Supporting Information

Evaluating Ammonia as Green Fuel for Power Generation: A Thermo-chemical Perspective

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1. Membrane Reactor Model

In the decomposition membrane reactor, ammonia is converted to nitrogen and hydrogen, according to the reaction S.1, and this component passes through the membrane and is separated in situ.

$$NH_3 \rightleftarrows \frac{1}{2}N_2 + \frac{3}{2}H_2 \tag{S.1}$$

The catalyst used in the decomposition section is Ni/Al_2O_3 and a Pd-Ag supported membrane is installed to recover the hydrogen from the decomposition of ammonia. The kinetics expression of the ammonia decomposition reaction is adapted from the Temkin expression [1,2]:

$$r = 3k_{reac}\left[K_p^2 a_{N_2}\left(\frac{a_{H_2}^3}{a_{NH_3}^2}\right)^{\alpha} - \left(\frac{a_{NH_3}^2}{a_{H_2}^3}\right)^{1-\alpha}\right]\Phi\Omega \tag{S.2}$$

Where k_{reac} is the kinetic constant of the reaction, K_p is the equilibrium constant, a_i is the activity of component i, Φ is the effectiveness factor, Ω is the catalytic activity and α is a kinetic parameter. To describe the permeation through the membrane, the following expression (S.2) is introduced using the gradient of pressure on both sides of the membrane as driving force [3].

$$r_{H_2}^p = \left(\frac{28.84\cdot 10^{-5}}{\delta}\right)\exp\left(\frac{-1888.381}{T}\right)\left(\sqrt{P_{H_2}^r} - \sqrt{P_{H_2}^p}\right) \tag{S.2}$$

Where δ is the thickness of the membrane, T is the reactor temperature and $P_{H_2}^j$ is the partial pressure of hydrogen on both sides of the membrane. The total pressure in the permeate side is set at 1 bar. In this work, an isotherm plug flow reactor is assumed to model this unit. The set of differential equations to describe the mass balances is as follows (S.3-S.5) [4]:

$$\frac{dF_{NH_3}}{dz} = -Ar_{NH_3} \tag{S.3}$$

$$\frac{dF_{N_2}}{dz} = \frac{1}{2}Ar_{NH_3} \tag{S.4}$$

$$\frac{dF_{H_2}}{dz} = \frac{3}{2}Ar_{NH_3} - L_{cir}\, r_{H_2}^p \tag{S.5}$$

Where A is the cross-sectional area of the reactor, L_{cir} is the cross-sectional length of the membrane and F_i is the molar flowrate of component i. The activity of each species is computed using the expression (S.6).

$$a_i = y_i \gamma_i P \tag{S.6}$$

The fugacity coefficients (γ_i) are calculated as a function of pressure and temperature using the correlations proposed by Dyson and Simon [2]. The kinetic constant (k_{reac}) is expressed as a function of the temperature according to equation (S.7).

$$k_{reac} = 8.849 \cdot 10^{14} \exp\left(\frac{-40765}{1.988T}\right) \tag{S.7}$$

The thermodynamic equilibrium constant is also computed as a function of the temperature of the reactor [5]:

$$\log_{10}\left(K_p\right) = \frac{2250.322}{T} - 0.85430 - 1.51049 \log_{10} T - 2.58987 \cdot 10^{-4} T + 1.48961 \cdot 10^{-7} T^2 \tag{S.8}$$

The initial velocity is an input parameter of this model. Based on this value, the cross-sectional area is calculated:

$$Q^0 = \frac{F_t^0}{\rho^0} \tag{S.9}$$

$$\rho^0 = \frac{P^0}{RT} \tag{S.10}$$

$$A = \frac{Q^0}{v^0} \tag{S.11}$$

Finally, to compute the pressure drop in the catalytic side, the Ergun equation is introduced:

$$\frac{dP}{dz} = -150 \frac{(1-\varepsilon)^2}{\varepsilon^3} \frac{\mu v}{d_p^2} - 1.75 \frac{(1-\varepsilon)}{\varepsilon^3} \frac{\rho v^2}{d_p} \tag{S.12}$$

2. Cost Estimation Procedure

With the results obtained in the optimization procedure, the economic analysis is carried out. First, the capital cost is estimated based on the factorial method proposed by Sinnot [6]. The first step consists of calculating the total purchase cost of the major equipment of the facility. For the basic units such as heat exchangers or compressors, the cost is estimated based on the correlations proposed by Almena and Martín [7]. In the ammonia decomposition reactor, the price of Ni/Al_2O_3 is set at 30€/kg [8] and the Pd/Ag supported membrane at 1500€/m^2 [9]. The costs of the gas and steam turbines are calculated as a function of the produced power [10]. The SCR treatment consists of a fixed bed reactor with a GHSV equal to 8000 h-1 [11]. The catalyst is Pd/Al_2O_3 with a price equal to 2501 €/kg [12]. With the total purchase cost of the major equipment, a detailed factorial estimation is applied to calculate the fixed capital of the facility including piping, instrumentation, erection, etc. For a facility working with fluids, the total factor is equal to 1.45.

Table S1: Summary of the operating cost calculations [6]

Variable Costs		
Raw materials		from flowsheet optimization
Miscellaneous materials		10% of Maintenance
Utilities		from flowsheet optimization
Fixed Costs		
Maintenance		5% of fixed capital
Labour		Estimated from correlations
Laboratory		20% of Labour
Supervision		20% of Labour
Plant Overheads		50% of Labour
Capital charges		10% of fixed capital
Insurance		1% of fixed capital
Taxes		2% of fixed capital

Operating cost is a sum of two terms: the fixed and variable costs (see Table S1). The fixed part includes maintenance, labor, capital charges, etc. and is estimated as a percentage of different items, as shown in Table S1. Labor costs are computed using the correlation proposed by Couper et al. [13]. On the variable side, the costs of the raw materials and utilities are included. The price of ammonia is fixed to 0.5 €/kg [14], however, the influence of the variation of this parameter is assessed in this work based on the different ammonia production technologies. The price of argon, nitrogen and hydrogen are set at 0.037 €/kg [15], 0.5

€/kg [16] and 4 €/kg [17], respectively. Finally, the cost of utilities are equal to 2.20 €/GJ for steam [18], 4.58 €/kt [18] for cooling water and 0.0787 €/kWh [19] for electricity.

3. Operating Conditions of the Gas Turbine

The inlet and outlet compositions of the combustion chamber in the gas turbine are presented here in terms of molar fraction.

Table S2: molar fraction of the inlet/outlet streams in the gas turbine

		A	B	C	D	E	F	G	H	I
Inlet Composition	H_2O	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	N_2	39.1	42.6	41.5	45.3	39.2	42.6	41.5	45.3	58.0
	O_2	10.5	11.5	10.6	11.6	10.5	11.5	10.6	11.6	14.9
	Ar	31.7	22.2	29.0	19.1	31.3	22.2	29.0	19.1	0.7
	H_2	5.6	7.1	5.7	7.2	5.7	7.1	5.7	7.2	7.9
	NH_3	13.1	16.6	13.2	16.8	13.3	16.6	13.2	16.8	18.5
	NO_x	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Outlet Composition	H_2O	20.5	21.8	20.6	22.0	20.5	21.8	20.6	22.0	28.6
	N_2	44.5	48.4	46.9	51.0	44.6	48.4	46.9	51.0	64.9
	O_2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	Ar	30.9	21.1	28.2	18.1	30.5	21.1	28.2	18.1	0.7
	H_2	4.1	8.7	4.2	8.8	4.4	8.7	4.2	8.8	5.8
	NH_3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	NO_x	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

4. Operating Conditions of the Rankine Cycle

In this section, the input/output pressures and temperatures of the different sections of the steam turbine are collected. This information complements that provided in Table 1 of the manuscript.

Table S3: Operating conditions of the different sections of the steam turbine

		A	B	C	D	E	F	G	H	I
High Pressure	Inlet P (bar)	125.0	125.0	125.0	125.0	125.0	125.0	125.0	125.0	125.0
	Inlet T (K)	782.0	991.6	785.9	785.9	782.7	991.6	785.9	782.7	785.9
	Outlet P (bar)	35.0	35.0	35.0	35.0	35.0	35.0	35.0	35.0	35.0
	Outlet T (K)	564.0	745.7	567.1	567.1	564.0	745.7	567.1	564.0	567.1
Intermediate Pressure	Inlet P (bar)	35.0	35.0	35.0	35.0	35.0	35.0	35.0	35.0	35.0
	Inlet T (K)	564.0	745.7	567.1	567.1	564.0	745.7	567.1	564.0	567.1
	Outlet P (bar)	5.0	9.5	9.5	9.5	5.0	9.5	9.5	5.0	9.5
	Outlet T (K)	425.5	621.6	451.3	451.3	425.5	621.6	451.3	425.5	451.3
Low Pressure	Inlet P (bar)	5.0	9.5	9.5	9.5	5.0	9.5	9.5	5.0	9.5
	Inlet T (K)	425.5	621.6	451.3	451.3	425.5	621.6	451.3	425.5	451.3
	Outlet P (bar)	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
	Outlet T (K)	399.1	569.3	401.8	401.8	399.1	569.3	401.8	399.1	401.8

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