Economic optimisation of local Australian ammonia production using plasma technologies with green/turquoise hydrogen

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ABSTRACT

Growing concern about the supply of goods under the COVID pandemic due to border restrictions and community lockdown has made us aware of the limitations of the global supply chain. Fertilisers are pivotal for the growth and welfare of humankind and there is more than a century history in industrial technology. Ammonia is the key platform chemical here which can be chemically diversified to all kinds of fertilisers. This paper puts a perspective on production technologies that can enable a supply of ammonia locally and on-demand in Australia, for the farmers to produce resilient and self-sustained fertilisers. To assess the validity of such a new business model, multi-objective optimisation has to be undergone, and computing is the solution to rank the millions of possible solutions. In this lieu, an economic optimisation framework for the Australian ammonia supply chain is presented. The model seeks to address the economic potential of distributed ammonia plants across Australia. Different techniques for hydrogen and related ammonia production such as thermal plasma, non-thermal plasma, and electrolysis (all typifying technology-disruption), and mini Haber-Bosch (typifying scale-disruption) are benchmarked to the central mega plant on a world-scale using conventional technology; verifying that 'Moore's Law'[1] of growing bigger and bigger is not the only path to sustainable agriculture. Results show that ammonia can be produced at $317/ton at a regional scale using thermal plasma hydrogen generation which could be competitive to the conventional production model, if credit in terms of lead time and carbon footprint could be taken into account.

Keywords: *ammonia; hydrogen; supply chain; plasma; optimisation; Australia*

INTRODUCTION

Ammonia is an essential nutrient for global food production and is one of the most important chemicals for today's industries.[2] Ammonia is essentially used to ensure the nitrogen levels required for human beings.[3] In farming activities, ammonia can be directly injected into the soils to be used as a nutrient for plants or to produce urea – one of the most popular fertilisers in the world.[4] In addition, ammonia can also be utilised as a precursor to nitrogenous commodity chemicals, to store energy, hydrogen, or can also be used as a coolant at low temperatures and reasonable pressures, and as a liquid fuel.[5] Undoubtedly, the demand for ammonia will significantly grow in the future to satisfy the need for food and other important applications.[6]

With the invention of the Haber-Bosch process in the early 20th century, ammonia has been mass-produced and considered a revolutionized industry.[7] The Haber-Bosch process uses hydrogen as a feedstock which is typically obtained from the processing of fossil fuels through steam reforming of methane or coal gasification. With an increase in food demand to feed a billion population world, more and more fossil resources are required to supply to the ammonia industry while it is reported that ammonia production is one of the main causes for greenhouse gas emissions, accounting for approximately 1% of total global GHG emissions.[8] Thus, to make the ammonia industry greener for a future sustainable world, new technologies need to be developed to reduce the dependence on fossil fuels.[9]

To assist the production of cleaner ammonia, a first-of-its-kind turquoise hydrogen pilot plant was built in 2014 at Redwood City Seaport, California by MONOLITH.[10] This plant produced hydrogen that is required for ammonia together with another valuable by-product, carbon black, through thermal plasma-powered pyrolysis of natural gas. Following MONOLITH, the pilot plant has successfully produced turquoise hydrogen at a production rate of 20 kg H_2/hr and the developed technology has been proven as commercially feasible. Following the success story of the pilot plant, in 2020, a 580-660 kg H_2/hr commercial plant was completed by MONOLITH at Olive Creek, Nebraska. Figure 1 shows the development plan of MONOLITH on a larger scale and three stages of their business development. Together with the turquoise hydrogen, it is expected that approximately 200,000 tons of carbon black can be co-produced annually through the Olive Creek facility which will significantly contribute to the reduction in the price of turquoise hydrogen. Following Monolith, thermal plasma needs an energy consumption of 10 kW/h hydrogens as compared to 60 kW/h hydrogens of water electrolysis.

Figure 1 *Key development plan for thermal plasma powered turquoise hydrogen production at MONOLITH.*[10]

Recently, plasma-catalytic ammonia synthesis has been reported worldwide.[11-17] With the assistant of catalyst, it is expected that plasma discharge can dissociate the reactants to form ammonia at milder temperatures and pressures.[13] The advantages of nonthermal plasma is that the reactive species, characterised by a nonthermal distribution of energy such as microwave and dielectric barrier discharge, etc., are available while the bulk gas temperature can be kept relatively low.[11, 14] In particular, the nonthermal-activated species, such as N_2, are expected to undergo lower dissociation barriers on the surface of the catalysts.[14] For the last 7 years, our group in Eindhoven and Adelaide have developed the technology to utilise non-thermal plasma for plasma-catalytic ammonia synthesis and also for plasma-catalytic NOx synthesis supplying nitrate fertilisers.[16-18] It is expected that the newly developed technique can produce ammonia at a distributed scale as opposed to operating at mega-scale and centralise ammonia production, and we have published techno--economic, environmental, and energy assessments of the new manufacturing approach.[19, 20] Recently, we have made one step further from the single process technologies and their assessments towards the integration of several new process technologies into a circular process chain, which has proven the thermodynamic feasibility.[15] The circular process comprised the manufacture of ammonia from manure through the plasma technologies considered here. We have also introduced quantitative circularity assessments (circularity transition indicators) to chemical manufacturing.[21, 22] Thus, we are now in the position to make complex assessments for those circular processes and can model real-world supply chains. While environmental assessments will be further assessed in future research, this paper is about a complex cost assessment of a real-world chain of the new technologies, translating into a real-world transformation of supply chains and business models.

Currently, ammonia production through conventional Haber-Bosch in a single chemical production plant can be as large as 2 million tons per year while the demand for nitrogen fertilisers is distributed across the countries.[5, 23] Especially, the smaller scale ammonia plants might be a solution for large-area countries such as Australia where transportation has a significant impact on retail cost while access to fertiliser is also limited in remote areas. It is expected that the production of ammonia at a smaller scale to supply the local markets can reduce transportation costs and shipping time to compensate for the relatively high investment cost due to early-stage technologies and scales.[24] In particular, the use of carbon-neutral renewable energy, such as solar or wind power, might contribute to the economic feasibility of such a smaller scale production of ammonia.[24-26]

In Australia, the consumption on a total nutrient (NPK) basis is over 1% of global consumption.[15] Yet the demand is expected to increase significantly due to the expansion of farming areas. This leads to a demand for inorganic fertilisers distributed in particular locations from the West to the East of Australia.[27] According to the Department of Agriculture, 58% of domestic land use and 59% of water extractions were used for agricultural purposes.[28] In the financial year between 2016 and 2017, about 57,300 Australian farmers utilized 5 million tons of fertiliser and the demand for ammonia is approximately 2.6 million tons. Ammonium phosphate is the most popular fertiliser in Australia, accounting for more than 13,000 thousand hectares, while urea is the widest applied fertiliser by smallholders across the country.[29] Those fertilisers demand a significant amount of ammonia which is currently centralised produced by Yara Australia in Pilbara, Western Australia. However, farmers in other states that are far away from Pilbara, such as Queensland and New South Wales, might have to pay more due to the expensive cost of the current supply chain network.[30]

Therefore, it is expected that the construction of new distribution centers or new distributed plants, based on state-of-the-art technologies, can reduce the cost of ammonia production and make it accessible for farmers in remote areas. To optimise the fertiliser supply chain network for Australia, Located Capacitated Plants and Warehouses Simultaneously problem (LCPWP)[31] will be applied in which parameters are collected from the Department of Agriculture. We will develop the mathematical formulation to minimise the supplying cost of ammonia from production to warehouse and market. The newly developed mathematic model will be then integrated into our Agile platform, developed by The Adelaide Teletraffic Centre (TRC), to form an application in which decision-makers can input data and get direct advice on potential plant locations and capacities.[32] Based on the demand for ammonia, two national central locations (Pilbara in Western Australia, and Alice Springs in The Northern Territory) and 7 regional locations (Streaky Bay in South Australia, Bendigo in Victoria, Moree in New South Wales, Brisbane in Queensland, Katherine in Northern Territory, Mandurah and Pilbara in Western Australia) were chosen for the optimisation model. Figure 2 shows the targeted locations for ammonia plant construction across Australia. In most cases, the plant locations were chosen based on the land-use planning of each state. Distances were calculated from the center of the location to the location.

Figure 2 *Targeted locations (✶) for ammonia supply chain network in Australia*

This article addresses two key questions concerning the economic potential of new renewable ammonia plants enabled by disruptive chemical processing technologies: Can such a renewable plant be economically competitive with existing conventional plants, and if so, what is needed to make such plants competitive at a regional scale? To this end, the remainder of this article proposes a general framework for analysing both conventional and renewable plants within the ammonia supply chain and is structured as follows. First, some background is presented that reviews existing research on sustainable supply chains and summaries the current state of the ammonia supply chain. Next, the general mathematical optimisation framework is introduced. We then present some preliminary data that will be used for the analysis of the case studies, which are centralised ammonia production and distributed plants across Australia. The results of these case studies are discussed in the following section. Finally, some concluding remarks and suggestions for future work are presented.

BACKGROUND

In Australia, The distribution of agricultural production is largely determined by the physical environment and climate. The traditional large farm system of wheat and sheep production is spread fairly uniformly between parts of New South Wales, Victoria, South Australia, and Western Australia. Sugarcane and large-scale vegetable production occur almost entirely in the tropical state of Queensland, while cotton is produced in both New South Wales and Queensland. Recently, the increasing number of farming lands in remote areas make it harder for farmers to access the fertiliser supplying system while the demands are also significantly different based on the locations. As a result, particular regions located across Australia require a consistent supply chain network that can offer quick delivery.

As a result of the large distances in Australia (roughly 4000 km from North to South and from West to East), transportation plays a key role in the supply chain, putting a negative effect on costs and environmental impact. A local supply would fundamentally change the role and impact of transportation.

In this work, we seek to develop a supply chain optimisation model which analyses an ammonia supply chain considering both existing conventional and new technologies with renewably generated hydrogen at both central and distributed locations. In this sense, supply chain optimisation is used here as a tool to provide a complete comparison of the economic potential of ammonia production through the two pathways. The traditional ammonia supply chain relies on centralised conventional plants where ammonia is produced in large quantities, transported, typically by train or truck, to local distribution centers, and then further transported by truck to local consumers. This work considers the possibility of introducing regional renewable ammonia plants into the traditional supply chain. Because these plants are being built locally, they can bypass the distribution centers and ship transport and instead deliver directly to the consumer, using either onsite storage or assuming the end-user has sufficient storage. The remainder of this article develops and uses an optimisation formulation to compare renewable and conventional ammonia production within the supply chain.

Problem Statement and data required

In this section, an optimisation framework is developed that considers the existing ammonia supply chain and decides if and where to build renewable plants among candidate location sites, as well as how to transport ammonia through the supply chain. The formulation uses steady-state mass balances throughout the supply chain; in practice, this would be accomplished through adequate storage at production, distribution, and end-use nodes. Ammonia can be purchased from existing conventional plants and then transported to one of the ammonia distribution centers.

A much more general form of the plant location model needs to be considered if the entire supply chain network from the supplier to the customer is designed. Location and capacity allocation decisions have to be made for both factories and warehouses. Multiple warehouses may be used to satisfy the demand for a market and multiple factories may also be used to replenish the warehouses.

Scope and Limitations

The scope of this study is based mainly on the current ammonia supply chain in Australia. The ultimate aim is to generate preliminary data to support decision-makers to develop a strategy for a greener and more sustainable ammonia supply chain network within Australia. The main focus will be to identify the potential locations for the distributed ammonia plants and their associated warehouses to satisfy the demand of local farmers while reducing transportation costs and lead time. However, the current study does not consider the uncertainty of ammonia demand due to the influence of weather, rainfall, seasons, and kind of crops, etc.

Table 1 shows the technologies considered for both H_2 and NH_3 production at two levels of centralisation which are national-scale plants and regional plants in state-wide farm areas. Data on steam methane reforming[33-35], thermal plasma methane pyrolysis[36-40], and water electrolysis to produce H_2[41-45] were collected from the literature review. We also introduced in this paper an oxygen credit of $1/kg of O_2 in case of the water electrolysis is applied for H_2 production[46] while a carbon credit of $1/kg carbon black (CB) will also be given to the scenarios where thermal plasma methane pyrolysis is used to produce turquoise hydrogen[47-50]. The price for $1/kg is conservative as typical Carbon Black prices are above $1.3/kg. Detailed information about cost analysis of hydrogen, nitrogen, and ammonia production is provided in Table S3 to S7 of the supporting materials.

Table 1 *Technologies considered for hydrogen and ammonia production at two levels of centralisation.*

Resources supply: **H_2 production**	**NH_3 synthesis:** **Reactor type**	**Location:** **Level of centralisation**
• Steam methane reforming • Thermal plasma-enabled methane pyrolysis • Water electrolysis	• Haber-Bosch • Mini Haber-Bosch • Non-thermal plasma	• National-scale plant • Regional plants in state farm areas

In terms of the potential locations for H_2 supply and ammonia production, at the national-scale plant, we will consider Pilbara (Western Australia) and Alice Springs (Northern Territory) as the centers for H_2 and NH_3 supply. 7 potential regional locations, based on the local demand for ammonia, will be assessed include Streaky Bay (South Australia), Mandurah and Pilbara (Western Australia), Katherine (Northern Territory), Moree (New South Wales), Brisbane (Queensland), and Bendigo (Victoria). The distances between potential plants to markets are shown in Table S2 (supporting materials).

MODEL FOR LOCATING CAPACITATED PLANTS AND WAREHOUSES SIMULTANEOUSLY

Notation for model

Index:

s: index of supplier s = 1…S

p: index of plant location including the potential location p = 1…P

c: index of class for plant c = 1…C

w: index of warehouse location including the potential location w = 1…W m: index of market m = 1… M

v: index of vehicle transportation method v = 1 …V

t: index of time slot t = 1…T

f: index of fertiliser f = 1…F

Parameters

α_{fspv} transportation cost α of materials transported from supplier s^{th} to plant p^{th} by mean of vehicle transportation v^{th} (AUD per ton)

β_{fpwv} transportation cost β of fertilizers transported from plants p^{th} to warehouse w^{th} by mean of vehicle transportation v^{th} (AUD per ton)

μ_{fpmv} transportation cost μ of fertilisers transported from plants p^{th} to market m^{th} by mean of vehicle transportation v^{th} (AUD per ton)

γ_{fwmv} transportation cost γ of fertilisers transported from warehouse w^{th} to market m^{th} by mean of vehicle transportation v^{th} (AUD per ton)

o_{fpc} unit operating cost of plant p^{th} for producing one ton of fertiliser at plant type c^{th}

w_w unit inventory cost of warehouse w^{th} for storing one ton of fertiliser during one timeslot

F_{fpc} fixed cost for investing plant p^{th} of type at capacity c^{th} for fertiliser sort f^{th}

f_w fixed cost for investing warehouse w^{th}

D_{fmt} demand for market m^{th} at timeslot t^{th}

DM_{xy} distance matrix from location x to location y

CP_{fpc} the maximum production capacity of potential plant p^{th}

CW_w the maximum storage capacity of potential warehouse w^{th}

CS_s maximum supplying capacity of the supplier s^{th}

To develop the formulation for cost optimisation, several parameters related to transportation need to be clarified. Regarding the mean of transportation, due to the specific geographical and product requirements, trains and container trucks are highly recommended. Therefore, parameters related to transportation cost are considered by the distance matrix (DM_{xy}) and unit cost ($truckcost\ and\ traincost$) are presented in Table 2.

Table 2. Parameters considered for the transportation cost

Parameter	Unit	Mean of Transportations	
		Container Truck	**Train**
α_{fspv}	AUD/ton	$truckcost * DM_{sp}$	$traincost * DM_{sp}$
β_{fpwv}	AUD/ton	$truckcost * DM_{pw}$	$traincost * DM_{pw}$
μ_{fpmv}	AUD/ton	$truckcost * DM_{pm}$	$truckcost * DM_{pm}$
γ_{fwmv}	AUD/ton	$truckcost * DM_{wm}$	$traincost * DM_{wm}$

In all cases, the unit cost of transportation by train will be significantly lower than the truck if the initial fixed cost is not considered. Therefore, the cost of purchasing a truck, hiring a container, etc. will be considered in case of transportation by truck to ensure a real scenario.

Decision Variables

Y_{fpc} $\quad Y_{fpc} = 1$ if plant at the location p^{th} with type c^{th} for fertiliser sort f^{th} is chosen to invest else $Y_{fpc} = 0$

y_w $\quad y_w = 1$ if warehouse at the location p^{th} is chosen to invest else $y_w = 0$

$x\alpha_{fsptv}$ $\quad$ materials quantity shipped from the supplier $s^{\ th}$to plant $p^{\ th}$at timeslot $t^{\ th}$ using vehicle transportation v^{th}

$x\beta_{fpwtv}$ $\quad$ fertiliser quantity shipped from the plant $p^{\ th}$to warehouse $w^{\ th}$at timeslot $t^{\ th}$ using vehicle transportation v^{th}

$x\mu_{fpmtv}$ $\quad$ fertiliser quantity shipped from the plant $p^{\ th}$to market $m^{\ th}$at timeslot $t^{\ th}$ using vehicle transportation v^{th}

$x\gamma_{fwmtv}$ $\quad$ fertiliser quantity shipped from the warehouse $w^{th}$to market $m^{\ th}$at timeslot $t^{\ th}$ using vehicle transportation v^{th}

$o\alpha_{fpct}$ $\quad$ operating cost at site p^{th} at timeslot t^{th} integrated with all quantities manufactured by type c^{th}

Mathematical Formulation of Locating Capacitated Plants and Warehouses

Objective function: to minimize the cost of production and supply of ammonia in Australia, we have developed the mathematical model as seen in Eq. 1. The equation was then coded and built to the Agile platform which was constructed by the Teletraffic Research Centre at The University of Adelaide. The objective of the simulation is to minimize the cost obtained through the utilization of equation 9.

$$\begin{aligned}
&\sum_t\sum_f\sum_p\sum_c F_{fpc}Y_{fpc} + \sum_t\sum_w f_w y_w \\
&+\sum_f\sum_s\sum_p\sum_t\sum_v(\alpha_{fspv}x\alpha_{fsptv} + v_v min(x\alpha_{fsptv},1)) + \sum_f\sum_p\sum_w\sum_t\sum_v(\beta_{fpwv}x\beta_{fpwtv} + v_v min(x\beta_{fpwtv},1)) \\
&+\sum_f\sum_w\sum_m\sum_t\sum_v(\gamma_{fwmv}x\gamma_{fwmtv} + v_v min(x\gamma_{fwmtv},1)) + \sum_f\sum_p\sum_m\sum_t\sum_v(\mu_{fpmv}x\mu_{fpmtv} + v_v min(x\mu_{fpmtv},1)) \\
&+\sum_f\sum_p\sum_c\sum_t o\alpha_{fpct} + \sum_w\sum_w il_{wt}w_w
\end{aligned} \quad (1)$$

Subject to:

$$\sum_f\sum_p\sum_v x\alpha_{fsptv} \le CS_s \qquad \forall s,t \quad (2)$$

$$\sum_s\sum_v x\alpha_{fsptv} - \sum_w\sum_v x\beta_{fpwtv} - \sum_m\sum_v x\mu_{fpmtv} \ge 0 \qquad \forall f,p,t \quad (3)$$

$$\sum_w\sum_v x\beta_{fpwtv} + \sum_m\sum_v x\mu_{fpmtv} \le \sum_c CP_{fpc}Y_{fpc} \qquad \forall f,p,t \quad (4)$$

$$il_{wt} = il_{w,t-1} + \sum_f\sum_p\sum_v x\beta_{fpwtv} - \sum_f\sum_m\sum_v x\gamma_{fwmtv} \qquad \forall w,t:t>1 \quad (5)$$

$$il_{wt} = \sum_f\sum_p\sum_v x\beta_{fpwtv} \qquad \forall w,t:t=1 \quad (6)$$

$$\sum_f\sum_m\sum_v x\gamma_{fwmtv} = 0 \qquad \forall w,t:t=1$$

$$0 \le il_{wt} \le CW_w y_w \qquad \forall w,t \quad (7)$$

$$\sum_{f}\sum_{m}\sum_{v} x\gamma_{fwmtv} \leq CW_w y_w \qquad \forall w,t \tag{8}$$

$$\sum_{w}\sum_{v} x\gamma_{fwmtv} + \sum_{p}\sum_{v} x\mu_{fpmtv} \geq D_{fmt} \qquad \forall f,m,t \tag{9}$$

$$\sum_{f}\sum_{c} Y_{fpc} \leq 1 \qquad \forall p \tag{10}$$

$$o\alpha_{fpct} \geq max(o_{fpc}(\sum_{w}\sum_{v} x\beta_{fpwtv} + \sum_{m}\sum_{v} x\mu_{fpmtv}) - BigM(1 - Y_{fpc}), 0) \qquad \forall f,p,c,t \tag{11}$$

The objective of the model is to recognise which methodology would offer the producer the slightest fetched paying for contributing and transporting in the supply chain. The main purpose is to minimise all existing costs including fixed investing, variable operational, and variable shipping ones with various indexes. In constraint (2), total materials for fertiliser manufacturing shipped to plants from suppliers must be less or equal to the capacity of that block. Constraint (3) ensure the feasibility between inbound and the outbound of all factories which is supposed to be consistent with each other. To be more specific, the quantity of fertiliser produced in any factory must be consistent with manufacturing type, location, and capacity. This statement is ensured by constraint (4). Concerning the warehouse, in constraints (5) to (7), the quantity of fertiliser received and stored must be the upper bound of the quantity delivered to markets for financial purposes. Similar to constraints (4), the capacity constraint in the warehouse block is satisfied in constraint (8). Total demands at a particular market are the upper bound of the quantity shipped from warehouses in (9). At a single potential location for the plant, only one decision for different tuples (product, location, capacity) is made in constraint (10). Constraint (11) is linearised from the non-linear form:

$$o\alpha_{fpct} \geq \max\left(o_{fpc}Y_{fpc}\left(\sum_{w}\sum_{v} x\beta_{fpwtv}\right), 0\right) \forall\, p,f,c,t \tag{12 }$$

The constraint (12) is an equivalent form of (11), but it is much easier for the readers to follow. This auxiliary constraint generates an operating cost for a particular plant site based on the output quantity of that plant, decision of investing, and operating cost parameter. This constraint is strongly bonded to the operating variable costs in the objective function (1).

Case study: Optimisation supply chain network for plasma-fertiliser in Australia

In Australia, consumption on a total nutrient (NPK) basis is over 1% of global consumption. Yet the demand is expected to increase significantly due to the expansion of farming areas. In the period between 2018 and 2019, approximately 57,300 Australian farmers utilised about 1.6 million tons of ammonia (in form of urea, ammonium phosphate, etc.) for a total area of 50 million hectares across the country. Taking the Western area of Australia as an example, inorganic fertilisers were applied for the largest agricultural land of Australia, with statistics being 19 million hectares or 37% of the total land used for agriculture, in the same period between 2018 and 2019. As previously mentioned, the establishment of new farmlands located in remote regions across Australia seems not to be beneficial from the current ammonia supply chain network [51]. Therefore, demand is given for either new distribution centers or new distributed plants to improve the supplying capacity while reducing cost and lead time. In this regard, Located Capacitated Plants and Warehouses Simultaneously problem (LCPWP)[31] appears to be a potential solution. Two levels of centralisation are shown in Figure 3 and the demand for ammonia in 7 main farming locations across Australia is also shown in Table 3.

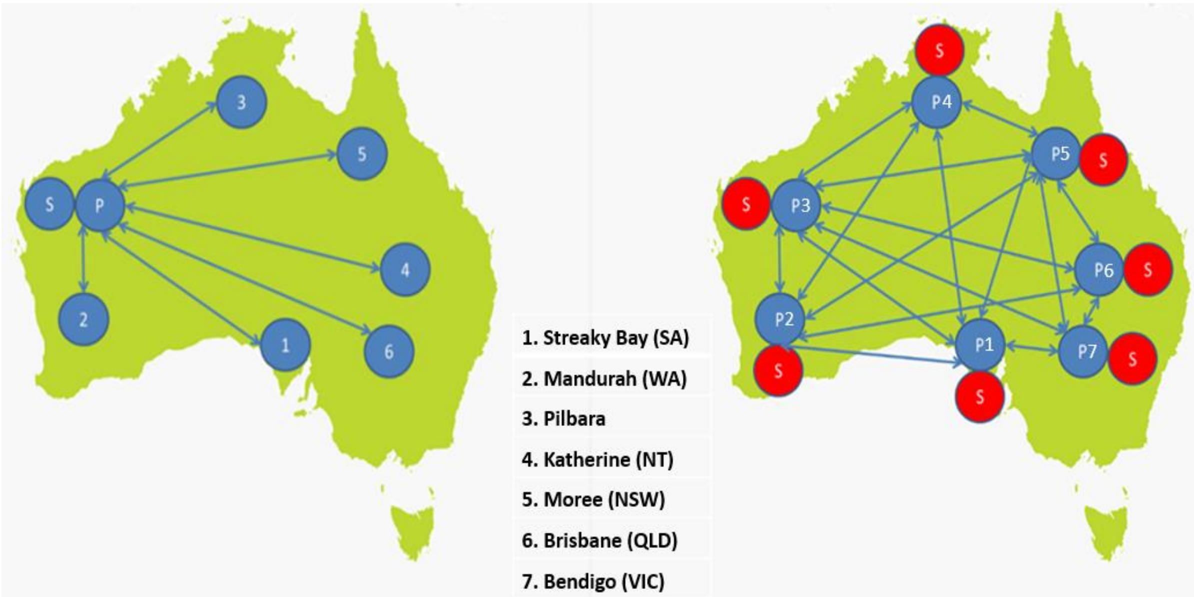

Figure 3 *Examples of two levels of centralisation (S: suppliers; P: plant; and 1-6 are the markets).*

Table 3 *Ammonia demand in main Australian farming regions and two levels of plant capacities considered* [28, 52].

Location	**Market location**	**Demand ammonia-related fertiliser, tons**	**Plant capacity 1, tons/year**	**Plant capacity 2, tons/year**
1	Streaky Bay (SA)	255,000	300,000	450,000
2	Mandurah (WA)	345,000	350,000	450,000
3	Pilbara	300,000	350,000	450,000

4	Katherine (NT)	1,500	2,000	5,000
5	Moree (NSW)	350,000	350,000	450,000
6	Brisbane (QLD)	100,000	150,000	250,000
7	Bendigo (VIC)	250,000	300,000	400,000
Total		1,601,500		

Although the cost of conventional ammonia production and transportation could be obtained through running the LPWP, the use of advanced, appropriate technology is the key to cost-effectiveness and flexible plant capacity to satisfy the local demand. In this sense, we will consider the new technologies developed for H_2 generation such as water electrolysis and thermal plasma methane pyrolysis as well as for NH_3 generation such as non-thermal plasma-assisted ammonia synthesis, respectively. Nevertheless, state-of-the-art reactor technology for ammonia synthesis brought to a new format and operating with renewable energy, such as mini Haber-Bosch for NH_3 generation will also be taken into account. Table 4 shows the variables associated with the technologies applied for NH_3 and H_2 production (X_1), potential H_2 supplier location (X_2), potential plant location at two levels (X_3), the potential for warehouse construction (X_4), and operating cost deduction factor to further explore the benefits of technological development in the future (X_5).

Table 4 *Variables considered for cost simulation and optimisation*

Independent variables	Coded Variables	Values
NH_3 + H_2 plant technology	X_1	Haber-Bosch + Conventional steam reforming; Mini Haber-Bosch + High thermal plasma (HTP); Mini Haber-Bosch + Water electrolysis; Non-thermal plasma (19% yield) + Water electrolysis
Supplier Location	X_2	Alice Springs; Pilbara; 7 regional locations
Plant Location	X_3	Alice Springs; Pilbara; 7 regional locations
Warehouse	X_4	Yes; No
Operating cost (OPEX)	X_5	50%; 75%; 100%

Based on Table 4, 120 scenarios have been considered for the cost optimisation simulation. Details of the scenarios with specific parameters are shown in Table S1 of the supporting materials. As given in the scenarios vary in the kind of technologies applied, the location of chemical plants, the use of warehouses (or not) and their locations, and the OPEX costs. The latter was reduced from 100% to 75% and 50% of the real value obtained through market analysis and literature review as shown in Table S5 of the supporting materials, respectively, to account for – in a lumped-sum manner – for possible ‘credits’. First of all carbon credits for the use of clean energy and the sales of activated carbon (for the thermal plasma), and also oxygen credits in the case of water electrolysis, which co-produces oxygen. It accounts further for costs for soil corrosion (because of using not the best fertiliser types for the given soil), and economic benefits for creating new local jobs in a high-technology field (to operate the local chemical plants). The new technologies and their local use also open the path to a bespoke use of fertilisers in terms of flexibility of time, amount (at a day), and fertiliser mix/type – assisted by data and artificial intelligence gathered by weather stations, (soil) sensing, drones or satellites. The result is a higher fertiliser efficiency, and thus a reduced need for fertiliser amount.

RESULTS AND DISCUSSIONS

Based on Table 4, 120 simulations have been run through the supply chain optimisation software on the Agile platform developed by The Adelaide Teletraffic Centre (TRC) to minimise the supplying cost of ammonia, using the mathematical model as seen in Eq. 9. The results were then validated by the IBM ILOG CPLEX Optimisation Studio (CPLEX). The obtained results allow us to compare the economic potentials of the newly developed technologies with the conventional ones and identifies the plant locations that will minimise warehouse and transportation costs.

Ammonia production based on central plant

Figure 4 shows the supply chain of centralised ammonia production developed under Located Capacitated Plants and Warehouses Simultaneously Problem (LCPWP). In these scenarios, ammonia is produced by a mega plant, whether in Pilbara or Alice Springs with different technologies, before supplying to the markets at 7 locations as described in Table 3.

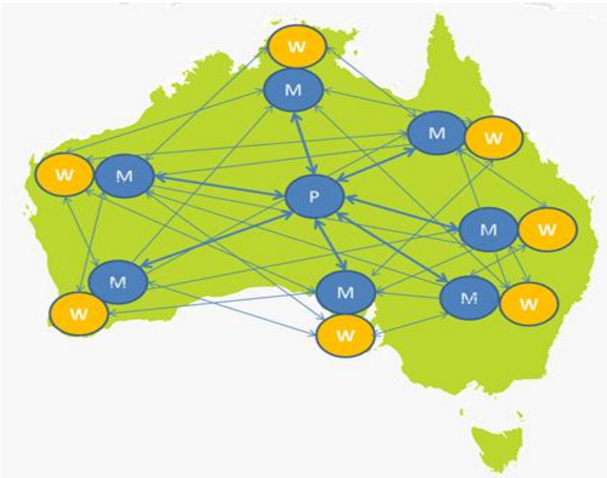

Figure 4 *Schematic diagram of centralised ammonia production in Alice Springs (P: plant; W: warehouse; and M: market).*

Figure 5 shows supplying costs of ammonia associated with 48 scenarios considered for the mega central plant. As can be seen in Figure 6, centralised production of ammonia in Alice Springs using Mini Haber-Bosch with hydrogen supplied by high thermal plasma (scenarios 7 to 12) can be competitive with the traditional production routes (scenarios 1 to 6). In most cases, ammonia can be supplied at around \$230/ton (scenarios 9 and 11 with 100% operating cost) if the thermal plasma methane pyrolysis could be adopted for the production of hydrogen. It should be noticed that we have already taken into account the carbon black credit, which can be sold conservatively at $1/kg, while the carbon footprint credit and higher carbon black credit could be further explored to make thermal plasma methane pyrolysis a more economically attractive process. Generation of hydrogen by water electrolysis (scenarios 13 to 24 and 37 to 48) appears to be not economically effective at a larger production scale, approximately 2.5 times higher the production cost delivered through high thermal plasma methane pyrolysis, although oxygen credit has been given to the cost calculation. This relatively high production cost is caused by the expensive plant investment and relatively high energy consumption.

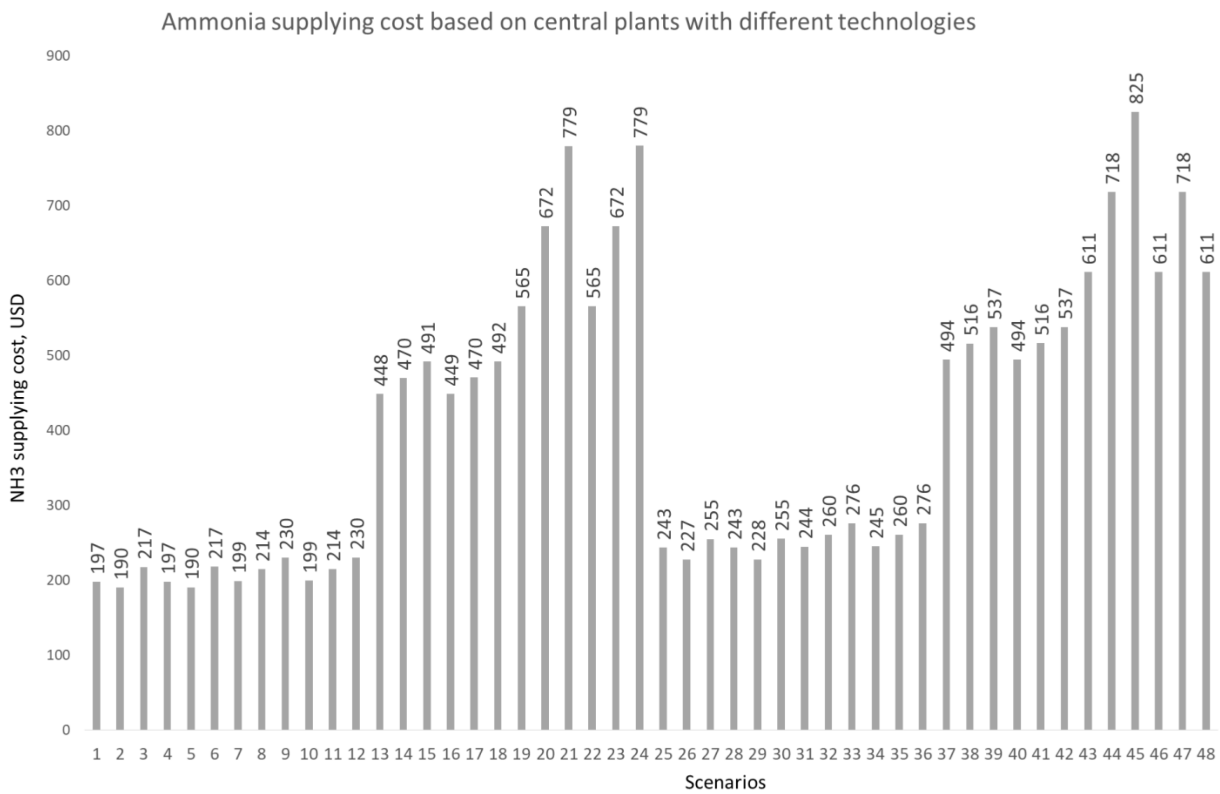

Figure 5 *Supplying costs of ammonia produced by the mega central plants.*

Scenario 1 to 6: Haber-Bosch ammonia + Conventional steam reforming hydrogen both in Alice Springs; 7 to 12: Mini Haber-Bosch ammonia and Thermal plasma hydrogen both in Alice Springs; 13 to 18: Mini Haber-Bosch ammonia and Water electrolysis hydrogen both in Alice Springs; 19 to 24: Non-thermal plasma ammonia and Water electrolysis hydrogen both in Alice Springs; 25 to 30: Haber-Bosh ammonia in Alice Springs and Conventional steam reforming hydrogen in Pilbara; 31 to 36: Mini Haber-Bosch ammonia in Alice Springs and thermal plasma hydrogen in Pilbara; 37 to 42: Mini Haber-Bosch ammonia in Alice Springs and water electrolysis hydrogen in Pilbara; 43 to 48: Non-thermal plasma ammonia in Alice Springs and Water electrolysis hydrogen in Pilbara.

In contrast and actually as to be expected, the production of ammonia using non-thermal plasma technology seems to be the most expensive. In its best case, the supply cost of ammonia is 3 times higher in comparison to the conventional Haber-Bosch, although oxygen credit has already been taken into account. This relatively high cost can be explained as non-thermal plasma synthesis of ammonia is still under development, and has not moved from laboratory scale to pilot scale; unlike all other technologies considered here which are at near-production scale. It should be noted that the performance of the non-thermal plasma technology was assumed to be according to best literature results and their optimistic trajectories; assuming that can be transferred to a large scale (which has not been done so far). Differently, in all other cases, real-world production data were considered. Accordingly, there is still room for future improvement for the non-thermal plasma technology before the developed technique could be economically competitive.

Ammonia production based on distributed plant

Figure 6 shows the map of distributed ammonia plants considered in this study. At each location, two capacities of plants are considered in order to supply for the local demand and can also be transported to the surrounding markets if required.

Figure 6 *Schematic diagram of distributed ammonia production across Australia (P: plant; S: supplier).*

In terms of the supply, hydrogen can be centralised produced in Pilbara and Alice Springs or be included as part of the distributed plants in 7 locations.

Distributed plants in 7 locations with central hydrogen suppliers in Pilbara and Alice Springs

Figure 7 shows the supplying cost of ammonia produced in distributed plants across Australia with central hydrogen suppliers in Pilbara and Alice Springs. It can be seen that building regional plants without a local supplier of hydrogen is not a good option since even at the best case (scenario 56: ammonia production by Haber-Bosch at Streaky Bay, Pilbara, Katherine, Moree, and Bendigo and hydrogen supplier is in Pilbara), the supplying cost of ammonia is still 50% higher in comparison to ammonia production based on the central plant ($190 in scenario 2 vs. $275 in scenario 56).

In terms of the plant locations, the developed mathematical suggests that it is not economical to build the plant in Mandurah and Brisbane, while ammonia supplied to those areas can be transported from Pilbara and Moree, respectively.

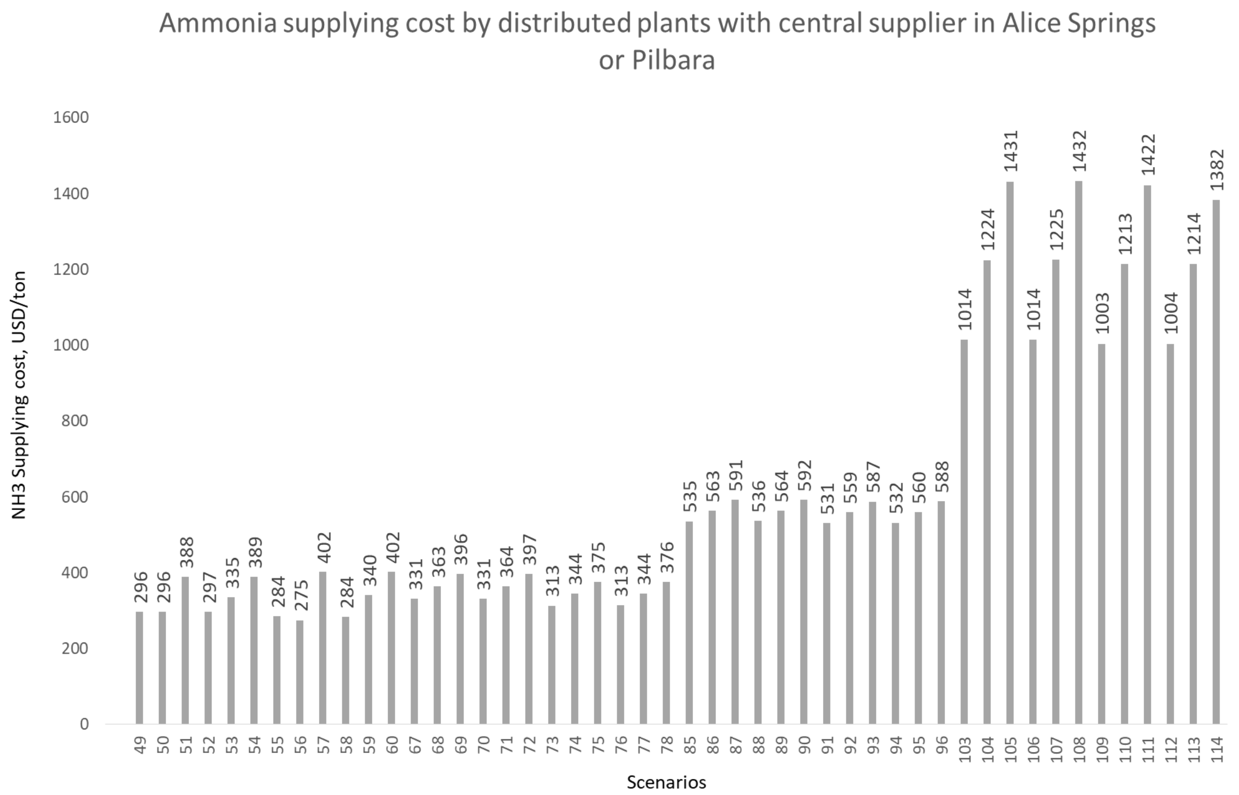

Figure 7 *Supplying costs of ammonia produced by the distributed plants with central supplier.*

Scenario 49 to 60: Haber-Bosch ammonia in 7 locations and Conventional steam reforming hydrogen in Pilbara or Alice Springs; 67 to 78: Mini Haber-Bosch ammonia in 7 locations and High thermal plasma hydrogen in Pilbara or Alice Springs; 85 to 96: Mini Haber-Bosch ammonia in 7 locations and Water electrolysis hydrogen in Pilbara or Alice Springs; 103 to 114: Non-thermal plasma ammonia in 7 locations and Water electrolysis hydrogen in Pilbara or Alice Springs

In terms of cost-effectiveness, similar to the ammonia production based on the central plant at national-scale, the production of ammonia by mini Haber-Bosch in 7 locations with high thermal plasma hydrogen suppliers in Pilbara or Alice Springs shows a competitive price, only 13% higher in comparison to one of conventional Haber-Bosch in both best scenarios. Further prospects can be expected by improvements of the technology in the case of non-thermal plasma-assisted ammonia production and water electrolyser in order to reduce the supplying cost of ammonia.

Water electrolysis can significantly contribute by oxygen credits.[46] That might make the economic competitiveness of the scenarios using water electrolysis even more. We will deliver a report on this effect in a future paper.

Distributed plants in 7 locations with local suppliers

Figure 8 shows the supplying cost of ammonia produced in distributed plants across 7 locations in Australia. It can be observed from the Figure that producing ammonia in 7 locations using the local hydrogen supplier results in approximately 14% higher cost in comparison to the central plant in Alice Springs. This 14% gap is mainly caused by the investment of individual plants across the 7 locations. However, it should be taken into account that the distributed production model significantly reduces the transportation time and CO_2 emissions interstate which might provide further credits that reward the higher cost of investment, and we will report in the very next time on that.

Conventional steam reforming combined with Haber-Bosch in 7 locations has comparable costs to the high thermal plasma combined with mini Haber-Bosch in 7 locations. Ammonia production based on water electrolysis combined with mini Haber-Bosch in 7 locations is higher, and water electrolysis combined with non-thermal plasma in 7 locations is still much higher and currently not economically competitive.

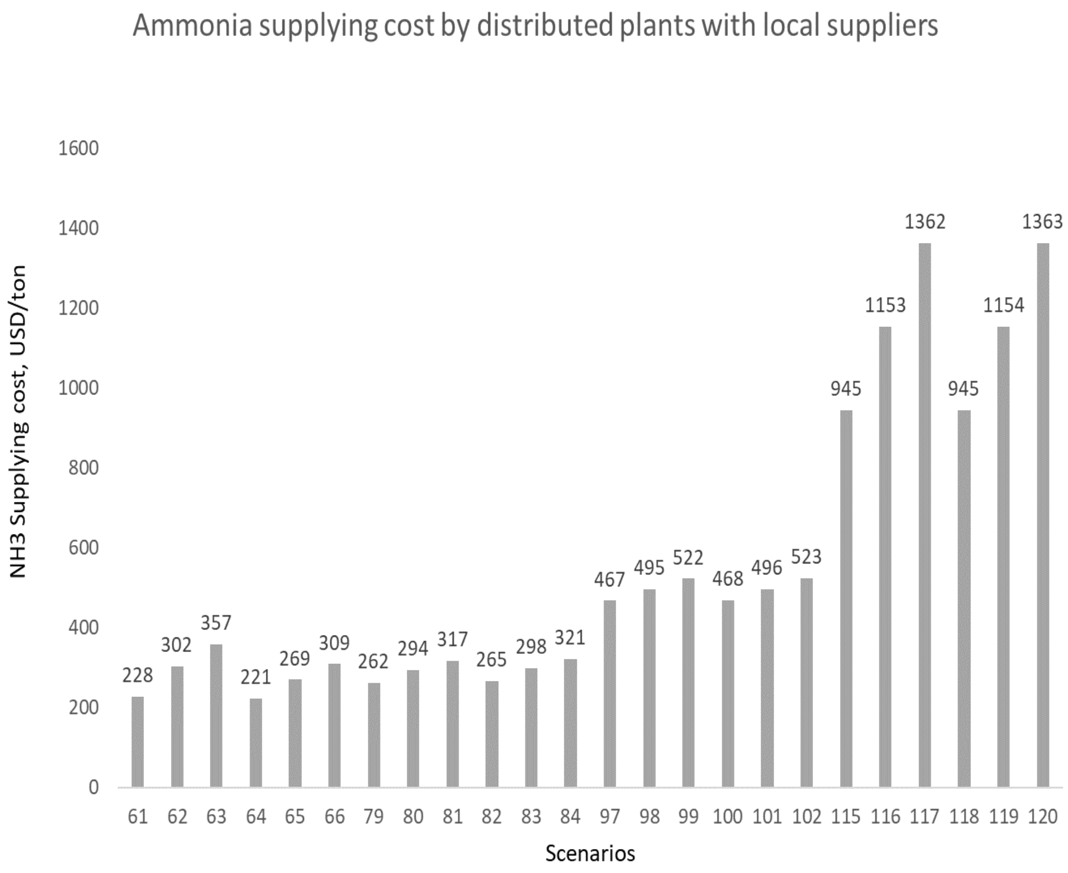

Figure 8 *Supplying costs of ammonia produced by the distributed plants integrated with hydrogen supplier. Scenarios 61 to 66: Integrated Haber-Bosch ammonia and conventional steam reforming hydrogen in 7 locations ; 79 to 84: Integrated mini Haber-Bosch ammonia and high thermal plasma hydrogen in 7 locations; 97 to 102: Integrated mini Haber-Bosch ammonia and water electrolysis hydrogen in 7 locations; 115 to 120: Integrated non-thermal plasma ammonia and water electrolysis hydrogen in 7 locations.*

Significantly, the production cost of ammonia, in case of hydrogen supplied through high thermal plasma methane pyrolysis, can be further reduced if carbon black, co-produced with turquoise hydrogen, is utilised as a soil amendment or for other local applications. This option should be explored in future studies regarding the distributed model.

CONCLUSIONS

This paper puts a perspective on production technologies that can enable a supply of ammonia locally and on-demand in Australia, for the farmers to produce resilient and self-sustained fertilisers. To assess the validity of such a new business model, economic screening optimisation has been performed to assess 120 scenarios in which ammonia and hydrogen are produced by different techniques at two levels of centralisation include national-scale and regional scale plants. We accounted for credits in a lumped way by setting operating costs to 50, 75, and 100% of the real value, respectively. Local plants profit from lower transportation costs and production of biogas (RNG) requires that feedstock be sourced nearby (e.g. landfill, agriculture waste, animal waste, etc). It will be harder to utilise renewable feedstocks in the centralised production model. The regional production may allow for the greater integration/use of renewable feedstocks (such as biomethane). This would enable greater amounts of CO2 credit to further offset the cost of production. Yet distributed plants are generally disadvantaged by the economy of scale, as they have to operate at lower productivity. New technologies can be disruptive and potentially break the economy of scale (Moore's law); at least to a part. The hypothesis of this paper is that 'credits' such as carbon credits and other benefits (e.g. transportation reduction) can partly compensate for the remaining economic deficiency after disruption, so that Moore's law in essence can be broken. This paper makes lumped sum estimates of those credits, as detailed above; yet, on a background of rough calculations.

Water electrolysis, thermal plasma, and non-thermal plasma lead to technology disruption, meaning they provide massive process intensification at potentially higher costs and scale up differently, e.g. by numbering up and thus also benefit from modularisation. Mini Haber Bosch technology keeps the reactor technology conventional, but benefits from the use of clean renewable energies; this is termed here scale-disruption, to account for the miniaturisation of productivity and reactor dimensions as the main effect.

Results show that the distributed plants using thermal plasma for hydrogen generation might compete with the conventional plants if transportation time (lead time) and CO_2 emissions could be taken into account. Distributed plants with water electrolysis are less economic, yet also not far away from the economics of thermal plasma. As we use only lumped sum credit estimations, in the real world, the actual credits will decide if water electrolysis or thermal plasma perform better; we will publish those exact calculations in the future. Regardless of such future evaluation, this paper shows that a local production with disruptive technologies can be competitive to a central world-scale plant; at least for a large-area country and continent such as Australia which consumes large amounts of fertilisers. That kind of evidence may open new business models and enable new supply chains. Future studies should focus on the assessment of the environmental impacts to provide a full picture of ammonia production at the two levels.

SUPPORTING INFORMATION

Scenario distributions; Distances between 7 market-plant locations (km); Cost of hydrogen production; Cost of nitrogen production; Cost of ammonia production by different technologies; Cost of ammonia production through conventional world-scale Haber-Bosch supplied by steam methane reforming; Cost of ammonia production through high thermal - Haber-Bosch; and Cost of NH3 storage by different publications

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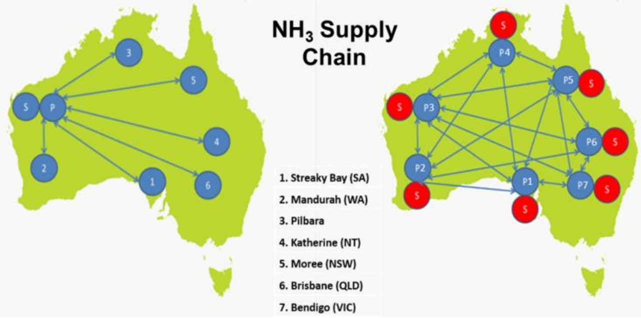

Centralised vs. decentralised production of ammonia in Australia by different technologies.