand, the chemical to power conversion efficiency could be determined by multiplying the fuel utilization factor (U_f) with Eq. (7a) or Eq. (7b). The oxygen utilization factor is defined as the ratio of oxygen consumed in the cathode to the total oxygen supplied (Fig. 2B) at the cathode inlet ($(n_1 - n_1)/n_1$).

Overall LECAPP System Power Generation Efficiency. Overall LECAPP system power generation efficiency (the net power efficiency) is defined as a ratio of net power produced over the total fuel consumed in the system.

$$\eta_{System} = \frac{P_{MCFC} + \sum \dot{W}_{TURB} - \sum \dot{W}_{COMP} - \sum \dot{W}_{FAN} - P_{ASU}}{LHV_{NGorplastic} \times W_8 + LHV_{NG} \times W_{10} + LHV_{NG} \times W_{13}}$$
(8)

where $\sum \dot{W}_{TURB}$ is the total power generation from ST; $\sum \dot{W}_{COMP}$ is the sum of power consumed by the compressors used in the CPU; $\sum \dot{W}_{FAN}$ is the sum of power consumption by the induced draft fans within the LECAPP system; P_{ASU} is the power consumption of the air separation unit (ASU) for oxygen production and w_i are the mass flow rates of fuels in the hydrogen generator and furnaces as shown in Fig. 1 where the subscripts denote the flow stream numbers.

Emissions Allocation and Total CO₂ Avoided. Without the LECAPP system, the total direct CO₂ emission flow rate (tCO_2/hr) of the clinker-making plant (**Stream 1**) is *e*_{direct.ref}. The reference emission

intensity (*I*) of clinker $(tCO_2/t \text{ clinker})$ of the cement industry with a clinker production rate of TPH (tonne per hour) was estimated as:

$$I_{direct,clinker,ref} = \frac{e_{direct,ref}}{TPH}$$
(9a)

Depending on the type of fuel used in power plants, the reference emission intensity ($I_{direct,power,ref}$) of electricity generation may vary from 25 to 1,152 kgCO₂/MWh [44]. Therefore, the CO₂ avoided may change accordingly. As a case study, this study used the reference emission intensity of a natural gas-fired combined cycle power plant of 331 kgCO₂/MWh [45].

The total direct CO₂ emissions (in tCO₂/hr) of the LECAPP system integrated clinker-making plant includes the reference case CO₂ emissions from the clinker-making ($e_{direct,ref}$), the CO₂ emissions related to the fuel consumed by the LECAPP system ($e_{fuel,LECAPP}$) and the residual CO₂ leaving the LECAPP system ($e_{direct,after}$). Since the integrated system produces two final saleable products, i.e., clinker (TPH) and net exportable power (P_{net} in MW), the residual CO₂ emissions ($e_{direct,after}$) could be allocated proportionally to the two products (CO₂ Allocation Method 1) as shown below:

$$I_{residual,clinker} = \frac{e_{direct,ref}}{e_{fuel,LECAPP} + e_{direct,ref}} \times e_{direct,after} \times \frac{1}{TPH}$$
(9b)

$$I_{residual,power} = \frac{e_{fuel,LECAPP}}{e_{fuel,LECAPP} + e_{direct,ref}} \times e_{direct,after} \times \frac{1}{P_{net}}$$
(9c)

Alternately, the residual CO_2 emission could be allocated solely to either the clinker or the power. The former approach results in emission intensities (CO_2 Allocation Method 2) as:

$$I_{residual,clinker} = \frac{e_{direct,after}}{TPH}$$
(9d)

$$I_{residual,power} = 0 \tag{9e}$$

The latter approach (CO₂ Allocation Method 3) results in:

$$I_{residual,clinker} = 0 \tag{9f}$$

$$I_{residual,power} = \frac{e_{direct,after}}{P_{net}}$$
(9g)

Irrespective of the approaches described above, the total CO_2 avoided from the LECAPP system integrated clinker-making plant (t CO_2 /hr)

Table 1

Material flow data of major streams in the LECAPP system with NG-based SG (Stream numbers are shown in Fig. 1).

Stream	T, °C	p, bar	m, kg/s	M, kmole/s	Molar composition, %						
					CH ₄	H ₂	H ₂ O	CO_2	CO	N ₂	02
1	200	1.10	90.9	2.92	0.0	0.0	14.7	27.9	0.0	55.7	1.0
2	650	1.07	330.8	11.39	0.0	0.0	10.0	10.3	0.0	70.5	8.9
3	650	1.06	267.5	9.81	0.0	0.0	11.7	1.2	0.0	81.9	5.0
4	650	1.15	17.3	1.65	0.2	63.9	16.0	4.3	15.6	0.0	0.0
5	650	1.05	80.6	2.71	0.0	6.5	42.4	47.6	3.5	0.0	0.0
6	920	1.04	85.8	2.74	0.0	0.0	48.4	50.6	0.0	0.0	1.0
7	28	96.36	61.9	1.42	0.0	0.0	0.1	97.9	0.0	0.0	1.9
8	25	1.30	5.3	0.33	1.0	0.0	0.0	0.0	0.0	0.0	0.0
9	25	1.30	11.9	0.66	0.0	0.0	1.0	0.0	0.0	0.0	0.0
10	25	1.30	3.2	0.20	1.0	0.0	0.0	0.0	0.0	0.0	0.0
11	75	1.09	63.2	2.19	0.0	0.0	0.0	0.0	0.0	0.8	0.2
12	850	1.08	66.4	2.39	0.0	0.0	16.7	8.3	0.0	72.4	2.6
13	25	1.30	2.5	0.16	1.0	0.0	0.0	0.0	0.0	0.0	0.0
14	75	1.09	50.3	1.74	0.0	0.0	0.0	0.0	0.0	0.8	0.2
15	650	1.08	52.9	1.90	0.0	0.0	16.7	8.3	0.0	72.4	2.6
16	335	1.10	38.4	1.33	0.0	0.0	0.0	0.0	0.0	0.8	0.2
17	125	1.09	82.3	2.85	0.0	0.0	0.0	0.0	0.0	0.8	0.2
18	267	1.10	267.5	9.81	0.0	0.0	11.7	1.2	0.0	81.9	5.0
19	28	1.00	23.9	1.32	0.0	0.0	100.0	0.0	0.0	0.0	0.0

 Table 2

 Material flow data of major streams in the LECAPP system with HDPE-based SG (Stream numbers are shown in Fig. 1).

Stream	T, °C	p, bar	m, kg/s	M, kmole/s	Molar composition, %						
					CH ₄	H ₂	H_2O	CO_2	CO	N_2	02
1	200	1.10	90.9	2.92	0.0	0.0	14.7	27.9	0.0	55.7	1.0
2	650	1.07	340.2	11.73	0.0	0.0	10.1	10.2	0.0	70.7	8.9
3	650	1.06	275.8	10.12	0.0	0.0	11.7	1.2	0.0	81.9	5.0
4	650	1.15	25.0	1.94	0.1	55.2	19.0	7.0	18.6	0.0	0.0
5	650	1.05	89.4	3.02	0.0	7.8	40.1	47.6	4.5	0.0	0.0
6	943	1.04	96.4	3.05	0.0	0.0	47.5	51.5	0.0	0.0	1.0
7	28	95.40	70.3	1.61	0.0	0.0	0.1	98.0	0.0	0.0	1.9
8	25	1.01	7.0	Not Applicable							
9	25	1.30	18.0	1.00	0.0	0.0	1.0	0.0	0.0	0.0	0.0
10	25	1.30	3.5	0.22	1.0	0.0	0.0	0.0	0.0	0.0	0.0
11	75	1.09	70.0	2.43	0.0	0.0	0.0	0.0	0.0	0.8	0.2
12	850	1.08	73.6	2.65	0.0	0.0	16.7	8.3	0.0	72.4	2.6
13	25	1.30	2.5	0.16	1.0	0.0	0.0	0.0	0.0	0.0	0.0
14	75	1.09	50.1	1.74	0.0	0.0	0.0	0.0	0.0	0.8	0.2
15	650	1.08	52.6	1.89	0.0	0.0	16.7	8.3	0.0	72.4	2.6
16	335	1.10	38.4	1.33	0.0	0.0	0.0	0.0	0.0	0.8	0.2
17	125	1.09	84.8	2.94	0.0	0.0	0.0	0.0	0.0	0.8	0.2
18	311	1.10	275.8	10.12	0.0	0.0	11.7	1.2	0.0	81.9	5.0
19	28	1.00	26.1	1.45	0.0	0.0	100.0	0.0	0.0	0.0	0.0

should be the same and can be calculated as:

$$CO_{2,avoided} = (I_{direct,clinker,ref} - I_{residual,clinker}) \times TPH + (I_{direct,power,ref} - I_{residual,power}) \times P_{net}$$
(10)

Specific Primary Energy Consumption for CO2 Avoided (SPECCA). The SPECCA is one way to characterize the efficacy of a CO₂ capture system by evaluating its energy efficiency and net intrinsic energy requirements for making cleaner products [26,46]. In the LECAPP system integrated clinker-making plant, the total energy input includes the energy needed to produce clinker (thermal and electrical) and the thermal energy supplied to operate the LECAPP system. Since the thermal energy supplied to the LECAPP system not only captures CO₂ emissions but also cogenerates low-carbon power, an imaginary reference system is created. This reference system includes the clinkermaking plant and a reference power plant without CO₂ capture. A reference power plant is also selected to estimate the thermal energy demand (Ethermal for power, ref in GJ/hr) needed to produce the same power P_{net} as the LECAPP system and its resulting CO₂ emissions $(e_{power,ref}$ in tCO₂/hr). The description of the imaginary reference system as compared with the LECAPP system integrated clinker-making plant,

and their respective energy and CO_2 emissions flows are illustrated in Fig. 3. Using the sum of energy (*E*) flows in GJ/hr and the sum of CO_2 emissions (*e*) flow in tCO₂/hr in the reference and LECAPP scenarios, the SPECCA can be estimated as:

$$SPECCA\left(\frac{GJ}{tCO_2}\right) = \frac{\sum \left(E_{after} - E_{ref}\right)}{\sum \left(e_{ref} - e_{after}\right)} \left(\frac{\frac{GJ}{hr}}{\frac{tCO_2}{hr}}\right)$$
(11)

The subscript 'after' denotes the LECAPP system integrated clinkermaking plant. The subscript 'ref' describes two separate reference systems: the clinker-making plant and the reference power plant (PP) with an efficiency of η_{pp} without CO₂ capture. As shown in Fig. 3, the LECAPP system does not affect the thermal energy and electricity demands in the clinker-making plant and their CO₂ emissions flows. Therefore, the overall SPECCA of the LECAPP system was evaluated by applying and simplifying Eq. (11) as:

$$SPECCA_{overall} = \frac{E_{thermal,LECAPP} - E_{thermal \ for \ power,ref}}{e_{direct,ref} + e_{power,ref} - e_{direct,after}}$$
(12)

In addition to the overall SPECCA of the LECAPP system, this study

Table 3

Major characteristics of MCFC and their comparison between two examined LECAP systems.

Item	Parameter	Unit	Case 1	Case 2		
			NG-	HDPE-		
			Daseu 30	Dased 3G		
1	CO ₂ transfer from	kmole/hr	3,798	3,866		
	Cathode to Anode	014	050			
2	Change in enthalpy	GJ/hr	-958	-983		
3	Change in Gibbs free		-751	-766		
4	Ideal efficiency	%	78.4	77.9		
5	Reversible cell voltage	V	1.025	1.026		
6	Nernst voltage loss factor		0.070	0.075		
7	Nernst cell voltage		0.954	0.952		
8	Other cell voltage losses		0.203	0.200		
9	Actual cell voltage		0.752	0.751		
10	Voltage efficiency	%	73.3	73.2		
11	Fuel cell efficiency (DC)		57.5	57.0		
12	Fuel cell AC power	MW	145	148		
13	Fuel cell efficiency (AC)	%	54.6	54.2		
14	Chemical energy flowing into MCFC	GJ/hr	1,191	1,310		
15	Chemical energy flowing out from MCFC		250	344		
16	Fuel utilization factor	%	79.0	73.8		
17	Chemical to electricity		43.2	40.0		
	conversion efficiency					
18	Oxygen utilization factor		51.8	51.5		
19	Oxygen demand in oxy-	tO ₂ /day	451	599		
	boiler					
Footno	otes by item numbers:					
1: Fron	n the Aspen Model	7: Item 5 – Item 6	13: Calcula (7b)	ted using Eq.		
2: Calculated using Eq. (4b)		8: Calculated using Eq. (6a)	14–15: Fro Model	m the Aspen		
3: Calculated using Eq. (4a)		9: Item 7 – Item 8	16: (Item 1 ∸ Item 14	4 – Item 15)		
4: Item 3 ÷ Item 2 (%)		10: Item 9 ÷ Item 5 (%)	- Item 14 17: Item 13 (Fraction)			
5: Calc	ulated using Eq. (5c)	11: Item $10 \times \text{Item}$	18–19: From the Aspen			
6: Calc	ulated using Eq. (5b)	12: Calculated using Eq. (7c)	mouci			

also evaluates the SPECCA for the clinker-making plant and power plant separately. In order to do that, the total thermal energy supplied to the LECAPP system ($E_{thermal.LECAPP}$ in GJ/hr) is needed to be distributed to clinker and power. This was done in two ways: (a) In proportion to the respective CO₂ emissions input to the LECAPP system as described in the CO₂ Allocation Method 1, and (b) To match the efficiency of displaced grid power. The first energy allocation method results in:

$$E_{thermal,power} = \frac{e_{fuel,LECAPP}}{e_{fuel,LECAPP} + e_{direct,ref}} \times E_{thermal,LECAPP}$$
(13a)

$$E_{thermal,clinker} = \frac{e_{direct,ref}}{e_{fuel,LECAPP} + e_{direct,ref}} \times E_{thermal,LECAPP}$$
(13b)

The second energy allocation method results in:

$$E_{thermal,power} = \frac{P_{net}}{\eta_{PP}} \times 3.6 \tag{14a}$$

$$E_{thermal,clinker} = E_{thermal,LECAPP} - \frac{P_{net}}{\eta_{PP}} \times 3.6$$
(14b)

Therefore, the SPECCA for clinker either using the first or the second energy allocation method was estimated by applying and simplifying Eq. (11) only to the clinker-making plant before and after the LECAPP

Table 4

Energy and $\rm CO_2$ flows in HDPE- vs NG-based SG subsystems for the 4,200 t/day clinker-making plant.

Item	Parameter	Unit	Case 1	Case 2				
			NG-based	HDPE-				
			SG	based SG				
1	Steam Supply	tH ₂ O/day (kgH ₂ O/t clinker)	1,032 (246)	1,556 (370)				
	Total Fuel Supply	102						
2	NG for H ₂ production	GJ/hr (GJ/t	958 (5.48)	0				
3	HDPE for H ₂	clinker)	0	1,087				
4	production		E7E (2.20)	(6.21)				
4 5	NG for Furnace 2		458 (2.62)	456 (2.60)				
6	Total energy in		1,992	2,181				
			(11.38)	(12.46)				
	Electrical Power							
7	MCFC	MW (kWh/t	145.4	147.9				
	a	clinker)	(831)	(845)				
8	Steam turbine		63.0 (360)	64.1 (366)				
9	Gross generation		208	(1 211)				
10	Air separation unit		-3.8	-5.0(-29)				
	···		(-21)					
11	Compressor for		-22.3	-25.3				
	purification		(-127)	(-145)				
12	Induction fan		-6.6	-7 (-42)				
12	Net generation		(-38)	174 (007)				
15	Net generation		(1.004)	1/4 ())/)				
14	Net Power Efficiency	%	31.8	28.8				
	CO ₂ Balance							
15	In CO ₂ from clinker-	tCO2/day (kgCO2/	3 098	3 098				
10	making	t clinker)	(738)	(738)				
16	CO ₂ added to the		2,621	3,340				
	LECAPP system		(624)	(795)				
17	From NG in SMR		1,261 (300)	0				
18	From NG in Furnace 2		757 (180)	839 (200)				
19	From NG in Furnace 2		603 (144)	600 (143)				
20	From HDPE in SG		0	1,901 (453)				
21	Total CO ₂ in		5.719	6.438				
			(1,362)	(1,533)				
	Out							
22	CO ₂ liquid for storage	tCO ₂ /day (kgCO ₂ /	5,273	5,984				
	2 1 0	t clinker)	(1,255)	(1,425)				
23	$\rm CO_2$ in the condensed		0.06	0.07				
	water		(0.015)	(0.016)				
24	CO ₂ in stack		446 (106)	454 (108)				
25	Total CO ₂ out		5,719	0,438				
26	% of CO ₂ in the stack	%	7.8	7.0				
27	% of the total CO ₂	%	92.2	93.0				
	capture rate							
Footno	tes by item numbers:							
1–5: Fr	om the Aspen Model	16: Items (17 + 18 +	19 + 20)					
6: Item	s(2+3+4+5)	17–20: From the Asp	en Model					
7-9: Fr 9: Sum	on the Aspen Model of Items $(7 + 8)$	21: Item 15 + Item 1 22-24: From the Asp	o en Model					
10-12:	From the Aspen Model	22-24: From the Aspen Model 25: Items $(22 + 23 + 24)$						
13: Iter	n 9 – Items (10 + 11 +	26: Item 24 ÷ Item 21 (%)						
12)	10 (7) (1000							
14: Iter 3600	n 13 ÷ (Item 6 × 1000 ÷) (%)	27: 100 – Item 26 (%)					
15: Fro	m the Aspen Model							

system as:

$$SPECCA_{clinker} = \frac{E_{thermal,clinker}}{e_{direct,ref} - \frac{e_{thermal,clinker}}{e_{forter,fort,ref} + e_{direct,after}} \times e_{direct,after}}$$
(15a)

Applying and simplifying Eq. (11) only to the power plant, the



Fig. 4. Energy and CO₂ flow diagrams for LECAPP system with A) NG-based SG and B) HDPE-based SG subsystems. [Note: ASU-Air separation unit, COMP.-Compressors in CPU, F1-Furnace 1, F2-Furnace 2, FANs-Induction fans power, HDPE-High-density polyethylne, MCFC-Molten carbonate fuel cell, P-Electrical Power, ST-Steam turbinel

SPECCA for power was evaluated as: -

$$SPECCA_{power} = \frac{E_{thermal,power} - E_{thermal for power,ref}}{e_{fuel,LECAP}} \times e_{direct,after}$$
(15b)

-

2.5. ASPEN Plus process modeling

ASPEN Plus version 10 was used to develop a process model of the LECAPP system. Peng Robinson calculation method was deployed to examine thermodynamic and chemical analyses. As Case 1 did not need to handle non-conventional solids such as ash and HDPE, but still required to handle conventional solid like pure carbon (C), the MIXCISLD stream class in ASPEN Plus (Mixed and Conventional Inert Solid) was selected. In Case 2, the MIXCINC stream class in ASPEN Plus (Mixed, Conventional Inert Solid and Non-conventional Solid) was used in the simulation to handle non-conventional solids.

The syngas generator (SG), furnaces and oxy-boiler used in the simulation were represented by Gibbs Reactor Module from ASPEN Plus. Since there is no separate module for the MCFC subsystem in Aspen Plus, the anode chamber of the MCFC was simulated as an equilibrium Gibbs Reactor Module. In the anode chamber, the input light syngas and the CO2 and O2 in the carbonate ions transferred from the cathode underwent simultaneous chemical reactions such as oxidation to form steam, reforming of unconverted CH₄ to form H₂, and water gas shift of CO to

Table 5

CO2 emissions distribution and CO2 avoided in HDPE- vs NG-based SG integrated LECAPP systems.

Item	Allocation Methods	Unit	Case 1	Case 2
			NG-based SG	HDPE-based SG
	1. Allocation to Clink	er and Electricity ir	n Proportion to th	eir Respective CO ₂ Inputs
1	Clinker	kgCO ₂ /t clinker	57	52
2	Electricity	kgCO ₂ /MWh	48	56
	CO2 Avoided			
3	Clinker	kgCO ₂ /t clinker	680	686
4	Electricity	kgCO ₂ /MWh	283	275
5	Total CO ₂ avoided	tCO ₂ /day	4,048	4,030
	2. Allocated only to c	linker		
6	Clinker	kgCO ₂ /t clinker	106	108
7	Electricity	kgCO ₂ /MWh	0	0
	CO ₂ Avoided	-		
8	Clinker	kgCO ₂ /t clinker	631	630
9	Electricity	kgCO ₂ /MWh	331	331
10	Total CO ₂ avoided	tCO ₂ /day	4,048	4,030
	3. Allocated only to e	electricity		
11	Clinker	kgCO ₂ /t clinker	0	0
12	Electricity	kgCO ₂ /MWh	106	108
	CO ₂ Avoided	0 -		
13	Clinker	kgCO ₂ /t clinker	738	738
14	Electricity	kgCO ₂ /MWh	225	223
15	Total CO ₂ avoided	tCO ₂ /day	4,048	4,030
Footn	otes by item numbers:			
1: Calo	culated using Eq. (9b)	6: Calculated usir	ng Eq. (9d)	11: No CO ₂ assigned to clinker (Eq. (9f))
2: Calo	culated using Eq. (9c)	7: No CO ₂ assigne	ed to electricity	12: Calculated using Eq. (9g)
	0 1 1	(Eq. (9e))	5	
3: Clin	ker reference	8: Clinker referen	ce emission	13: Clinker reference emission intensity (738 kgCO ₂ /t Clinker)– Item 11
emis	sion intensity (738	intensity (738 kg	CO ₂ /t Clinker)–	
kgC0	O ₂ /t Clinker)– Item 1	Item 6		
4: Elec	tricity reference	9: Electricity refe	rence emission	14: Electricity reference emission intensity (331 kgCO ₂ /MWh) – Item 12
emis	sion intensity (331	intensity (331 kg	CO ₂ /MWh) –	
kgC0	D ₂ /MWh) – Item 2	Item 7		
5: Calo	culated using Eq. (10)	10: Calculated us	ing Eq. (10)	15: Calculated using Eq. (10)

 $\rm H_2$ to achieve chemical equilibrium at 650 °C. Additionally, the MCFC cathode chamber was modeled as a Gas Separator Module in ASPEN Plus in which a portion of the carbon dioxide from the supplied flue gases and the oxygen in the air input was separated in proportion to the number of electrons transferred from the anode to form carbonate ions. The carbonate ions then transferred to the anode chamber. The remaining CO₂ and air then left the cathode chamber at 650 °C as CO₂ lean gas.

While the steam reforming of NG could be carried out easily in the Gibbs Reactor Module in a single step, the steam gasification of HDPE required a couple of steps. Firstly, the HDPE was defined as a non-conventional solid fuel according to its elemental compositions, proximate analysis and pyritic sulfur contents. Secondly, the HDPE composition was then converted into conventional components using an R-Yield Reactor Module of the ASPEN Plus, making the converted HDPE compositions suitable for gasification reactions in the Gibbs Reactor Module.

The inert ash from HDPE was separated (in Case 2) from the syngas (**Stream 4**) using the SSplit Module of the ASPEN Plus (See Fig. S3A). Other Modules of the ASPEN Plus such as Heat Exchanger, Turbine and Pump were deployed in the Rankine cycle to generate power from both the CO_2 rich and lean gas streams as shown in Fig. 1. The cooled CO_2 rich stream was then purified in the CPU by using Compressors, Coolers, and Liquid-Gas Separators Modules of the ASPEN Plus as shown in Figs. S2C (Case 1) and S3C (Case 2).

3. Result and discussions

3.1. Material flows through the LECAPP system

Case 1. (*LECAPP with NG-based SG*) In this case, a steam methane reformer was used to represent the SG subsystem. Other heat integrations and linkages between other subsystems of the LECAPP system are shown in Fig. S2.

The combined CO_2 at the cathode inlet would be the source of CO_2 for the MCFC operation, where the CO_2 concentration ([CO_2]) is diluted to 10.3% (**Stream 2**) from 27.9% in the clinker flue gas (**Stream 1**) by ambient air added to increase the oxygen supply (refer to Table 1). Thus, a total of 4,458 tCO₂/day (**Stream 2**, Table 1) from the combined flue gases enters the cathode including about 70% (3,098 tCO₂/day, **Stream 1**) from clinker production, with the balance coming from the LECAPP system. To achieve a 90% capture of the combined CO_2 inputs to the LECAPP system, a larger capacity (145 MW) of the MCFC subsystem is required, which is an increase of 44% relative to that for only capturing 90% CO_2 from the clinker flue gas.

The results of the simulation show that the steam methane reformer consumes 460 t/day of NG to produce 184 t/day of H₂ that is needed to operate the MCFCs subsystem, which is equivalent to 0.40 kg of H₂/kg of NG reformed, close to the published yield in the literature [47]. In addition, 276 t/day and 220 t/day of NG are needed respectively in



Fig. 5. Comparison of the estimated SPECCA for clinker, power, and overall LECAPP system NG-based SG using natural gas combined cycle (NGCC) and ultra supercritical coal fired power plants for two energy input allocation methods: Proportion to CO₂ managed (A and B) and Matching efficiency of displaced grid power (C and D).



Fig. 6. Comparison of the estimated SPECCA for clinker, power, and overall LECAPP system with HDPE-based SG using natural gas combined cycle (NGCC) and ultra supercritical coal fired power plants for two energy input allocation methods: Proportion to CO₂ managed and Matching efficiency of displaced grid power.

Furnace 1 to provide thermal energy demand in the steam methane reformer, and in Furnace 2 to preheat the mixture of gases to 650 $^\circ\text{C}.$

The gases leaving the cathode of the MCFCs has only 1.2% [CO₂], defined here as a CO₂ lean gas stream (**Stream 3**). The gases leaving the anode of the MCFC (**Stream 5**) consists of 47.6% [CO₂], defined as a CO₂ rich gas stream. Both outlet streams of the fuel cells are at 650 °C and

available for waste heat recovery power plants.

It is also noted here that in the anode chamber, the following three reactions occur: (1) Oxidation of H_2 by O_2 dissociated from the CaCO₃²⁺ ions to form steam, (2) Reforming of the residual CH₄ to produce more H_2 , CO and CO₂, and (3) The water–gas shift reaction to convert CO and steam to produce more H_2 . Because of the above reactions, there is some

unused H_2 in the anode outlet stream (**Stream 5**, Table 1). To recover the chemical energy from residual H_2 , CO and CH₄, the anode outlet stream is combusted in an oxy-boiler with oxygen instead of air to avoid diluting the CO₂ rich gas stream with N₂. The temperature of the CO₂ rich gas stream (**Stream 6**) after the oxy-boiler increases to about 920 °C. The sensible heat available from the CO₂ rich and lean gas streams could operate the ST cycle with a total steam flow rate of 202 t/ hr at 540 °C (Power generation will be discussed later).

As shown in Fig. 1, 7,413 t/day of the cooled CO_2 rich stream after waste heat recovery power plants enters the CO_2 purification unit (CPU), resulting in a 5,348 t/day of liquid CO_2 stream (**Stream 7**) with a purity of 98%, which meets the purity specification of CO_2 pipeline for geological storage [48].

About 23,112 t/day of the CO₂ lean stream (**Stream 18**) after the waste heat recovery power plant was also used to preheat the furnace combustion air (**Streams 11 & 14**) and cathode ambient air requirements (**Stream 17**) as shown in Fig. 1 as well as the raw materials for the clinker-making plant (see Fig. S2D). The cooled CO₂ lean stream containing 446 t/day of CO₂ at 267 °C was then released to the atmosphere through the stack (**Stream CL12** in Fig. S2D).

Case 2. (*LECAPP with HDPE-based SG*) In this case, a steam gasifier was deployed as the SG in the LECAPP system. Details of heat integration and linkages to other subsystems of the LECAPP system are shown in Fig. S3. To ensure 90% of the CO₂ supplied to the cathode chamber would migrate to the anode chamber of the MCFC, the composition of syngas and its flow rate needed at the anode inlet of the MCFCs are summarized in Table 2.

The simulation of the steam gasification of HDPE results in 0.31 kg of H₂/kg of HDPE gasified, which is 23% lower compared to Case 1. The dry molar composition of H₂ resulted in this study is 68.1%, close to the 62% [H₂] of experimental result that was published for the steam gasification of plastic waste in a spouted bed reactor at the steam-to-plastic waste ratio of 2 and temperature of 900 °C [49].

The lower H₂ yield in the steam gasifier compared to that in the steam methane reformer means more HDPE is needed to be gasified to meet the H₂ demand in the MCFCs subsystem, thereby increasing the heat demand for H₂ production in the SG as well as the CO₂ emissions associated with the HDPE. For instance, the NG demand in Furnace 1 is 306 t/day for the steam gasifier compared to 276 t/day for the steam methane reformer, resulting in a higher CO₂ molar flow rate in the flue gas (Stream 12) by 10.8% relative to Case 1. The total combined CO₂ flow rate to the cathode inlet (Stream 2) is 4,537 t/day, marginally higher than that in Case 1. The increased NG demand in Furnace 1 would raise the temperature of the mixed flue gas (Stream 2' in Fig. 1) because Furnace 1 produces 10.8% more flue gas (6,358 t/day in Case 2) at 850 °C (Stream 12) relative to 5,736 t/day of flue gas in Case 1. This increased in flue gas flow would reduce the NG demand of Furnace 2 which is needed to increase the temperature of the mixture of clinker flue gas and air (sum of Streams 1, 16, & 17) to 650 °C. This also explains why there is only a marginal increase in CO₂ entering the cathode inlet (Stream 2) by 1.8% in Case 2 relative to 4,458 tCO₂/day in Case 1.

The following are noteworthy points between the two cases, i.e., replacing NG with HDPE. The use of 603 t/day of dry HDPE in steam gasification could replace 460 t/day of NG. This makes it possible to divert 144 kg HDPE/t clinker, or 220 thousand tonnes of HDPE wastes from landfills annually. Similarly, a higher exhaust gas flow rate at the cathode outlet (**Stream** 3) as well as at the exit of the oxy-boiler (**Stream** 6) relative to Case 1, result in slightly more power recovery from the waste heat power generation systems. In Case 2, the steam flow rate in

the ST cycle increases to 204 t/hr from 202 t/hr in Case 1.

3.2. Energy and carbon flow comparison for Cases 1 and 2

The MCFC Subsystem. As noted previously, when the HDPE is used, there is a minor increase in the molar CO₂ flow (by 1.8%) from the cathode to the anode of the cell. This would increase the Faradaic current generation, hence 3 MW greater power generation by the MCFCs as presented in Table 3 (Item 12). Results also suggest that there is a slight decrease in the ideal efficiency of about 0.5% (Table 3, Item 13). The Nernst voltage loss factor increases by 5 mV per cell (Table 3, Item 6), which has a negligible adverse impact on the actual cell voltage (Table 3, Item 9), resulting in a very similar voltage efficiency of about 73% as the NG-based SG (Table 3, Item 10).

The use of HDPE decreases the fuel utilization factor from 79.0% to 73.8% (Table 3, Item 16), reducing the chemical to electricity conversion efficiency of the MCFC from 43.2% (Case 1) to 40.0% (Case 2) (Table 3, Item 17). This increases the unused H₂, CO, and CH₄ in Stream 5, thereby resulting in a larger oxy-boiler system relative to the NG-based SG subsystem (Fig. 1). This can be related to the estimated increase in the oxygen demand (Stream O2ASU in Figs. S2Aand S3A) in the oxy-boiler by 32.8% in Case 2 (to 599 tO₂/day) relative to 451 tO₂/ day in Case 1 (Table 3, Item 19).

Overall LECAPP System. Table 4 compares the overall performance of the LECAPP system for Case 1 (NG-based SG) and Case 2 (HDPE-based SG). Since the HDPE-based SG has a higher flue gas flow rate and oxygen demand in the oxy-boiler compared to the NG-based SG (Table 3, Item 19), more CPU and ASU powers would be needed in Case 2 (Table 4, Items 10–12). However, the increased hot gas flow rate also results in slightly more power generation from the waste heat as discussed in **subsection 3.1**, thereby increasing the gross power generation capacity from 208 MW in Case 1 to 212 MW in Case 2 (Table 4, Item 9).

Since more amount (or energy) of HDPE must be gasified than NG reformed to produce the necessary H₂ (Table 4, Items 2 & 3), the LECAPP system with the HDPE-based SG requires 1,556 t/day of steam, an increase of 51% compared to the NG-based SG (Table 4, Item 1). This steam demand, however, could be more than fulfilled from the condensed water recovered in the CPU subsystem of 2,065 t/day in Case 1 and of 2,255 t/day in Case 2 (Tables 1 and 2, Stream 19).

Recall that the CO_2 entering the LECAPP system from the clinkermaking plant remains the same at 3,098 tCO₂/day for both cases (Table 4, Item 15). The CO₂ emission from the fuel supplied to the LECAPP system adds an additional 3,340 tCO₂/day for the HDPE-based SG compared to 2,621 tCO₂/day for the NG-based SG (Table 4, Item 16), in part due to a higher carbon intensity for HDPE (73 kgCO₂/GJ_{LHV}) compared to NG (57kgCO₂/GJ_{LHV}) [2], and due to higher fuel demand for hydrogen production (Table 4, Items 2 & 3). It should be noted that from the total CO₂ balance, both cases have a similar total capture rate (Table 4, Item 27).

Fig. 4 provides an overview of the energy and CO_2 flows per tonne of clinker for the two cases incorporating the LECAPP system. Note that the energy input for Case 2 (12.46 GJ/t clinker) is about 9.5% higher than that for Case 1 (11.38 GJ/t clinker). Taking into consideration the electricity demand to support the LECAPP system, the net efficiency for power generation and export to grid is 32% (1,004 kWh/t Clinker) for Case 1 and 29% (997 kWh/t clinker) for Case 2 (Fig. 4A1 & 4B1).

For carbon flows, Case 2 (HDPE-based SG) processes 1,534 kgCO₂/t clinker, 13% more than the 1,362 kgCO₂/t Clinker that is processed in Case 1 (NG-based SG) (Fig. 4A2 & 4B2). Of this carbon, 92–93% can be captured and geologically sequestered.

3.3. CO₂ emissions intensities and total CO₂ avoided

Emissions Stored and Residual Emissions. The LECAPP system adds 2,621–3,340 tCO₂/day (Table 4, **Item 16**) of additional emissions on the 3,098 tCO₂/day that is produced by the clinker production plant (Table 4, **Item 15**). But more than 92% (Table 4, **Item 27**) of total CO₂ is captured and sequestered, leaving residual emissions of 446–454 tCO₂/ day (Table 4, **Item 24**) to the atmosphere. However, the clinker production plant plus the LECAPP system now generates two products: clinker for cement making and electricity for the public grid. In the following sections we explore three strategies for allocating the residual CO₂ emissions between clinker production and power generation:

(a) CO₂ Allocation Method 1: CO₂ emissions are allocated in the proportion of carbon in CO₂ entering the MCFC from the clinker plant (assigned to clinker production) versus the carbon in fuel to run the LECAPP system (assigned to the grid power generated) (see Eqs. (9b) and (9c)).

In Case 1, the clinker accounts for 54.2% (Table 4, Item 15/Item 21) of the total CO₂ input to the LECAPP system. Therefore, the clinker is responsible only for 242 tCO₂/day of the total residual emissions, resulting in emission intensity of 57 kgCO₂/t clinker. The remaining residual emissions (204 tCO₂/day) are assigned to the net power (176 MW, Table 4, Item 13) produced by the LECAPP system, resulting in an electricity emission intensity of 48 kgCO₂/MWh (Table 5, Item 2). For Case 2, calculated emission intensities for clinker and electricity production are 52 kgCO₂/t clinker and 56 kgCO₂/MWh, respectively (Table 5, Item 1 & 2).

In both cases, the emission intensities are less than 8% of that for the reference NG-fired clinker plant (738 kgCO₂/t clinker), and less than 17% of that for an NG-fired combined cycle power plant (331 kgCO₂/MWh).

The total CO₂ avoided through the use of the LECAPP system range from 680 to 686 kg CO₂/t clinker (Table 5, Item 3), and 275 to 283 kg CO₂/MWh (Table 5, Item 4) for Case 1 and 2, respectively. For a cement plant producing 4,200 t clinker, and a LECAPP system producing 174 to 176 MW of grid power, the total CO₂ avoided is estimated to be 4,030 to 4,048 tCO₂/day (Table 5, Item 5).

- (b) CO₂ Allocation Method 2: CO₂ emissions are allocated only to clinker production. This results in carbon-free electricity production (Table 5, Item 7), and emission intensity for clinker production of about 107 kgCO₂/t clinker (Table 5, Item 6), representing an 86% reduction compared to the reference clinker plant.
- (c) CO₂ Allocation Method 3: CO₂ emissions are allocated only to power production. This results in carbon-free clinker production (Table 5, Item 11), and emission intensity of about 107 kgCO₂/ MWh (Table 5, Item 12), representing a 68% reduction compared to the reference combined cycle power plant.

Our assessment is that CO_2 Allocation Method 1 is the fairest representation, but regional policies, tax regimes or market forces could justify other strategies for allocating residual CO_2 emissions.

3.4. SPECCA of the LECAPP system

The specific primary energy consumption for CO₂ avoided (SPECCA),

defined in **subsection 2.4**, can be used to compare the performance of carbon capture technologies. Since the efficiency of the reference power plant and its emission intensity could affect the thermal energy demand and the CO_2 avoided, two reference power plants were selected: (a) a 53.1% efficient natural gas-fired combined-cycle power plant (NGCC), and (b) a 39.5% efficient ultra-supercritical coal-fired power plant (USC) [50]. The reference emission intensity was assumed to be 331 kgCO₂/ MWh for NGCC [45] and 830 kgCO₂/MWh for USC [51].

Fig. 5 shows a summary of the estimated SPECCA of the LECAPP system with NG-based SG. When the total thermal energy input is allocated to the clinker and power in proportion to CO_2 managed (Fig. 5A & 5B), the SPECCA for clinker is 9.07 GJ/tCO₂ for both NGCC and USC power plants. However, the SPECCA for power is estimated to be -5.63 GJ/tCO₂ for NGCC and -5.01 GJ/tCO₂ for USC. The negative SPECCA for power indicates that the LECAPP system is more efficient in terms of energy expended per tonne of CO₂ emitted in generating the same amount of power vis-à-vis the reference power plants (refer to **Table S3**).

When the thermal energy input is allocated to both clinker and power to match the efficiency of displaced grid power (Fig. 5C & 5D), the SPECCA for clinker is 6.72 GJ/tCO_2 and 3.28 GJ/tCO_2 respectively for NGCC and USC. The lower SPECCA for clinker for USC indicates that the less efficient USC power plant requires more thermal energy to produce the same power as the NGCC, resulting in more energy allocation to the power than to the clinker. Under this energy allocation method, since the thermal energy allocated to power in the LECAPP system would be the same as the thermal energy needed in the reference power plant, the SPECCA for the power would be zero.

To incorporate the CO₂ avoided from both clinker and power, the overall SPECCA was also determined by combining the clinker-making plant and power generation plant into one system. For both energy allocation methods, the overall SPECCA of the LECAPP system is estimated to be 4.74 GJ/tCO_2 and 1.52 GJ/tCO_2 respectively for NGCC and USC.

Fig. 6 shows the SPECCAs for clinker, power, and overall LECAPP system for Case 2 (with HDPE-based SG). Since the thermal energy demand in Case 2 increases by 9.5%, thereby emitting 1.8% more CO₂ to the atmosphere compared to Case 1, the overall SPECCA increases to 5.94 GJ/tCO_2 for NGCC relative to 4.74 GJ/tCO_2 in Case 1, and 2.32 GJ/tCO_2 for USC relative to 1.52 GJ/tCO_2 in Case 1.

Here, the range of the overall SPECCA of the LECAPP system from 1.52 to 5.94 GJ/tCO₂ is compared with other capture technologies. It is much lower than the thermal energy demand of 8.81 GJ/tCO₂ captured by direct air capture [52]. With respect to other commercial capture technologies, the overall SPECCA of the LECAPP system is comparable to oxy-fuel (1.62 to 2.20 GJ/tCO₂) and chilled Ammonia (2.43 to 3.79 GJ/tCO₂) but superior to MEA (3.78 to 7.08 GJ/tCO₂) [8]. It also performs well against nascent capture technologies such as membrane assisted CO₂ liquefaction technology (2.80 to 3.58 GJ/tCO₂) [8] and calcium looping (3.8 to 4.9 GJ/tCO₂) [53]. However, the overall SPECCA of the LECAPP system estimated here is higher than the estimate by Spinelli et al. [26]. The difference could be attributable to the higher energy requirements in the LECAPP design with MCFCs using external syngas generator (SG) to accommodate both gaseous and solid fuels, and to a higher CO₂ capture rate of 90%.

3.5. Regional fit for the LECAPP system

When combined with a cement plant producing 4,200 t clinker/day,

the LECAPP system requires a geological storage capacity of 5,273 or 5,984 tCO₂/day for Case 1 and Case 2, respectively (Table 4, Item 22). That translates to 1.9 to 2.2 MtCO₂/year, or 76 to 88 MtCO₂ over a 40-year life for the facility.

Not all nations and regions of the world have geological storage potential sites capable of managing this quantity of CO_2 , but many do including Western Canada (3.7 GtCO₂) [54], Indonesia (163 GtCO₂), China (403 GtCO₂), the USA (812 GtCO₂), Russia (1,234 GtCO₂) and Africa (1,563 GtCO₂) [55]. In the global transition to net-zero emissions, it is likely that regions with geological storage capacity will have a significant competitive advantage for clinker production.

The LECAPP system developed here is also fuel flexible, so it could also be deployed in other parts of the world like where natural gas cost is expensive [56] or in countries like China that produces 59 million tonnes of plastic wastes per year [57].

4. Conclusions

The low emissions cement and power production (LECAPP) system described here offers a promising technology for decarbonizing both cement production and power generation in the global transition to netzero emissions. It can be added onto existing clinker production facilities to address both process and energy emissions, thereby reducing the carbon intensity of clinker production by over 92%, while generating exportable electricity with a carbon intensity of only 13% of that from a natural gas-fired, combined-cycle power plant.

While the LECAPP system must have access to sites for large scale utilization/storage of the $\rm CO_2$ stream, the external syngas generator

Appendix A. Derivation of enthalpy and entropy changes

The enthalpy change of the generalized cell reaction was estimated as:

$$\Delta H^{o}(T) = \left(\sum n_{j}h_{j}^{o}(T)\right)_{Product} - \left(\sum n_{k}h_{k}^{o}(T)\right)_{Reactant}$$
(A.1)

The specific enthalpy (J/mole) of gas at any temperature T can be estimated as:

$$h^{o}(T) = h^{o}_{298} + \int_{298}^{T} C_{p}(T) dT$$
(A.2)

Substituting Eq. (A.2) in Eq. (A.1) and simplifying, we get

$$\Delta H^{o}(T) = \Delta H^{o}(298) + (\dot{m_{5}} - m_{5}) \times I(C_{p})^{T}_{H_{2}O} + (\dot{m_{1}} - m_{4} + \dot{n_{2}} - n_{2}) \times I(C_{p})^{T}_{CO_{2}} + (\dot{m_{1}} - m_{1}) \times I(C_{p})^{T}_{H_{2}} + (\dot{m_{2}} - m_{2}) \times I(C_{p})^{T}_{CH_{4}} + (\dot{m_{3}} - m_{3}) \times I(C_{p})^{T}_{CO} + (\dot{n_{1}} - n_{1}) \times I(C_{p})^{T}_{O_{2}}$$
(A.3)

where

$$\Delta H^{o}(298) = (m_{5}^{'} - m_{5}) \times \left[h_{298,H_{2}O}^{o} - I(C_{p})_{H_{2}O}^{298}\right] + (m_{4}^{'} - m_{4} + n_{2}^{'} - n_{2}) \times \left[h_{298,CO_{2}}^{o} - I(C_{p})_{CO_{2}}^{298}\right] + (m_{1}^{'} - m_{1}) \times \left[h_{298,H_{2}}^{o} - I(C_{p})_{H_{2}}^{298}\right] + (m_{2}^{'} - m_{2}) \times \left[h_{298,CO_{2}}^{o} - I(C_{p})_{CO_{2}}^{298}\right] + (m_{1}^{'} - m_{1}) \times \left[h_{298,CO_{2}}^{o} - I(C_{p})_{O_{2}}^{298}\right] + (m_{2}^{'} - m_{2}) \times \left[h_{298,CO_{2}}^{o} - I(C_{p})_{CO_{2}}^{298}\right] + (m_{1}^{'} - m_{1}) \times \left[h_{298,O_{2}}^{o} - I(C_{p})_{O_{2}}^{298}\right]$$
(A.4)

$$I(C_p)_s^{298} = A_s T + \frac{B_s T^2}{2} + \frac{C_s T^3}{3} + \frac{D_s T^4}{4} \quad at \ T = 298K$$
(A.5)

$$I(C_p)_s^T = A_s T + \frac{B_s T^2}{2} + \frac{C_s T^3}{3} + \frac{D_s T^4}{4} \quad at \ any \ temperature \ T(K)$$
(A.6)

The entropy change of the generalized cell reaction was estimated as:

$$\Delta S^{o}(T) = \left(\sum n_{j} s_{j}^{o}(T)\right)_{Product} - \left(\sum n_{k} s_{k}^{o}(T)\right)_{Reactant}$$
(A.7)

means that the system is fuel-flexible, capable of using waste streams such as plastics or biomass, thereby reducing demand for landfill. If biomass is used, there is the potential to create zero or negative emission electricity or clinker.

Further studies should explore the levelized cost of CO_2 avoided, including the estimates of capital and operational costs of a LECAPP system.

CRediT authorship contribution statement

Daya R. Nhuchhen: Conceptualization, Data curation, Formal analysis, Investigation, Methodology, Software, Validation, Visualization, Writing - original draft, Writing - review & editing. Song P. Sit: Conceptualization, Methodology, Project Administration, Supervision, Validation, Writing - review & editing. David B. Layzell: Conceptualization, Funding acquisition, Resources, Supervision, Visualization, 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.

Acknowledgements

The authors are grateful for the financial support of LafargeHolcim Inc, the Transition Accelerator, and Natural Resources Canada.

D.R. Nhuchhen et al.

(A.8)

The specific entropy (J/mol/K) of a gas at any temperature T can be estimated as:

$$s^o(T) = s^o_{298} + \int_{298}^T rac{C_p(T) dT}{T}$$

Substituting Eq. (A.8) in Eq. (A.7) and simplifying, we get

$$\Delta S^{o}(T) = \Delta S^{o}(298) + (\dot{m_{5}} - m_{5}) \times I\left(\frac{C_{p}}{T}\right)_{H_{2}O}^{T} + (\dot{m_{4}} - m_{4} + \dot{n_{2}} - n_{2}) \times I\left(\frac{C_{p}}{T}\right)_{CO_{2}}^{T} + (\dot{m_{1}} - m_{1}) \times I\left(\frac{C_{p}}{T}\right)_{H_{2}}^{T} + (\dot{m_{2}} - m_{2}) \times I\left(\frac{C_{p}}{T}\right)_{CH_{4}}^{T} + (\dot{m_{3}} - m_{3}) \times I\left(\frac{C_{p}}{T}\right)_{CO}^{T} + (\dot{n_{1}} - n_{1}) \times I\left(\frac{C_{p}}{T}\right)_{O_{2}}^{T}$$
(A.9)

where

$$\Delta S^{o}(298) = (\dot{m_{5}} - m_{5}) \times \left[s_{298,H_{2}O}^{o} - I\left(\frac{C_{p}}{T}\right)_{H_{2}O}^{298} \right] + (\dot{m_{4}} - m_{4} + \dot{n_{2}} - n_{2}) \times \left[s_{298,CO_{2}}^{o} - I\left(\frac{C_{p}}{T}\right)_{CO_{2}}^{298} \right] + (\dot{m_{1}} - m_{1}) \times \left[s_{298,H_{2}}^{o} - I\left(\frac{C_{p}}{T}\right)_{H_{2}}^{298} \right] + (\dot{m_{2}} - m_{2}) \times \left[s_{298,CO_{2}}^{o} - I\left(\frac{C_{p}}{T}\right)_{CO_{2}}^{298} \right] + (\dot{m_{1}} - m_{1}) \times \left[s_{298,O_{2}}^{o} - I\left(\frac{C_{p}}{T}\right)_{O_{2}}^{298} \right] + (\dot{m_{2}} - m_{2}) \times \left[s_{298,CO_{2}}^{o} - I\left(\frac{C_{p}}{T}\right)_{CO_{2}}^{298} \right] + (\dot{m_{1}} - n_{1}) \times \left[s_{298,O_{2}}^{o} - I\left(\frac{C_{p}}{T}\right)_{O_{2}}^{298} \right]$$
(A.10)

$$I\left(\frac{C_p}{T}\right)_s^{298} = A_s \ln(T) + B_s T + C_s \frac{T^2}{2} + D_s \frac{T^3}{3} at T = 298K$$
(A.11)

$$I\left(\frac{C_p}{T}\right)_s^T = A_s \ln(T) + B_s T + C_s \frac{T^2}{2} + D_s \frac{T^3}{3} \quad at \quad any \quad temperature \quad T(K)$$
(A.12)

Appendix B. Validation of MCFC model

The generalized MCFC model derived here was compared and validated with the existing model that was developed for an ideal cell reaction Eq. (1). Table B.1 presents gas flows and their composition at the inlet and outlet of the fuel cell anode and cathode. Since the Gibbs free energy change affects other fuel cell parameters, its method of calculation is summarized in Table B.2.

The validation of the Gibbs free energy change, Nernst cell voltage, Nernst voltage loss factor and the actual cell voltage for two examined cases (Case 1 & Case 2) are presented in Table B.3. It shows that the existing model for the Gibbs free energy change, which is approximated only as a temperature function, can not incorporate the changes in the gas composition in the MCFCs. Since the existing model does not incorporate the concentration of all gas composition, it predicts a higher Nernst voltage loss factor of 109 mV compared to 73 mV predicted by the new model. As this generalized model incorporates all chemical activities of different gas species coming into the MCFC from the supplied syngas, it provides an accurate estimation of the Nernst voltage loss factor, thereby resulting in a better prediction of the Nernst cell voltage and the actual cell voltage. To validate this, the actual cell voltage predicted by the existing and proposed (present) models was compared with the experimental value published in the literature [42]. Results of the percentage error showed that the new model developed here predicted more accurately than the existing model.

Table B1

```
Summary of major gas flows and its composition to the fuel cell: I) Case 1: NG-based SG, and II) Case 2: HDPE-based SG
```

	I) Case 1: NG only					II) Case 2: NG + HDPE			
	Parameter	Anode In	Anode Out	Average		Parameter	Anode In	Anode Out	Average
	Pressure (atm)	1.1350	1.0361	1.0856		Pressure (atm)	1.1350	1.0363	1.0856
	Mole flow, k-mole/s	1.6512	2.7132	2.1822		Mole flow, k-mole/s	1.9442	3.0234	2.4838
	Gas composition					Gas composition			
	H ₂	0.6390	0.0648	0.3519		H ₂	0.5523	0.0781	0.3152
	CH ₄	0.0021	0.0000	0.0011		CH ₄	0.0014	0.0000	0.0007
	CO	0.1559	0.0352	0.0956		CO	0.1856	0.0448	0.1152
	CO ₂	0.0428	0.4759	0.2594		CO ₂	0.0701	0.4757	0.2729
	H ₂ O	0.1601	0.4241	0.2921		H ₂ O	0.1905	0.4013	0.2959
	Parameter	Cathode In	Cathode Out	Average		Parameter	Cathode In	Cathode Out	Average
	Pressure (atm)	1.0559	1.0460	1.0509		Pressure (atm)	1.0560	1.0461	1.0511
	Mole flow, k-mole/s	11.3934	9.8107	10.6020		Mole flow, k-mole/s	11.7302	10.1195	10.9249
	Gas composition					Gas composition			
	02	0.0894	0.0500	0.0697		O ₂	0.0889	0.0500	0.0695
	CO ₂	0.1029	0.0119	0.0574		CO ₂	0.1017	0.0118	0.0568
	Molar flow	In (kmole/s)	Out (kmole/s)			Molar flow	In (kmole/s)	Out (kmole/s)	
Anode	H ₂	1.05512	0.17584		Anode	H ₂	1.07383	0.23626	
	CH_4	0.00349	0.00002			CH ₄	0.00279	0.00006	
	CO	0.25745	0.09547			CO	0.36084	0.13549	
	CO ₂	0.07070	1.29126			CO ₂	0.13635	1.43826	
	H_2O	0.26443	1.15064			H ₂ O	0.37035	1.21337	
Cathode	O ₂	1.01809	0.49053		Cathode	O ₂	1.04289	0.50597	
	CO ₂	1.17236	0.11724			CO ₂	1.19315	0.11931	

Table B2	
Summary of Gibbs free energy change calculation using enthalpy and entropy change of the overall cell reaction Eq. (2) for I) Case 1: NG-based SG, and II) Case 2: HDPE-based SG.	

	I) Case 1: NG only	Standard enth of formation	Standard enthalpy and entropy of formation		Constants for Cp in J/mole/K		Cp in J/mole/K Temper		ture (K)	Change in enthalpy (kW)		Change	in entropy (kW)			
	Gas	hº298 (J/ mole)	s ^o 298 (J/ mole/K)	А	$\begin{array}{c} B \times \\ 10^{-3} \end{array}$	$\begin{array}{c} C\times \\ 10^{-6} \end{array}$	$\begin{array}{c} D\times\\ 10^{-9}\end{array}$	Ref. (K)	Cell (K)	I (Cp) _{Ref}	I(Cp) _T	ΔH _{Ref} (kW)	$n \times I(Cp)_T$ (kW)	I(Cp/ T) _{Ref}	I(Cp/ T) _T	ΔS _{Ref} (kW/K)	$n imes I(Cp/T)_T$ (kW/K)
Anode Cathode	H_2 CH_4 CO CO_2 H_2O O_2 CO_2	0 -74,873 -110,527 -393,522 -241,826 0 -393,522	131 186 198 214 189 205 214	27 19 31 20 32 28 20	9 52 -13 73 2 0 73	-14 12 28 -56 11 17 -56	8 -11 -13 17 -4 -11 17	298 298 298 298 298 298 298 298	923 923 923 923 923 923 923	8,391 8,136 8,832 8,706 9,781 8,523 8,706	26,767 41,076 27,989 38,059 32,704 28,608 38,059 Sum	7,378 288 19,333 -490,944 -222,978 4,496 424,399 - 258,027 ΔH_T (kW)	-23,536 -142 -4,534 46,453 28,983 -15,092 -40,157 -8,025 -266,052	157 126 173 132 185 161 132	190 182 207 184 226 197 184	$\begin{array}{c} 23 \\ 0 \\ -4 \\ 99 \\ 4 \\ -23 \\ -86 \\ {\color{red} 13} \\ \Delta S_T \ (kW/K) \end{array}$	-167 -1 -34 224 200 -104 -194 - 75 -62
	II) Case 2: NG + HDPE	Standard en entropy of fe	thalpy and ormation	Con	stants for	Cp in J/m	ole/K	Tempera	ture (K)	Change	in enthalp	до _т (кw) у (kW)	-200,040	Change	in entropy	(kW)	
	Gas	hº298 (J/ mole)	sº298 (J/ mole/K)	A	$\begin{array}{c} B \times \\ 10^{-3} \end{array}$	$\begin{array}{c} C\times\\ 10^{-6}\end{array}$	$\begin{array}{c} D\times\\ 10^{-9}\end{array}$	Ref. (K)	Cell (K)	I (Cp) _{Ref}	I(Cp) _T	ΔH _{Ref} (kW)	$n \times I(Cp)_T$ (kW)	I(Cp/ T) _{Ref}	I(Cp∕ T) _T	ΔS _{Ref} (kW/K)	$n \times I(Cp/T)_T$ (kW/K)
Anode	H ₂ CH ₄ CO CO ₂ H ₂ O	0 -74,873 -110,527 -393,522 -241,826	131 186 198 214 189	27 19 31 20 32	9 52 -13 73 2	-14 12 28 -56 11	8 -11 -13 17 -4	298 298 298 298 298 298	923 923 923 923 923 923	8,391 8,136 8,832 8,706 9,781	26,767 41,076 27,989 38,059 32,704	7,028 227 26,897 -523,663 -212,112	-22,420 -112 -6,307 49,549 27,571	157 126 173 132 185	190 182 207 184 226	22 0 -6 106 3	-159 0 -47 239 190
Cathode	O ₂ CO ₂	0 -393,522	205 214	28 20	- 0 73	17 56	-11 17	298 298	923 923	8,523 8,706	28,608 38,059 Sum	4,576 431,925 - 265,122 ΔH_T (kW) ΔG_T (kW)	-15,360 -40,869 - 7,948 -273,070 -212,668	161 132	197 184	-24 -87 15 ΔS _T (kW/ K)	-106 -197 - 80 -65

D.R. Nhuchhen et al.

Table B3

Comparison of the results of the derived MCFC model with existing model and validation with experimental cell voltage [Cell temperature of 650 °C and current density of 1,500 Ampere/m²].

Parameter	Case 1: NG-based SG		Case 2: HPDE-based SG			
	Existing studies	Present study	Existing studies	Present study		
Gibbs free energy change, (kW)	199,720	208,648	199,720	212,668		
Reversible cell voltage (V)	1.035	1.025	1.035	1.026		
Nernst voltage loss (mv)	105	70	112	75		
Nernst cell voltage (V)	0.930	0.954	0.923	0.952		
Actual cell voltage (V)	0.727	0.751	0.719	0.748		
Actual cell voltage [experimental*] (V)	0.794					
% error (%)	-8%	-5%	-9%	-6%		

*Milewski et al. [42].

Appendix C. Supplementary material

Supplementary data to this article can be found online at https://doi.org/10.1016/j.apenergy.2021.118001.

References

- IISD. 73 Countries Commit to Net Zero CO2 Emissions by 2050. International Institute for Sustainable Development; 2019. Retrieved online at https://sdg.iisd. org;443/news/73-countries-commit-to-net-zero-co2-emissions-by-2050/.
- [2] Nhuchhen DR, Layzell DB, Sit SP. Alternative Fuels in Cement Making: An Energy and Material Flow Model. Fuel 2020;295:120544–59. https://doi.org/10.1016/j. fuel.2021.120544.
- [3] Summerbell DL, Barlow CY, Cullen JM. Potential reduction of carbon emissions by performance improvement: A cement industry case study. J Cleaner Prod 2016; 135:1327–39. https://doi.org/10.1016/j.jclepro.2016.06.155.
- [4] IEA. Technology Roadmap Low-Carbon Transition in the Cement Industry. International Energy Agency; 2018. Retrieved online at https://www.iea.org/publi cations/freepublications/publication/TechnologyRoadmapLowCarbonTransiti onintheCementIndustry.pdf.
- [5] Ishak SA, Hashim H. Low carbon measures for cement plant a review. J Cleaner Prod 2015;103:260–74. https://doi.org/10.1016/j.jclepro.2014.11.003.
- [6] Markewitz P, Zhao L, Ryssel M, Moumin G, Wang Y, Sattler C, et al. Carbon capture for CO₂ emission reduction in the cement industry in Germany. Energies 2019;12 (12):2432–56. https://doi.org/10.3390/en12122432.
- [7] Schakel W, Hung CR, Tokheim LA, Strømman AH, Worrell E, Ramírez A. Impact of fuel selection on the environmental performance of post-combustion calcium looping applied to a cement plant. Appl Energy 2018;210:75–87. https://doi.org/ 10.1016/j.apenergy.2017.10.123.
- [8] Voldsund M, Anantharaman R, Berstad D, De Lena E, Fu C, Gardarsdottir SO, et al. CEMCAP Comparative Techno-economic Analysis of CO2 Capture in Cement Plants. SINTEFF Energy Research; 2019, Report D4.6. Retrieved online at https://www.zenodo.org/record/2605128#.XwS9PihKiUk.
- [9] Ellis LD, Badel AF, Chiang ML, Park R-Y, Chiang Y-M. Toward electrochemical synthesis of cement—An electrolyzer-based process for decarbonating CaCO₃ while producing useful gas streams. Proc Natl Acad Sci 2020;117(23):12584–91. https:// doi.org/10.1073/pnas.1821673116.
- [10] Halliday C, Hatton TA. The potential of molten metal oxide sorbents for carbon capture at high temperature: Conceptual design. Appl Energy 2020;280: 116016–31. https://doi.org/10.1016/j.apenergy.2020.116016.
- [11] Wang Fu, Deng S, Zhang H, Wang J, Zhao J, Miao He, et al. A comprehensive review on high-temperature fuel cells with carbon capture. Appl Energy 2020;275: 115342. https://doi.org/10.1016/j.apenergy.2020.115342.
- [12] Sartori da Silva F, Matelli JA. Exergoeconomic analysis and determination of power cost in MCFC – steam turbine combined cycle. Int J Hydrogen Energy 2019; 44(33):18293–307. https://doi.org/10.1016/j.ijhydene.2019.05.156.
- [13] Mehr AS, Lanzini A, Santarelli M, Rosen MA. Polygeneration systems based on high temperature fuel cell (MCFC and SOFC) technology: System design, fuel types, modeling and analysis approaches. Energy 2021;228:120613–39. https://doi.org/ 10.1016/j.energy.2021.120613.
- [14] Campanari S, Chiesa P, Manzolini G. CO₂ capture from combined cycles integrated with Molten Carbonate Fuel Cells. Int J Greenhouse Gas Control 2010;4(3):441–51. https://doi.org/10.1016/j.ijggc.2009.11.007.
- [15] Duan L, Sun S, Yue L, Qu W, Yang Y. Study on a new IGCC (Integrated Gasification Combined Cycle) system with CO₂ capture by integrating MCFC (Molten Carbonate Fuel Cell). Energy 2015;87:490–503. https://doi.org/10.1016/j. energy.2015.05.011.
- [16] Carapellucci R, Cipollone R, Di Battista D. Modeling and characterization of molten carbonate fuel cell for electricity generation and carbon dioxide capture. Energy Procedia 2017;126:477–84. https://doi.org/10.1016/j.egypro.2017.08.228.
- [17] Ghezel-Ayagh H. Electrochemical Membrane for Carbon Dioxide Capture and Power Generation. U. S. Department of Energy and Fuel Cell Inc.; 2017, Technical Report DOE-FCE–0007634-2. Retrieved online at https://www.osti.gov/biblio/1 414833-electrochemical-membrane-carbon-dioxide-capture-power-generation.

- [18] Spinelli M, Di Bona D, Gatti M, Martelli E, Viganò F, Consonni S. Assessing the potential of molten carbonate fuel cell-based schemes for carbon capture in natural gas-fired combined cycle power plants. J Power Sources 2020;448:227223–35. https://doi.org/10.1016/j.jpowsour.2019.227223.
- [19] Spinelli M, Campanari S, Romano MC, Consonni S, Kreutz TG, Ghezel-Ayagh H, et al. Molten carbonate fuel cells for retrofitting post-combustion CO2 capture in coal and natural gas power plants. 031001-031001–15 J Electrochem Energy Convers Storage 2018;15(3). https://doi.org/10.1115/1.4038601.
- [20] Campanari S, Manzolini G, Chiesa P. Using MCFC for high efficiency CO₂ capture from natural gas combined cycles: Comparison of internal and external reforming. Appl Energy 2013;112:772–83. https://doi.org/10.1016/j.apenergy.2013.01.045.
- [21] Falcucci G, Jannelli E, Minutillo M, Ubertini S, Han J, Yoon SP, et al. Integrated numerical and experimental study of a MCFC-plasma gasifier energy system. Appl Energy 2012;97:734–42. https://doi.org/10.1016/j.apenergy.2012.01.060.
- [22] Greppi P, Bosio B, Arato E. Feasibility of the integration of a molten carbonate fuelcell system and an integrated gasification combined cycle. Int J Hydrogen Energy 2009;34(20):8664–9. https://doi.org/10.1016/j.ijhydene.2009.08.012.
- [23] Manzolini G, Campanari S, Chiesa P, Giannotti A, Bedont P, Parodi F. CO₂ separation from combined cycles using molten carbonate fuel cells. J Fuel Cell Sci Technol 2012;9(1):0110181–8. https://doi.org/10.1115/FuelCell2011-54719.
- [24] Samanta S, Ghosh S. A thermo-economic analysis of repowering of a 250 MW coal fired power plant through integration of Molten Carbonate Fuel Cell with carbon capture. Int J Greenhouse Gas Control 2016;51:48–55. https://doi.org/10.1016/j. ijggc.2016.04.021.
- [25] Berlowitz PJ, Barckholtz TA, Lee AS. Integration of Molten Carbonate Fuel Cells in Cement Processing. Patent 2014, Publication Number US 2014/0261090 A1. Retrieved online at https://patents.google.com/patent/US20140261090.
- [26] Spinelli N, Romano MC, Consonni S, Campanari S, Marchi M, Cinti G. Application of molten carbonate fuel cells in cement plants for CO₂ capture and clean power generation. Energy Procedia 2014;63:6517–26. https://doi.org/10.1016/j. egypro.2014.11.687.
- [27] De Silvestri A, Stendardo S, Pietra MD, Borello D. Decarbonizing cement plants via a fully integrated calcium looping-molten carbonate fuel cell process: Assessment of a model for fuel cell performance predictions under different operating conditions. Int J Hydrogen Energy 2021;46(28):14988–5007. https://doi.org/ 10.1016/j.ijhydene.2020.12.024.
- [28] Baranak M, Atakül H. A basic model for analysis of molten carbonate fuel cell behavior. J Power Sources 2007;172(2):831–9. https://doi.org/10.1016/j. jpowsour.2007.05.027.
- [29] NETL. Fuel Cell Handbook. USA: U.S. Department of Energy, National Energy Technology Laboratory; 2004. Retrieved online at https://www.osti.gov/servlets /purl/834188.
- [30] Dayton DC, Ratcliff M, Bain R. Fuel Cell Integration A Study of the Impacts of Gas Quality and Impurities: Milestone Completion Report. Golden, CO., USA: National Renewable Energy Laboratory (NREL); 2001. Retrieved online at https://www.nre l.gov/docs/gen/fy01/30298.pdf.
- [31] Li X. Principles of Fuel Cells. London, New York: Taylor & Francis Group LLC; 2006.
- [32] Duan L, Zhu J, Yue L, Yang Y. Study on a gas-steam combined cycle system with CO2 capture by integrating molten carbonate fuel cell. Energy 2014;74:417–27. https://doi.org/10.1016/j.energy.2014.07.006.
- [33] Sors F, Holm P. Development of Steam Turbine Inlet Control Valve for Supercritical Pressure at Siemens Industrial Turbomachinery AB. Sweden: Master's Thesis, Linköping University; 2010. Retrieved online at https://www.diva-portal.org/sma sh/get/diva2:327829/FULLTEXT01.pdf.
- [34] Duan L, Xia K, Feng T, Jia S, Bian J. Study on coal-fired power plant with CO2 capture by integrating molten carbonate fuel cell system. Energy 2016;117: 578–89. https://doi.org/10.1016/j.energy.2016.03.063.
- [35] Hongliang H, Zhang H, Weng S, Su M. Dynamic numerical simulation of a molten carbonate fuel cell. J Power Sources 2006;161(2):849–55. https://doi.org/ 10.1016/j.jpowsour.2006.04.109.

- [36] Yoshiba Y, Koda E. Efficiency analyses of a coal gasification Molten Carbonate Fuel Cell With a gas turbine combined cycle including CO2 recovery. In Proceedings Series, Turbo Expo: Power for Land, Sea, and Air; 2008, p. 489–98 [Paper No: GT2008-50360]. https://doi.org/10.1115/GT2008-50360.
- [37] ECN. Phyllis2 Database for biomass and waste. Energy Research Centre of the Netherlands, Database for Biomass and Waste; 2019. Retrieved online at https://ph yllis.nl/.
- [38] Darde A, Prabhakar R, Tranier JP, Perrin N. Air separation and flue gas compression and purification units for oxy-coal combustion systems. Energy Procedia 2009;1(1):527–34. https://doi.org/10.1016/j.egypro.2009.01.070.
- [39] Revankar S, Majumdar P. Fuel Cells: Principles, Design, and Analysis. USA: Taylor Francis Group; 2014.
- [40] Sonntag RE, Borgnakke C. Fundamentals of Thermodynamics. 8th ed. USA: John Wiley & Sons Inc; 2013.
- [41] Mench MM, editor. Fuel Cell Engines. Hoboken, NJ, USA: John Wiley & Sons, Inc.; 2008.
- [42] Milewski J, Discepoli G, Desideri U. Modeling the performance of MCFC for various fuel and oxidant compositions. Int J Hydrogen Energy 2014;39(22):11713–21. https://doi.org/10.1016/j.ijhydene.2014.05.151.
- [43] Green RH, Perry DW. Perry's Chemical Engineers' Handbook. 8th ed. USA: McGraw-Hill Companies Inc.; 2008.
- [44] Moro A, Lonza L. Electricity carbon intensity in European Member States: Impacts on GHG emissions of electric vehicles. Transportation Research Part D: Transport and Environment 2018;64:5–14. https://doi.org/10.1016/j.trd.2017.07.012.
- [45] IEAGHG. Update Techno-economic Benchmarks for Fossil Fuel-fired Power Plants with CO₂ Capture. UK: IEA Environmental Projects Ltd., Technology Collaboration Programme Technical Report 2020-07; 2020.
- [46] De Lena E, Spinelli M, Gatti M, Scaccabarozzi R, Campanari S, Consonni S, et al. Techno-economic analysis of calcium looping processes for low CO₂ emission cement plants. Int J Greenhouse Gas Control 2019;82:244–60. https://doi.org/ 10.1016/j.ijggc.2019.01.005.
- [47] Boyano A, Blanco-Marigorta AM, Morosuk T, Tsatsaronis G. Exergoenvironmental analysis of a steam methane reforming process for hydrogen production. Energy 2011;36(4):2202–14. https://doi.org/10.1016/j.energy.2010.05.020.

- [48] Craig R, Butler D. Oil Sands CO2 Pipeline Network Study. Canada's Oil Sands Innovation Alliance; 2017. Retrieved online at https://www.cosia.ca/sites/defa ult/files/attachments/Final%20Report%20COSIA%2018%20July.pdf.
- [49] Erkiaga A, Lopez G, Amutio M, Bilbao J, Olazar M. Syngas from steam gasification of polyethylene in a conical spouted bed reactor. Fuel 2013;109:461–9. https:// doi.org/10.1016/j.fuel.2013.03.022.
- [50] EIA. Cost and Performance Characteristics of New Generating Technologies, Annual Energy Outlook 2020. U.S. Energy Information Administration; 2020. Retrieved online at https://www.eia.gov/outlooks/aeo/assumptions/pdf/table 8.2.pdf.
- [51] IPCC. AR5 Climate Change 2014: Mitigation of Climate Change: Chapter 7 Energy Systems. Intergovernmental Panel on Climate Change; 2014. Retrieved online at https://www.ipcc.ch/site/assets/uploads/2018/02/ipcc_wg3_ar5_chapter7.pdf.
- [52] Keith DW, Holmes G, Angelo DS, Heidel K. A Process for Capturing CO₂ from the Atmosphere. Joule 2018;2(8):1573–94. https://doi.org/10.1016/j. joule.2018.05.006.
- [53] De Lena E, Spinelli M, Martinez I, Gatti M, Scaccabarozzi R, Cinti G, et al. Process integration study of tail-end Ca-Looping process for CO₂ capture in cement plants. Int J Greenhouse Gas Control 2017;67:71–92. https://doi.org/10.1016/j. ijggc.2017.10.005.
- [54] Bachu S, Melnik A, Bistran R. Approach to evaluating the CO2 storage capacity in Devonian deep saline aquifers for emissions from oil sands operations in the Athabasca area. Canada. Energy Procedia 2014;63:5093–102. https://doi.org/ 10.1016/j.egypro.2014.11.539.
- [55] Kearns J, Teletzke G, Palmer J, Thomann H, Kheshgi H, Chen Y-H, et al. Developing a consistent database for regional geologic CO2 storage capacity worldwide. Energy Procedia 2017;114:4697–709. https://doi.org/10.1016/j. egypro.2017.03.1603.
- [56] Global Petrol Prices. Gasoline prices around the world. Website: GlobalPetrolPrices.com; 2021. Retrieved online at https://www.globalpetrolpric es.com/gasoline_prices/.
- [57] Ritchie H, Roser M. Plastic Pollution. Website: Our World in Data; 2018. Retrieved online at https://ourworldindata.org/plastic-pollution.