



**DLSU RESEARCH CONGRESS 2020**  
"Building Resilient, Innovative,  
and Sustainable Societies"  
June 17-19, 2020



## Optimal Integration of a Partial Chemical Looping Combustion and Iron Production Plant

John Patrick D Mercado<sup>1</sup> and Aristotle T. Ubando<sup>2\*</sup>

<sup>1,2</sup> De La Salle University-Manila, 2401 Taft ave. Malate, Manila 1002, Philippines)

\*Aristotle.ubando@dlsu.edu.ph

**Abstract:** This study proposed the optimal design of a partial chemical looping combustion (CLC) system integrated into an iron production plant (IPP). There have been numerous studies on chemical looping combustion, but none have studied a system incorporating a partial looping of iron oxides. The iron industry is one of the largest contributors to the carbon emissions worldwide. Much of the emissions come from the heat and power needed by the iron industry. The analysis considered to include the production of pig iron, power generation, and the reduction of hematite requirement through a stoichiometric ratio and effects analyses. A quadratic model that fully characterized the system was developed. The initial values for the system were based on a 10 MW power plant wherein the inputs and outputs of the plant were assumed invariant. Thus, allowing the integration of the system through the determination of the heat requirement of the iron production plant. The iron manufacturing case study of an iron manufacturing is adapted from Ubando et al (2019) along with the raw materials and product influx of the system. Lingo was used as a modelling software to implement the optimal integration of the system. The optimization model was able to successfully calculate the value of the hematite to magnetite ratio of the raw material entering the iron production plant. A case with a fixed pig iron output of 800t/h from and 10MW power production from the combined system found an optimum ratio of 75.32%

**Key Words:** Chemical looping combustion, partial loop, iron production, optimization,



## 1. INTRODUCTION

The iron industry is one of the largest industries in the world. It is seen as what drives the progress of economies. Despite being one of the most important industries, it also is one of the most significant contributors to the production of carbon dioxide. With the growing demand for iron in the infrastructure and automotive industries, the emissions of this industry are also expected to increase as well. This is of concern since it already amounts to 7% of global carbon dioxide emissions (Ubando et. al. 2019). The large amount of the emissions of this industry is from the power and heat requirement of the processes involved. Chemical looping combustion (CLC) is seen as a relatively new but promising prospect in power production due to its inherent carbon capture capabilities. CLC uses an oxygen carrier to transfer oxygen from the combustion air to the gaseous fuel. Through this process, the combustion air and fuel never mix, allowing for the gasses from the oxidation of the fuel to be extracted separately (Lyngfelt et. al, 2001). There have been numerous studies on this process exploring various fuels and oxygen carriers (Jerndal et. al., 2006). The carbon capture capability of CLCs is mostly due to the high purity of the carbon dioxide being produced from the process (Abad et. al, 2007). There are also various other chemical looping processes such as chemical looping gasification (Zhao et al., 2017). There have also been studies that explored the various oxygen carriers (Matzen et. al., 2017). Hematite is viewed as one of the more promising oxygen carriers because of its relatively low cost and high reactivity. There were also various studies about the use of Iron ores specifically, hematite as an oxygen carrier in CLC though the studies focused on its use along with solid fuels (Gu et. al., 2011). This study aims to demonstrate how iron manufacturing and CLC can be integrated into each other to maximize the profits generated. It was noted through multiple searches through various databases that such a study with an open loop chemical looping

combustion was yet to be made. This study is intended to fill this gap and show the potential of such a system.

## 2. METHODOLOGY

### 2.1 Iron Production Plant

The data on the iron production plant was derived from the paper of Ubando et al. (2019). The iron production plant was simplified into a single unit for ease in coding as seen in fig.1. The exhaust gasses and their prices were added together as well as the additives for the iron production plant. The five process units were put together and the only outputs and inputs considered were those that exited the system. This is possible because it is assumed that the relationships between those process units were linear

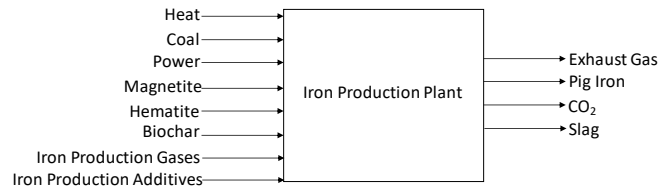


Fig.1 The iron production plant and its products

and scaling one would scale the other proportionally as much. It is also assumed that the amount of slag produced by a constant amount of input, regardless of the type of iron ore being used, would remain the same. This means that as long as the sum of the different kinds of iron is the same, the amount of slag would remain the same. The same relation is assumed to hold true for the other inputs and outputs of the system. There is also a stream of magnetite entering the system and it is assumed that it has a 10% greater

$$q = \frac{\dot{m}_h}{\dot{m}_m} \quad (\text{Eq.1})$$

$$q \geq 0; q \leq 1 \quad (\text{Eq.2})$$

where:

$q$  = Ratio of hematite to magnetite

$\dot{m}_h$  = Mass flux of hematite

$\dot{m}_m$  = Mass flux of magnetite



price than regular hematite. It is also assumed that there is a 12.5 % increase in the amount of pig iron produced for a system that purely uses magnetite as an input. The 12.5% is determined through the ratio of the amount of iron in magnetite to hematite. It was seen that magnetite has 12.5% more iron content than hematite. These assumptions are made considering everything else remains constant. A variable  $q$  was introduced and represented the ratio of hematite to magnetite entering the iron production plant. The variable is initialized as seen in Eq.1 and 2

## 2.2 CLC Plant

The CLC plant is also governed by multiple assumptions to make the calculations simpler. The initial values of the OC, power produced, and amount of fuel was adopted from Porrizzo et al (2016). The values used were for a 10 MW<sub>th</sub> power plant but was then scaled up to 500 MW<sub>th</sub> the up scaling of the plant was assumed to be linear for all variables. The paper mentioned that the plant was able to achieve 52% thermal efficiency without CO<sub>2</sub> emissions to the atmosphere. The main assumptions made for the CLC system are as follows: the power generator with a 52% efficiency is incorporated into the system, the power was assumed to all be produced in the Air reactor (AR) and the power produced was directly related to the fraction of magnetite coming in from the fuel reactor (FR). The flow rate of air was neglected in the model since it was not significant to the quantities being analyzed. It is also assumed that the fuel reactor fully converts the hematite into magnetite. The amount of magnetite exiting the fuel reactor was two thirds of the amount of hematite entering it due to the loss of oxygen. The amount of magnetite entering the air reactor then decreased due to part of it going to the iron production plant. In order to properly observe the effect of the flow of magnetite into the iron production plant, the capacities of the plants were held constant. The system can be seen in fig.2.

## 2.3 Optimization Model

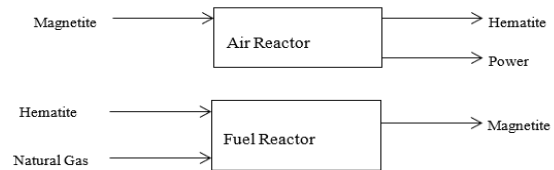


Fig 2 The two reactors of the CLC system

The scenario for this model is that there is an iron production plant with an output capacity of 800 tons per hour of pig iron. There is also a CLC plant with an power output capacity of 10MW. The two plants are in close proximity to each other. The owners want to work together to increase their profit through a direct exchange of products between. This study aims to find out the proportion of hematite to reduced iron ore, also known as magnetite within an integrated iron and energy production system based on CLC. The final products considered in this system are pig iron, heat, and electricity. The next paragraphs will describe the multiple assumptions made in modeling the system. The model that was developed is a quadratic program that analyzes only the product stream and omits the capital costs.

The model considered in this system had an objective function as shown in Eq. 3 and 4. The data used for the price vector is presented in Table 1 and the data used in the product streams are seen in Table 2.

$$\max = R \quad (\text{Eq. 3})$$

$$R = \sum_{i=1}^n P_i y_i \quad (\text{Eq. 4})$$

where:

- $R$  = Profit
- $P_i$  = Price Vector
- $y_i$  = Product Output Vector
- $n$  = Number of product streams



Table 1. Products and their prices

Product	Price	Units
Magnetite	85.03	\$/ton
Hematite/ Iron Ore	77.3	\$/ton
Pig Iron	711.16	\$/ton
Natural gas	145.87	\$/ton
Power	92.1	\$/MWh
CO <sub>2</sub>	0	\$/m <sup>3</sup>
Heat	51.58	\$/MWh
Coal	63.8	\$/ton
Biochar	329	\$/ton
Slag	0	\$/ton
Exhaust gasses	0	\$/ton
Iron production gasses	8.24	\$/m <sup>3</sup>
Iron production additives	223.95	\$/ton

Table 2. The products and their quantities

Product	IPP	FR	AR	Units
Magnetite	0	833.3	-833.3	t/h
Hematite/ Iron Ore	-990.4	-1250	1250	t/h
Pig iron	800	0	0	t/h
Natural gas	0	-190	0	t/h
Power	-16.2	0	260	MW
Heat	-111.2	0	0	MW
CO <sub>2</sub>	292.9	0	0	m <sup>3</sup>
Coal	-661.1	0	0	t/h
Biochar	-284.8	0	0	t/h
Slag	229.6	0	0	t/h
Exhaust gas	1061.9	0	0	t/h
Iron production gasses	-1726.7	0	0	\$/m <sup>3</sup>
Iron Production additives	-1120.4	0	0	t/h

$$\sum_{j=1}^n A_j x_j = y_i \quad (\text{Eq. 5})$$

where:

- $A_j$  = Product streams
- $x_j$  = Process scaling factor

$$(v_3 + v_3 * q * .125) * x_1 = y_3 \quad (\text{Eq. 6})$$

where:

- $y_1$  = Pig iron product stream
- $v_2$  = Pig iron exiting the Iron plant

For each output vector  $y$ , a material and energy balance is made throughout the system as seen in eq. 5.

The model maximized the profit. It then displayed value of  $q$  corresponds to the max profit. In addition, the pig iron produced from the iron production plant, the fuel consumption, and power produced from the CLC were the constraints.

The model ran using an educational version of Lingo. To better understand the assumptions and their relationships, the individual product streams will be analyzed. The full system being analyzed is shown in figure 3.

Equation 6 shows the pig iron product stream where the assumption made was that the fraction of magnetite input into the system increased the amount of pig iron produced by the system by 12.5%, also assuming most other factors in the IPP remained the same regardless of the type of ore used.



$$-v_5 * x_1 + \left( \frac{\frac{2}{3} * v_2 - q * v_1}{\frac{2}{3} v_2} \right) * v_6 * x_3 = y_5 \quad (\text{Eq. 7})$$

where:

- $y_5$  = Power product stream
- $v_5$  = Power entering the Iron plant

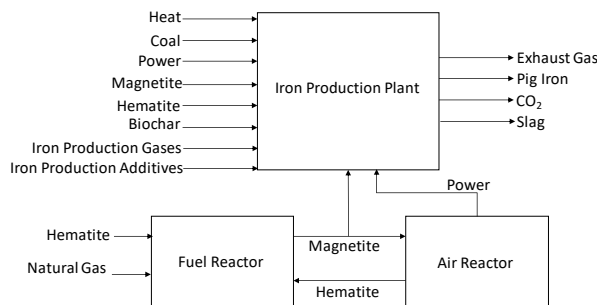


Fig.3 The full system being analyzed

Equation 7 shows the power product stream where it is assumed that all the power is produced in the AR and that the amount of power produced is proportional to the ratio of the magnetite entering it to the amount of magnetite exiting the FR. This assumption is made for the sake of simplification of the model and to consider the decrease in the amount of power produced due to the reduction of magnetite in circulation in the system.

An additional important constraint added to the model was that the process vectors of the AR and FR,  $x_2$  and  $x_3$  are set to be equal since they essentially function as a pair always. The constraints added were that the amount of fuel input to the CLC remained the same and that the amount of pig iron produced remained the same.

### 3. RESULTS AND DISCUSSION

The constraints added to the system were a fixed pig iron output of 800t/h from the IPP and 10MW power production from the CLC. The results of the run on the system showed that for the assumptions made, the value of  $q$  that gave the highest profit while the amount of pig iron produced and amount of fuel input remained constant, was around 75.32%. The local optimum was found and the objective value, or the profit gained, was 76,726\$. The model was able to calculate the optimal  $q$  for the chosen case. It was also noticed that as the power increased, the pig iron remained constant, and the ratio of hematite to magnetite decreased. Thus, more magnetite from the CLC is being diverted to the iron plant to produce the same amount of pig iron at a lower cost. These are all the effects of the assumptions previously made during the modelling of the system.

### 4. CONCLUSIONS

The study showed a methodology on modelling an iron production plant with a fixed output with the optimal integration of a partial chemical looping combustion system. It was also shown that benefits are gained by allowing a portion of the reduced magnetite to be utilized in the IPP. The assumptions on the relationships of the processes could be also further improved using empirical results from actual experiments.





## 5. ACKNOWLEDGEMENTS

The authors acknowledge the Department of Science and Technology – Science Education Institute (DOST-SEI) and the Engineering Research and Development for Technology (ERDT) program for the support provided to the author in seeking a Master of Science in Mechanical Engineering degree at De La Salle University-Manila.

## 6. REFERENCES

- Abad A, Mattisson T, Lyngfelt A, Johansson M. The use of iron oxide as oxygen carrier in a chemical-looping reactor. *Fuel*. 2007;86(7-8):1021–35.
- Chen H, Zheng Z, Chen Z, Bi XT. Reduction of hematite ( $\text{Fe}_2\text{O}_3$ ) to metallic iron (Fe) by CO in a micro fluidized bed reaction analyzer: A multistep kinetics study. *Powder Technology*. 2017;316:410–20.
- Clark J. The Extraction of Iron [Internet]. Chemistry LibreTexts. Libretxts; 2019 [cited 2019Dec15]. Available from: [https://chem.libretexts.org/Courses/Westminster\\_College/CHE\\_180\\_-\\_Inorganic\\_Chemistry/10:\\_Chapter\\_10\\_-\\_The\\_Transition\\_Metals/10.1:\\_Properties\\_of\\_Transition\\_Metals/Metallurgy/The\\_Extraction\\_of\\_Iron](https://chem.libretexts.org/Courses/Westminster_College/CHE_180_-_Inorganic_Chemistry/10:_Chapter_10_-_The_Transition_Metals/10.1:_Properties_of_Transition_Metals/Metallurgy/The_Extraction_of_Iron)
- Gu H, Shen L, Xiao J, Zhang S, Song T. Chemical Looping Combustion of Biomass/Coal with Natural Iron Ore as Oxygen Carrier in a Continuous Reactor. *Energy & Fuels*. 2011;25(1):446–55.
- Jerndal E, Mattisson T, Lyngfelt A. Thermal Analysis of Chemical-Looping Combustion. *Chemical Engineering Research and Design*. 2006;84(9):795–806.
- Lyngfelt A, Leckner B, Mattisson T. A fluidized-bed combustion process with inherent  $\text{CO}_2$  separation: application of chemical-looping combustion. *Chemical Engineering Science*. 2001;56(10):3101–13.
- Monazam ER, Breault RW, Siriwardane R. Reduction of hematite ( $\text{Fe}_2\text{O}_3$ ) to wüstite (FeO) by carbon monoxide (CO) for chemical looping combustion. *Chemical Engineering Journal*. 2014;242:204–10.
- Ponomar V, Brik O, Cherevko Y, Ovsienko V. Kinetics of hematite to magnetite transformation by gaseous reduction at low concentration of carbon monoxide. *Chemical Engineering Research and Design*. 2019;148:393–402.
- Porrazzo R, White G, Ocone R. Techno-economic investigation of a chemical looping combustion based power plant. *Faraday Discussions*. 2016;192:437–57.
- Shen L, Wu J, Xiao J, Song Q, Xiao R. Chemical-Looping Combustion of Biomass in a 10 kWth Reactor with Iron Oxide As an Oxygen Carrier. *Energy & Fuels*. 2009;23(5):2498–505.
- Steel manufacture [Internet]. [www.steelconstruction.info](http://www.steelconstruction.info). ArcelorMittal; [cited 2019Dec15]. Available from: [https://www.steelconstruction.info/Steel\\_manufacture](https://www.steelconstruction.info/Steel_manufacture)
- Ubando AT, Chen WH, Tan RR, Naqvi SR. Optimal integration of a biomass-based polygeneration system in an iron production plant for negative carbon emissions. *International Journal of Energy Research*. 2019;