

# Exergy, Economical and Environmental Analysis of a Natural Gas Direct Chemical Looping Carbon Capture and Formic Acid-Based Hydrogen Storage System

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**ABSTRACT:** Chemical looping combustion is one of the novel technologies in energy, which can co-generate hydrogen and power with an efficient carbon capture process to control the system's emission. This system's carbon capture process is one of the main processes to achieve the United Nations' environmental goals and other climate change control agencies. This paper aims to study Designing a Natural Gas Direct Chemical Looping Carbon capture and Formic acid Hydrogen storage system for a combined cycle power plant and analyze it with energy, exergy, and environmental factors. The model was implemented on a 500 MW combined cycle power plant unit in Iran, and the results show that if the model is implemented on the plant, overall energy efficiency can be increased by 33%. Furthermore, according to the references, carbon emissions decreased by more than 93%, which is achievable using Chemical looping combustion.

**KEYWORDS:** Formic acid synthesis; Natural gas direct chemical loop; Carbon dioxide utilization; Combustion looping; Solar fuel; Hydrogen carrier.

## INTRODUCTION

Climate change is becoming a severe issue and has attracted much attention toward the low carbon and green technologies to reduce the carbon dioxide emission of the industry and energy sectors. In this matter, coal plays the most crucial role [1]. Most developing countries such as India and China use coal as their main primary energy supply [2]. To meet the coal-fired power plants' emissions, the researchers developed a set of carbon capture technologies. These technologies are implementable in different sectors. These technologies aim to prevent

industrial CO<sub>2</sub> emissions from entering the atmosphere [3]. Furthermore, the carbon captured during this process can be reused in chemical processes to synthesize hydrocarbons and other useful products. This process is called carbon utilization (CU), gaining much attention in recent years [4].

Some researchers [5, 6] studied various conventional carbon capture technologies and reported them. Another research [7] stated that conventional carbon capture methods have a great energy penalty. Considering

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the conventional carbon capture processes' energy penalty, a novel Chemical Looping Combustion (CLC) method is introduced. CLC is an innovative and novel carbon capture method that reduces energy consumption to negligible amounts [8,9]. A study[10] introduced the CLC implementation for energy and fuel in the combustion process. A researcher [11] stated that several recent publications studied power and hydrogen co-generation using gas and liquid fuel CLC processing. But the main gap in this field is the CLC application for soiled fuel processing, which is the main emission source globally. The hydrogen and power co-generation in solid fuels such as coal and biomass is necessary for the future of the coal burnt industries. Comparing the Coal Direct Chemical Looping (CDCL) with the gaseous fuel CLC shows that the process efficiency is much higher than the conventional CLC processes [12]. Another study[13] also stated that the O<sub>2</sub> demand of the Coal DCL is lower than the gaseous CLC process. The Natural-Gas Direct Chemical Looping (NDCL) is limited but in 2011, A research project [14] studied a 0.5 GW power plant for combined hydrogen and power generation. In this study, different fuels such as natural gas and coal were studied. Another researcher[15] studied power plants in terms of their fuels and CLC process efficiency. A study conducted in 2012[16] designed and developed a reactor based on its thermodynamic assumptions and kinetic status. They analyzed the performance of the conversion and conservation processes in air, fuel, and steam reactors. The simulation of the NDCL process shows that the plant has 78% thermal efficiency and 90% carbon capture plant. Also, another author from Canada[17] developed a CHP plant with hydrogen generation in various case studies. In this study, an exergy analysis was conducted for those case studies, and also, many parametric approaches were considered. They noted a 13.86% efficiency reduction in hydrogen and CHP compared to stand-alone power generation.

The oxygen carrier plays an essential role in the efficiency of the NDCL process. A researcher[18] studied metallic elements for the NDCL process. In the NDCL process, despite its higher efficiency, the overall performance of the classic materials such as Fe<sub>2</sub>O<sub>3</sub> as an oxygen carrier is low for the coal-based fuel CLC process. In another study [19], the copper oxide impact on improving the iron oxide coal reaction performance and the rate was studied.

This study noted that a mixture of the CuO (5% wt) in the Fe<sub>2</sub>O<sub>3</sub> (means adding a share of CuO to the oxygen carrier equal to the 5%wt of the total Fe<sub>2</sub>O<sub>3</sub>) enhances the reaction's performance and the rates. This is why, in this paper, a bimetallic oxygen carrier is used for the NDCL process.

However, the Carbon emission capture technology makes nearly 100% capture available in the newer technologies; the safety of the climate system in all of its aspects such as biosphere, geosphere, cryosphere, hydrosphere, and atmosphere is a significant issue, and the aim of all experts [20-22]. Because of the noted issues and needs, there is an interest in researching the fields of carbon utilization. Carbon dioxide can be utilized for fuel conversion and other chemicals such as formaldehyde, formic acid, methanol, and urea [23, 24]. Also, newer studies[25] investigated carbon dioxide utilization to produce more useful chemicals and fuels such as methane, methanol, formic acid, and dimethyl carbonates. They also reviewed the CLC technologies of carbon capture and other emission control technologies. This study showed that the combined CLC and hydrothermal technology would lead to the production of heat, power, and chemicals to reduce carbon emissions. Another study[26] has reviewed the methanol production in solid fuel-power plants of 33 MW electricity and 207.99 tons/d methanol generation. This study concluded that potential improvements in efficiency and performance occur while using carbon utilization methods to produce more valuable chemical products than conventional methods. Also, a researcher [27] developed coal gasification and hydrogen production using wind power. This process leads to carbon emission reduction and methanol synthesis. These noted facts state that carbon utilization is a more prominent and implementable carbon emission reduction than carbon capture and storage. In this study, formic acid synthesis from a co-generation system is being studied.

Formic acid (FA) is beneficial in the petrochemical industry, food industry, textile industry, etc. Due to the robust acidic nature and reductant components and characteristics, the FA synthesis is economically feasible. A study[28] states that FA synthesis from CO<sub>2</sub> is feasible when the CDCL method is implemented. FA is very useful in refining heavy oil to the crude oil quality. The FA's global demand was 710000 tons in 2017, and it is predicted to reach 880000 tons by 2023 (the annual

**Table 1: Shows the details of each case study (technical scenario).**

Case	plant	Oxygen carrier	Carbon capture	FA production plant
1	CCPP	-	No	No
2	NDCL	Fe <sub>2</sub> O <sub>3</sub>	Yes	No
3	NDCL	Bimetallic	Yes	Yes

**Table 2: The details of the natural gas supplied to the plant according to ASTM standard test.**

Proximate analysis	Wt%	Ultimate analysis	Wt%
Volatile matter	~100	Carbon	74.8
Fixed carbon	~0	Hydrogen	25.17
Ash	~0	Oxygen	~0
Moisture (as received)	~0	Nitrogen	~0
Heat Value (LHV) [MJ/kg]	44	Sulfur	~0
-	-	Ash	~0

\*This table is adapted from the ASTM standard test for natural gas combustion results [36]

\*\* The input fuel is assumed to be a refined natural gas in which only hydrocarbons are accountable, and other elements such as sulfur or oxygen are negligible[36].

growth of 3.74% in 2018-2023) [29]. FA 85% wt is more dominant in the market, but 90%, 94%, and 99% are also demanded. The formic acid's overall market value was 619 million \$ in 2019 [29]. Patents developed in the FA carbon utilization[30-33] show that the FA synthesis process prevents carbon dioxide emission to the atmosphere in the DCL process.

They consider the growing climate change issue, the urgent need for carbon utilization to make greater-scale carbon capture available. The 1.5°C threshold introduced by the COP21 makes Carbon utilization even more necessary [34]. Hydrogen is one of the reactants of FA synthesis. Because of this fact, hydrogen production is also considered in the NDCL process. This research paper studies the hydrogen and power co-generation NDCL method using iron oxide and bimetallic oxygen carriers. In this study, the feasibility and environmental effects of the FA NDCL process are also studied. The limitation of references in the power generation combined with the FA synthesis plant is also one of the leading research gaps in this field, which this paper answers. This paper aims to evaluate and compare the efficiency of the NDCL plant coupling with CU technology. This process is studied in terms of energy, exergy, and hydrogen production efficiency. This model's innovation was to implement the feedwater heater to preheat the water before entering

the boiler to enhance the overall efficiency of the CCU process. Also, in this paper, the NDCL plant, coupled with the CU plant, is analyzed as energetic, economic, and environmentally compared to the NDCL process without the CU plant.

## EXPERIMENTAL SECTION

three different technical cases (as illustrated in Table 1) have been considered and modeled to demonstrate the technical feasibility (This analysis is a new feasibility study approach in which a case is studied considering both economic and technical aspects using new thermodynamical methods (i.e 4E) [35].) of formic acid synthesis at the NDCL co-generation plant using Aspen Plus and CHEMCAD. A 500 MW Combined Cycle Power Plant (CCPP) substation is typically simulated for Tehran-based climatic conditions and is utilized to compare with other cases[33]. The analysis of Iranian natural gas supplied to the Damavand combined cycle in Tehran is shown in Table 2. A constant natural the gas flow of 6.13 kg/s was selected for all cases to provide constant input energy to the plants. NDCL cases are analyzed against conventional CCPP without CO<sub>2</sub> capture and its use to estimate the energy penalties associated with CO<sub>2</sub> use and other energy, exergy, and techno-environmental indexes.

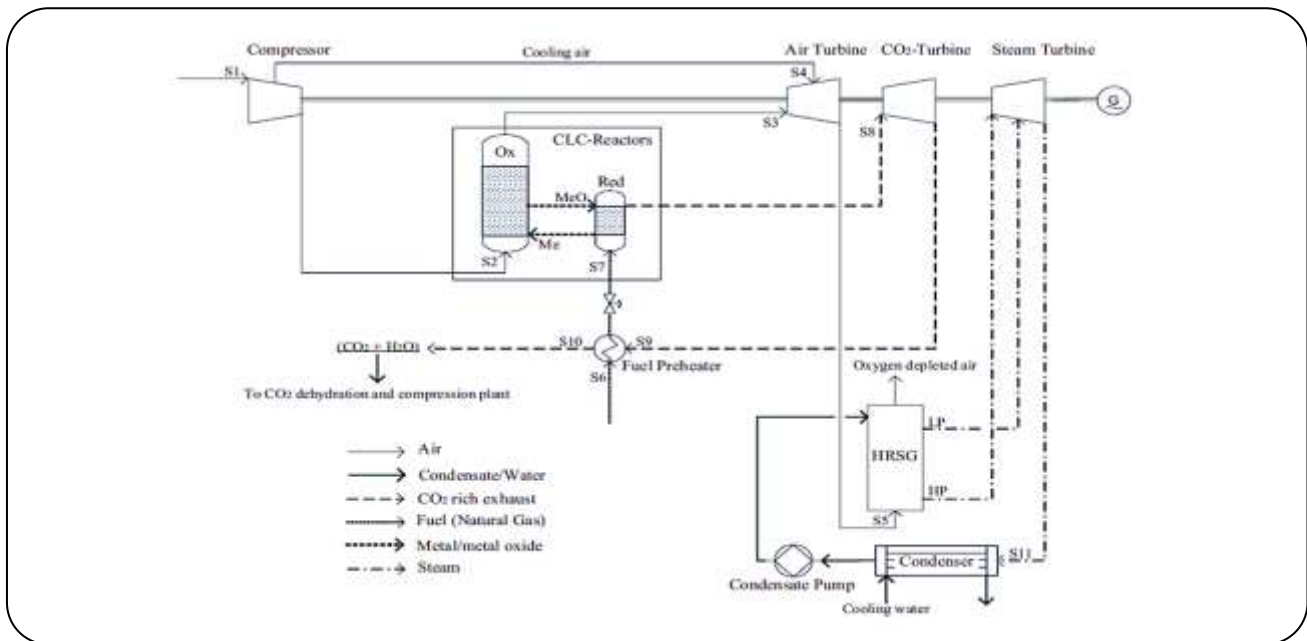


Fig. 1: Configuration of a natural-gas chemical looping system.

A simple block diagram of NDCL plants using CO<sub>2</sub> for the formic acid synthesis of H<sub>2</sub> and CO<sub>2</sub> (for cases 2 and 3) is shown in Fig. 1. Illustrates the details of this process:

#### NCL configuration and model

The combined cycle differs from a conventional one because air and fuel flow are kept in separate Bryton cycles using a separate air and CO<sub>2</sub> turbine. It is assumed that the air compressor, air turbine, and CO<sub>2</sub> turbine are in the same shaft, while it can be assumed that the air turbine drives the compressor. The fuel is assumed to be under pressure, so no fuel compressor is included[11]. The air enters the CLC oxidation reactor as it exits the compressor, which reacts with the reduced metal, while the fuel reacts with a metal oxide in the reduction reactor simultaneously in a continuous operation[22]. To prevent any gas leakage between the two reactors, maintaining the same pressure of the gases in the ducts where the CLC reactors' connection is significant for the transport of solids. These conduits are necessarily those through which solids separated from oxygen-contaminated air enter the fuel reactor's cyclone system. If there is a pressure difference in the ducts, the gas may leak between the two reactors. Therefore, it is desirable to obtain the same pressure at the output of the redox reactors. This is done by controlling the pressure at the inlet of the reduction reactor using a pressure control valve.

Pressure varies according to the pressure at the oxidation reactor's outlet and the pressure drop through the reduction reactor [34].

The low-pressure hot oxygen air coming out of the oxidation reactor enters the air turbine and is mixed with the compressor's cooling air [24]. Due to the pressure drop in the heat recovery steam generator (HRSG), the air expands somewhat above atmospheric pressure. The air turbine exhaust passes the HRSG to produce steam at two pressure levels. The high-pressure steam enters the steam turbine 60 bar and expands to 5 bar where the low-pressure steam is accepted. Then the entire vapor expands to the condenser pressure. In the reduction reactor, the fuel's reaction with the metal oxide results in CO<sub>2</sub> exhaust and steam being reduced at the reactor temperature and pressure[35]. The exhaust in the CO<sub>2</sub> turbine expands slightly above atmospheric pressure due to the pressure drop in the fuel preheater, which causes fuel propellant, minimizes exergy loss, cools the exhaust flow, and reduces body dehydration in the high-temperature stream when the fuel heater exits are selected so that there is no risk of steam condensation [17].

#### CLC reactor configuration and model

Fig. 2 illustrates the principle of Chemical Loop Combustion (CLC). The fuel conversion is achieved by two intermediate reactions oxidation and reduction [9].

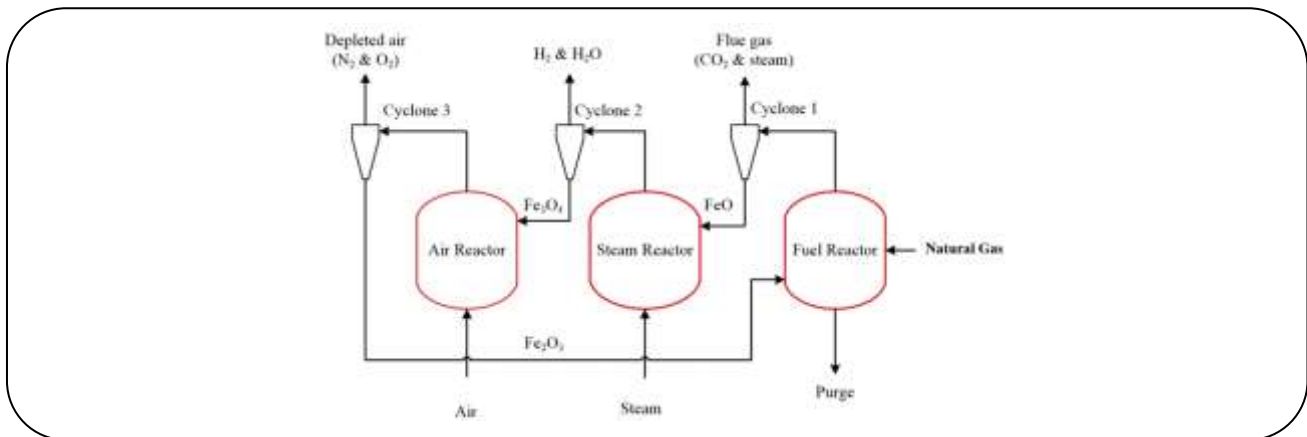
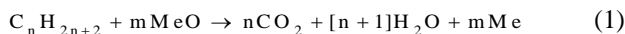


Fig. 2: The schematics of the CLC reactor.

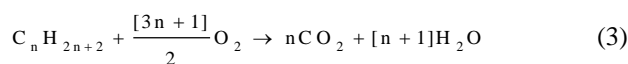
To explain the concept of chemical loop combustion and understand how it is implemented in power cycles, it is necessary to have a practical understanding of the heterogeneous solid-gas reactions simultaneously in two reactors in continuous operation. The fuel reacts with the oxygen in the metal oxide to a stoichiometric ratio in the reduction reactor, reducing the metal oxide to metal. This is represented by equation 1 [7]:



Metal oxide also transfers the chemical energy in the fuel to the air in sensible heat. In the oxidation reactor, the oxygen in the air oxidizes the metal to metal oxide. The reduced metal oxide circulates in the oxidation reactor as it reacts with air. The oxidation reaction is presented in equation 2 [36]:



The metal oxide is reduced inside the reactor, transferring oxygen and sensible heat to the fuel. The fuel conversion reaction's net heat is the same as in a direct, ordinary combustion reaction, and the reaction redox's sum. Eq. (3) shows the net heat dissipation reaction [3, 16].



In Equations (1, 2), and (3),  $MeO$  is a metal oxide,  $Me$  is a metal, and  $C_n H_{2n+2}$  is a hydrocarbon fuel molecule. At the same time,  $m$  and  $n$  are stoichiometric factors [37-44]. The metal oxide, called "oxygen carrier," is bonded to an inert solid that does not participate in chemical

reactions but provides mechanical stability and increases the heat transfer capacity of solids. The oxidation reaction is exothermic for metal and results in heat release, thereby releasing oxygen-depleted air at elevated temperatures [5]. If the reactors are pressurized, oxygen discharged air into the gas turbine can be expanded to generate power. Due to the nature of the metal oxide used, the solids reduction reaction needs a high temperature to occur. And if the reduction is endothermic, the reaction's required heat flux is provided by the oxidation reaction's exothermic nature. Carbon dioxide-rich exhaust gas is also available at high temperatures (and pressures in pressurized reactors) and can also generate electricity by developing in the turbine or producing steam in the steam recovery steam generator. If the reactors are not pressurized (atmospheric reactors), the available heat can be extracted to produce steam, generating power in a Rankin cycle [45-49].

$CO_2$  is available in the exhaust stream due to the higher concentration in the mixture with high partial pressure ( $P_0=0.12\text{MPa}$ ,  $T_0=408\text{K}$ ). After extracting the heat in the exhaust, the flow can be compressed for component separation using water in the process. The stream remains with pure  $CO_2$ , which can be compressed and converted to liquid  $CO_2$ , which is more portable for storage. In this method, the energy penalty for  $CO_2$  sequestration and compression is lower than the penalty for  $CO_2$  capture in a conventional power plant where  $CO_2$  is diluted with other combustion products and lower than the partial pressure CLC ( $P=106.4\text{ bar}$ ,  $T=338.2\text{K}$ ). The Oxygen and Hydrogen streams are also produced as the by-products and separated in the Chemical looping process [50].

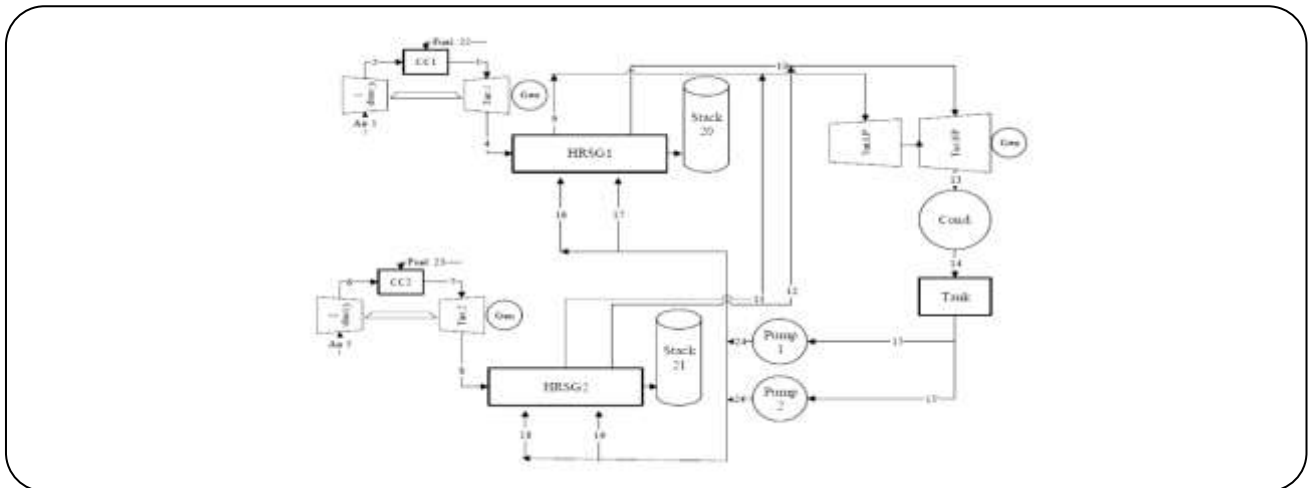


Fig. 3: The schematics of the Damavand power plant.

### Thermodynamical configuration and model of CCPP

As a case study, Damavand's CCPP has been investigated in this work. Damavand CCPP, also known as the Pakdasht Shahdawai Power Plant, has been operational since 2005[20]. Damavand was the largest power plant in the Middle East at the time of construction. Damavand CCPP has a rated capacity of 2868 MW consisting of twelve units of 159 MW V94.2 gas turbine units and six units of 160 MW steam turbine units[36]. The average power production is 2366 MW, 2532 MW in winter, and 2172 MW in summer. The average operating capacity of each gas and steam unit is 124.8 MW and 144.7 MW, respectively. The main fuel of the units is natural gas, and diesel fuel is gasoline. The plant uses a dry cooling tower (Heller) that supplies electricity at two 230 and 400 kV substations. Some assumptions have been made to formulate a model for this combined cycle power plant [19].

- All processes are steady-state
- Air and exhaust gas fuels are considered ideal gases ( $Z_{air@inlet}=0.96$ ,  $Z_{exhaustgas@outlet}=0.97$ )
- All processes in pipes, lines, and heat exchangers with ambient pressure and low pressure are considered.
- Dead state is considered as strip  $P_0 = 1.01$  and  $T_0 = 293.2$  K

One of the units (2 gas + 1 steam station) is analyzed in this research. The thermodynamic model of the unit is summarized in table 3 below:

### NDCL configuration and model

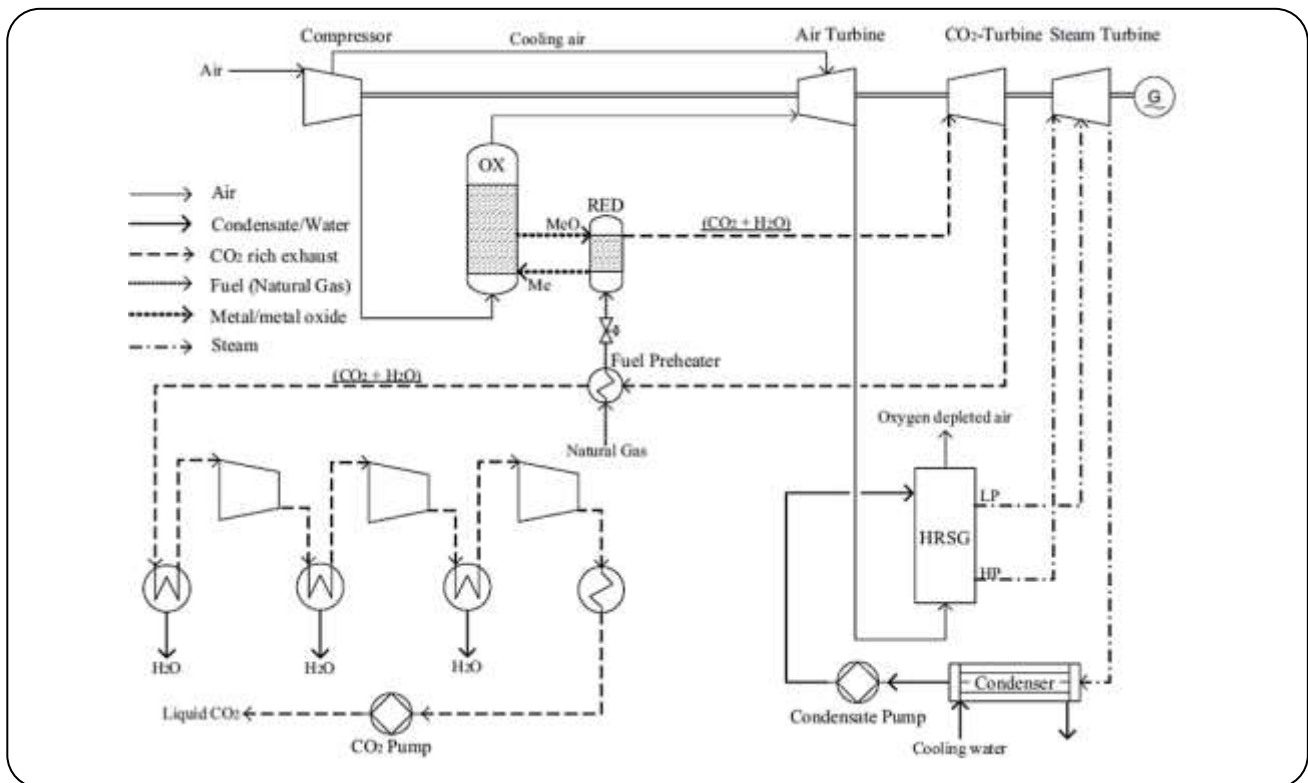
The subcritical CCPP is replaced by conventional CCPP combustion by air reactor, steam reactor, and fuel

reactor loop in the NDCL plant[51-55]. Figure 4 shows the process flow chart of the NDCL system for  $H_2$  generation and power generation. Gas products are separated from each reactor (air, fuel, and steam reactor) using cyclone separators[56]. Flue gases (mainly  $CO_2$  and steam) and hydrogen-rich currents are sent from the steam and steam reactors to the Heat Recovery Steam Generating (HRSG) unit to recover heat while the oxygen discharged by oxygen first passes through the air reactor the is sent to the Gas Turbine (GT) unit to generate power and then to the HRSG unit. MHeatX models are used to model HRSG units (i.e., evaporator, superheater, heater, and equalizer)[57]. Because the hydrogen produced by this plant requires further compression for formic acid synthesis, the Hydrogen-rich current is not transmitted through the GT/expander. Instead, the flue gas stream passes through the HRSG via the air-compressor train, and  $CO_2$  is separated and compressed at a pressure of 105 bar[58]. The steam and carbon dioxide is recycled to the steam reactor ( $31^\circ C$ ) and fuel reactor ( $190^\circ C$ ) from the intermediate stage of HRSG. The superheat and heated steam are generated in sub-critical conditions in the HRSG and pass through the High-Pressure (HP) and medium-pressure turbines, respectively. Two HP and three Low-Pressure FWH (LP) series with air vents are designed to preheat the feed and improve thermal efficiency[59].

In this study, a bimetallic oxygen carrier (5% CuO in  $Fe_2O_3$  by weight percent) supported on  $Al_2O_3$  is considered in case 3. Steady-state simulation for thermodynamic analysis of the NDCL process using CHEMCAD complies with the assumptions are listed in Table 4. The main design assumptions

**Table 3: The thermodynamical exergy, energy, and environment, the economic model of the CCPP.**

Description	Equation
Power consumption in Air compressor	$W_{AC} = m_a(h_2 - h_1)$
Power generation in Air turbine	$W_{GT} = m_g(h_3 - h_4)$
HRSG thermal model	$m_g C_p g(T_a - T_b) = m_w H_P(h_u - h_t)$
Efficiency ratio of the steam cycle	$\eta_{ST} = \left(\frac{W_{ST,act}}{W_{ST,is}}\right)$
Pumping system performance ratio	$\eta_{pump} = \left(\frac{h_{15,is} - h_{24}}{h_{15} - h_{24}}\right)$
Exergy balance	$Ex_Q + \sum m_i ex_i = \sum m_e ex_e + Ex_w + Ex_D$
Exergy equation	$ex = ex_{ph} + ex_{ch}$
Physical exergy	$ex_{ph} = (h - h_0) + T_0(s - s_0)$
Chemical exergy	$ex_{ch}^{mix} = \sum X_i ex_i^{ch} + RT_0 \sum X_i \ln X_i$
Exergy of the fuel	$\zeta = \frac{ex_f}{LHV_f}$



**Fig. 4: The schematics of the CCPP + CLC [37].**

are to describe units for the development of the NDCL process flash page. Table 5 describes the NDCL plant steam and fuel reactors are modeled as moving bed reactors (RGibbs Multistage), and the air reactor is modeled as a single RGibbs model. The results of these three reactors' equilibrium mass and energy are confirmed by the results available in the literature [38-40]. Besides, the PR-BM and

STEAMNBS property methods for determining flue gases, solids, water, and steam are considered[60-66].

**The formic acid synthesis unit**

This study simulates the homogeneous catalytic process for producing formic acid from captured H<sub>2</sub> and CO<sub>2</sub>. The process sheet has been validated by references [37, 38].

**Table 4: The assumptions which are being made to the model in CHEMCAD.**

Class	Assumption
Non-Conventional Solid	None
Conventional Solid	Fe <sub>2</sub> O <sub>3</sub> , Fe, FeO, Fe <sub>3</sub> O <sub>4</sub> , FeS, Cu, CuO, Al <sub>2</sub> O <sub>3</sub> , Cu <sub>2</sub> O, Cu <sub>2</sub> S,
Property mode	PR-BM
Solution	Sequential model
Fuel and steam reactor	Multi-stage RGibbs (Moving bed)
Air reactor	Multi-stage RGibbs (Moving bed)
Gas turbine (Combustion)	RGibbs
Mixer	mixer
separator	Sep/flash
Pressure controlling systems	Air compressor/Pumps/Gas compressor/turbines
Heat Exchangers	Heater/HeatX/MHeatX
Reference Environment	T=293.2 K and P=1.01 bar
Chemical property of the reference	75.62% N <sub>2</sub> , 20.3% O <sub>2</sub> , 3.12% H <sub>2</sub> O, 0.03% SO <sub>2</sub> , 0.92% (He, Ar, H <sub>2</sub> , CO <sub>2</sub> )
$\Delta T_{\text{compressor}}$	10 K
Pinch point (FWHs)	3 K
Auxiliary power Demand	7.5%
Pumping system performance	85%

**Table 5: The critical design assumptions.**

Class	Assumption
Air compressor	Compressor pressure ratio: 18 NDCL: 31.41 bar
Combustion chamber	Operating Pressure: 18.2 bar Operating temperature: 1440.7°K Excess air: 20% Calculation Option: chemical and phase equilibrium
Air reactor	Oxidation Temperature: 1472 K Solids entrainment ratio: 0.25 Calculation Option: chemical and phase equilibrium
Fuel reactor	Reduction Temperature: 1250 K Degree of reduction (Xred): 0.3 Calculation Option: chemical and phase equilibrium
Gas Turbines	GT/expander number: 2 Discharge pressure: 1.01bar Turbine inlet temperature: 1410 k The outlet temperature of the turbine: 800-830°K Isentropic efficiencies: 90%
HRSG and steam turbine	Three level pressures (HP/IP/LP): 166.7 bar/39.7 bar/7.3 bar Steam temperature (HP/IP/LP): 537°C/537°C/303.3°C Isentropic efficiencies (HPT/IPT/LPT): 89.0%/90.3%/85.1%
Condenser	Condenser pressure: 0.103 bar Pinch Temperature: 10°C
Carbon compressor	mixer Delivery pressure: 106.4 bar Compressor efficiency: 85% Delivery temperature: 40°C
Steam Reactor	Oxygen carrier to support ratio: 70 to 30 (wt. %) Operating temperature: 1050° K Calculation Option: chemical and phase equilibrium



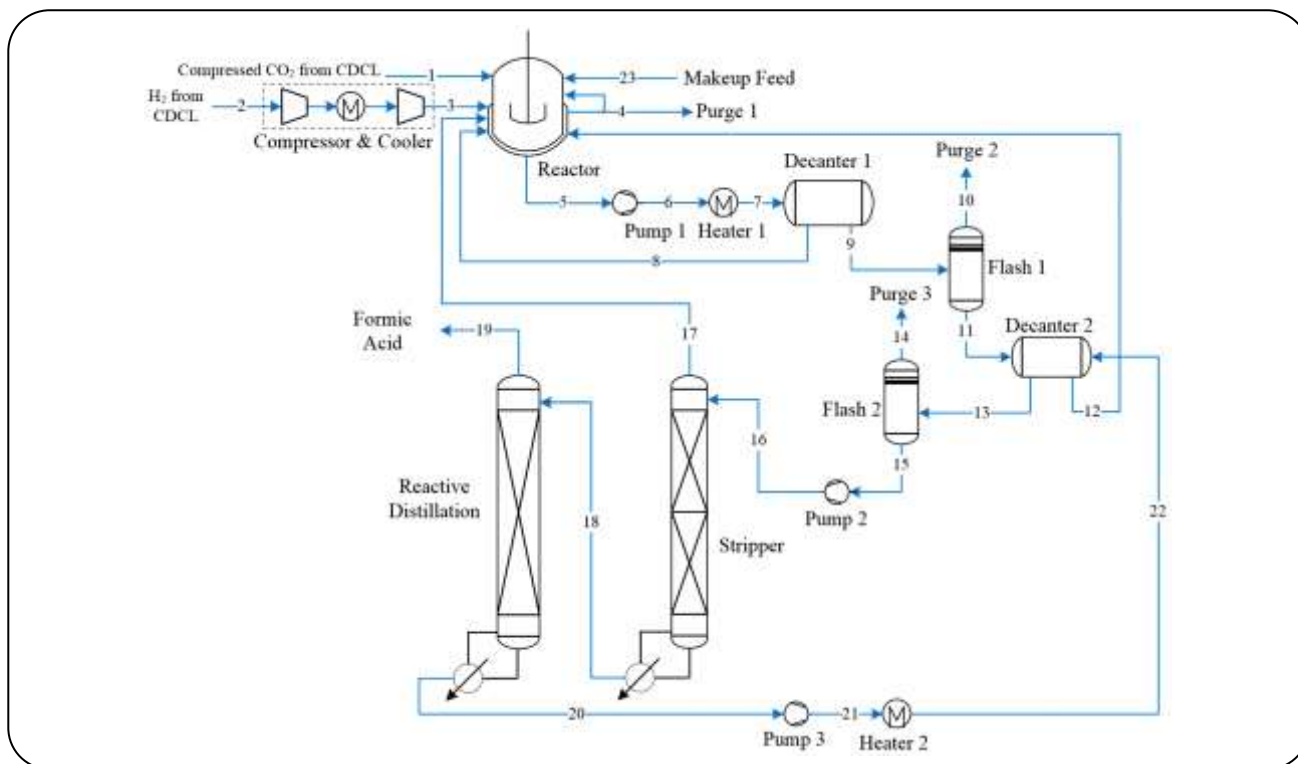
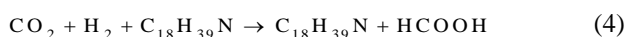


Fig. 5: The schematics of FA plant.

Fig. 5 shows a flow chart of the process of formic acid synthesis from the captured CO<sub>2</sub> used in this study. Hydrogen is produced from this NDCL plant with the power and production of H<sub>2</sub> for this synthesis process [67].

The formic acid synthesis process is divided into five main sections: Compression stage: Before feeding CO<sub>2</sub> and H<sub>2</sub> to the reaction stage, these gases must be liquid by compressing them to 105 bar and cooling them to 33°C. In this study, CO<sub>2</sub> was prepared for NDCL secretion at 105 bar and 33°C. At the same time, hydrogen is available at 30.9 bar and 25°C. Therefore, the hydrogen produced is compressed up to 105 bar (to avoid exergy destruction during the mixing process). Reaction phase: In the reaction phase, the homogeneous reaction of the liquid CO<sub>2</sub> and H<sub>2</sub> to form a compound additive acid (e.g., formic acid) in the presence of polar solvent (water and methanol mixture), phosphine, and ruthenium-based catalysts, as shown in Eq. (4) [68]:



Since the stoichiometric ratio of CO<sub>2</sub> and H<sub>2</sub> is the same, hydrogen production from the NDCL plant is adjusted to meet the molar CO<sub>2</sub> flow rate in the flue gas. The

additional heat required to maintain the reactor temperature at 90°C comes from the NDCL plant. Hydrogen-free CO<sub>2</sub> and H<sub>2</sub> released from the reactor are recycled after flashing a small amount (1% split fraction, mass basis) to avoid inert accumulation and non-return components. Catalyst Recovery Stage: Since catalysts are expensive[41], a set of two decanter systems working at 130 and 70 bar are used to achieve maximum recovery. After forming and purifying formic acid, a portion of the amine is recycled to the reactor to achieve maximum catalyst recovery. This study yields almost 100% catalyst recovery. Stripping step: Methanol is recovered using a balance-based stripping column operated on three strips. Light gases are separated from the feed stream using a flash vessel that works under atmospheric pressure before being fed to the column. The strip's low product purity is adjusted to obtain the desired product purity of 85% formic acid. The top products of the column (Water, methanol, and dissolved gases) are cooled and recycled into the reactor. Reactive Distillation Stage: Formic acid is formed and purified in a reactive distillation column. The current entering the reaction distillation column is 0.25 bar and 180°C. Under these conditions, the additive amine acid's

Table 6: The performance factor of the NDCL plant.

Factor	Formula
Energy performance plant	$\eta_{\text{Gross}} = \frac{W_{\text{gross}}}{m_{\text{fuel}} * \text{LHV}_{\text{fuel}}} * 100$
Hydrogen efficiency	$\eta_{\text{H}_2} = \frac{\text{LHV}_{\text{H}_2} \cdot m_{\text{H}_2}}{m_{\text{fuel}} * \text{LHV}_{\text{fuel}}} * 100$
Carbon capture efficiency	$\eta_{\text{CO}_2} = \frac{\text{CO}_{2,i} - \text{CO}_{2,o}}{\text{CO}_{2,i}}$
Specific carbon dioxide emission	$E_{\text{CO}_2} = \frac{m_{\text{CO}_2\text{emit}}}{W_{\text{net}}}$
Annual CO <sub>2</sub> emissions rate	$\varepsilon_{\text{fCO}_2} = \frac{m_{\text{CO}_2\text{emit}}}{3.6 * E_{\text{chf}}}$
Exergy efficiency of the plant	$\text{ExE} = \frac{\xi_{\text{H}_2} \cdot \text{LHV}_{\text{H}_2} \cdot m_{\text{H}_2} + \xi_{\text{FA}} \cdot \text{LHV}_{\text{FA}} \cdot m_{\text{FA}}}{\text{Electricity consumption}}$

separation forms the amine compound into formic acid and amine. Because the reaction is endothermic, adding heat to the column reboiler maintains the column temperature at 180°C. Formic acid is collected from the top product and cooled, while the amine from the bottom product is collected and recycled to the secondary decanter, as shown in Fig. 5. The performance parameters of this plant can be described using the following indexes mentioned in Table 6.

## RESULTS AND DISCUSSION

The mass and energy equilibrium is needed to evaluate plants' overall performance by simulating three plant configurations (i.e., conventional CCPP, NDCL with H<sub>2</sub> and power generation, and formic acid synthesis using captured CO<sub>2</sub> and produced H<sub>2</sub>). The simulation of these plants is confirmed separately from the literature results [17, 25, 37, 39]. The cases considered in this study are listed in Table 2, and a comparative analysis of the results obtained for these cases is discussed below.

### Technical Analysis

#### NDCL unit Vs. conventional CCPP

The key performance indicators of the NDCL plant with H<sub>2</sub> generation and power generation (Case 2) and conventional substation (Case 1) are summarized in Table 7. Simulation results of the conventional CCPP power plant and efficiency (Case 1) are consistent with studies in the literature [17, 21]. Since case 1 is not equipped with a carbon capture system, it emits all carbon dioxide (44.79 kg/s) from this plant, while the NDCL plant captures all CO<sub>2</sub> in the flue gas. The gross electricity generation capacity of conventional power plants and NDCL is 457.9 MWe and 202.6 MWe, respectively. Although the NDCL plant

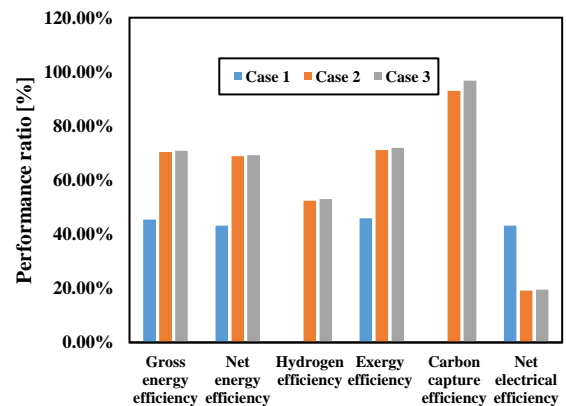


Fig. 6: Compares the results of each case of CCPP or NDCL.

efficiency is about half of the conventional CCPP's net electrical power generation. Because hydrogen is generated using the power at the NDCL power plant, the reduced oxygen carrier from the fuel reactor rather than air is oxidized by steam, resulting in an electrical energy penalty [32]. Hence, a penalty of 22.1% in net electrical efficiency is observed for case 2 compared to case 1, as shown in Fig. 6. Since hydrogen is also a good energy source, hydrogen efficiency is calculated based on its heating value. The value, LHV 141.9 MJ/kg [33, 68-70]. For hydrogen production of 526.33MW, hydrogen efficiency is estimated to be 52.44%. Total net energy efficiency is estimated as the sum of electric and hydrogen efficiency and is 70.33%. The hydrogen and net electrical efficiency values from the other studies reported in the literature are shown in Table 8. The higher the hydrogen production, the lower the electrical efficiency of the plant. It can be noted that the energy efficiency obtained in the present study is comparable with the other studies[71-75].

**Table 7: The results of the simulation of the NDCL cases and CAPP.**

Parameter	Case 1	Case 2	Case 3
Gross energy efficiency	45.4%	70.3%	70.9%
Net energy efficiency	43.2%	68.8%	69.2%
Hydrogen efficiency	0%	52.5%	53.0%
Exergy efficiency	45.8%	71.0%	71.9%
Carbon capture efficiency	0%	93.0%	96.7%
Net electrical efficiency	43.2%	19.1%	19.6%
Thermal input energy	1059.7	1059.7	1059.7
Net gas turbine output	332	106.3	110.7
Steam turbine output	163	96.3	96.7
Net power consumption	37.1	28.9	29.8
Net electricity output	457.9	202.6	207.4
Hydrogen production rate	0	526.3	526.0

**Table 8: The results of the other studies in this field.**

Carbon capture efficiency	Hydrogen efficiency	Net electrical efficiency	Fuel LHV [MJ/kg]	Reference
~78%	77%	3%	27	Zeng et al. (2012)
~90%	85%	1%	27	Fanxing (2013)
~89%	25%	23%	26	Dincer (2014)
~98%	19%	31%	29	Cristian Cormos (2014)
~100%	51%	13%	16	SURYWANSHI (2019)
~94%	52%	19%	44	This paper

**Monomethalic NDCL vs. bimetallic NDCL**

Because CO<sub>2</sub> control is essential to solving environmental problems [36], the plant's performance for NDCL is evaluated with and without a CDU that synthesizes formic acid from captured CO<sub>2</sub> and H<sub>2</sub>. Table 8 compares plant performance for NDCL with and without CDU by production and energy consumption. As the Natural input (1055 MJ/s) is maintained constant for all loads, CO<sub>2</sub> production is constant for all cases. Therefore, a constant amount of hydrogen (526.33 MW with a hydrogen efficiency of 52.44%) is necessary to synthesize formic acid. It is worth mentioning that the oxygen carrier used in this reaction is Fe<sub>2</sub>O<sub>3</sub>. Therefore, it produces general heat similar to an air reactor, a fuel reactor, and a carbon reactor. This results in a similar net gas turbine output of 96.30 MW output. Reactors, heaters, quarter-collector columns, and more, are suitable

energy units available in formic acid synthesis plants [38,72-76]. Besides, pumps and compressors also contribute to net power consumption. Therefore, there is excess energy consumption in the formic acid synthesis process and the difference between pure energy and water consumption capacity. This reduces the net power output of 67.5 MW and an increase of 0.50 MW of net energy consumption in case 3 compared to case 2. The gross and net electrical efficiency is calculated and shown in Fig. 6. Therefore, the integration of CDU into NDCL components has a gross and net energy penalty of 5.5 and 5.9, respectively. One of this study's main goals is to highlight the potential improvement in overall plant performance for high energy use. To achieve the aims, plans are performed with a bimetallic oxygen carrier to increase the exchange rate of fuel using CuO (5% wt) and Fe<sub>2</sub>O<sub>3</sub> (90% wt) oxygen carriers.

Different metal oxides have been proposed in the literature as possible candidates for the CLC process were determined as CuO, CdO, NiO, Mn<sub>2</sub>O<sub>3</sub>, Fe<sub>2</sub>O<sub>3</sub>, and CoO[1-5]. To increase the reactivity and durability of the oxides, the particles have been doped with several inserts such as Al<sub>2</sub>O<sub>3</sub>, YSZ, TiO<sub>2</sub>, or MgO, which act as porous support. Ref. [6] showed a review of the literature data on oxygen carriers in CLC[77].

CuO is one of the cheapest materials and has the highest oxygen transport capacity among the possible metal oxides. Several investigations in the literature related Cu as an oxygen carrier for CLC. Ref. [5, 7] at TDA Research developed Cu-based sorbents in their sorbent energy transfer system, a type of CLC where the power cycle operates in a very conventional manner. The copper-containing oxygen carriers demonstrated excellent chemical stability.

Experimental studies of CLC systems with iron oxide showed lower reaction rates than oxygen carriers like copper oxide [41]. An additional benefit of containing CuO is to convert sulfur to Cu<sub>2</sub>S in the fuel reactor where the quality of natural gas is low, and there is a higher amount of Sulfur content in it, preventing the formation of H<sub>2</sub>S and SO<sub>x</sub> in the flue gases. Cu<sub>2</sub>S can then easily be oxygenated to the CO and SO<sub>x</sub> gases in the air reactor. In practice, the presence of H<sub>2</sub>S provides oxygen transport activity to be manipulated to the other unwanted reactions causing an impairment that can be avoided using a proper natural gas refinery plant. As shown in Table 7, rather than Fe<sub>2</sub>O<sub>3</sub> (case 2), a bimetallic oxygen carrier (Case 3) increases gross and net electrical energy generation by 4.7 MW and 11.3 MW, respectively, thus, a 0.4% increase in the net energy performance. This improvement occurs mainly during oxidation in the air reactor. This is due to increased exothermic heat in copper oxide compared to iron oxide reactions [27, 28, 32]. It has been concluded that even though copper oxide is not involved in hydrogen formation, a small fraction of copper in Fe<sub>2</sub>O<sub>3</sub> can increase the system's total performance (see Fig. 7).

### Environmental Analysis

The primary role of NDCL technology is to reduce carbon emissions, so plant performance is also compared based on ecological assessment, as shown in Table 9. The most important factors determining each system's environmental performance are Carbon capture efficiency

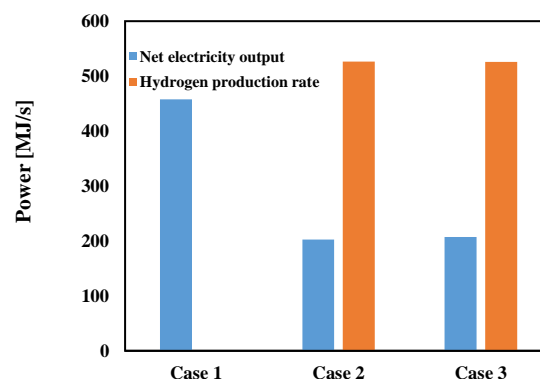


Fig. 7: Compares the results of bimetallic or monometallic oxygen carriers on the energy performance of the system.

and levelized carbon dioxide emissions. The levelized carbon dioxide for conventional CCPP is 381 kgCO<sub>2</sub>/MWh. The annual CO<sub>2</sub> capture rate is estimated to be 7,000 hours a year [22]. Similar to traditional CCPP, environmental assessments are intended for both oxygen carriers. Because CLC technology is used for cases 2 and 3, 93 and 96.7% of emissions were calculated. The integration of CDU with the NCDL plant using Fe<sub>2</sub>O<sub>3</sub> increased the net electrical output per unit of captured CO<sub>2</sub> to 1.59 MW/kgCO<sub>2</sub>. A slight improvement was observed in a bimetallic oxygen carrier compared with monometallic iron oxide as an oxygen carrier [34,78-102].

### Economics analysis

The cost values listed in Table 10 for the different scenarios of equipment were used to calculate different stages of capital cost(CAPEX) estimates using the method described in Sec. 2. The effect of the scaling factor on the cost of the reactors was also examined and is shown in Figure 8. The results show that the reactor cost increases from \$0.7 million to about \$1.76 million when the scaling factor increases from 0.4 to 0.7[11, 66]. Although the scaling factor influences the reactor cost, it does not significantly affect the overall cost of equipment as the reactors account for only about 2% of the total cost of equipment. Hence, the recommended scaling value of 0.56 was used for further economic analysis. The results of all cost estimations are shown in Table 11. In this table, different cost levels described earlier for the CAPEX estimation are written in normal letters, while the cost components which make up the subsequent cost levels are highlighted in italics. The table shows the capital cost economic details for the CLC system. The results show

**Table 9: The environmental analysis of the systems.**

Parameter	Case 1	Case 2	Case 3
Total carbon emission, kgCO <sub>2</sub> /s	46.7	1.89	1.27
Carbon capture efficiency, %	0.0	93	96.7
Levelized carbon emission, kg/MWh	381	26.7	12.6
Carbon emission per Fuel energy, kg/GJfuel	0.0	69.3	69.3
Net power per kg Carbon captured, MW/kgCO <sub>2</sub>	0.0	1.59	1.65

**Table 10: System equipment cost estimates.**

Item	Cost estimate (million \$)
Air compressor	40
Air reactor	1.3
Fuel reactor	1.5
Separators	0.9
Heat exchangers	5.1
Turbines	135
Pumps	0.4
Instrumentation and control	33.2
Piping	66.7
electrical system	50.1
Buildings	62
Yard improvement	27
Service facilities	101
Land	14.3
CO <sub>2</sub> separation and compression system	18.9
Formic Acid system	102

that the plant components cost is about \$716.9 million while the total CAPEX is \$947.4 million at the base case conditions and prices.

Furthermore, the calculation of the operational cost (OPEX) costs was also undertaken. The two major categories of OPEX costs, which are direct and indirect production costs, were calculated. The costs were calculated by estimating different OPEX costs as percentages of fixed costs. Table 7 shows the percentage ranges for the items contained in the OPEX and the selected percentage values.

These ranges were sourced from literature as described earlier. The results show the total annual OPEX cost is about \$195.08 million. The fuel cost accounts for a significant portion of the OPEX cost. The CAPEX and OPEX costs were used to carry out several economic metric performances. The CAPEX and OPEX for the two NGCC power plants (with and without CO<sub>2</sub> capture) were also calculated by adjusting the National Energy Technology Laboratory [37]. This was done by changing the input price of natural gas, the base year \$, and adding the cost of overheads to make a fair comparison. It should be mentioned that there is a minor difference in the capacities of the three plants. However, this difference is very small (0.005%) and has a negligible effect on economic comparison [102-127].

The percentages of the major annual cost components for the plants were also calculated to understand the role of each cost component on the CAPEX for the three power plants. The results show that the most significant cost is the fuel cost. Figure 8 shows the percentages of the most significant costs on the CAPEX. The results show that the fuel costs account for 53.4, 54.2, and 65.2% for the NGCC, NGCC with carbon capture, and NGCC with capture and formic acid plants. The next significant cost is the annual CAPEX cost, accounting for about 15.2, 16.5, and 9.85% for the NGCC, NGCC with carbon capture, and NGCC with capture and formic acid plants, respectively. The other three most significant costs are maintenance, overheads, local taxes, and insurance costs. Table 12 shows the difference between the major costs of electricity and carbon capture for the three power plants. The cost analysis contributes to developing a better understanding of the effect of changes in prices of any cost components on the CAPEX and the cost of CO<sub>2</sub> capture [127-141].

Table 11: Capital cost for the system.

Cost Item	Value (million \$)
Bare erected costs (BEC)	625
Engineering, procurement, and construction (EPC)	93
Engineering, procurement, and construction cost (EPCC)	717
Process contingency	33
Project contingency	33
Total plant costs (TPC)	886
Owner's costs	79
Total overnight costs (TOC)	861
Escalation costs	86
Total as-spent costs (TASC)	1062

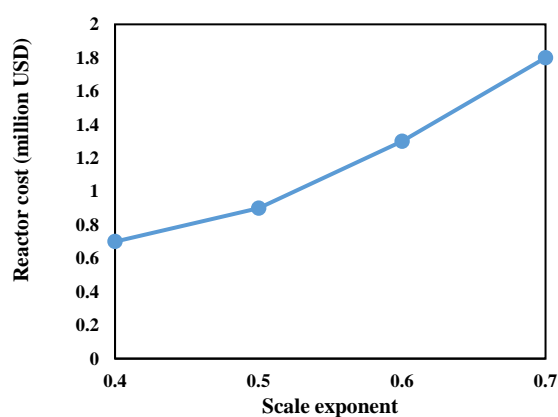


Fig. 8: Scaling impacts the costs of the system.

The results of the economic analysis of each case are presented in Table 13. The results show that the payback period of case 1 is the least among the other cases. However, cases 2 and 3 are also economically feasible due to their acceptable payback period. Also, the results of the economic analysis are aligned with the results of the literature [70-78].

## CONCLUSIONS

In this paper, a steady flow model of the NDCL process with  $H_2$  and co-generation of electricity was simulated using CHEMCAD to explore the technical and thermodynamical feasibility of coupling FA synthesis with the plant to utilize carbon capture. Also, this study examined the technical feasibility of oxygen removal features of copper to promote the reactions of natural gas and  $Fe_2O_3$ . This case was studied by taking the different plant settings as examples into account. These plants' performance was compared with conventional CCPPs

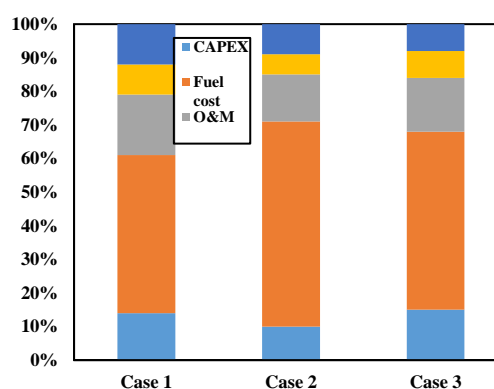


Fig. 9: Portfolio of the costs in each case.

based on overall electricity and energy production, plant efficiency, and environmental assessment. All NDCL plants resulted in 90-100%  $CO_2$  capture. A penalty of 19% is observed in net electrical efficiency with NDCL compared to conventional CCPP. However, the overall net energy efficiency of the NDCL plant increased by 32% due to the production rate of 526.3 MW of hydrogen compared to CCPP. The present study also shows that integrating formic acid synthesis as a scheme of carbon dioxide used in NDCL resulted in a 4.6% penalty in electrical and overall energy efficiency.

On the other hand, an improvement of overall and net electrical efficiency of 0.38 for bimetallic oxygen carriers compared to  $Fe_2O_3$  is observed. Besides, the environmental evaluation also showed an improvement in net electrical efficiency per kg of  $CO_2$  captured for the bimetallic oxygen carrier. In the end, economic analysis shows an acceptable financial output for the two proposed cases. However, it is suggested that an exergoeconomic

**Table 12: Total investment cost and system performance for the CLC and NGCC power plant.**

Item	Case 1	Case 2	Case 3
Cost of electricity (U.S. cents/kWh)	4.5	6.2	6.2
Cost of CO <sub>2</sub> captured (\$/ton)	—	28	24
CAPEX cost	490	948	1062
Fuel flow rate (kg/h)	74,450	84,135	76,500
Annual fuel cost (Million \$)	108.2	123	111
Annual Ni cost (Million \$)	—	—	2.4
Annual OPEX	145	176	200

**Table 13. Payback time (return on investment) analysis.**

Item	Case 1	Case 2	Case 3
Electricity produced (MW)	457.9	202.6	207.4
CO <sub>2</sub> captured efficiency	0%	93.0%	96.7%
Annual electricity revenue (Million \$)	371.2	178.2	180.5
Annual CO <sub>2</sub> revenue (Million \$) <sup>1</sup>	-	34.8	40.1
Hydrogen Revenue (Million \$)	-	168.9	-
Formic Acid Revenue (Million \$)	-	-	81.2
Hydrogen Carrier Revenue (Million \$) <sup>2</sup>	-	-	93.1
Total annual revenue (Million \$)	371.2	381.9	394.9
Annual OPEX (Million \$)	168.3	221.4	234.7
Annual profit (Million \$)	202.9	160.5	160.2
Payback period (years)	2.5	5.9	6.6

1) Green Tax and Carbon market

2) Using formic acid as a hydrogen carrier decreases the hydrogen transportation costs to 35% of the original cost.

analysis be performed on these cases to give a deeper insight into the feasibility of the proposed systems.

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