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Product carbon footprint methodology for ammonia production by conventional steam reforming–A case study

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ABSTRACT

There are 10 nitrogen fertilizer companies in Egypt with 14 production lines, the majority of which are ammonia/urea plants and only four ammonia/nitric acid/ammonium nitrate plants. In 2020, Egypt produced 6.7 million tons of urea of which 4.7 million were exported making it the world's 5th largest exporter with 40.00% exported to European Union. The introduction of European carbon border adjustment mechanism (CBAM), which may trigger similar actions in other is a real threat to Egyptian fertilizers exports. According to CBAM, the importer will pay a tax proportional to the difference between ammonia embedded emissions and the free allowance set by relevant regulations. There are general guidelines for estimation of embedded emissions, however, detailed industry specific calculations have not yet been developed. Estimation of ammonia embedded emissions takes into consideration both the fuel used within the ammonia plant system boundary and that used for exported steam and for electricity generation. There will be two different values for ammonia embedded emissions based on whether or not exported energy takes place: 1.62 $tCO_2/t\ NH_3$ in the case of ammonia/urea plants and 2.52 in the case of ammonia/nitric acid plants, where no steam or CO_2 exports takes place. Since embedded emissions directly impact the competitiveness of the Egyptian fertilizers, a rigorous methodology is proposed that takes into consideration all these aspects compared to other estimation techniques using different levels of approximation and exclusions. The impact of different decarbonization measures on embedded emissions and CBAM cost is also investigated taking into consideration the phaseout of free allowances.

Keywords: product carbon footprint, carbon allocation, conventional steam reforming, embedded carbon, CBAM methodology, free allowance

INTRODUCTION

In Egypt, the energy-intensive industries represent 68.47% of the total energy consumption of the industrial sector. The nitrogen fertilizer industry is energy intensive and ammonia production is the main contributor to carbon emissions, which led the GOE to include in its nationally determined contributions (NDCs), a decarbonization target of 10.00% for the industry by 2030. According to the second updated NDC for Egypt (NDC, 2023), Egypt plans to decarbonize the industrial sector by reducing its energy intensity, using renewable and alternative fuels, and introducing low carbon process improvements, primarily through the decrease in the average specific thermal energy consumption by 10.00% for three energy intensive industries (iron and steel, fertilizers, and ceramic tiles industries). However, at the level of each facility, this decrease is not enough to breach the gap between the embedded emissions and the benchmark for free allowance as the latter is planned to decrease to reach zero in 2035 according to the European Green Deal (Pinsent Masons, 2023).

The European emission trading system (ETS) sets a cap on the amount of green house gases that can be released from an industrial installation. If emissions are higher than the cap, allowances are bought from ETS market. Carbon border adjustment mechanism (CBAM) is based on ETS system and its free allowances, but it will progressively replace it (CELEX 32021R0447, 2021). Current CBAM obligations are calculation by evaluating embedded emissions in imported goods to European Union (EU), then deducting the free EU ETS (2023) allocation emission, which is 0.157 in the case of ammonia. This value is then multiplied by the tons of imports and by average weekly EU ETS (2023) price. If a carbon tax is paid in the country of origin it is subtracted for adjustment. Since such tax does not currently exist in Egypt, the European importer will have to pay the whole value of ETS cost for CO_2 exceeding the allowable benchmark. In 2022, the average price was €80/t CO_2 (EU ETS, 2023). For fertilizers containing ammonia such as urea, ammonium nitrate and mixed fertilizers CBAM cost will be based on the percentage of ammonia within the imported good: 57.00% in urea, 28.00% in nitric acid and 42.00% in ammonium nitrate.

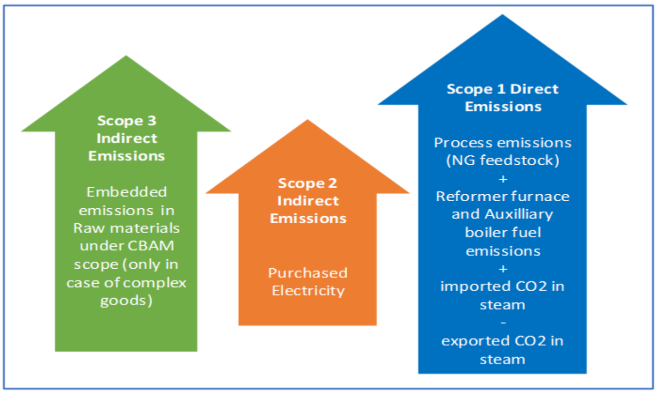

Figure 1. Embedded emissions scope under CBAM (CBAM Guidelines, 2023)

CBAM methodology (CBAM Guidelines, 2023) is different from the cradle-to-gate approach (BASF, 2021) in that it does not include the upstream activities related to extraction, manufacturing, and transportation of inputs to the factory and it also subtracts any exported embedded CO_2. This results in a lower CBAM value for embedded emissions. **Figure 1** presents the scope of CBAM carbon emissions (CBAM Guidelines, 2023). Under CBAM, ammonia is defined as a simple good since the input materials used for its production (natural gas and fuel) have no embedded emissions. In Egypt, 90.00% of ammonia production lines use UHDE technology for conventional steam reforming. Production capacity of lines is between 1,100 and 1,400 t NH_3/d and natural gas feedstock is about 685 m^3 NG/t NH_3 corresponding to a steam to carbon ratio of 2.5 (UNIDO, 2014). Specific energy of NG feedstock is 26 GJ/t NH_3, which is higher than BAT value of 22.1 (IPPC BREF LVIC, 2007).

COMPLEXITY OF N-FERTILIZER STEAM CYCLE

Ammonia line is both a producer and consumer of thermal energy. HP steam is generated mainly from the exothermic reactions taking place in the secondary reformer, the water gas shift reactors, and ammonia synthesis reactor as well as the auxiliary boiler. Thermal energy is consumed in the primary reformer as direct combustion of natural gas but at the same time steam is generated from waste heat in flue gases. As presented in **Figure 2**, steam generated from the reformer flue gases is used as process steam and to heat combustion air to reformer, NG feedstock, and air feed to secondary reformer.

High pressure steam from all sources in an HP steam header from which it is distributed to various activities: electricity generation (part of which is exported to the urea plant), export to urea plant, driving the ammonia compressor and the CO_2 compressor, and other motors within the system boundary of the ammonia plant. HP steam is made up of a mixture of zero carbon and fossil carbon steam and will therefore have embedded emissions that should be estimated to allow deduction of CO_2 exported to the urea plant as per CBAM methodology (**Figure 1**). In the case of ammonia/nitric acid plants there is no export of steam or CO_2 such a step will not be needed. EU Commission will be developing tailored certification methodologies for the different types of carbon removal activities (EU Commission, 2022). Minimizing assumptions and exclusion of energy streams and taking into consideration embedded carbon in steam and energy exports will result in a higher degree of accuracy.

ESTIMATION OF AMMONIA EMBEDDED EMISSIONS

Setting Boundary Around Ammonia Production Line

Figure 2 shows the system boundary, where the inputs consist of NG feedstock, NG fuel to reformer, NG fuel to auxiliary boiler, and grid electricity. The outputs are ammonia, exported CO_2, steam and electricity to the urea plant. The PCF under cradle-to-grave methodology returns an inflated value for carbon emissions as exported emissions are not deducted.

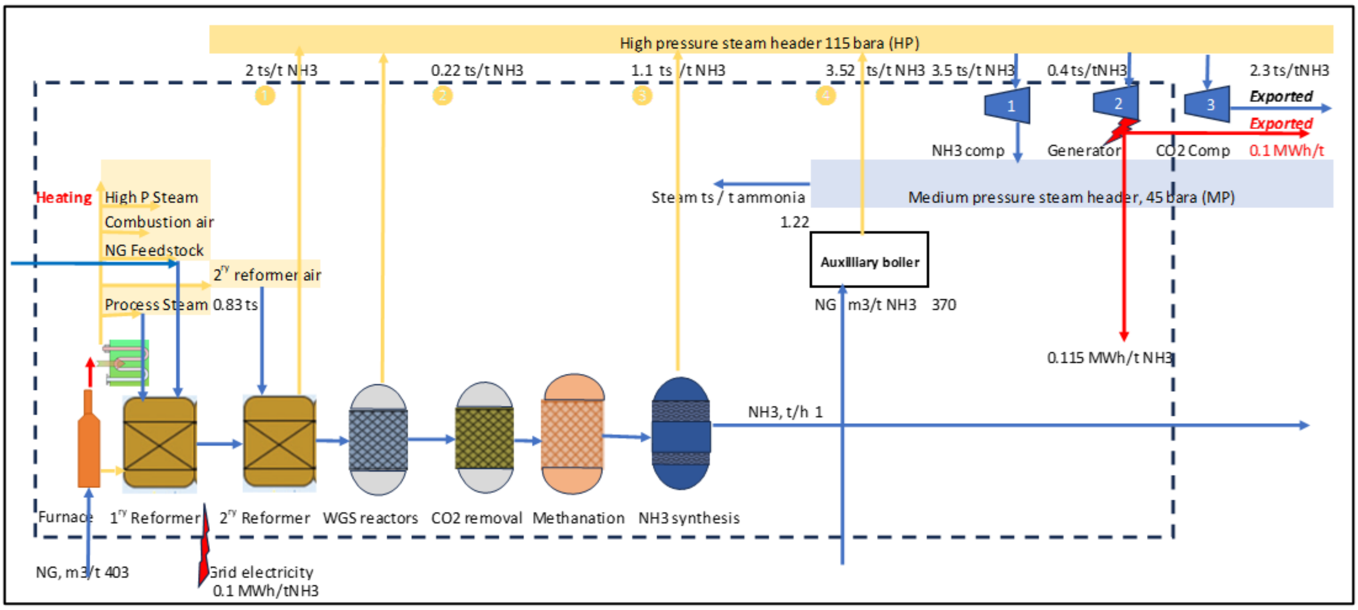

Figure 2. Schematic diagram showing system boundary & interacting surroundings (Source: Author's own elaboration)

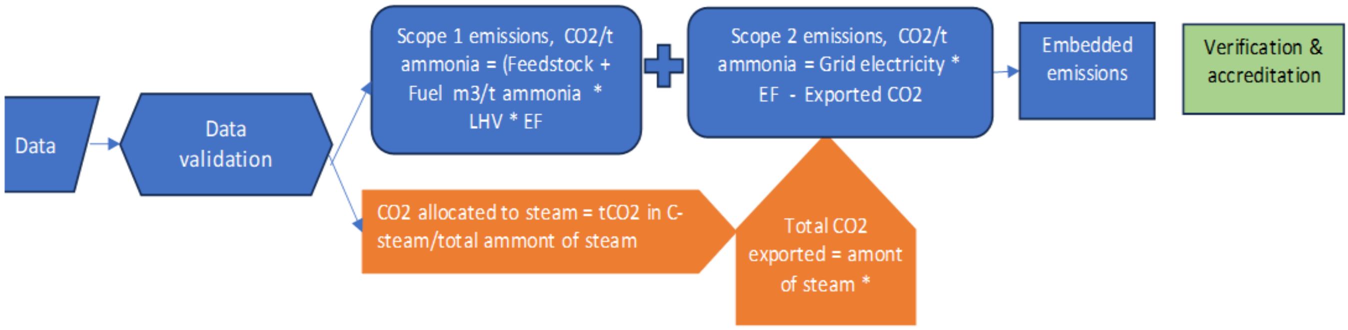

Figure 3. Flowchart for calculation steps (Source: Author's own elaboration)

Although the reformer furnace and auxiliary boiler are located at the ammonia plant the fuel used provides energy in excess to that needed for the production line be used by other plants, which is accounted for by deduction under CBAM.

Steps for Estimation of Embedded Emissions

The required calculation steps are presented in the flowchart of **Figure 3**.

Estimation of embedded CO_2 in steam from auxiliary boiler & waste heat of reaction

The first step is to calculate embedded CO_2 in steam. It is therefore important for the steam cycle to be well defined. Necessary data about steam generation consist of amount of HP steam generated from flue gases of secondary reformer furnace (1), water gas shift reactors (2), ammonia synthesis reactor (3), and HP steam from the auxiliary boiler (4). Steam consumption consist of steam used for driving ammonia compressor, electricity generator and CO_2 compressor as well as amount of fuel used for boiler and reformer furnace. MP process steam is calculated from NG feedstock and S/C ratio, which is specific to plant or from steam cycle diagram of company. Auxiliary boiler is dedicated to production of HP steam. Heat content of NG consumed in the boiler can be calculated from amount of NG (FNG_b) and its HHV (38 kJ/m^3):

ΔHNG_b (MJ/d)=FNG_b×38/1,000,

where FNG_b is volumetric flowrate of NG fed to boiler at NTP.

For a boiler efficiency of 80.00%, the enthalpy of generated steam is, as follows:

ΔHs (MJ/d)=0.8×FNG_b×38/1,000

From steam tables, the specific enthalpy of HP steam is 2,693 MJ/t from which the amount of steam generated is, as follows:

t_{sb} (t/d)=0.8×FNG_b×(38/1,000)/2,693

CO_2 emissions from boiler NG are calculated using IPCC default value for the emission factor for combustion of NG, which is 56.1 t CO_2/TJ. This amount of CO_2 will be embedded in the generated steam.

t CO_2/d=ΔHs (MJ/d)×56.1/1,000,000,

where t CO_2/d is CO_2 emissions allocated to HP steam from boiler. Embedded emissions in HP steam are calculated from the amount of CO_2 allocated HP steam from boiler divided by the total amount of steam fed to the header, estimated in t CO_2/t steam.

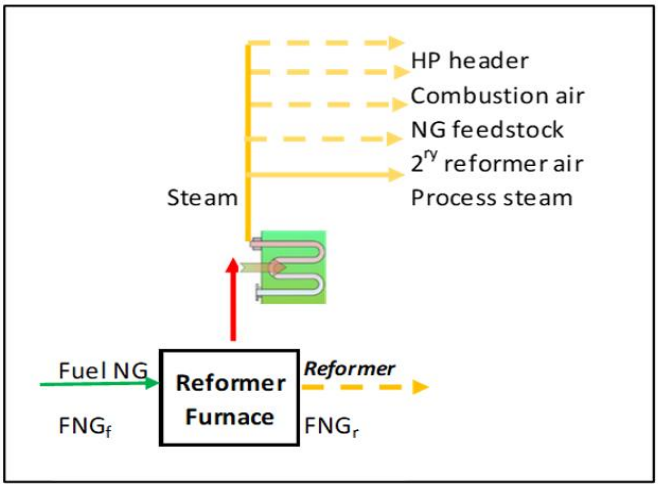

Figure 4. Heat balance on reformer furnace (- - thermal energy) (Source: Author's own elaboration)

Embedded emissions of steam in HP header or EmE_s can be computed, as follows:

EmE_s=CO_2 allocated to boiler steam/(t_{s1}+t_{s2}+t_{s3}+t_{sb})=0.115 t CO_2/t steam (as per case study data),

where t_{s1}, t_{s2}, t_{s3}, and t_{sb} are the tons of steam generated from secondary reformer, water gas shift reactors, ammonia synthesis, and auxiliary boiler respectively.

Estimation of steam generated from reformer flue gases

The primary reformer furnace main function is to provide the necessary heat for the endothermic reaction occurring in the reformer (Elnashaie, 2022). The hot flue gases are used to generate HP steam, using a waste heat boiler (**Figure 4**).

NG feedstock is mixed with process steam (MP) and the preheated mixture enters the primary reformer at a temperature in the range of 400-600 °C. The overall reaction is highly endothermic:

$CH_4+H_2O \rightarrow CO+3H_2$ and ΔHo=206 kJ/mol,

where ΔH_r at 600 °C was estimated to be 14.6 kJ/mol.

The number of moles reacting (Ng) is calculated from the flowrate of NG feedstock used and multiplied by the heat of reaction. However, since the conversion in the primary reformer is 60.00%, the required heat is, as follows:

Q=0.6×Ng×214.6/1,000 MJ/d

Amount of FNG_r generating this energy can be estimated by dividing it by the HHV of NG.

Table 1. Input data

Input to ammonia line	
Ammonia production=1,240 t/d	
NG feedstock=685 m^3/t NH_3	
Process steam=0.83 t/t NH_3	
NG fuel to reformer furnace=403 m^3/t NH3	
NG fuel to auxiliary boiler=370 m^3/t NH_3	
Grid electricity=0.1 MWh t NH_3	
Self-generated power, MW=11	
Fraction used by ammonia line=0.53	
Boiler efficiency=80.00%	
General assumptions	
LHV for NG=38 MJ/m^3	
Steam cycle data	
Input steam flowrate to HP header	
From secondary reformer=2 t/t NH_3	
From WGSR=0.22 t/t NH3	
From ammonia synthesis=1.1 t/t NH_3	
From boiler=3.52 t/t NH_3	
Embedded emissions in HP steam=0.115 t CO_2/t NH_3	
Output steam flowrate from HP header	
To ammonia synthesis compressor=3.5 t/t NH_3	
To electricity generator=0.4 t/t NH_3	
To CO_2 compressor, 2.3 t/t NH_3	

$FNG_{r\,(}m^3/d)=Q\times1{,}000/38$

Energy content of NG fed to reformer furnace with a flowrate of FNG_f m^3/d:

ΔHNG_f (MJ/d)=$FNG_f\times38/1{,}000$

Thermal energy in generated steam=$\Delta HNG_f\times$MJ/d-Q(MJ/d).

All the thermal energy provided by reformer flue gases is used for heating input air, input NG feed and as steam drivers. It is not collected in the HP steam header.

Estimation of CO_2 emissions exported to urea plant

Exported steam:

- Steam used to generate 0.1 MWh/t NH_3=0.18 t steam/t NH_3
- Steam used to drive CO_2 compressor in urea plant=2.3 t steam/t NH_3

Exported CO_2:

- In steam=2.48 t steam×EF of steam
- Process CO_2 assuming all process CO_2 from ammonia plant used in urea plant under BAT conditions=1.24 t CO_2/t NH_3

Estimation of ammonia embedded emissions

Scope 1 emissions:

Process emissions from feedstock (t CO_2/d)=Feedstock (m^3/d)×LHV (MJ/m^3)×56.1 (t CO2/TJ)/10^6=1.44 t CO_2/tNH_3 (case study)

Fuel emissions (t CO_2/d)=(NG to reformer furnace+NG to boiler)×LHV (MJ/m^3)×56.1 (t CO_2/TJ)/10^6=1.66 t CO_2/t NH_3

Scope 2 emissions:

CO_2 from consumed grid electricity-exported CO_2=Consumption of grid electricity×0.411 t CO_2/MWh (EF of Egyptian grid)-exported CO_2

Scope 3 emissions=0 under CBAM

Table 2. Case study results

Scope 1		
	Energy input, GJ/t NH_3	t CO_2/t NH_3
Feedstock (process)	26.1	1.44
Reformer fuel	15.3	0.86
Boiler fuel	14.1	0.788
Total scope 1	55.1	3.1
Scope 2		
	t CO_2/t NH_3	
Grid electricity	0.0411	
CO_2 exported to urea	-1.24	
Steam exported to urea	-0.286	
Total scope 2	-1.48	
Ammonia embedded emissions: 1.62 t CO_2/t NH_3		

CASE STUDY RESULTS

Methodology was applied to the set of input data, which represent the average performance of six production lines (UNIDO, 2014) as well as theoretical derivations (**Table 1**).

Data Validation (BASF, 2021)

1. Input/output monthly flowrates are requested to check for deviations >15.00% and get the average.
2. A mass balance is performed to check the compatibility of process steam flowrate with S/C ratio as well as the amount of steam exported.
3. Check CO_2 allocation factors.
4. Heat balance around the reformer and the auxiliary boiler was performed to check the company data regarding steam production and consumption and efficiency of energy generating equipment.

The results obtained by applying CBAM methodology are given in **Table 2**.

IMPACT OF DECARBONIZATION MEASURES

A number of decarbonization options have been proposed for the fertilizer industry (Fertilizer Europe, 2022), some of more applicable for Egypt are analyzed below.

Impact on Embedded Emissions

Implementation of energy efficiency projects such as hydrogen recovery from purge gas, minimizing steam losses, increase efficiency of generator, boiler and furnace can reduce fuel consumption by about 2.00-3.00%. Ammonia embedded emissions will be reduced from 1.62 to 1.58 t CO_2/t NH_3.

Reaching BAT benchmark for process emissions (1.24 t CO_2/t NH_3) by maximizing ammonia production through replacement of catalysts to increase conversion efficiency, ammonia recovery from purge gas, optimize operating conditions in reactors. Total emissions will be reduced from 1.62 to 1.42 t CO_2/t NH_3.

The impact of ***replacing 15.00% of hydrogen used for ammonia synthesis by green hydrogen*** can be calculated, as follows: Each kg of grey ammonia requires 4.5 kg NG (NREL, 2009) and a reduction of 15.00% of grey hydrogen will reduce

Table 3. Impact of decarbonization on current deviation of embedded emissions from free allowance (1.57 t CO_2/t NH_3)

Product	Embedded emissions, t CO_2/t NH_3					Deviation from free allowance	CBAM cost €/ t NH_3
	Current	Energy efficiency	Lower process emissions	15% green hydrogen	All three measures		
Ammonia (A/U plants)	1.62	1.58	1.48	1.37	1.13	-0.44	0
Ammonia (A/NA lants)	2.52	2.49	2.32	2.27	2.17	1.60	128

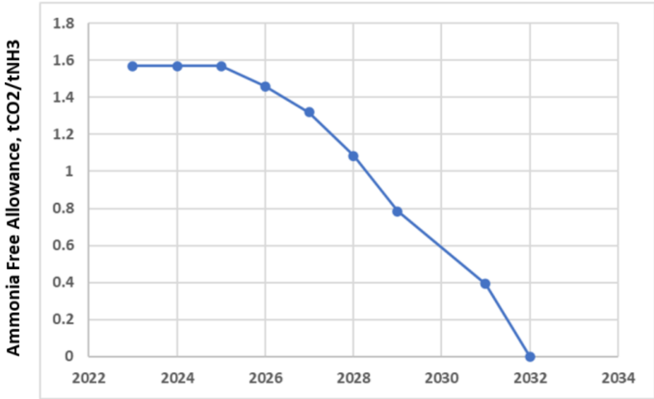

Figure 5. Phasing out of ammonia free allowance (EU ETS News, 2023)

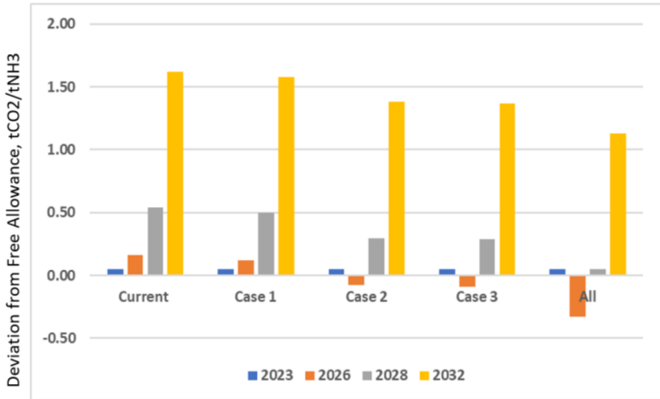

Figure 6. Increase in deviation from free allowance with time (Source: Author's own elaboration)

requires NG by 15.00%=4.5×0.15=0.675 t NG corresponding to a CO_2 reduction of 0.25 t CO_2/t NH_3 causing a reduction in CO_2 embedded emissions from 1.62 to 1.37 t CO_2/t NH_3.

By applying all three measures, the ammonia embedded emissions will become 0.92 t CO_2/t NH_3.

Impact on CBAM Cost

Since CBAM cost is proportional to the deviation between current embedded emissions and free ETS free allowance, the smaller the deviation the lower CBAM cost (**Table 3**). However, with the phasing out of free allowances (Pinsent Masons. 2023) the deviations, and consequently CBAM cost, will increase. **Figure 5** presents the planned phasing out of free allowance (EU ETS News, 2023) and **Figure 6** the impact of phasing out on deviations from free allowance.

DISCUSSION

The results indicate that estimated ammonia embedded emissions of 1.62 t CO_2/t NH_3 is higher than European free allowance of 1.57 t CO_2/t NH_3. Process emissions from feedstock are used for the production of urea and the contribution of consumed grid electricity is only 2.50% of the total embedded emissions. The highest contribution comes from fuel. By implementing the presented decarbonization measures, ammonia embedded emissions will become 1.13 for ammonia/urea plants, which is less than the free allowance of 1.57 t CO_2/t NH_3 and will remain so until 2026. With the phasing out of free allowance the gap between embedded emissions and free allowance and continues to grow from 0.05 in 2028 to 1.13 t CO_2/t NH_3 in 2032 and consequently CBAM cost will increase to reach 4 €/t NH_3 in 2028 and 90.4 €/t NH_3 in 2032 assuming the ETS cost for CO_2 remains at 80 €/t CO_2. For ammonia/nitric acid/ammonium nitrate plants, embedded emissions after implementation of the three presented decarbonization measures will be much higher 2.17 compared to 1.33 t CO_2/t NH_3. More drastic decarbonization projects will need to be implemented.

CONCLUSIONS

The calculation of embedded emissions has been used to identify areas that can be targeted for reduction of CO_2 emissions. Egyptian companies are currently developing their carbon footprint and have received reporting templates from their exporting agents. They are also assessing the various decarbonization measures: energy efficiency, capturing CO_2 in urea, melamine or soda ash, partial replacement of NG with green hydrogen.

The assessment will be based on the estimation of embedded emissions for each option and the corresponding ETS cost reduction. The financial feasibility will include factors such as capital expenditure for each planned decarbonization project and operating costs, potential for tapping into non-EU markets, current and future CBAM costs.

It is clear from the results that the minimum embedded emissions that can be reached with capital expenditures affordable by the Egyptian industry will not lead to zero emissions. Other proposed measures such as the use green electricity instead of steam to drive motors and turbines and to be used for heating purposes. Clearly the operating cost for such a measure will be prohibitive specially in the case of Egypt, where the cost electricity is much higher than NG.

It is not expected for the coming 20 years that Egypt will shut down its grey ammonia lines (lifetime over 50 years) but could install dedicated green ammonia lines in parallel with the existing ones. However, there are plans to produce green ammonia to be exported as fuel and off takers are starting to contact the companies.

Chemical industries holding company, sovereign fund of Egypt, and Ministry of Electricity are to sign a partnership agreement with benchmark power international, to launch a green ammonia plant at semadco fertilizer plant in Suez (Semadco, 2023). Scatec will partner Egyptian government entities to develop a million-ton-per-year green ammonia plant in Ain Sokhna (Ammonia Energy, 2022).

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Data sharing statement: Data supporting the findings and conclusions are available upon request from author.

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