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# 1 Economies of scale in ammonia synthesis loops embedded with iron- and ruthenium-based 2 catalysts

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9  
10 Keywords: Ammonia synthesis process, cost analysis, economy of scales, ruthenium catalyst,  
11 renewable energy

## 12 13 Abstract (150 words)

14 The economies of scale were analyzed in ammonia synthesis loops embedded with iron-based catalysts  
15 (Fe) and ruthenium-based catalysts (Ru/C). Aspen Plus<sup>®</sup> was utilized to simulate the synthesis and  
16 separation processes with the product range from ammonia 0.1-500 tonne/day. The detailed kinetic  
17 models, the Temkin equation and the modified one, were employed to evaluate catalytic activity in  
18 reactors precisely. The result shows the cost advantage of Ru/C on a small scale. Besides, on a small  
19 scale, the costs of heat exchangers and reactors are dominant, while the catalyst cost of Ru/C itself is  
20 not dominant on any scales. For the ammonia synthesis based on renewable energy, Ru/C catalyst  
21 under mild pressure, i.e., Ru/C-50bar, is preferable. The direction of the future research on the catalyst  
22 of ammonia synthesis from the viewpoint of cost is also discussed.

## 23 24 1. Introduction

25 Ammonia is indispensable for human beings as an artificial fertilizer and is one of the most produced  
26 chemicals. The amount of ammonia production is more than 182 million tonnes in 2019 and is  
27 expected to increase by a total of 4% during the next four years [1]. Furthermore, ammonia is a carrier  
28 of renewable energy because ammonia can be synthesized from the hydrogen gas prepared by water  
29 electrolysis based on renewable energy. Ammonia is promising as a carrier because it readily becomes  
30 a liquid state under less than 10 atm at room temperature, and liquid ammonia has a high energy  
31 density in weight and volume [2-7]. Liquid ammonia is suitable for a portable fuel because nitrogen  
32 gas can be emitted into the air without pollution and obtained everywhere. It means no need to recover  
33 nitrogen gas after the utilization and send back to the location that generates hydrogen from renewable  
34 energy, which omits the cost and energy for recovery and transportation. The market size of ammonia  
35 has an enormous potential to expand in the near future.

36 Industrial production of ammonia is operated through the following exothermic reaction:  $N_2 + 3H_2$

37  $\rightarrow 2\text{NH}_3$   $\Delta H = -92$  kJ/mol [8]. The production usually employs the Haber-Bosch process, where the  
38 catalyst is iron-based one, and the operation condition is harsh: 350-525 °C and 100-300 atm [9].  
39 Although the lower temperature is favorable in terms of equilibrium, the reaction temperature must be  
40 high to accelerate the reaction. The cost of equipment, including reactors and compressors, is much  
41 expensive to endure the severe condition. These costs are usually cut down by the economy of scale  
42 [10], and thus the plant of ammonia production has been generally large and centralized, e.g., 1000  
43 tonne/day [11].

44 Recently, the small-scale plants get attention, such as the plant, which produces 3, 10, and 60  
45 tonne/day of ammonia and consumes 1.5, 5-6, and 25-30 MW, respectively [12]. The small-scale plant  
46 can reduce risks of capital investment and enables localized production. Thus, the transportation cost  
47 decreases, the safety consideration and the worse accessibility are mitigated. The local community  
48 obtains self-sufficiency and independence, avoids ammonia price fluctuations, and ensures the security  
49 of ammonia supply [12-14]. Moreover, renewable energy, which is characterized as highly distributed,  
50 is efficiently utilized in rural areas for the small-scale of ammonia synthesis [12, 14, 15]. However,  
51 the small plant sacrifices the benefits of scale, and the equipment for the harsh operating condition  
52 induces high cost. To realize the small-scale and localized plants, the moderate condition for ammonia  
53 synthesis is desired, which reduces the extreme robustness of the equipment.

54 The suitable catalyst for mitigating the reaction condition is ruthenium supported by graphitized  
55 carbon (Ru/C). In 1972, an alkali promoted Ru/C was invented by the Ozaki group and showed high  
56 activity at moderate conditions [16]. Plenty of researches has developed Ru/C, and its reactivity is  
57 much higher than conventional iron-based catalyst [17-25] even though the operation condition is  
58 mild: 325-450 °C and  $\leq 100$  atm [9]. Besides, recent researches significantly developed the ruthenium-  
59 based catalysts and achieved high reactivity at a surprisingly mild condition in a lab-scale [26-30].  
60 The catalysts with various metals also show excellent activity at ambient conditions [31-37].

61 Ru/C has already been realized in Kellogg Advanced Ammonia Process (KAAP) process, and there  
62 are enough datasets to model a reactor based on Ru/C [41, 48]. However, the plant scale of KAAP is  
63 enormous; around 2000 tonne/day [11]. In addition, the number of plants is only seven in the world,  
64 and the conventional iron-based catalysts have been still general [11]. Although many reports simulate  
65 and optimize the processes of the plants on small-scales, they employ the harsh condition needed by  
66 iron-based catalysts or assume equilibrium without consideration of real catalytic activities [13, 38-  
67 45]. The detailed kinetic model must be employed to evaluate the advantage of the Ru/C catalyst in  
68 the reaction. Furthermore, the optimization and analysis of the plants based on Ru/C are scarce, with  
69 only two literatures [46, 47]. One focuses on the optimization of the reaction [46]. The other analyzed  
70 the cost of the polygeneration process for natural gas and ammonia with the up-to-date models for  
71 Ru/C [47]. To the best of our knowledge, no research investigates the economies of scale in the plant  
72 embedded with ruthenium-based catalysts and clarify the advantage of ruthenium-based catalysts on

73 a small scale. The ruthenium is expensive, considered as the fatal drawback of Ru/C [9, 18]. If Ru/C  
 74 mitigates reaction conditions, the cost of equipment and operation should decrease. Thus, these are a  
 75 trade-off, which is influenced by the economies of scale. The quantitative investigation is required to  
 76 seize the potential of ruthenium-based catalysts for small-scale plants.

77 In this study, we examined the economies of scale in ammonia synthesis loops embedded with Ru/C.  
 78 As a comparison, the loops with the commercialized iron-based catalysts, KM1R (Fe), were also  
 79 investigated. Aspen Plus<sup>®</sup> was utilized to simulate the loops and changed the amount of ammonia  
 80 production scale. We implemented the detailed kinetic models as explained later to evaluate catalytic  
 81 activity in reactors precisely. Several reaction conditions, including severe conditions, are assumed to  
 82 compare with Fe. Based on the results, we quantitatively elucidated the advantage of Ru/C on a small  
 83 scale, and identified the impact of ruthenium cost and the cost relation for electricity and equipment  
 84 against scales. The direction of future research on a catalyst of ammonia synthesis from the viewpoint  
 85 of cost was also suggested.

86

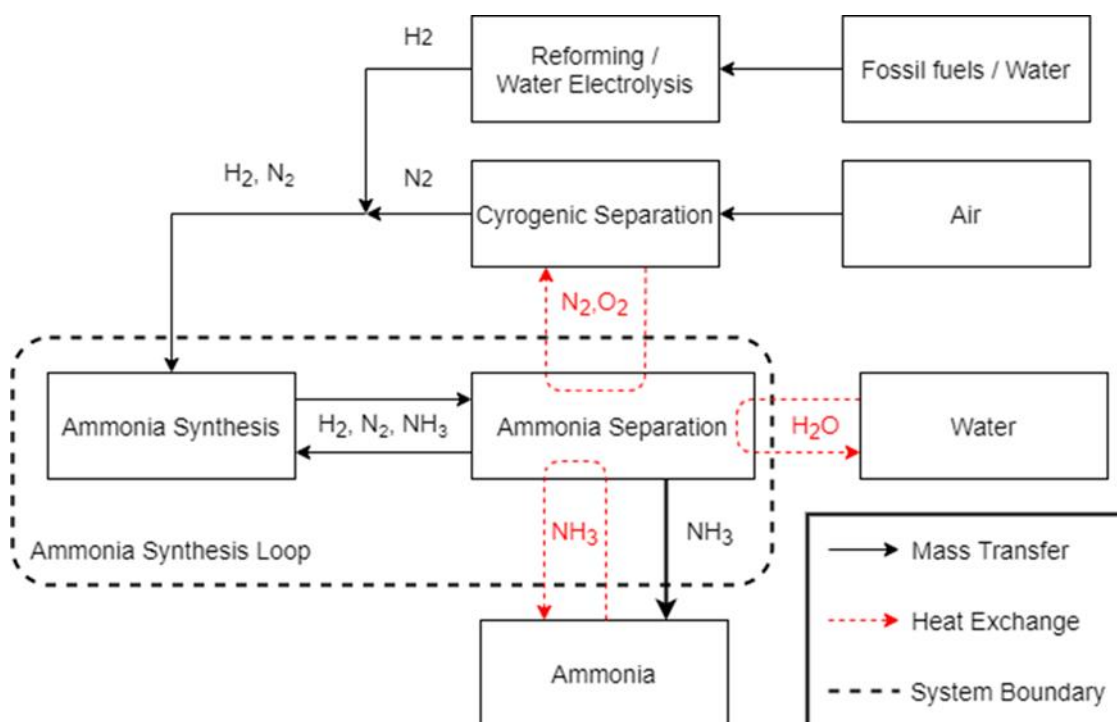
## 87 **2. Method**

### 88 2.1 Whole scheme of the ammonia synthesis loop

89 Figure 1 shows the system boundary of this study. An ammonia production plant consists of a hydrogen  
 90 and nitrogen production and an ammonia synthesis loop. We focused on ammonia synthesis loop  
 91 because the purpose was to evaluate the impact of the mild reaction condition achieved by Ru/C on  
 92 the ammonia synthesis loop. Although the cost for hydrogen and nitrogen production process is  
 93 essential, it does not change the conclusion of the comparison among all types of plants because the  
 94 amount of hydrogen and nitrogen gas is the same. Therefore, in this study, the cost calculation was  
 95 made for the interior of the system, the ammonia synthesis loop, while mass transfer and heat exchange  
 96 took place across the boundaries of the system. (Fig1). Cryogenic air separation is suitable for  
 97 preparing nitrogen gas because of high purity of nitrogen [13, 48], since the catalysts for ammonia  
 98 synthesis are readily poisoned by H<sub>2</sub>O and O<sub>2</sub> [49]. Pressure swing adsorption is not suitable because  
 99 it cannot achieve high purity for ammonia synthesis, although it seems preferable for small-scale  
 100 production. We assumed to utilize the cold heat of O<sub>2</sub> and N<sub>2</sub> in the cryogenic air separation to cool  
 101 down ammonia for the separation.

102





103  
104 Fig. 1. The system boundary of this study, where the cost calculation was conducted for the ammonia  
105 synthesis loop.  
106

107 Aspen Plus<sup>®</sup> was employed to simulate the whole processes of the ammonia synthesis loop. The loop  
108 was based on the template of the ammonia synthesis plant in Aspen Plus<sup>®</sup> with some modification (Fig.  
109 2) [50]. The properties of gas and liquid were from the database in Aspen Plus<sup>®</sup>. The plant scales were  
110 0.1, 1, 10, 100, and 500 tonne/day. The loops were almost the same to the plants with Fe and Ru/C to  
111 estimate how the different reaction conditions change the cost of the operation and equipment,  
112 including the catalyst cost. The inlet gas is the stoichiometric ratio of ammonia,  $H_2/N_2 = 3$ .

113  
114 2.2 Multi catalyst beds and cooling system

115 The operation temperature in the reactor needs to be high to accelerate the reaction, although ammonia  
116 synthesis is an exothermic reaction. It means as the reaction proceeds, the temperature increases to be  
117 close to the equilibrium, and the reactivity slows down. Therefore, the reactor needs to cool down  
118 when the temperature is too high. The plant generally employs a multi-bed reactor and removes the  
119 heat in the outlet of each reactor. In this study, three beds system was applied because the three-bed  
120 reactor system was found to be the most efficient in terms of  $NH_3$  production, energy savings, capital,  
121 and maintenance cost [51]. The three-bed reactor system consisted of three reactors and two heat  
122 exchangers (Fig. 2(b)).

123 The reactant gas before the inlet cooled the gas at the outlet of the reactor (Fig. 2(b)). The inlet and  
124 the maximum temperature (in the outlet) of each reactor were 400 °C and 490 °C for Fe and, 370 °C

125 and 460 °C for Ru/C, which keeps  $\Delta T < 100$  K for safety [10]. These operation temperatures were  
 126 determined by the available experimental data [52, 53].

127 In the case that the ammonia concentration is close to equilibrium, the reaction rate slows down and  
 128 redundantly increases the reactor volume, resulting in high cost. Hence, the general way to determine  
 129 the volume was employed, which stops the reaction when the product concentration reached 90% of  
 130 the equilibrium under adiabatic conditions [54]. In all cases we simulated, the reactor reached to 90%  
 131 of the equilibrium at the third one. The reaction was stopped when the  $\Delta T$  increased to = 90 K, or the  
 132 ammonia concentration in a reactor reached 90% of the equilibrium, which determines the volume of  
 133 reactors.

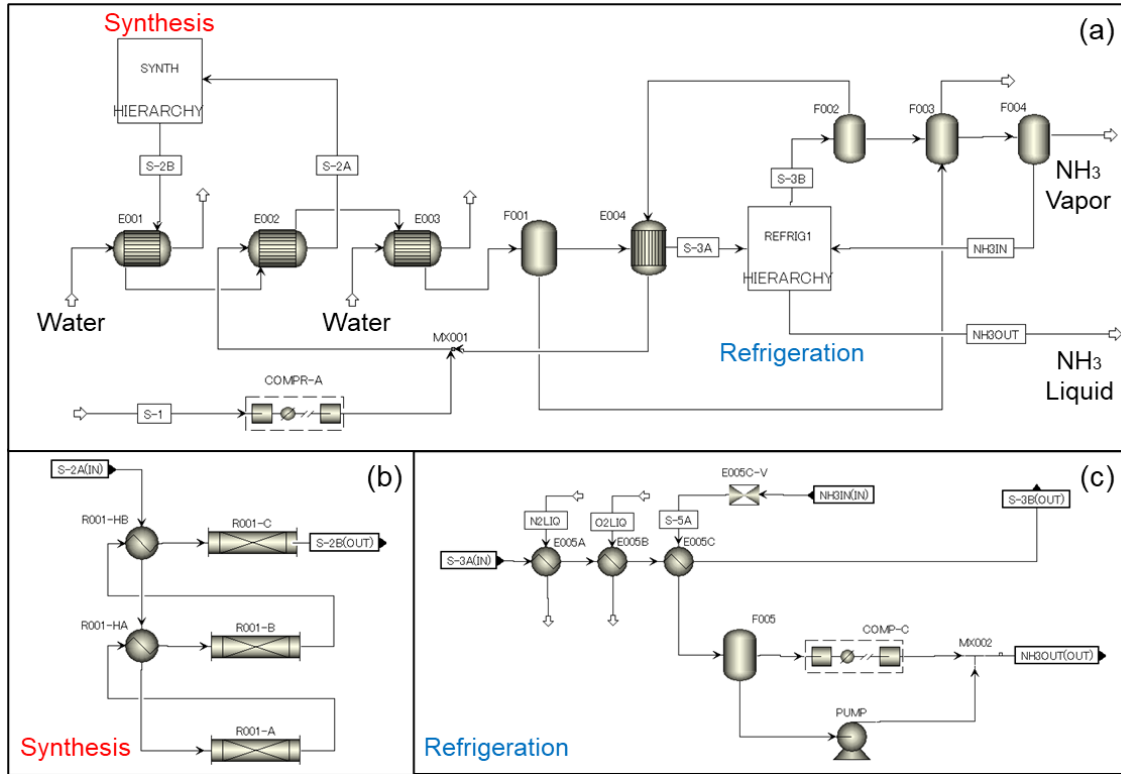
134 The operation pressures were 150 and 300 bar for Fe, and 50 and 100 bar for Ru/C (hereafter Fe-  
 135 150bar, Fe-300bar, Ru/C-50bar, and Ru/C-100bar, respectively), where the operation conditions are  
 136 similar to the experimental data [52, 53]. The amount of produced ammonia in each scale is slightly  
 137 different among the four loops, within 3%, where we considered negligible errors. The loop embedded  
 138 with Ru/C under 75 bar (Ru/C-75bar) was also simulated for additional analysis.

139

### 140 2.3 Separation of ammonia by refrigeration

141 The ammonia concentration at equilibrium is small under high temperatures. Then, plenty of  $H_2$  and  
 142  $N_2$  remains unreacted and need to be recycled from the viewpoint of cost. For the recycle, we employed  
 143 a general method in ammonia synthesis, refrigeration under high pressure, to make ammonia liquid  
 144 and separate the product liquid and the reactant gases. The refrigeration temperature is 11.5 °C at 300  
 145 bar, -2.7 °C at 150 bar, -10.5 °C at 100 bar, and -26.0 °C at 50 bar, which was adjusted to bring the  
 146  $NH_3$  molar concentration at the reactor inlet to 3 %. Water was utilized to initial cooling to room  
 147 temperature (30 °C), and the cooled gases in cryogenic air separation were used in the second. To  
 148 decrease temperature lower, the pressure of the  $NH_3$  product was released, and its latent heat and cold  
 149 heat were utilized, followed by the compression of the product to be liquid under 20 atm at room  
 150 temperature, 30 °C (Fig. 2(c)). In the Fe-300 bar, the refrigeration process differs from others because  
 151 the high pressure does not require much lower temperatures for ammonia separation (See Section A in  
 152 the Supplementary Information).

153



154

155 Fig. 2. (a) Overall layout of the ammonia synthesis loop simulation in Aspen Plus<sup>®</sup>. (b) Flowsheet of  
 156 the ammonia synthesis process: the details of the “SYNTH” block in the overall flowsheet. (c)  
 157 Flowsheet of the ammonia refrigeration process for separation of the product NH<sub>3</sub>: the details of the  
 158 “REFRIG1” block in the overall flowsheet.

159

#### 160 2.4 Kinetics in a reactor

161 Plenty of experimental kinetic data for Fe is represented by the following simple Temkin equation [55-  
 162 57]:

$$163 \quad r_{\text{NH}_3} = k_r \left( K_a^2 a_{\text{N}_2} \left[ \frac{(a_{\text{H}_2})^3}{(a_{\text{NH}_3})^2} \right]^\alpha - \left[ \frac{(a_{\text{NH}_3})^2}{(a_{\text{H}_2})^3} \right]^{1-\alpha} \right) \quad (1)$$

164 where,  $r_{\text{NH}_3}$  is the reaction rate in  $\text{kmol}_{\text{NH}_3}/\text{hr}/\text{m}^3$  of catalyst beds,  $k_r$  is a kinetic constant of the  
 165 reverse reaction,  $K_a$  is the equilibrium constant of the reaction,  $a_i$  ( $i = \text{H}_2, \text{N}_2, \text{and } \text{NH}_3$ ) is the  
 166 activity of component  $i$ ,  $\alpha$  is an adaptive parameter to be set at a constant value. In this study, we  
 167 utilized the parameters,  $\alpha$  and  $k_r$ , determined by Dyson et al. [55] based on the experimental kinetic  
 168 data obtained by Nielsen et al. [52].  $\alpha$  is 0.5 and  $k_r$  is expressed as follows:

$$169 \quad k_r = 1.7698 \times 10^{15} \exp\left(-\frac{40765}{R_c T}\right) \quad (2)$$

170 where  $R_c$  is the gas constant in  $\text{cal}/\text{K}/\text{mol}$ , the unit of the temperature  $T$  is Kelvin.

171 The Temkin equation (1) cannot represent the experimental kinetic data for Ru-based catalysts well  
172 because the reaction over Ru-based catalysts is inhibited by hydrogen poisoning [53, 58] while the  
173 reaction over Fe-based catalysts is inhibited by ammonia poisoning [59]. Buzzi et al. considered 23  
174 possible kinetic models by the Langmuir-Hinshelwood-Hougen-Watson (LHHW) approach, which  
175 separates the reaction into elementary reaction steps and expresses the overall reaction rate as the  
176 slowest step rate [60]. Rossetti et al. modified the Temkin equation to successfully represent the  
177 experimental kinetic data for Ru/C catalyst by the LHHW approach, which takes into account  
178 hydrogen poisoning [53]. The modified-Temkin equation under the condition of the feeding ratio  
179  $H_2/N_2 = 3$  is the following:

$$180 \quad r_{N_2} = k_f \frac{\left( (a_{N_2})^{0.5} \left[ \frac{(a_{H_2})^{0.375}}{(a_{NH_3})^{0.25}} \right] - \frac{1}{K_a} \left[ \frac{(a_{NH_3})^{0.75}}{(a_{H_2})^{1.125}} \right] \right)}{1 + K_{H_2} (a_{H_2})^{0.3} + K_{NH_3} (a_{NH_3})^{0.2}} \quad (3)$$

181 where  $r_{N_2}$  is the reaction rate in  $\text{kmol}_{N_2}/\text{hr}/\text{m}^3$  of catalyst beds,  $k_f$  is a kinetic constant of the  
182 forward reaction,  $K_{H_2}$  and  $K_{NH_3}$  are the adsorption equilibrium constants for hydrogen and ammonia,  
183 respectively. The kinetic and thermodynamic parameters of Ru/C catalyst,  $k_f$ ,  $K_{H_2}$ , and  $K_{NH_3}$ , have  
184 been calculated from experimental data [46, 53]:

$$185 \quad k_f = 9.02 \times 10^8 \exp\left(-\frac{23000}{R_c T}\right) \quad (4)$$

$$186 \quad \log_e K_{H_2} = -\frac{56.9024}{R} + \frac{37656}{RT} \quad (5)$$

$$187 \quad \log_e K_{NH_3} = -\frac{34.7272}{R} + \frac{29228}{RT} \quad (6)$$

188 where  $R$  is the gas constant in J/K/mol.

189 The equilibrium constant  $K_a$  was calculated according to Gillespie and Beattie [53, 55, 61]:

$$190 \quad \log_{10} K_a = -2.691122 \log_{10} T - 5.519265 \times 10^{-5} T \\ 191 \quad + 1.848863 \times 10^{-7} T^2 + \frac{2001.6}{T} + 2.6899 \quad (7)$$

192 For gases, the activity of a component can be expressed as follows:

$$193 \quad a_i = \frac{f_i}{P^\ominus} \quad (8)$$

194 where,  $f_i$  is the fugacity of component  $i$ , and  $P^\ominus$  is the standard pressure. Choosing  $P^\ominus$  as equal  
195 to 1 atm, one can be written as:

$$196 \quad a_i = f_i = \varphi_i y_i P \quad (9)$$

197 where  $\varphi_i$  is the fugacity coefficient of component  $i$ ,  $y_i$  is the molar fraction of component  $i$ ,  $P$   
198 is the pressure in atm. We employed the fugacity coefficients calculated by Cooper and Shaw et al.  
199 for hydrogen and by Cooper and Newton for nitrogen and ammonia [53, 55, 62, 63].

$$\varphi_{\text{H}_2} = \exp \left\{ \exp(-3.8402T^{0.125} + 0.541)P - \exp(-0.1263T^{0.5} - 15.980)P^2 \right. \\ \left. + 300[\exp(-0.011901T - 5.941)] \left[ \exp\left(-\frac{P}{300}\right) \right] \right\} \quad (10)$$

$$\varphi_{\text{N}_2} = 0.93431737 + 0.3101804 \times 10^{-3}T + 0.295896 \times 10^{-3}P \\ - 0.2707279 \times 10^{-6}T^2 + 0.4775207 \times 10^{-6}P^2 \quad (11)$$

$$\varphi_{\text{NH}_3} = 0.1438996 + 0.2028538 \times 10^{-2}T - 0.4487672 \times 10^{-3}P \\ - 0.1142945 \times 10^{-5}T^2 + 0.2761216 \times 10^{-6}P^2 \quad (12)$$

The reaction kinetics, Eq. (1) for Fe-based catalysts and Eq. (3) for Ru/C catalysts, were implemented by user Fortran subroutines of the Plug flow reactor (RPlug) model in Aspen Plus<sup>®</sup>, and the “RPlug” model was adopted in adiabatic conditions.

209

## 2.5 Economic analysis

The total cost for the loops is separated into a capital cost,  $C^{cap}$ , and an operation cost,  $C^{op}$ .  $C^{cap}$  was estimated by the following equations [10]:

$$C^{cap} = \sum_j C_j \quad (13)$$

$$C_j = C_{j,fix} + LM \times \frac{\text{CEPCI in 2019}}{1000} \times AF \times C_{j,ref} \times \left( \frac{s_j}{s_{ref}} \right)^{n_j} \quad (14)$$

$C_j$  is the Free On Board (FOB) cost for equipment  $j$ .  $C_{j,fix}$  is the cost of the control system of  $j$ .  $LM$  is the cost of labor and management.  $AF$  is an alloy factor, which is determined by the cost of materials.  $C_{j,ref}$  is the FOB cost for  $j$  in a reference scale,  $s_{ref}$ .  $s_j$  is the actual scale of  $j$ .  $n_j$  is a parameter that determines the influence of a scale. The parameters in the equation (14) for each equipment,  $j$ , are given in Table 1 with the assumption that CEPCI is 1000. Pressure adjustment in Table 2 is multiplied to the reactor cost in a reference scale,  $C_{reactor,ref}$ . Stainless steel (SUS 304) was employed for the material for reactors, compressors, and heat exchangers (shell and tube) with the alloy factor, 2.75 for reactors and compressors and 2.80 for heat exchangers [10]. It is because SUS 304 is durable for the temperature and the pressure required for the plants and is tolerant for hydrogen embrittlement [64, 65]. Chemical plant cost indexes (CEPCI) in 2019, 607.5 was utilized.

225

226 Table 1. Summary of the parameter for eq. (14) [10]

Unit	Basis	$C_{j,fix}$	$C_{j,ref}$	$s_{ref}$	$n_j$	$LM$	$AF$
Reactor	Volume (m <sup>3</sup> )	63,000	110,000	20	0.52	2.3	2.75
Compressor, Low	Rated Power (kW)	7,000	1,350,000	1000	0.9	2.15	2.75
Compressor, High	Rated Power (kW)	7,000	10,300,000	10000	0.71	2.15	2.75
Heat Exchanger	Area (m <sup>2</sup> )	27,000	70,000	100	0.71	2.8	2.8

227

Table 2 Pressure adjustment for reactor

P (bar)	Pressure adjustment
300	6.1
150	3.4
100	2.3
75	1.9
50	1.6

 228  $C^{op}$  was calculated by the following equation [10]:

$$229 \quad C^{op} = \sum_{t=1}^{year} \frac{1}{(1+d)^{t-1}} C_{elec} E_{comp} \quad (15)$$

230 where the duration of the operation,  $year$ , is assumed as 20 years.  $d$  is the discount rate, 2.25%, and  
 231  $C_{elec}$  is the cost for electricity, 0.0683 USD/kWh, assuming the price for the industrial sector in 2019  
 232 in the USA [66]. The energy required to compressor per year,  $E_{comp}$ , is estimated by the output from  
 233 Aspen Plus<sup>®</sup>.

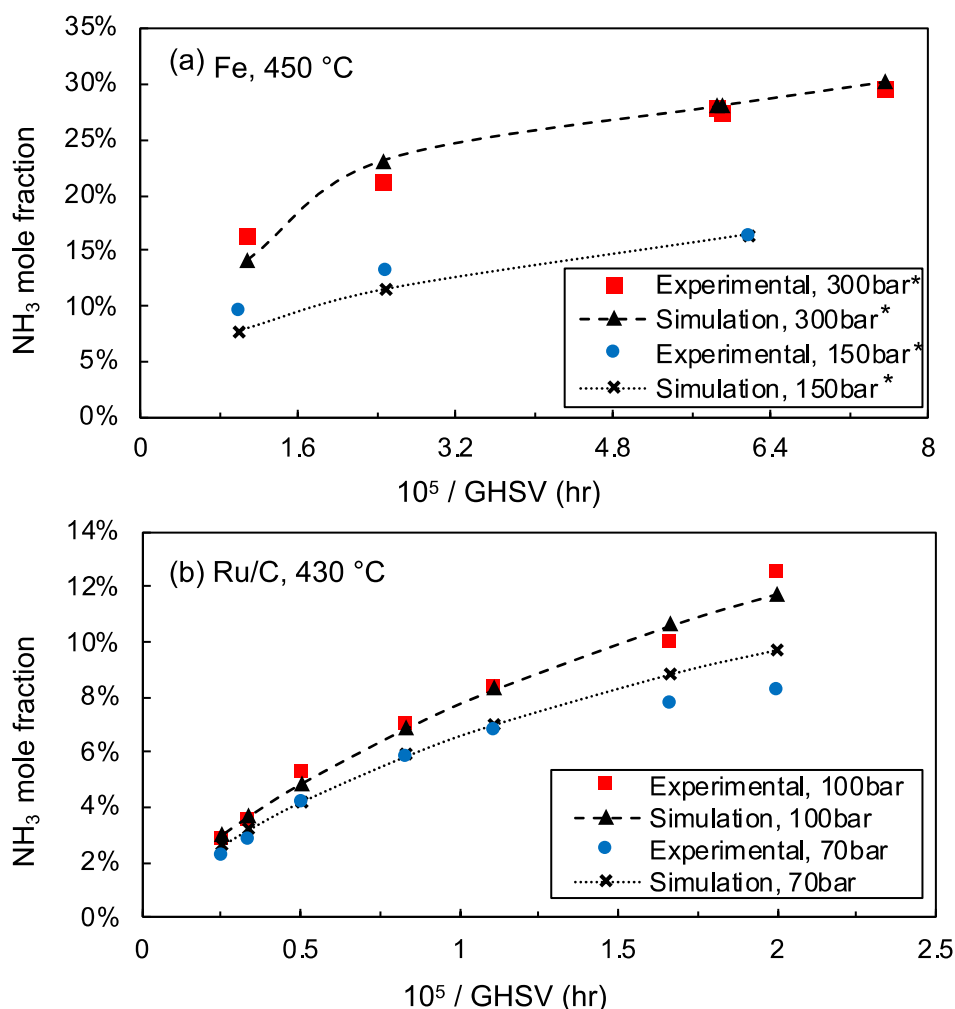
234 The catalyst cost is generally estimated by weight and material cost per weight without the economy  
 235 of scale [67]. In this study, the cost of the Fe and Ru/C catalysts are 0.18 USD/kg [68] and 321.04  
 236 USD/kg, respectively. The cost of Ru/C is calculated by the price of ruthenium (9730 USD/kg) and  
 237 graphene (10 USD/kg) respectively [69, 70]. The Ru content was 3.2 wt% [53]. The bulk density of  
 238 the Fe catalyst is 2.8 g/cm<sup>3</sup>, and that of the Ru/C catalyst is 0.8 g/cm<sup>3</sup> [71]. The duration of the catalysts  
 239 is assumed as ten years based on the data in the literature [17].

240

### 241 3. Results

#### 242 3.1 Configurations of the simulated reactors

243 Figure 3 shows the comparison of the experimental data with the result of a single pass over the reactor  
 244 simulation for validation. In the verification, a single reactor was used to investigate the ammonia  
 245 conversion rates by varying the Gas Hourly Space Velocity (GHSV) at a specific temperature, pressure,  
 246 and a molar ratio of hydrogen to nitrogen under experimental conditions [52, 53]. The results indicated  
 247 that the conversion rates of ammonia in the simulated reactor for Fe and Ru/C were a good  
 248 approximation of the ammonia conversion rates in the experiment. Therefore, the models we  
 249 constructed were sufficiently accurate to describe the ammonia synthesis loops.



250

251 Fig. 3. Comparison of the experimental data with the reactor simulation results of a single pass over  
 252 a reactor, (a) for Fe at  $T = 450\text{ }^{\circ}\text{C}$ ,  $*P = 304\text{ bar}$  (=300 atm) and 152 bar (=150 atm), and  $\text{H}_2/\text{N}_2 =$   
 253 3.0 [52], (b) for Ru/C  $T = 430\text{ }^{\circ}\text{C}$ ,  $P = 100\text{ bar}$  and 70 bar, and  $\text{H}_2/\text{N}_2 = 3.0$  [53].

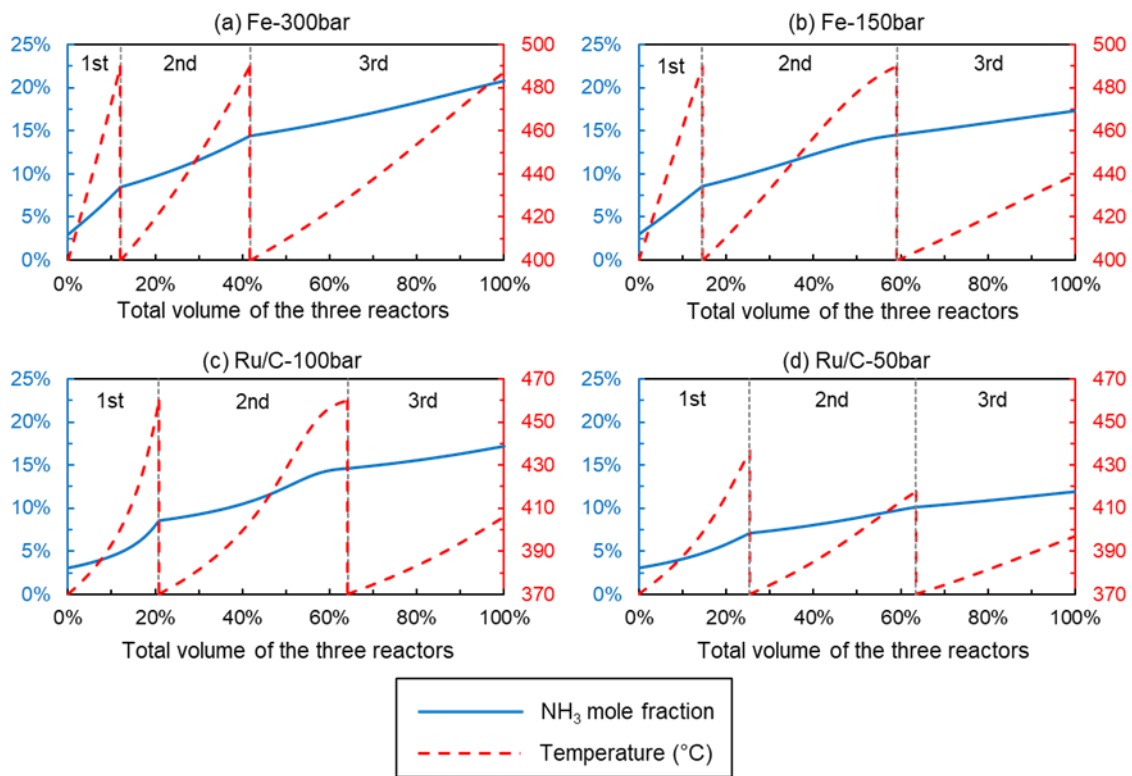
254

255 Figure 4 shows the ammonia concentration and temperature change in the three-bed reactor in the  
 256 ammonia synthesis loops. The ammonia concentration at the three-bed reactor outlet is highest at Fe-  
 257 300 bar, lowest at Ru/C-50bar, and close to that at Fe-150bar and Ru/C-50bar. The total reactor size  
 258 in Ru/C-100bar is smaller than that in Fe-150bar because the activity of the Ru/C catalyst at 100 bar  
 259 is greater than that of the Fe-based catalyst at 150 bar (Table 3).

260

261 The tendencies in these reactors are explained by the characteristics of these catalysts and ammonia  
 262 as follows. As the reactor pressure decreases, the ratio of the first bed volume to the total reactor  
 263 volume tends to decrease. For Fe-300bar and Fe-150bar, the proportion of the second and third beds  
 264 is large due to the reaction rate reduced by ammonia poisoning, which is severe at high pressure [59].  
 Then, it increases residence time and expands the volume of the second and third beds. In contrast,

265 Ru/C we employed tends to suffer from hydrogen poisoning rather than ammonia poisoning [58],  
 266 which induces a slow reaction rate in the first reactor enriched by hydrogen but fast in the third one  
 267 with a high concentration of ammonia. Hence, Ru/C results in a large volume in the first reactor and  
 268 a small volume in the third one. In the comparison between Ru/C-100bar and Ru/C-50bar, the low  
 269 pressure in Ru/C-50bar seems unfavorable for equilibrium to obtain a high concentration of ammonia  
 270 because the reaction of Ru/C-50bar is stopped by the reason that ammonia concentration reaches 90%  
 271 of equilibrium rather than  $\Delta T = 90\text{K}$  even at the first and second stage. Especially,  $\Delta T$  in the second  
 272 reactor is small, which stops its reaction early and results in a small volume against the total. Therefore,  
 273 the tendencies in these reactors are reasonable, and thus our models can well describe the properties  
 274 of these catalysts.



275

276 Fig. 4.  $\text{NH}_3$  concentration and temperature change in the simulated three-bed reactor system in the  
 277 ammonia synthesis loops, (a) Fe-300bar, (b) Fe-150bar, (c) Ru/C-100bar, (d) Ru/C-50bar.

278



279 Table 3. The results in the reactor system in different plant types at the scale of 100 tonne/day.

Plant type	Temperature (°C)	Total volume of the reactors (m <sup>3</sup> )	Catalyst weight (tonne)	GHSV* <sup>1</sup> (10 <sup>4</sup> /hr)	Affluent NH <sub>3</sub> (vol.%)	Productivity* <sup>2</sup> (mmol/hr/g <sub>cat</sub> )
Fe-300bar	400-490	1.15	3.23	3.28	20.79	76.94
Fe-150bar	400-490	4.22	11.81	1.09	17.36	21.23
Ru/C-100bar	370-460	3.95	3.16	1.18	17.17	79.42
Ru/C-50bar	370-437	7.05	5.64	1.18	11.96	44.64

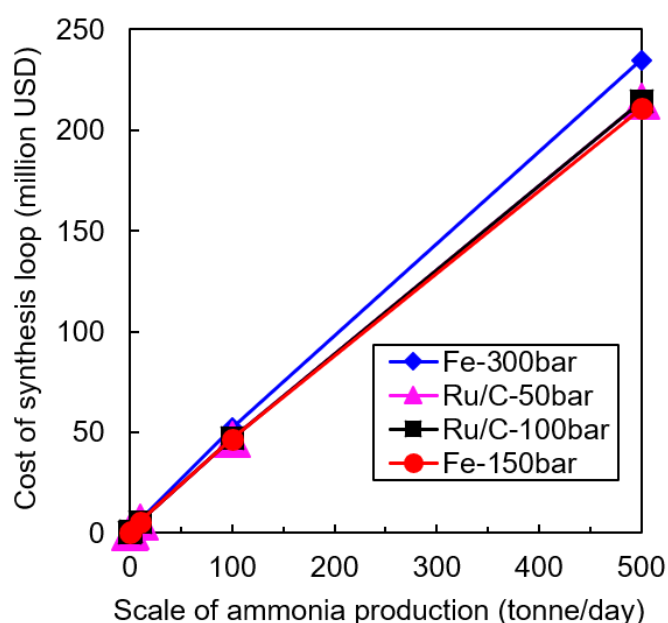
280 \*<sup>1</sup> GHSV was calculated based on the total volume of the reactors (m<sup>3</sup>) and the volume flow rate  
281 (m<sup>3</sup>/hr) of the gas flowing into the reactor system under the standard condition of 0 °C and 1 atm.

282 \*<sup>2</sup> Productivity was calculated based on the catalyst weight (g<sub>cat</sub>) and the molar increase in NH<sub>3</sub>  
283 (mmol/hr) in the gas between the reaction system inlet and outlet.

284

### 285 3.2 Overall cost of ammonia synthesis loop

286 Figure 5 shows the overall cost of the ammonia synthesis loops embedded with Fe and Ru/C with  
287 various scales of ammonia production. Figure 6 exhibits the ratio of the total cost per the cost of Ru/C-  
288 100bar. The total costs are mostly linear with the scale. Fe-300bar has the highest cost over the scale  
289 of 1 tonne/day. It is noted that Fe-150bar shows the lowest cost in the scale at 500 tonne/day, and  
290 Ru/C-50bar has the lowest cost at 100 tonne/day, and Ru/C-100bar shows the lowest cost below the  
291 10 tonne/day scale. Therefore, it is correct that Ru/C is more advantageous than Fe in the small scale  
292 of ammonia production, particularly below 100 tonne/day. However, the difference is not so large with  
293 the current condition.



294

295

Fig. 5 The total cost of the ammonia synthesis loop against the production scale.

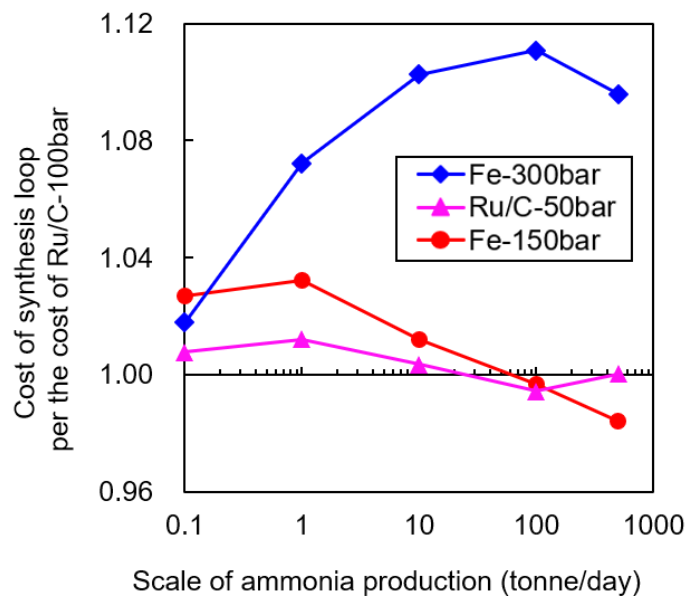
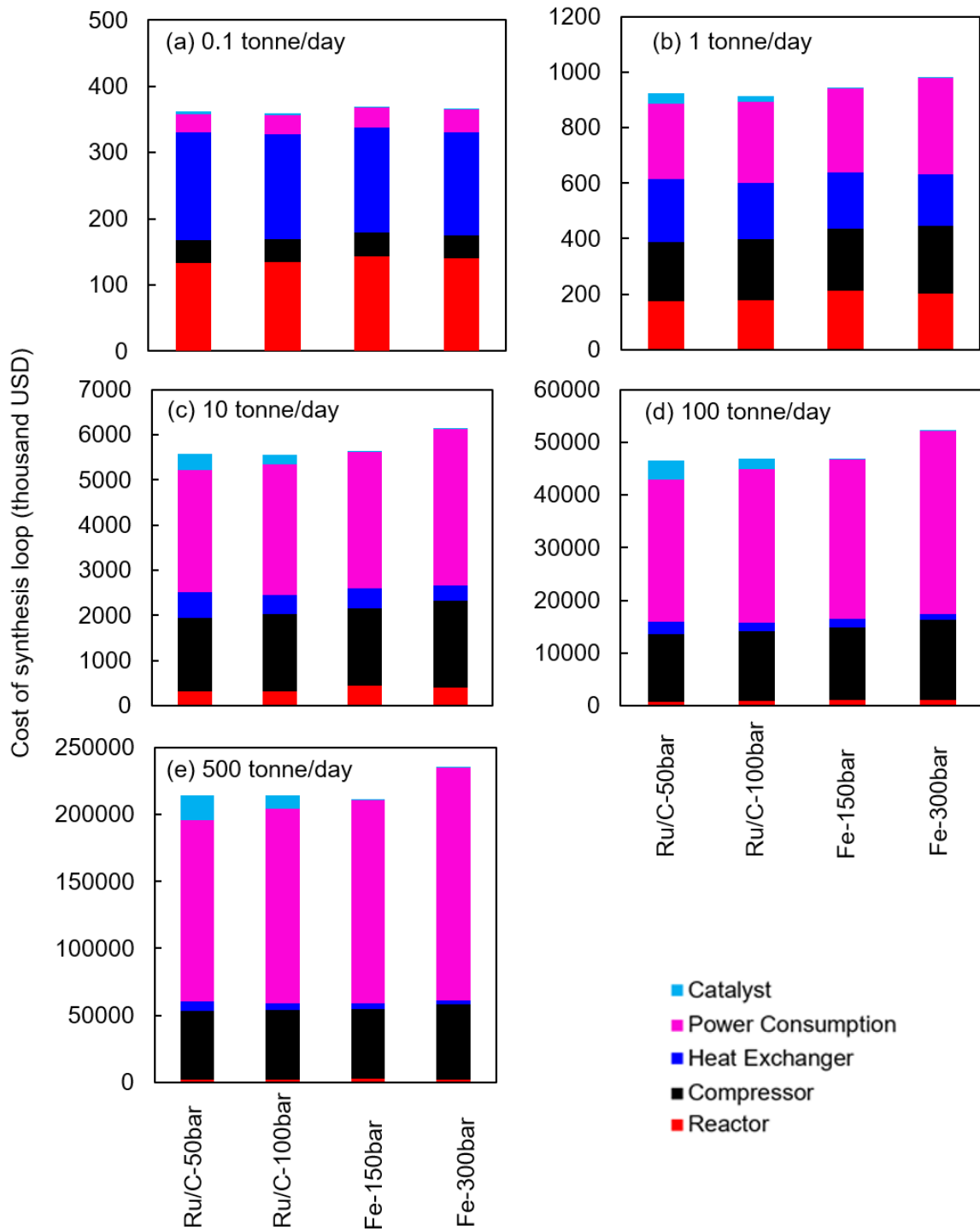


Fig. 6 The total cost of the ammonia synthesis loop per the cost of Ru/C-100bar against the production scale.

### 3.3 Breakdown of loop cost at different scales

The breakdowns of the cost of these ammonia synthesis loops are shown in Fig. 7. As general tendencies, the costs of energy consumption dominate on large scales, explaining the linear relation between the total costs and the scale because energy consumption shows mostly monotonic increases of cost. In contrast, the costs of reactors and heat exchangers are dominant on small scales. The origin that Ru/C-100bar is lower cost than Fe-150bar in the 0.1-10 tonne/day scale is all components except for catalysts are cheaper in the Ru/C-100bar than those in the Fe-150bar, and the cost of catalysts are not dominant.



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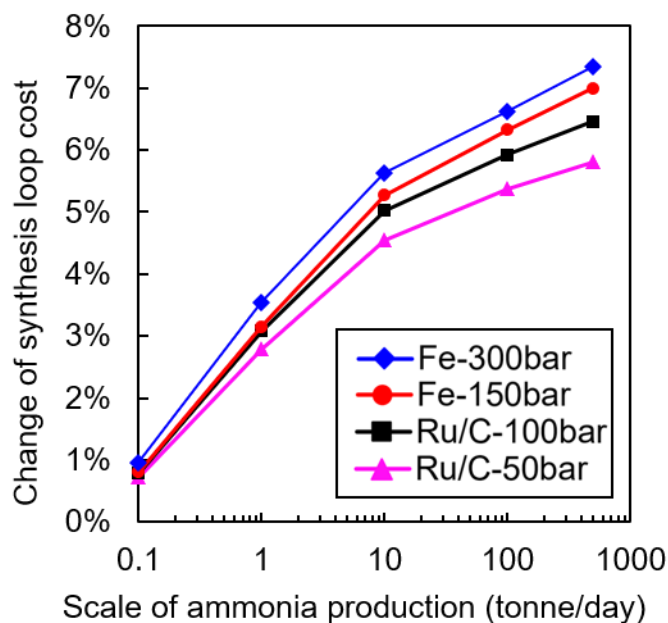
Fig. 7 Breakdown of the cost of ammonia synthesis loop in different scales, (a) 0.1 tonne/day, (b) 1 tonne/day, (c) 10 tonne/day, (d) 100 tonne/day, (e) 500 tonne/day.

312 The difference between Ru/C and Fe is that Fe requires large energy consumption for the harsh  
313 condition, and Ru/C induces high costs for the catalyst itself. However, the cost ratio of catalysts in  
314 Ru/C is 9 % at most, and thus the catalyst cost does not matter. Although the catalyst cost of Ru is said  
315 too expensive to be fatal, our results show that other components are higher cost. Currently, we  
316 assumed that the durability of catalysts is ten years. The other publications indicate that the catalysts  
317 can last longer than ten years [17], and then the cost ratio of catalysts will be less than 9 %. Therefore,  
318 it is concluded that the utilization of Ru metals as Ru/C is not problematic in terms of cost.

319

### 320 3.4 Sensitivity to the electricity price, catalyst cost, and pressure

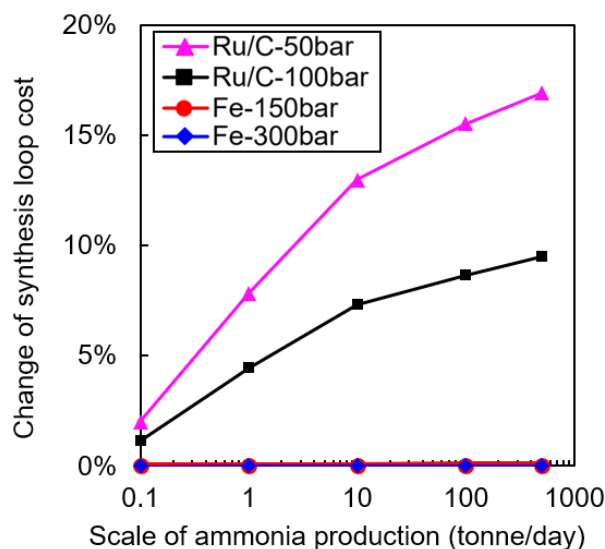
321 This section analyzes the sensitivities of parameters in each case, and preferable cases are suggested  
322 in the different conditions. The energy consumption is dominant, more than 30%, except for a tiny  
323 scale, 0.1 tonne/day. Then, we analyzed the change of sensitivity against energy price. The current  
324 price of electricity is assumed to be the industrial price in the USA, which is variable based on  
325 locations. Figure 8 exhibited the change in total cost when the energy price increased to 110%. The  
326 least sensitive one to energy price is the loop with Ru/C-50bar. It means that Ru/C is advantageous in  
327 the case that the price of electricity is high. When the energy price increased to 106.3%, i.e., 0.0726  
328 USD/kWh, the cost of Ru/C-50bar is the same as the cost of Ru/C-100bar at the scale of 10 tonne/day.  
329 Hence, if the price is more than 0.0726 USD/kWh, Ru/C-50bar is the cheapest at a 10 tonne/day scale.



330

331 Fig. 8. The sensitivities of synthesis loop cost when energy price increases by 10% (i.e., the case that  
332 the energy price increased from 0.0683 USD/kWh to 0.07513 USD/kWh).

333 The catalyst cost for Ru/C-50bar is relatively high. Figure 9 indicates the sensitivities on the cost  
334 where the catalyst cost is twice, or the loading amount of the catalyst is double, or the lifetime of the  
335 catalyst becomes half. In this case, with Ru/C-50bar, the catalyst cost at a 500 tonne/day scale is 17%  
336 in the total and cannot be ignored.



337

338

Fig. 9. The sensitivities of synthesis loop cost due to the twice cost for catalyst

339

340 Figure 10 shows the cost of each component against pressure at the loop embedded with Ru/C. The  
341 costs of power consumption and compressor are high at high pressure. The catalyst cost is small at  
342 high pressure because the reaction rate is fast at the condition, and fewer catalysts are required. It is  
343 noted that the cost of heat exchangers increases when the pressure is mild. It is derived from that the  
344 unreacted gas increases due to slow reaction rate at small pressure, and needs to be more recycled, and  
345 thus the total volume in the loop also increases (Table 4). In contrast, the difference in the cost of the  
346 reactors among three pressure is within 1% even though the volume of a reactor also increases due to  
347 low pressure. It is because of the pressure adjustment, which is applied for the only reactor.

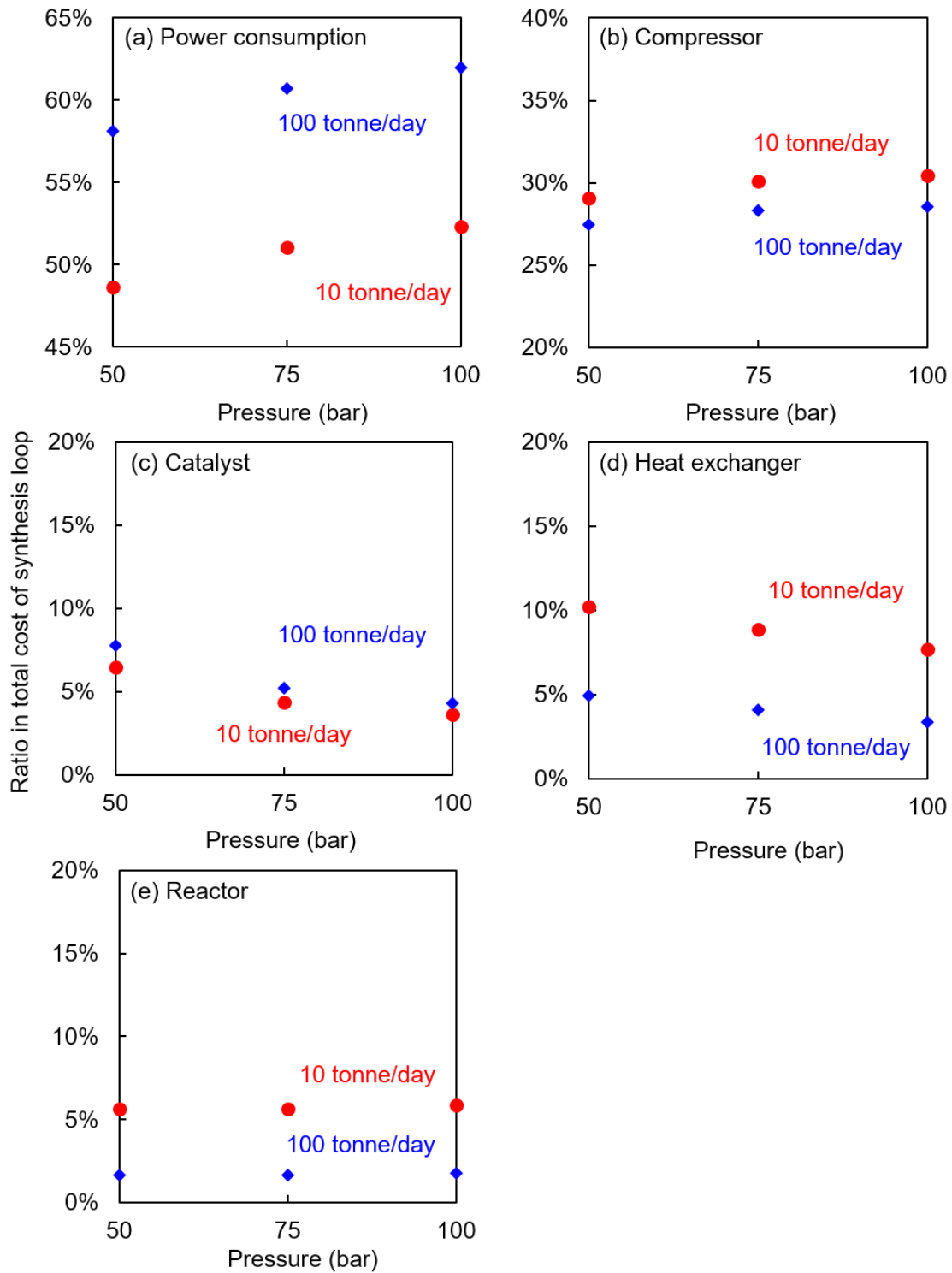
348 As a summary of this section, in the case that electricity price is high, the mild pressure achieved by  
349 Ru/C is preferable to reduce energy consumption. Still, it requires more catalysts and a large volume  
350 of a heat exchanger, resulting in a high cost. These are in the trade-off relation.

351

352 Table 4. Scales of reactors and heat exchangers in the loop embedded with Ru/C (Please see Table  
353 A.2. in Supplementary Information for details)

		10 tonne/day			100 tonne/day		
	Unit	100 bar	75 bar	50 bar	100 bar	75 bar	50 bar
Reactor	Total volume (m <sup>3</sup> )	0.395	0.477	0.705	3.954	4.770	7.050
Heat exchanger	Total area (m <sup>2</sup> )	38.9	53.2	68.4	388.6	531.6	684.4
Molar flow rate*	10 <sup>5</sup> mol/hr	2.08	2.50	3.15	20.80	24.97	31.51

354 \* The molar flow rate of gas into the reactor system

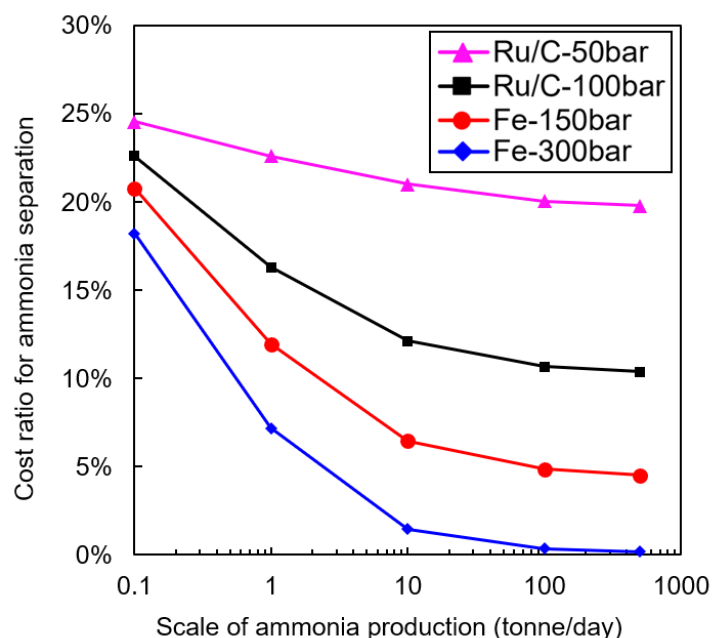


355  
356  
357  
358

Fig. 10. The ratio of each component in the total cost of the synthesis loop against operating pressure, (a) Power consumption, (b) Compressor, (c) Catalyst, (d) Heat exchanger, (e) Reactor.

359 3.5 Disadvantage of low pressure for ammonia separation

360 Ru/C successfully makes the reaction condition mild and decreases the cost of components. It reduces  
361 the cost of power consumption to compress inlet gas. However, the cost reduction was not drastically  
362 because low pressure is not favorable for the separation step. High pressure or low temperature are  
363 required to make ammonia liquid state, which results in large power consumption. Figure 11 indicates  
364 the total cost for ammonia separation, including heat exchanger, compressor, and power for a  
365 compressor in the separation step (See Section B in the Supplementary Information). The low pressure  
366 at milder conditions suffers from the high cost for the separation, especially in lower scales. Therefore,  
367 the cost reduction based on a milder condition in reactors is the trade-off relation with separation cost.  
368 It is derived from the property of ammonia and is inevitable without another approach, such as  
369 adsorbent. The adsorbent can separate ammonia regardless of operation pressure and release ammonia  
370 by waste heat from the loop, which is promising to reduce the power consumption for the separation.



371  
372  
373  
374

Fig. 11. Cost ratio for ammonia separation



## 375 4. Discussion

### 376 4.1 Suitable catalyst and condition for ammonia synthesis at various scales and locations

377 The analysis of loop cost and the cost structure against different scales reveals that the suitable catalyst  
 378 and operation condition differs on the required scale and the energy prices. With the current  
 379 assumption, Fe-150bar has the lowest cost in the range of over 100 tonne/day while Ru/C-50bar  
 380 exhibits the lowest cost at 100 tonne/day, and Ru/C-100bar shows the lowest cost below the scale of  
 381 10 tonne/day. According to chapter 9 in the literature [17], small- and medium-scale plants employ  
 382 higher operation pressure than large-scale plants. Although the reason was not clearly shown in the  
 383 literature, the tendency is the same with our results where Ru/C-100bar is cheaper than Ru/C-50bar at  
 384 the scale below 10 tonne/day due to the separation process. It suggests the industrial design requires  
 385 high pressure at a small scale due to the ammonia separation and support the validity of our results.

386 It is noted that the cost structure is different from each other. As indicated in section 3.4, Ru/C-50bar  
 387 is less sensitive to the cost of energy consumption. In the location that the price of electricity is high,  
 388 Ru/C-50bar will be preferable, whereas the mild pressure induces high catalyst costs. Renewable  
 389 energy tends to be expensive than the electricity generated by fossil fuels and is distributed with low  
 390 energy density, which results in small scales. In small scales, the catalyst cost of Ru/C is not dominant,  
 391 as mentioned in section 3.3. Therefore, we can conclude that the loop embedded with high loading  
 392 Ru/C catalyst at mild pressure is the best for small-scale production based on renewable energy.

393 Recently, the cost of renewable energy is decreasing significantly. The project-level levelized cost  
 394 of electricity generated by solar photovoltaics is 0.0680 USD/kWh in 2019, calculated with “*a real*  
 395 *weighted average cost of capital; 7.5% for Organization for Economic Co-operation and Development*  
 396 *(OECD) countries and China and 10% for the rest of the world*” [72]. It is very close to the price  
 397 employed in the model is 0.0683 USD/kWh. The low cost is usually derived from the large-scale  
 398 installation, which is different from the small-scale production mentioned above. Ru/C catalyst will  
 399 be practical for the ammonia synthesis by the distributed generation of electricity based on renewable  
 400 energy.

401

### 402 4.2 Direction for future research of ammonia synthesis

#### 403 *4.2.1 Mild condition for ammonia synthesis achieved by recent ruthenium-based catalysts*

404 Here we discuss the cost reduced by the other promising catalysts. Recent progress on the ruthenium-  
 405 based catalysts enables ammonia synthesis at remarkably mild conditions, such as 50 °C at 1 atm ( $\approx$   
 406 1bar) [26]. In that condition, hydrogen embrittlement will not occur, which is fatal in the harsh  
 407 condition. We currently employ SUS 304, which is durable in severe conditions and tolerant for  
 408 hydrogen embrittlement. The alloy factor of SUS 304 is around 2.8, which means if the mild condition  
 409 is achieved, the alloy factor decrease to 1.0 [10]. Otherwise, the materials with high thermal  
 410 conductivity, such as aluminum or copper, can be utilized for heat exchangers. These can reduce the

411 cost of equipment. Under a small scale such as 1 tonne/day, the cost of component is more dominant  
412 than that of energy consumption. Therefore, the reduced alloy factor or the material with high thermal  
413 conductivity will be a significant impact on the total cost on a small scale. In addition, low pressure  
414 does not require the high energy to compress a gas, and then is suitable for the ammonia synthesis  
415 based on expensive energy, i.e., renewable energy.

416 However, low pressure induces the difficulty of ammonia separation, as shown in section 3.5.  
417 Although these are in the trade-off relation, moderate pressure, such as 10 bar, would be preferable  
418 rather than 1 bar.

419 As for ammonia separation, absorbent could be helpful, which can catch ammonia even under low  
420 pressure and release it by waste heat of the loop [73, 74]. Absorbent has an impact on mitigating the  
421 demerit of reduced pressure.

422

#### 423 *4.2.2 Alternative metals for ruthenium*

424 Recent researches also focus on alternative catalyst metal instead of ruthenium [31, 32, 75-77]. If the  
425 ruthenium-based catalysts are durable over ten years, the cost of ruthenium is not dominant, as shown  
426 in section 3.3. However, if they deactivate within ten years or the loading amount is much more than  
427 3.2 wt%, the catalyst impacts the total cost. Then, research to achieve a long lifetime of catalysts and  
428 reduce the loading amount of ruthenium should be focused on as well as the search for alternative  
429 metals. The cost reduction based on decreasing the amount of ruthenium and using alternative metal  
430 is the trade-off with the reactivity of the catalyst.

431 In the case that the energy price is high such as the usage of renewable energy, milder pressure is  
432 preferred, but more amount of catalysts is required. Thus, the recent study on making synthesis  
433 condition mild is suitable for the synthesis based on renewable energy.

434

#### 435 *4.2.3 Catalyst without ammonia poisoning*

436 As shown in Fig. 4, ammonia concentration is finally high in the third reactors. Fe has a negative  
437 reaction order for ammonia [59], which means Fe is poisoned by ammonia and is not suitable for the  
438 synthesis at a high ammonia concentration. Remarkable catalysts in the recent researches have a  
439 negative order [29, 31, 32], as well as Fe. In contrast, Ru/C has almost zero reaction order for ammonia  
440 and is ideal for the third reactor [58]. The catalysts without ammonia poisoning should be invented for  
441 efficient synthesis. With this point of view, the catalyst, Ru/Ba/LaCeO, has almost zero-order and is  
442 promising [78].

443

### 444 **5. Conclusion**

445 This study performed the economic analysis of the ammonia synthesis loops embedded with Fe and  
446 Ru/C at a broad production scale under several operating conditions. It elucidated that Fe-150bar is

447 the lowest cost on a large scale, 500 tonne/day range. Ru/C-50bar is the lowest at 100 tonne/day scale,  
448 and Ru/C-100bar exhibits the lowest cost under a 100 tonne/day scale. These suggest that Ru/C is  
449 advantageous on the small scales, especially below 100 tonne/day scale. Furthermore, in contrast to  
450 the general idea that ruthenium is too expensive, the catalyst cost of ruthenium is not dominant on any  
451 scale. If the recent ruthenium-based catalyst has a short lifetime, or the loading amount of ruthenium  
452 is much more than 3.2%, the research of alternative metal to reduce the catalyst cost of ruthenium is  
453 practical. The research on the new catalyst to mitigate the operation condition is promising to reduce  
454 the cost of reactor and heat exchanger, but too small pressure also induces the high cost. Moderate  
455 pressure, such as 10 bar, will be preferable, which is also advantageous to separate ammonia. For the  
456 ammonia synthesis based on renewable energy, which is distributed and expensive, Ru/C catalyst  
457 under mild pressure, i.e., Ru/C-50bar, is preferable. The other promising catalysts in the recent  
458 researches are also beneficial to mitigate the condition and reduce the cost, which will be the focus of  
459 the next research. This study clarified the clear and quantitative advantage of Ru/C catalysts at small  
460 scales. It provides the direction for future research on the economic-effective catalyst for ammonia  
461 synthesis.

462

#### 463 **Author Contributions**

464 †M. Y. and T. O. contributed equally to this work

465

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469

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## 660 **Supplementary Information**

661

### 662 **Economies of scale in ammonia synthesis loops embedded with iron- and ruthenium-based** 663 **catalysts**

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#### 672 **A. Explains and results of the ammonia synthesis loop simulation in Aspen Plus<sup>®</sup>**

673 Aspen Plus<sup>®</sup> was employed to simulate the whole processes in the loop of ammonia synthesis. The  
 674 process was based on the template of an ammonia synthesis plant in Aspen Plus<sup>®</sup> with some  
 675 modification (Fig. 2) [50]. The RKS-BM (Redlich-Kwong-Soave with Boston-Mathias modification)  
 676 property method was chosen for the description of the thermodynamic properties of the high-  
 677 temperature, high-pressure conditions in ammonia synthesis loops. The physical properties were taken  
 678 from the database in Aspen Plus<sup>®</sup>. An explanation of the overall process and the assumptions put in  
 679 this simulation is as follows (Figure A.1, and Table A.1, A.2):

- 680 1. It was assumed that the nitrogen feedstock gas was obtained by a cryogenic air separation process  
 681 supplying the same amount of nitrogen [13, 48].
- 682 2. The feedstock consisted of hydrogen and nitrogen in a molar ratio of 3:1, and the pressure was  
 683 raised by a centrifugal compressor from 1 atm to the reaction pressure.
- 684 3. The feedstock was mixed with the reactant gases in the ammonia synthesis loop and fed into the  
 685 synthesis process (Figure A.1.c).
- 686 4. The syngas is cooled to room temperature by preheating the reactant gas and cooling with water  
 687 and then fed to the refrigeration process (Figure A.1.a and A.1.d).
- 688 5. Liquid ammonia and the unreacted gas are separated by refrigeration, and the gas is reused in an  
 689 ammonia synthesis loop. In some cases, liquid ammonia is used as a refrigerant for the separation  
 690 of ammonia then recovered (Figure A.1.b).
- 691 6. The pressure drop in reactors and heat exchangers was set to zero for simplicity.

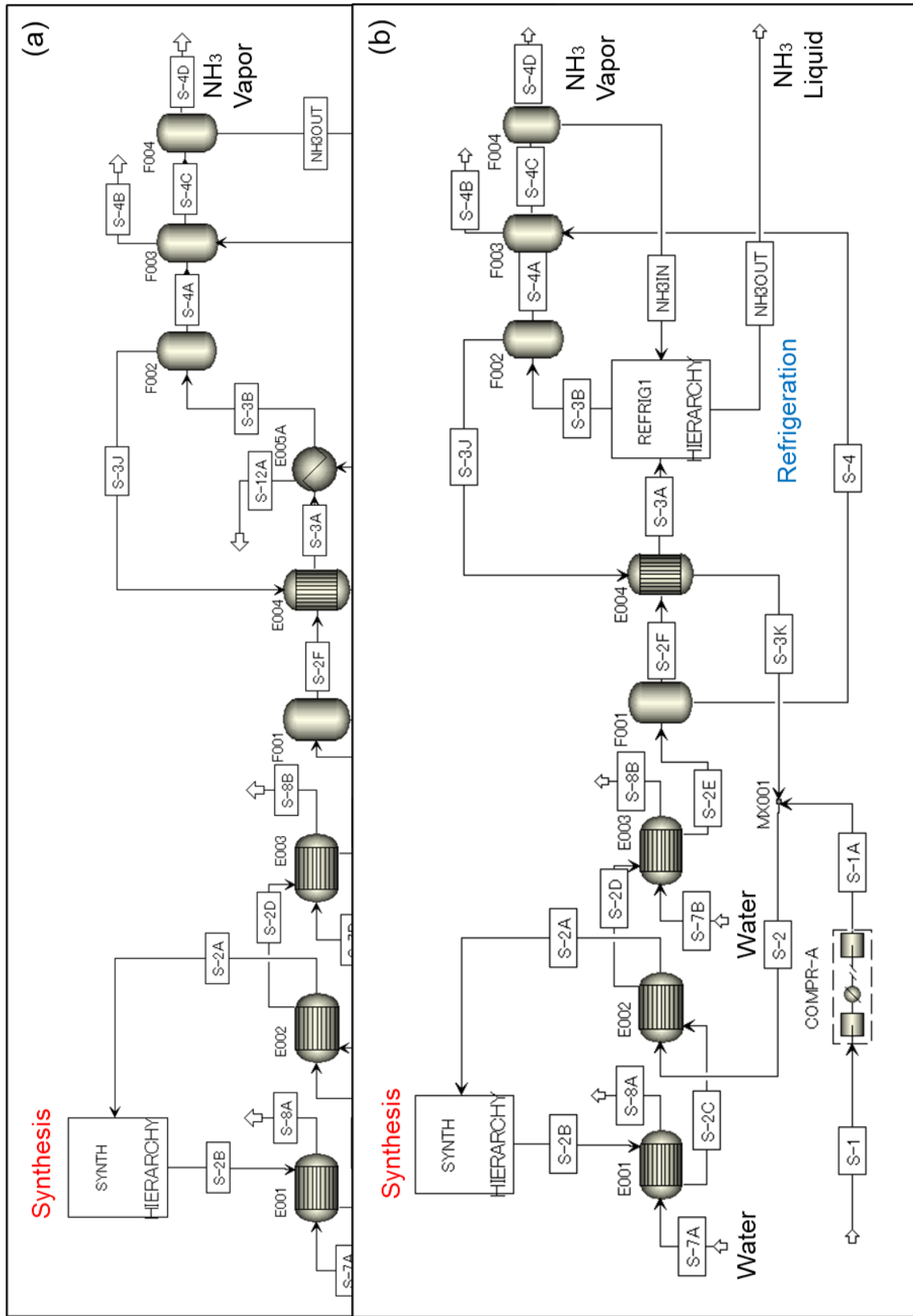
692 In this study, the loops with Fe (KM1R) and Ru/C catalysts as catalysts for ammonia synthesis were  
 693 simulated, respectively [52, 53]. The reaction conditions depend on the different catalysts. For the Fe  
 694 catalyst, two types of simulations were performed at reactor temperatures of 400–490°C, 300 bar and

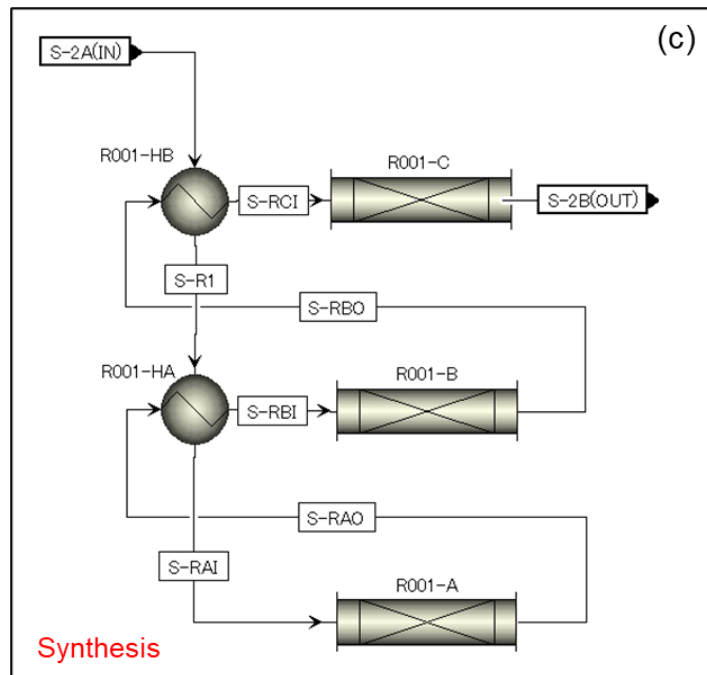
695 150 bar. On the other hand, the Ru/C catalyst was simulated at 370-460°C in the reactor at 100 bar  
696 and 50 bar [52, 53].

697 Differences in pressure affect the process because the cooling temperature required for ammonia  
698 separation is dependent on the loop pressure. The Fe-300bar process (Fig. A.1.a) differs from the other  
699 processes in the refrigeration part, where the Fe-300bar process involves only liquid nitrogen cooling  
700 for ammonia separation. Figure A.1.d shows the details of the “REFRIG1” block in the main flowsheet  
701 of the other processes (Fig. A.1.b). In the “REFRIG1” block, the ammonia gas in the synthesis loop is  
702 liquefied by evaporation of liquid nitrogen, liquid oxygen, and pressure-released NH<sub>3</sub> product.

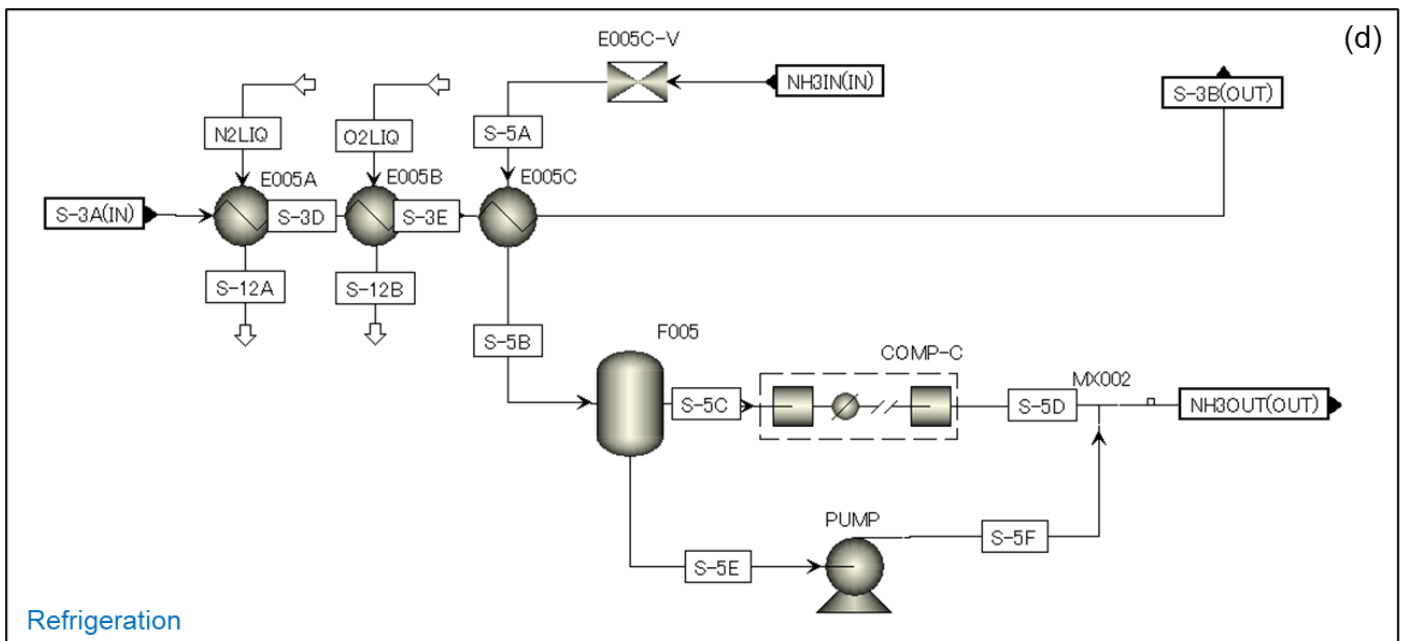
703 Table A.1 shows the summary of the stream results in a simulation of a 100 tonne/day plant for Fe  
704 and Ru/C. Also, Table A.2 provides a summary of the results for the blocks (equipment) for all types  
705 of loops at the scale of 100 tonne/day. In this study, the plant scale, i.e., the flow rate of the product  
706 ammonia, was varied from 0.1 tonne/day to 1000 tonne/day. In the Aspen Plus<sup>®</sup> simulations, extensive  
707 variables such as streamflow rate, reactor volume, heat exchanger area, and compressor rated power  
708 varied equally as the plant scale changed. For example, when the product ammonia flow rate increased  
709 by a factor of 10, these extensive variables also increased by a factor of 10. On the other hand, intensive  
710 variables such as temperature, pressure and molar ratio remained constant as the plant scale changed.

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714 Fig. A.1. (a) Overall layout of the ammonia synthesis loop simulation in Fe-300bar. (b) Overall layout  
715 of the ammonia synthesis plant simulation in Fe-150bar, Ru/C-100bar, Ru/C-75bar and Ru/C-50bar.  
716 (c) Flowsheet of the ammonia synthesis process, the details of the “SYNTH” block in the main  
717 flowsheet A.1.b. (d) Flowsheet of the ammonia refrigeration process for separation of the product NH<sub>3</sub>,  
718 the details of the “REFRIG1” block in the main flowsheet A.1.b.  
719

720 Table A.1. Summary of the stream results in the simulation at the scale of 100 tonne/day  
 721 ammonia production.

Fe-300bar								
Process	Stream ID	Phase	Temperature °C	Pressure bar	Molar flow rate 10 <sup>5</sup> mol/hr	H <sub>2</sub>	N <sub>2</sub>	NH <sub>3</sub>
						mole fraction		
Main Flowsheet	<b>NH3OUT</b>	<b>L</b>	<b>30.3</b>	<b>20</b>	<b>2.447</b>	<b>0.001</b>	<b>0.000</b>	<b>0.999</b>
	<b>S-1</b>	<b>V</b>	<b>33.0</b>	<b>1</b>	<b>5.033</b>	<b>0.750</b>	<b>0.250</b>	<b>0.000</b>
	S-1A	V	30.0	300	5.033	0.750	0.250	0.000
	S-2	V	26.4	300	16.896	0.734	0.236	0.030
	S-2A	V	223.0	300	16.896	0.734	0.236	0.030
	S-2B	V	487.4	300	14.408	0.602	0.190	0.208
	S-2C	V	300.0	300	14.408	0.602	0.190	0.208
	S-2D	V	92.3	300	14.408	0.602	0.190	0.208
	S-2E	L+V	30.0	300	14.408	0.602	0.190	0.208
	S-2F	V	30.0	300	12.257	0.704	0.223	0.073
	S-3A	L+V	23.6	300	12.257	0.704	0.223	0.073
	S-3B	L+V	11.5	300	12.257	0.704	0.223	0.073
	S-3J	V	11.5	300	11.863	0.727	0.230	0.043
	S-3K	V	25.0	300	11.863	0.727	0.230	0.043
	S-4	L	30.0	300	2.151	0.017	0.006	0.976
	S-4A	L	11.5	300	0.394	0.012	0.004	0.984
	S-4B	V	30.5	30	0.092	0.423	0.146	0.431
	S-4C	L	30.5	30	2.453	0.001	0.001	0.998
	S-4D	V	30.3	20	0.007	0.276	0.107	0.617
	N2LIQ	L	-196.0	1	1.258	0.000	1.000	0.000
S-12A	V	-149.6	1	1.258	0.000	1.000	0.000	
SYNTH	S-2A	V	223.0	300	16.896	0.734	0.236	0.030
	S-2B	V	487.4	300	14.408	0.602	0.190	0.208
	S-R1	V	310.8	300	16.896	0.734	0.236	0.030
	S-RAI	V	400.0	300	16.896	0.734	0.236	0.030
	S-RAO	V	490.0	300	16.042	0.693	0.222	0.085
	S-RBI	V	400.0	300	16.042	0.693	0.222	0.085
	S-RBO	V	489.9	300	15.206	0.649	0.207	0.145
	S-RCI	V	400.0	300	15.206	0.649	0.207	0.145

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Fe-150bar								
Process	Stream ID	Phase	Temperature °C	Pressure bar	Molar flow rate 10 <sup>5</sup> mol/hr	H <sub>2</sub>	N <sub>2</sub>	NH <sub>3</sub>
						mole fraction		
Main Flowsheet	<b>NH3IN</b>	<b>L</b>	<b>16.3</b>	<b>20</b>	<b>2.499</b>	<b>0.001</b>	<b>0.000</b>	<b>0.999</b>
	<b>NH3OUT</b>	<b>L+V</b>	<b>4.8</b>	<b>20</b>	<b>2.499</b>	<b>0.001</b>	<b>0.000</b>	<b>0.999</b>
	<b>S-1</b>	<b>V</b>	<b>33.0</b>	<b>1</b>	<b>5.033</b>	<b>0.750</b>	<b>0.250</b>	<b>0.000</b>
	S-1A	V	30.0	150	5.033	0.750	0.250	0.000
	S-2	V	26.2	150	20.501	0.739	0.231	0.030
	S-2A	V	223.0	150	20.501	0.739	0.231	0.030
	S-2B	V	439.6	150	17.998	0.633	0.194	0.174
	S-2C	V	300.0	150	17.998	0.633	0.194	0.174
	S-2D	V	91.5	150	17.998	0.633	0.194	0.174
	S-2E	L+V	30.0	150	17.998	0.633	0.194	0.174
	S-2F	V	30.0	150	16.747	0.679	0.208	0.113
	S-3A	L+V	21.1	150	16.747	0.679	0.208	0.113
	S-3B	L+V	-2.7	150	16.747	0.679	0.208	0.113
	S-3J	V	-2.7	150	15.468	0.735	0.225	0.040
	S-3K	V	25.0	150	15.468	0.735	0.225	0.040
	S-4	L	30.0	150	1.252	0.010	0.003	0.987
	S-4A	L	-2.7	150	1.279	0.005	0.002	0.993
	S-4B	V	16.2	30	0.028	0.533	0.187	0.280
	S-4C	L	16.2	30	2.503	0.001	0.001	0.998
S-4D	V	16.3	20	0.003	0.426	0.166	0.408	

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725

Fe-150bar								
Process	Stream ID	Phase	Temperature °C	Pressure bar	Molar flow rate 10 <sup>5</sup> mol/hr	H <sub>2</sub>	N <sub>2</sub>	NH <sub>3</sub>
						mole fraction		
SYNTH	S-2A	V	223.0	150	20.501	0.739	0.231	0.030
	S-2B	V	439.6	150	17.998	0.633	0.194	0.174
	S-R1	V	311.0	150	20.501	0.739	0.231	0.030
	S-RAI	V	400.0	150	20.502	0.739	0.231	0.030
	S-RAO	V	490.0	150	19.461	0.698	0.217	0.085
	S-RBI	V	400.0	150	19.461	0.698	0.217	0.085
	S-RBO	V	490.0	150	18.440	0.654	0.201	0.145
	S-RCI	V	400.0	150	18.440	0.654	0.201	0.145
REFRIG1	NH3IN	L	16.3	20	2.499	0.001	0.000	0.999
	NH3OUT	L+V	4.8	20	2.499	0.001	0.000	0.999
	N2LIQ	L	-196.0	1	1.258	0.000	1.000	0.000
	O2LIQ	L	-196.0	1	0.339	0.000	0.000	0.000
	S-12A	V	8.7	1	1.258	0.000	1.000	0.000
	S-12B	V	4.9	1	0.339	0.000	0.000	0.000
	S-3A	L+V	21.1	150	16.746	0.679	0.208	0.113
	S-3B	L+V	-2.7	150	16.747	0.679	0.208	0.113
	S-3D	L+V	9.7	150	16.746	0.679	0.208	0.113
	S-3E	L+V	5.9	150	16.746	0.679	0.208	0.113
	S-5A	L+V	-3.1	4	2.499	0.001	0.000	0.999
	S-5B	L+V	-2.8	4	2.499	0.001	0.000	0.999
	S-5C	V	-2.8	4	0.616	0.003	0.001	0.996
	S-5D	L+V	25.0	20	0.616	0.003	0.001	0.996
	S-5E	L	-2.8	4	1.883	0.000	0.000	1.000
S-5F	L	-2.1	20	1.883	0.000	0.000	1.000	

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(Continued))

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Ru/C-100bar								
Process	Stream		Temperature	Pressure	Molar flow rate	H <sub>2</sub>	N <sub>2</sub>	NH <sub>3</sub>
	ID	Phase	°C	bar	10 <sup>5</sup> mol/hr	mole fraction		
Main Flowsheet	<b>NH3IN</b>	<b>L</b>	<b>-1.7</b>	<b>20</b>	<b>2.513</b>	<b>0.001</b>	<b>0.000</b>	<b>0.999</b>
	<b>NH3OUT</b>	<b>L</b>	<b>9.9</b>	<b>20</b>	<b>2.513</b>	<b>0.001</b>	<b>0.000</b>	<b>0.999</b>
	<b>S-1</b>	<b>V</b>	<b>33.0</b>	<b>1</b>	<b>5.033</b>	<b>0.750</b>	<b>0.250</b>	<b>0.000</b>
	S-1A	V	30.0	100	5.033	0.750	0.250	0.000
	S-2	V	26.2	100	20.803	0.727	0.243	0.030
	S-2A	V	193.0	100	20.803	0.727	0.243	0.030
	S-2B	V	405.9	100	18.293	0.620	0.208	0.172
	S-2C	V	300.0	100	18.293	0.620	0.208	0.172
	S-2D	V	122.8	100	18.293	0.620	0.208	0.172
	S-2E	L+V	30.0	100	18.293	0.620	0.208	0.172
	S-2F	V	30.0	100	17.887	0.634	0.213	0.153
	S-3A	L+V	21.8	100	17.887	0.634	0.213	0.153
	S-3B	L+V	-10.5	100	17.887	0.634	0.213	0.153
	S-3J	V	-10.5	100	15.770	0.719	0.241	0.040
	S-3K	V	25.0	100	15.770	0.719	0.241	0.040
	S-4	L	30.0	100	0.407	0.006	0.003	0.991
	S-4A	L	-10.5	100	2.117	0.003	0.001	0.996
	S-4B	V	-1.9	30	0.010	0.610	0.239	0.150
	S-4C	L	-1.9	30	2.515	0.001	0.000	0.999
S-4D	V	-1.7	20	0.002	0.543	0.237	0.220	

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(Continued)

729



Ru/C-100bar								
Process	Stream ID	Phase	Temperature °C	Pressure bar	Molar flow rate 10 <sup>5</sup> mol/hr	H <sub>2</sub>	N <sub>2</sub>	NH <sub>3</sub>
						mole fraction		
SYNTH	S-2A	V	193.0	100	20.803	0.727	0.243	0.030
	S-2B	V	405.9	100	18.293	0.620	0.208	0.172
	S-R1	V	280.7	100	20.803	0.727	0.243	0.030
	S-RAI	V	370.0	100	20.805	0.727	0.243	0.030
	S-RAO	V	460.0	100	19.743	0.685	0.229	0.086
	S-RBI	V	370.0	100	19.743	0.685	0.229	0.086
	S-RBO	V	460.0	100	18.703	0.640	0.214	0.146
	S-RCI	V	370.0	100	18.703	0.640	0.214	0.146
REFRIG1	NH3IN	L	-1.7	20	2.513	0.001	0.000	0.999
	NH3OUT	L	9.9	20	2.513	0.001	0.000	0.999
	N2LIQ	L	-196.0	1	1.258	0.000	1.000	0.000
	O2LIQ	L	-196.0	1	0.338	0.000	0.000	0.000
	S-12A	V	12.5	1	1.258	0.000	1.000	0.000
	S-12B	V	9.7	1	0.338	0.000	0.000	0.000
	S-3A	L+V	21.8	100	17.888	0.634	0.213	0.153
	S-3B	L+V	-10.5	100	17.888	0.634	0.213	0.153
	S-3D	L+V	13.5	100	17.888	0.634	0.213	0.153
	S-3E	L+V	10.7	100	17.888	0.634	0.213	0.153
	S-5A	L+V	-11.0	3	2.513	0.001	0.000	0.999
	S-5B	L+V	-10.4	3	2.513	0.001	0.000	0.999
	S-5C	V	-10.4	3	1.390	0.001	0.001	0.998
	S-5D	L+V	25.0	20	1.390	0.001	0.001	0.998
	S-5E	L	-10.4	3	1.123	0.000	0.000	1.000
S-5F	L	-9.7	20	1.123	0.000	0.000	1.000	

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(Continued)

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732

Ru/C-100bar								
Process	Stream		Temperature	Pressure	Molar flow rate	H <sub>2</sub>	N <sub>2</sub>	NH <sub>3</sub>
	ID	Phase	°C	bar	10 <sup>5</sup> mol/hr	mole fraction		
SYNTH	S-2A	V	193.0	100	20.803	0.727	0.243	0.030
	S-2B	V	405.9	100	18.293	0.620	0.208	0.172
	S-R1	V	280.7	100	20.803	0.727	0.243	0.030
	S-RAI	V	370.0	100	20.805	0.727	0.243	0.030
	S-RAO	V	460.0	100	19.743	0.685	0.229	0.086
	S-RBI	V	370.0	100	19.743	0.685	0.229	0.086
	S-RBO	V	460.0	100	18.703	0.640	0.214	0.146
	S-RCI	V	370.0	100	18.703	0.640	0.214	0.146
REFRIG1	NH3IN	L	-1.7	20	2.513	0.001	0.000	0.999
	NH3OUT	L	9.9	20	2.513	0.001	0.000	0.999
	N2LIQ	L	-196.0	1	1.258	0.000	1.000	0.000
	O2LIQ	L	-196.0	1	0.338	0.000	0.000	0.000
	S-12A	V	12.5	1	1.258	0.000	1.000	0.000
	S-12B	V	9.7	1	0.338	0.000	0.000	0.000
	S-3A	L+V	21.8	100	17.888	0.634	0.213	0.153
	S-3B	L+V	-10.5	100	17.888	0.634	0.213	0.153
	S-3D	L+V	13.5	100	17.888	0.634	0.213	0.153
	S-3E	L+V	10.7	100	17.888	0.634	0.213	0.153
	S-5A	L+V	-11.0	3	2.513	0.001	0.000	0.999
	S-5B	L+V	-10.4	3	2.513	0.001	0.000	0.999
	S-5C	V	-10.4	3	1.390	0.001	0.001	0.998
	S-5D	L+V	25.0	20	1.390	0.001	0.001	0.998
	S-5E	L	-10.4	3	1.123	0.000	0.000	1.000
S-5F	L	-9.7	20	1.123	0.000	0.000	1.000	

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Ru/C-75bar								
Process	Stream		Temperature	Pressure	Molar flow rate	H <sub>2</sub>	N <sub>2</sub>	NH <sub>3</sub>
	ID	Phase	°C	bar	10 <sup>5</sup> mol/hr	mole fraction		
Main Flowsheet	<b>NH3IN</b>	<b>L</b>	<b>-15.9</b>	<b>20</b>	<b>2.515</b>	<b>0.000</b>	<b>0.000</b>	<b>0.999</b>
	<b>NH3OUT</b>	<b>L</b>	<b>14.0</b>	<b>20</b>	<b>2.515</b>	<b>0.000</b>	<b>0.000</b>	<b>0.999</b>
	<b>S-1</b>	<b>V</b>	<b>33.0</b>	<b>1</b>	<b>5.033</b>	<b>0.750</b>	<b>0.250</b>	<b>0.000</b>
	S-1A	V	30.0	75	5.033	0.750	0.250	0.000
	S-2	V	26.0	75	24.975	0.719	0.251	0.030
	S-2A	V	228.0	75	24.975	0.719	0.251	0.030
	S-2B	V	405.1	75	22.462	0.631	0.223	0.145
	S-2C	V	300.0	75	22.462	0.631	0.223	0.145
	S-2D	V	87.2	75	22.462	0.631	0.223	0.145
	S-2E	L+V	30.0	75	22.462	0.631	0.223	0.145
	S-2F	V	30.0	75	22.462	0.631	0.223	0.145
	S-3A	L+V	13.6	75	22.462	0.631	0.223	0.145
	S-3B	L+V	-17.5	75	22.462	0.631	0.223	0.145
	S-3J	V	-17.5	75	19.942	0.711	0.251	0.038
	S-3K	V	25.0	75	19.942	0.711	0.251	0.038
	S-4	L	na	75	0.000	na	na	na
	S-4A	L	-17.5	75	2.520	0.002	0.001	0.997
	S-4B	V	-16.2	30	0.004	0.644	0.270	0.086
	S-4C	L	-16.2	30	2.516	0.001	0.000	0.999
	S-4D	V	-15.9	20	0.001	0.595	0.279	0.126

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(Continued)

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Ru/C-75bar								
Process	Stream ID	Phase	Temperature °C	Pressure bar	Molar flow rate 10 <sup>5</sup> mol/hr	H <sub>2</sub>	N <sub>2</sub>	NH <sub>3</sub>
						mole fraction		
SYNTH	S-2A	V	228.0	75	24.975	0.719	0.251	0.030
	S-2B	V	405.1	75	22.462	0.631	0.223	0.145
	S-R1	V	280.7	75	24.975	0.719	0.251	0.030
	S-RAI	V	370.0	75	24.975	0.719	0.251	0.030
	S-RAO	V	460.0	75	23.699	0.677	0.238	0.085
	S-RBI	V	370.0	75	23.699	0.677	0.238	0.085
	S-RBO	V	423.8	75	22.947	0.650	0.229	0.121
	S-RCI	V	370.0	75	22.947	0.650	0.229	0.121
REFRIG1	NH3IN	L	-15.9	20	2.514	0.000	0.000	0.999
	NH3OUT	L	14.0	20	2.514	0.000	0.000	0.999
	N2LIQ	L	-196.0	1	1.259	0.000	1.000	0.000
	O2LIQ	L	-196.0	1	0.339	0.000	0.000	0.000
	S-12A	V	6.5	1	1.259	0.000	1.000	0.000
	S-12B	V	4.5	1	0.339	0.000	0.000	0.000
	S-3A	L+V	13.6	75	22.463	0.631	0.223	0.145
	S-3B	L+V	-17.5	75	22.462	0.631	0.223	0.145
	S-3D	L+V	7.5	75	22.463	0.631	0.223	0.145
	S-3E	L+V	5.5	75	22.463	0.631	0.223	0.145
	S-5A	L+V	-20.2	2	2.514	0.000	0.000	0.999
	S-5B	L+V	-19.2	2	2.514	0.000	0.000	0.999
	S-5C	V	-19.2	2	1.858	0.001	0.000	0.999
	S-5D	L+V	25.0	20	1.858	0.001	0.000	0.999
	S-5E	L	-19.2	2	0.656	0.000	0.000	1.000
S-5F	L	-18.5	20	0.656	0.000	0.000	1.000	

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(Continued)

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740

Ru/C-50bar								
Process	Stream		Temperature	Pressure	Molar flow rate	H <sub>2</sub>	N <sub>2</sub>	NH <sub>3</sub>
	ID	Phase	°C	bar	10 <sup>5</sup> mol/hr	mole fraction		
Main Flowsheet	<b>NH3IN</b>	<b>L</b>	<b>-25.1</b>	<b>20</b>	<b>2.519</b>	<b>0.000</b>	<b>0.000</b>	<b>0.999</b>
	<b>NH3OUT</b>	<b>L</b>	<b>15.4</b>	<b>20</b>	<b>2.519</b>	<b>0.000</b>	<b>0.000</b>	<b>0.999</b>
	<b>S-1</b>	<b>V</b>	<b>33.0</b>	<b>1</b>	<b>5.033</b>	<b>0.750</b>	<b>0.250</b>	<b>0.000</b>
	S-1A	V	30.0	50	5.033	0.750	0.250	0.000
	S-2	V	25.8	50	31.506	0.727	0.243	0.030
	S-2A	V	257.0	50	31.506	0.727	0.243	0.030
	S-2B	V	396.9	50	28.990	0.660	0.220	0.120
	S-2C	V	300.0	50	28.990	0.660	0.220	0.120
	S-2D	V	58.6	50	28.990	0.660	0.220	0.120
	S-2E	V	30.0	50	28.990	0.660	0.220	0.120
	S-2F	V	30.0	50	28.992	0.660	0.220	0.120
	S-3A	L+V	-0.7	50	28.992	0.660	0.220	0.120
	S-3B	L+V	-26.0	50	28.994	0.660	0.220	0.120
	S-3J	V	-26.0	50	26.473	0.723	0.241	0.036
	S-3K	V	25.0	50	26.473	0.723	0.241	0.036
	S-4	L+V	na	50	0.000	na	na	na
	S-4A	L	-26.0	50	2.522	0.001	0.000	0.999
	S-4B	V	-25.4	30	0.001	0.683	0.259	0.057
	S-4C	L	-25.4	30	2.520	0.001	0.000	0.999
	S-4D	V	-25.1	20	0.001	0.641	0.275	0.084

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(Continued)

742

Ru/C-50bar								
Process	Stream ID	Phase	Temperature °C	Pressure bar	Molar flow rate 10 <sup>5</sup> mol/hr	H <sub>2</sub>	N <sub>2</sub>	NH <sub>3</sub>
						mole fraction		
SYNTH	S-2A	V	257.0	50	31.506	0.727	0.243	0.030
	S-2B	V	396.9	50	28.990	0.660	0.220	0.120
	S-R1	V	304.1	50	31.506	0.727	0.243	0.030
	S-RAI	V	370.0	50	31.507	0.727	0.243	0.030
	S-RAO	V	436.5	50	30.313	0.697	0.233	0.071
	S-RBI	V	370.0	50	30.313	0.697	0.233	0.071
	S-RBO	V	417.9	50	29.464	0.674	0.225	0.102
	S-RCI	V	370.0	50	29.464	0.674	0.225	0.102
REFRIG1	NH3IN	L	-25.1	20	2.519	0.000	0.000	0.999
	NH3OUT	L	15.4	20	2.519	0.000	0.000	0.999
	N2LIQ	L	-196.0	1	1.258	0.000	1.000	0.000
	O2LIQ	L	-196.0	1	0.339	0.000	0.000	0.000
	S-12A	V	-6.2	1	1.258	0.000	1.000	0.000
	S-12B	V	-7.7	1	0.339	0.000	0.000	0.000
	S-3A	L+V	-0.7	50	28.993	0.660	0.220	0.120
	S-3B	L+V	-26.0	50	28.995	0.660	0.220	0.120
	S-3D	L+V	-5.2	50	28.993	0.660	0.220	0.120
	S-3E	L+V	-6.7	50	28.993	0.660	0.220	0.120
	S-5A	L+V	-27.1	2	2.519	0.000	0.000	0.999
	S-5B	L+V	-25.7	2	2.519	0.000	0.000	0.999
	S-5C	V	-25.7	2	2.014	0.000	0.000	0.999
	S-5D	L	25.0	20	2.014	0.000	0.000	0.999
	S-5E	L	-25.7	2	0.506	0.000	0.000	1.000
	S-5F	L	-25.0	20	0.506	0.000	0.000	1.000

743

744

745 Table A.2.

746 Summary of the block results in the simulation at the scale of 100 tonne/day ammonia production.

Equipment	Units	Block-ID	Fe-300bar	Fe-150bar	Ru/C-100bar	Ru/C-75bar	Ru/C-50bar
Reactor	m <sup>3</sup>	R001-A	0.139	0.609	0.825	1.200	1.784
		R001-B	0.344	1.887	1.711	1.721	2.689
		R001-C	0.673	1.721	1.418	1.849	2.578
Total volume	m <sup>3</sup>		1.155	4.217	3.954	4.770	7.050
Heat exchanger	m <sup>2</sup>	E001A	9.088	8.598	6.790	8.237	9.882
		E002	47.520	56.695	33.754	74.644	189.183
		E003A	159.276	136.520	93.852	83.999	84.090
		E004*	21.110	36.283	38.440	58.941	105.582
		E005A*	1.535	7.004	7.567	8.185	8.864
		E005B*	null	2.771	2.917	3.093	3.299
		E005C*	null	114.032	174.811	261.054	239.791
		R001-HB	16.787	20.254	20.342	24.394	30.842
R001-HC	8.347	10.030	10.088	9.072	12.835		
Total area	m <sup>2</sup>		263.664	392.187	388.561	531.620	684.368
Compressor	MW	COMPR-A	3.552	3.000	2.702	2.499	2.224
	MW	COMPR-B*	null	0.101	0.274	0.412	0.552
Pump	kW	PUMP*	null	4.253	2.652	1.624	1.254
Total rated power	MW		3.552	3.105	2.978	2.913	2.777

747 \* Blocks we defined as used for ammonia separation.

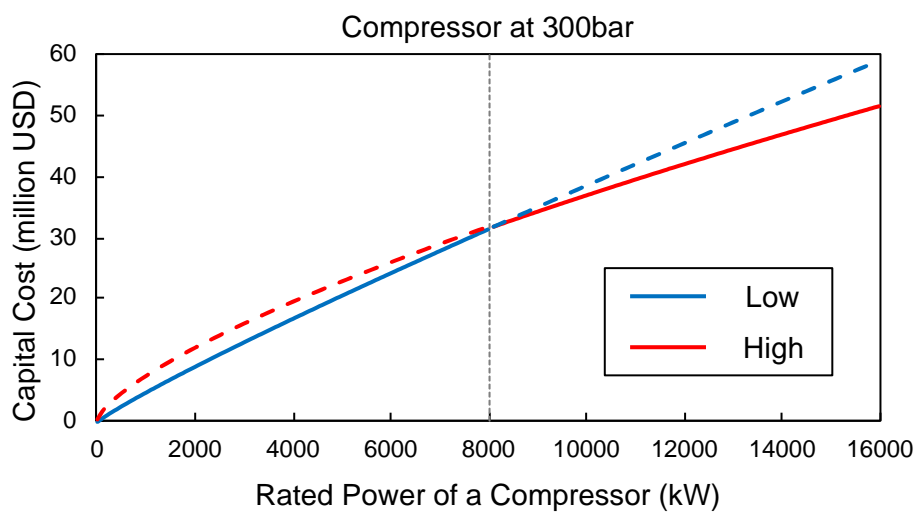
748



749 **B. Explains and results of the cost evaluation of the ammonia synthesis loop**

750 In this study, the pump, the block “PUMP” in the simulation, was excluded from the cost evaluation  
751 because the capital cost of pumps relative to the capital cost of compressors was negligible [10] and  
752 the rated power of the pump was at most 0.14 % of the total rated power in the all processes (Table  
753 A.2).

754 Two types of parameters were used to determine the capital cost of the compressor, “Low” and  
755 “High,” depending on the rated power of the compressor [10]. Since these two capital costs are  
756 intersected by approximately 8,000 kW of rated power (Fig B.1), 8,000 kW was set as the criterion  
757 for choosing between the two types of parameters.



758

759 Fig. B.1. The capital cost of a compressor by two types of parameters.

760

761 Table B.1 shows the sum of the basis of equipment, the total capital cost by equipment ty  
762 pe, the operation cost and the total cost of the ammonia synthesis loop. Tables B.2 represen  
763 ts the summary of the breakdown of the total loop cost on different scales. Table B.3 indica  
764 tes the total cost for ammonia separation, including heat exchanger, compressor, and power c  
765 onsumption for the compressor in the separation process (Table A.3).

766

767 Table B.1. Breakdown of the cost of ammonia synthesis loop at the scale of 100 tonne/day.

		Unit	Fe-300bar	Fe-150bar	Ru/C- 100bar	Ru/C- 75bar	Ru/C- 50bar
Reactor	Total volume	m <sup>3</sup>	1.155	4.217	3.954	4.770	7.050
	Total cost	million USD	1.063	1.166	0.816	0.773	0.778
Catalyst	Total weight	tonne	3.234	11.806	3.163	3.816	5.640
	Total cost	million USD	0.001	0.004	2.031	1.925	3.621
Heat exchanger	Total area		263.7	392.2	388.6	388.9	684.4
	Total cost	million USD	1.148	1.622	1.588	2.450	2.309
Compressor	Total rated power	MW	3.552	3.101	2.976	2.978	2.776
	Total cost	million USD	15.176	13.657	13.382	13.249	12.803
Power	Total rated power	MW	3.552	3.105	2.978	2.981	2.777
	Total cost	million USD	34.687	30.282	29.061	28.431	27.107
Total cost of ammonia synthesis loop		million USD	52.075	46.731	46.878	46.829	46.619

768

769

770 Table B.2. Summary of the breakdown of the total ammonia synthesis loop cost in  
 771 different scales.

Fe-300bar	Scale (tonne/day)	0.1	1	10	100	500
Reactor	million USD	0.141	0.201	0.401	1.063	2.304
Catalyst		0.000	0.000	0.000	0.001	0.006
Heat exchanger		0.155	0.186	0.343	1.148	3.283
Compressor		0.035	0.245	1.914	15.176	55.625
Power consumption		0.035	0.347	3.469	34.687	173.434
Total loop cost		0.365	0.978	6.127	52.075	234.651
Fe-150bar	Scale (tonne/day)	0.1	1	10	100	500
Reactor	million USD	0.144	0.211	0.432	1.166	2.543
Catalyst		0.000	0.000	0.000	0.004	0.021
Heat exchanger		0.159	0.204	0.435	1.622	4.770
Compressor		0.036	0.225	1.727	13.657	51.965
Power consumption		0.030	0.303	3.028	30.282	151.409
Total loop cost		0.368	0.942	5.623	46.731	210.708
Ru/C-100bar	Scale (tonne/day)	0.1	1	10	100	500
Reactor	million USD	0.134	0.179	0.327	0.816	1.735
Catalyst		0.002	0.020	0.203	2.031	10.156
Heat exchanger		0.158	0.202	0.429	1.588	4.664
Compressor		0.035	0.220	1.692	13.382	52.247
Power consumption		0.029	0.291	2.906	29.061	145.305
Total loop cost		0.359	0.913	5.556	46.878	214.107
Ru/C-75bar	Scale (tonne/day)	0.1	1	10	100	500
Reactor	million USD	0.133	0.175	0.314	0.773	1.636
Catalyst		0.002	0.024	0.245	2.450	12.250
Heat exchanger		0.161	0.215	0.494	1.925	5.722
Compressor		0.035	0.218	1.675	13.249	52.639
Power consumption		0.028	0.284	2.843	28.431	142.155
Total loop cost		0.360	0.917	5.572	46.829	214.402
Ru/C-50bar	Scale (tonne/day)	0.1	1	10	100	500
Reactor	million USD	0.133	0.175	0.315	0.778	1.647
Catalyst		0.004	0.036	0.362	3.621	18.107
Heat exchanger		0.164	0.230	0.569	2.309	6.926

Compressor	0.034	0.211	1.619	12.803	51.986
Power consumption	0.027	0.271	2.711	27.107	135.533
Total loop cost	0.362	0.924	5.576	46.619	214.199

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773

774

Table B.3. Total cost for ammonia separation in different scales.

Fe-300bar	Scale (tonne/day)	0.1	1	10	100	500
Total loop cost	million USD	0.365	0.978	6.127	52.075	234.651
Cost for separation		0.067	0.070	0.091	0.193	0.466
Ratio for separation	%	18.2	7.2	1.5	0.4	0.2
Fe-150bar	Scale (tonne/day)	0.1	1	10	100	500
Total loop cost	million USD	0.368	0.942	5.623	46.731	210.708
Cost for separation		0.077	0.112	0.364	2.278	9.523
Ratio for separation	%	20.8	11.9	6.5	4.9	4.5
Ru/C-100bar	Scale (tonne/day)	0.1	1	10	100	500
Total loop cost	million USD	0.359	0.913	5.556	46.878	214.107
Cost for separation		0.081	0.149	0.673	5.002	22.217
Ratio for separation	%	22.6	16.3	12.1	10.7	10.4
Ru/C-75bar	Scale (tonne/day)	0.1	1	10	100	500
Total loop cost	million USD	0.360	0.917	5.572	46.829	214.402
Cost for separation		0.085	0.182	0.937	7.251	32.539
Ratio for separation	%	23.8	19.8	16.8	15.5	15.2
Ru/C-50bar	Scale (tonne/day)	0.1	1	10	100	500
Total loop cost	million USD	0.362	0.924	5.576	46.619	214.199
Cost for separation		0.089	0.209	1.172	9.356	42.421
Ratio for separation	%	24.5	22.6	21.0	20.1	19.8

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