Thermal-plasma-assisted renewable hydrogen and solid carbon production from ionic liquid-based biogas upgrading: A process intensification study

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Nomenclature

[Bmim][PF$_6$]   1-butyl-3-methylimidazolium hexafluorophosphate

[Bmim][Tf$_2$N]   1-butyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide

[Bmim][DCA]   1-butyl-3-methylimidazolium dicyanamide

[Bmim][MeSO$_4$]   1-butyl-3-methylimidazolium methylsulfate

[Emim][Tf$_2$N]   1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide

[Emim][DEP]   1-ethyl-3-methylimidazolium diethylphosphate

[Emim][EtSO$_4$]   1-ethyl-3-methylimidazolium methylsulfate

[Hmim][Tf$_2$N]   1-hexyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide

[Hmim][B(CN)$_4$]   1-hexyl-3-methylimidazolium tetracyanoborate

[N$_{8,8,8,1}$][Tf$_2$N]   trioctylmethylammonium bis(trifluoromethylsulfonyl)imide

[S$_{2,2,2}$][Tf$_2$N]   triethylsulfonium bis(trifluoromethylsulfonyl)imide

Abstract

Considering the critical roles of hydrogen in energy transition and the renewable character of biogas, an integrated process linking ionic liquid (IL) based biogas upgrading and thermal plasma (TP) assisted hydrogen production is proposed and studied from the process intensification point of view. To select a practically suitable IL absorbent for biogas upgrading, an IL screening is first conducted from an experimental database exhaustively collected from the literature. Following the thermodynamic screening and the assessment of important physical properties, the retained IL is evaluated in a conceptual biogas upgrading process. The upgraded biogas, comprising high biomethane purity, is fed into a TP reactor for the production of hydrogen by decarbonisation, where solid carbon could be simultaneously obtained as a second product. The improvement of the combined process is further examined by strategies of heat and power integration. The configuration of the whole integrated process is finally presented, showing a promising scenario for energy efficient and sustainable production of hydrogen.

Keywords: hydrogen production; biogas upgrading; ionic liquid; thermal plasma; heat and power integration

1. Introduction

Due to many critical roles in renewable energy integration and decarbonisation of energy systems, hydrogen is regarded as the fundamental pillar of the energy transition from traditional energy systems to innovative and sustainable alternatives [1]. However, the current hydrogen production processes still heavily rely on non-renewable sources such as natural gas, coal gasification, and fossil fuel reforming, which unfavorably breach the sustainable and environmentally benign character of the obtained hydrogen. For truly renewable hydrogen production, several new technologies, for example, water electrolysis, biomass thermochemical conversion, biological method and photoelectrochemical method, have also been proposed and are under active development [1-5]. Among these different options, the thermal or thermocatalytic decomposition of methane (CH_4) into hydrogen (turquoise hydrogen) and carbon has attracted significant attention of researchers [3,6,7]. This process could not only be eight times less costly than water electrolysis but also simultaneously produce high value-added solid carbon that can be utilised in many applications [3]. Therefore, direct CH_4 decarbonisation is widely expected to be a promising option for hydrogen production.

To make the methane decarbonisation method more sustainable, it is highly desirable to reduce the dependency of this process on natural gas [1]. In this context, biogas can be considered as a renewable CH_4 source (always known as biomethane) as it can be abundantly obtained from the anaerobic digestion process of various wet biomass (animal waste, agricultural residues, landfills, etc.) [8]. Biogas is mainly composed of CH_4 (55% - 70%), carbon dioxide (CO_2, 30% - 45%), and traces of other gases such as hydrogen sulfide, ammonia, siloxanes, etc. Typically, after the anaerobic digestion, an initial biogas cleaning stage is employed to remove the trace impurities,

resulting in a mixture of CH_4 and CO_2. Before this mixture can be further exploited as a CH_4 source for hydrogen production, a proper biogas upgrading process should be developed to remove the unwanted CO_2 and achieve high CH_4 purity. So far, several technologies including water scrubbing, membrane separation, and amine scrubbing have been developed and commercialised for biogas upgrading [9, 10]. However, these technologies suffer from different deficiencies, such as low absorption capacity and mass transfer rate of CO_2 (water scrubbing), poor selectivity and high manufacture cost (membrane), intensive energy consumption as well as volatility, degradation and corrosion (amine scrubbing). Recently, ionic liquids (ILs) have attracted significant attention as solvents for various separations [11-16] due to unique properties such as negligible volatility, wide liquid range, easy structural tunability, etc. The carbon capture by ILs has been extensively studied [14, 17] and a few researchers have also demonstrated the great potential of ILs for the biogas upgrading process [18-20]. Nevertheless, one should note that the selection of ILs plays a decisive role in the process performance of IL-based biogas upgrading.

The second aspect in determining the sustainability of the methane decarbonisation approach is the primary energy source applied in the process [1]. Among the different possible options (biological, electrical, electrochemical, electrothermal, photochemical, etc.), thermal plasma (TP) provides many benefits for the conversion of electrical energy to chemical energy, offering a flexible, controllable and tunable heating source without direct CO_2 emissions. Moreover, it is particularly suitable for endothermic processes and cases requiring high temperatures, which are commonly met in most thermochemical processes [3]. Considering these advantages, substantial efforts have been made to explore the TP-based decomposition of hydrocarbons, including the plasma cracking of methane into hydrogen and carbon

black [21-23]. Therefore, it is worth studying the performance of TP assisted hydrogen production from upgraded biogas.

In addition to the selection of absorbent and energy source, several other process improvement techniques such as the integration of heat and power could also greatly improve the performance of the whole process, especially when streams of high temperature and pressure are involved. These strategies have been illustrated in an earlier work by using the IL [Bmim][PF$_6$] as the absorbent for biogas upgrading [24], and thus, are also worth investigating under the optimal selection of absorbent.

By considering all the essential aspects mentioned above, this work presents a process intensification study for the TP assisted renewable hydrogen and solid carbon production from IL-based biogas upgrading. An IL screening is first performed to select the best absorbent from an exhaustively collected experimental database. The selected IL is then evaluated in a biogas upgrading process, which is compared with that based on [Bmim][PF$_6$] as a reference. Finally, the biogas upgrading process is combined with a TP reactor for biomethane decarbonszation for the simultaneous production of hydrogen and solid carbon, where process integration techniques are further examined.

2. Biogas upgrading using ILs

2.1 Ionic liquids screening

It is without a doubt that the optimal screening of ILs will make a great effect on the performance of the biogas upgrading process. In literature, there are several studies on the theoretical screening or design of ILs for CO_2 capture [25-28]. However, to ensure a reliable process analysis subsequently, this work focuses on a practical IL screening for biogas upgrading from the ones that have experimental solubility data for both CO_2 and CH_4. So far, many different ILs have been experimentally studied for

CO₂ absorption whereas the solubility of CH₄ has only been measured in a relatively smaller number of ILs. Through an exhaustive search from the ILthermo database [29], only eleven ILs namely [Bmim][Tf$_2$N], [Bmim][DCA], [Bmim][MeSO$_4$], [Emim][Tf$_2$N], [Emim][DEP], [Emim][EtSO$_4$], [Hmim][Tf$_2$N], [Hmim][B(CN)$_4$], [N$_{8,8,8,1}$][Tf$_2$N], [S$_{2,2,2}$][Tf$_2$N], and [Bmim][PF$_6$] meet this criteria (see the full names of ILs in the Nomenclature). As the experimental gas solubilities in ILs were reported under different temperature and pressure conditions, the molality-based Henry's law constant (H_m) of ILs for CO$_2$ and CH$_4$ are derived as Eq. 1, and then used to evaluate the absorption capacity (C) and selectivity (S) of these ILs for the CO$_2$/CH$_4$ separation as Eqs. 2 - 3.

$$H_m(T) = \lim_{m \to 0} \frac{p}{m} \tag{1}$$

$$C(T) = 1/H_m^{CO2}(T) \tag{2}$$

$$S(T) = H_m^{CH4}(T)/H_m^{CO2}(T) \tag{3}$$

where m stands for the molality solubility (mol/kg) of gases (CO$_2$, CH$_4$) in ILs at a certain temperature (T) in K, p is the pressure in MPa; $H_m^{CO2}(T)$ and $H_m^{CH4}(T)$ are the H_m of ILs for CO$_2$ and CH$_4$ at T, respectively. According to the available experimental data (Table S1, Supporting Information), the corresponding results of C and S of the eleven ILs are listed in Table 1. It should be mentioned that due to the slight temperature differences in different experimental studies, the C and S of ILs at 293, 298, 303, and 313 K are calculated from the data within the temperature ranges of 290 - 295, 295 - 300, 300 - 305, and 310 - 315 K, respectively. As seen, [Bmim][DCA] is the optimal IL reaching a good balance between C and S, and is thermodynamically more promising than [Bmim][PF$_6$] that has been demonstrated to be a potential absorbent for the same process [20, 24]. Moreover, [Bmim][DCA] has a low viscosity of 0.0293 Pa.S at 298.15 K, which is almost one magnitude lower in comparison to [Bmim][PF$_6$] (0.246 Pa.S at

the same temperature) [29]; the toxicity of [Bmim][DCA] towards leukemia rat cell line (IPC-81) is also benign ($logEC_{50}$=3.14), comparable to that of [Bmim][PF$_6$] ($logEC_{50}$=3.10) [30]. In view of all these facts, [Bmim][DCA] is selected here as the absorbent for the biogas upgrading process.

Table 1. Comparison of *C* and *S* of ILs for CO_2/CH_4 separation derived from H_m. ("--" represents data unavailable from experimental solubility data.)

ILs	C(T)				S(T)			
	293	298	303	313	293	298	303	313
[Bmim][Tf$_2$N]	1.30	0.87	1.00	0.71	--	--	--	16.78
[Bmim][DCA]	1.11	0.91	0.94	0.74	46.97	--	39.80	31.46
[Bmim][MeSO$_4$]	0.59	--	--	0.41	27.28	--	--	--
[Emim][Tf$_2$N]	1.28	1.02	0.85	0.66	--	19.30	--	13.01
[Emim][DEP]	--	1.39	--	0.69	--	--	--	19.65
[Emim][EtSO$_4$]	--	--	0.52	0.34	--	--	--	--
[Hmim][Tf$_2$N]	1.04	0.88	0.98	0.69	17.08	--	--	--
[Hmim][B(CN)$_4$]	1.53	1.37	--	1.12	26.51	--	--	19.96
[N$_{8,8,8,1}$][Tf$_2$N]	--	--	0.55	0.47	--	--	5.34	4.80
[S$_{2,2,2}$][Tf$_2$N]	--	--	--	0.57	--	--	--	13.68
[Bmim][PF$_6$]	0.84	0.78	0.62	0.61	--	35.50	--	--

2.2 *Process simulation of IL-based biogas upgrading*

To better evaluate the practical application performance of the selected [Bmim][DCA], process simulation is performed for a conceptual biogas upgrading process (as shown in Figure 1) by using Aspen Plus (Version 10.0). As seen, after the biogas cleaning stage following the anaerobic digestion, the biogas is first compressed to 40 bar and cooled to 30 °C before entering the absorber. In the absorber, the biogas counter-currently comes into contact with the IL absorbent, where biomethane meeting the purity requirement flows out from the top as the product stream. The CO_2-rich IL collected from the bottom is fed to a series of three flash drums for IL recovery. The

finally recovered IL is then cooled to 30 °C and pumped to increase the pressure as the

recirculated absorbent stream together with a certain amount of solvent makeup.
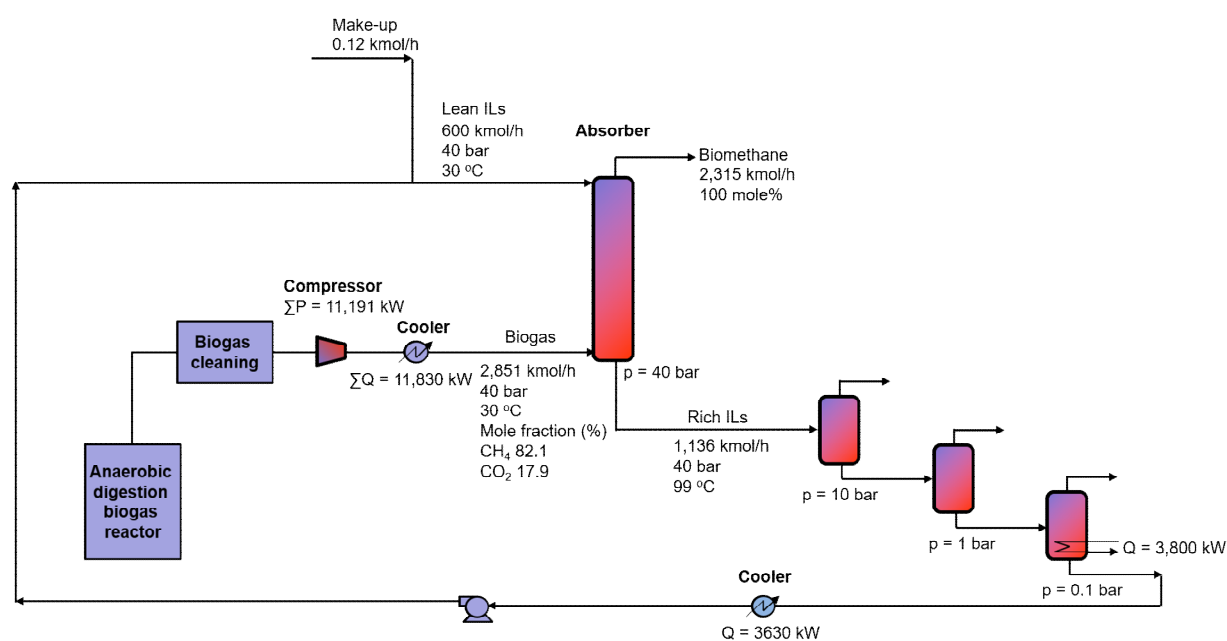
Figure 1. Conceptual flowsheet of the ionic liquid (IL)-based biogas upgrading process.

For the process simulation of [Bmim][DCA] based process, the IL is defined as

pseudo-component by specifying its molecular weight, density, normal boiling point,

critical properties, etc. This component definition approach for modeling IL-involved

process has been introduced in previous studies [11, 31-33]. The detailed information

for defining [Bmim][DCA] is taken from Huang et al. [34] and given in Table S2

(Supporting Information). For describing the phase behaviors in the absorber, the Peng-

Robinson (PR) equation of state model is selected as the thermodynamic method as it

has been demonstrated to be robust and present the minimum deviation for correlating

the VLE of IL-CO_2/CH_4 systems among three base models (PR, Redlich-Kwong, and

Soave-Redlich-Kwong) [20]. Based on the experimental solubility of CO_2 and CH_4 in

[Bmim][DCA], the PR binary interaction parameters of [Bmim][DCA]-CO_2 and

[Bmim][DCA]-CH_4 are regressed by the *Regression* module in Aspen Plus. The

obtained kA_{ij} of [Bmim][DCA]–CO_2 and [Bmim][DCA]–CH_4 are -0.8406 and 0.2737,

respectively. Figure 2 compares the experimental and PR correlated gas solubilities of CO_2 and CH_4 in [Bmim][DCA], where the data points are generally located in a close range around the diagonal, indicating a good model correlation performance for the studied system.
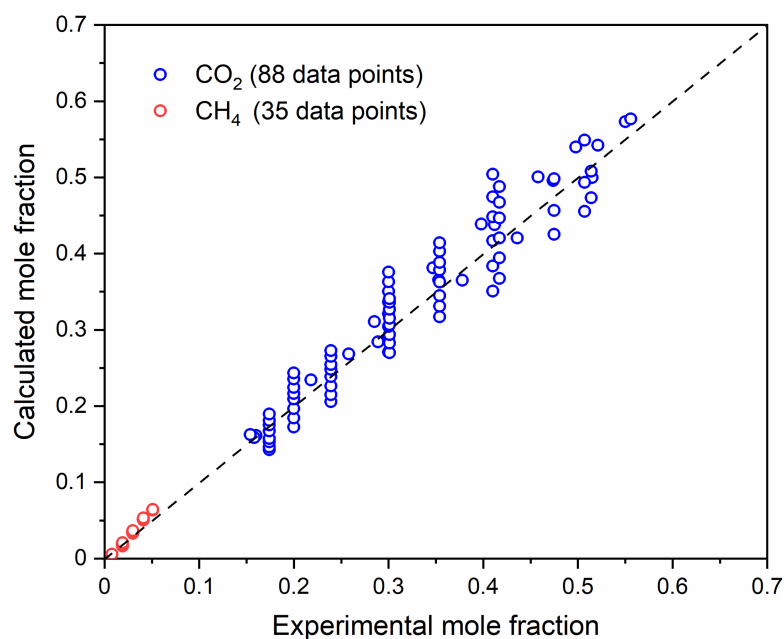

Figure 2. Comparison between experimental and PR correlated solubilities of (a) CO_2 and (b) CH_4 in [Bmim][DCA].

To make a fair comparison with earlier work [24] using [Bmim][PF_6], a model biogas of 82.1 mol% CH_4 and 17.9 mole% CO_2 is assumed as the feed gas of the absorber with a flowrate of 2,851 kmol/h; the operating pressures for the three flash drums are set as 10, 1, and 0.1 bar, respectively. It is found that with the same stages of the absorber, [Bmim][DCA] can recover 98.9% biomethane with a purity of 100 mole% when the absorbent flowrate is 600 kmol/h. In comparison, the recovery and purity of biomethane in the [Bmim][PF_6] based reference case is 96% and 99.8 mole% with an absorbent flowrate of 2,252 kmol/h, respectively. That is to say, the selected [Bmim][DCA] can achieve a higher recovery and purity of biomethane in the biogas upgrading process than [Bmim][PF_6] with only around one-quarter of the IL usage.

Regarding the IL recovery, a load of 3,800 kW was applied in the third flash drum to completely strip the gas, which is comparable to that of 3,150 kW in the [Bmim][PF$_6$] based reference case. The relatively higher load required for [Bmim][DCA] can be ascribed to its stronger absorption capacity. The main process simulation results are also given in Figure 1. From the process performance point of view, the above comparison validates that the selected [Bmim][DCA] is a practically suitable absorbent for the biogas upgrading task.

3. Hydrogen production using thermal plasma

A thermal plasma (TP) reactor is employed for hydrogen production from the upgraded biomethane (see Figure 3 for the conceptual flowsheet for this process). As seen, the upgraded biomethane is first heated to 600 °C before being fed into the TP reactor with two reaction zones. In zone 2, the biogas is thermally decomposed into hydrogen and solid carbon, and the outlet from zone 2 is fed into a heat exchanger to preheat the feed and then enters a separator to separate solid carbon and hydrogen. Solid carbon is collected from the bottom of the separator as a potential commercial product while a fraction of hydrogen is recycled to zone 1 to produce hydrogen radicals before entering zone 2. The splitting into two serial reaction zones is designed to increase the chemical yield of the TP reactor [3]. For modelling the TP assisted hydrogen production, the UNIQUAC properties package was employed [35].
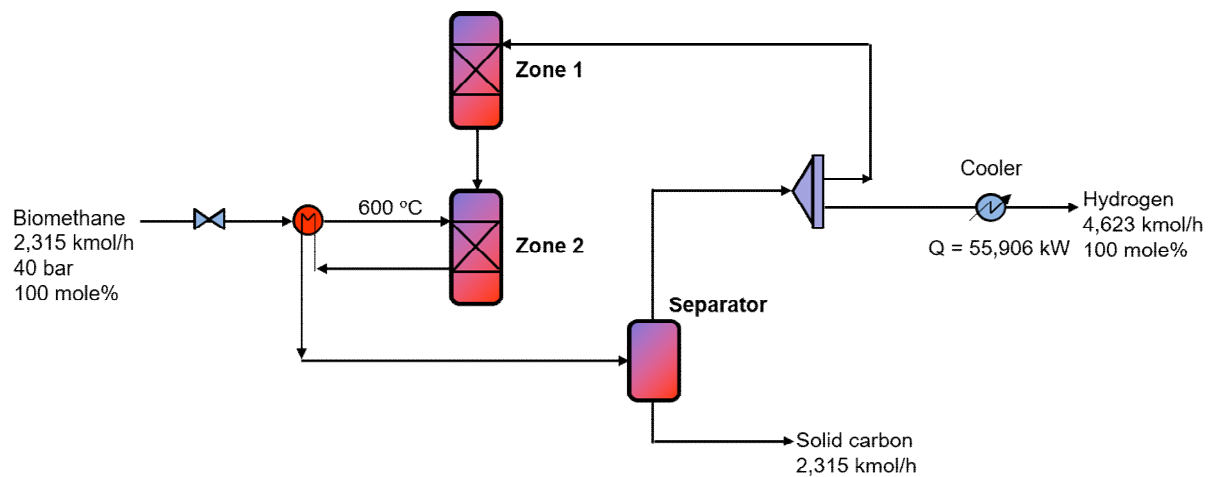
Figure 3. Conceptual flowsheet of the thermal plasma (TP)-assisted production of hydrogen and solid carbon from upgraded biogas.

Based on the upgraded biogas from above, 2,315 kmol/h biomethane of 100 mol% purity is introduced as the feed gas for the TP reactor. In comparison, the feed gas is 2,252 kmol/h biomethane of 99.8 mole% purity from the [Bmim][PF$_6$] based reference process, which is resulted from the higher performance of [Bmim][DCA] in the biogas upgrading. Consequently, 2,315 kmol/h solid carbon and 4,623 kmol/h hydrogen is produced by the TP-assisted process, which are also higher than 2,250 kmol/h and 4,502 kmol/h in the earlier [Bmim][PF$_6$]-based work.

4. Process improvement

To decrease the external energy demand, heat and power integration strategies could be applied in the integrated process, for instance, to increase the heat exchange simultaneously among process streams and to generate power from streams having high temperature and pressure.

First, as extra heat is available in the hydrogen product stream out of the Separator (Figure 3), it can be utilised for heating the third flash drum in the biogas upgrading part. Thus, a heat exchanger is used for heat integration between the hot stream of

hydrogen product and the cold stream of liquid in the third flash drum. The result shows that it is possible to save 3,800 kW power of this unit, which corresponds to 100% saving in terms of the flash drum duty.

Second, it is also possible to utilise heat from the condenser in the compression unit and the remaining heat from the outlet of the TP reactor to generate power. In particular, the hydrogen product stream can be used as a heat source to generate stream, which can then be used to drive the turbine to produce 4,284 kW power (Figure 4). The same approach can be adopted to utilise the heat from the cooler in the compression unit, which can generate 350 kW power. The generated power can be used to drive the compressors in the compression unit.
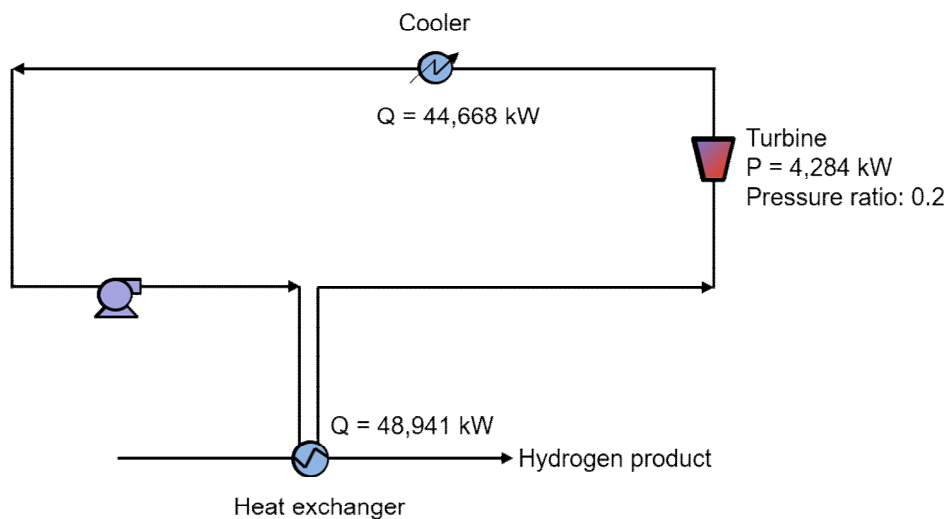
Figure 4. Conceptual flowsheet of the power generation system.

Third, considering the top stream of the absorber is working at high pressure, a turbine can be potentially used to drive a power generator. The force of the purified biomethane on the blades rotates the rotor shaft of the power generator. In turn, the generator converts the mechanical energy of the rotor into electrical energy. As a result, the use of turbine can generate 2,541 kW electricity. In this sense, 22.7% of the total compression power is saved for compressing the inlet biogas of the absorber.

By applying the above process intensification strategies, the configuration of the whole integrated process is shown in Figure 5. Total electricity energy that can be generated by utilising the high pressure of the absorber top stream, the heat from the condenser in the compression unit, and the remaining heat from the outlet of the TP reactor is 7,175 kW. These strategies afford a 64.1% saving in the power consumption in the compression unit. Notably, the saving in the heat duty of the third flash drum is 100%.
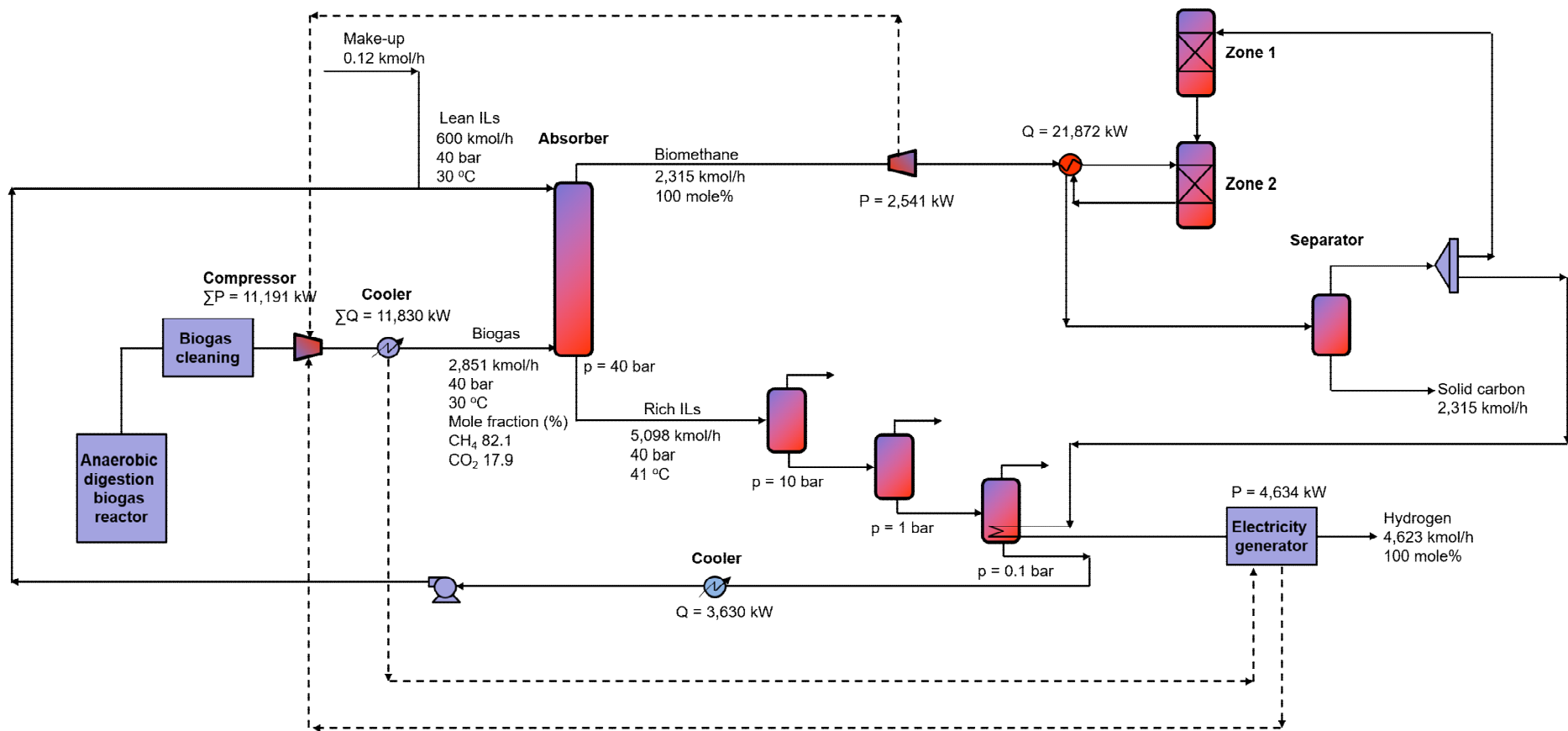
Figure 4. Configuration of the whole integrated process including ionic liquid (IL)-based biogas upgrading and thermal plasma (TP) assisted hydrogen production.

4. Conclusions

Motivated by the production of sustainable hydrogen, the IL-based biogas upgrading and TP assisted biomethane decarbonisation is linked as an integrated process, where the process intensification is realised by the selection of suitable IL absorbent, the application of TP reaction, and the heat and power integration. Based on an experimental database of CO_2 and CH_4 solubilities in eleven ILs, [Bmim][DCA] is selected as it reaches the best trade-off between CO_2 absorption capacity and selectivity, and outperforms the reference IL absorbent [Bmim][PF$_6$]. Combining with its low viscosity and toxicity, [Bmim][DCA] is subsequently evaluated in a conceptual biogas upgrading process, showing an excellent performance in terms of biomethane recovery and purity. Thanks to this merit, a larger amount of hydrogen and the second product of solid carbon can be obtained by the TP assisted decarbonisation. The implementation of heat and power integration effectively leads to 64.1% and 100% energy savings in the compression unit and the third flash drum, respectively. The whole integrated process demonstrates a promising combination of the efficient utilisation of biogas upgrading and the sustainable production of high value-added hydrogen and solid carbon.

References

1. Acar C, Dincer I. Review and evaluation of hydrogen production options for better environment. Journal of Cleaner Production, 2019, 218: 835-849.

2. Chi J, Yu H. Water electrolysis based on renewable energy for hydrogen production. Chinese Journal of Catalysis, 2018, 39(3): 390-394.

3. Gautier, M., Rohani, V., Fulcheri, L. Direct decarbonization of methane by thermal plasma for the production of hydrogen and high value-added carbon black. *International Journal of Hydrogen Energy*, 2017, *42*(47), 28140-28156.

4. Arregi A, Amutio M, Lopez G, et al. Evaluation of thermochemical routes for hydrogen production from biomass: A review. Energy conversion and management, 2018, 165: 696-719.

5. Ahmed M, Dincer I. A review on photoelectrochemical hydrogen production systems: challenges and future directions. International Journal of Hydrogen Energy, 2019, 44(5): 2474-2507.

6. Zhang J, Li X, Chen H, et al. Hydrogen production by catalytic methane decomposition: carbon materials as catalysts or catalyst supports. International Journal of Hydrogen Energy, 2017, 42(31): 19755-19775.

7. Dvoynikov M, Buslaev G, Kunshin A, et al. New concepts of hydrogen production and storage in arctic region. Resources, 2021, 10(1): 3.

8. Angelidaki I, Treu L, Tsapekos P, et al. Biogas upgrading and utilization: Current status and perspectives. Biotechnology Advances, 2018, 36(2): 452-466.

9. Lombardi L, Francini G. Techno-economic and environmental assessment of the main biogas upgrading technologies. Renewable Energy, 2020, 156: 440-458.

10. Baena-Moreno F M, le Saché E, Pastor-Pérez L, et al. Membrane-based technologies for biogas upgrading: a review. Environmental Chemistry Letters,

2020: 1-10.

11. Bedia J, Ruiz E, Riva J D, et al. Optimized Ionic Liquids for Toluene Absorption. Aiche Journal, 2013, 59(5):1648-1656.

12. Song Z, Zhou T, Zhang J, et al. Screening of ionic liquids for solvent-sensitive extraction–with deep desulfurization as an example. Chemical Engineering Science, 2015, 129: 69-77.

13. Liu X, Huang Y, Zhao Y, et al. Ionic liquid design and process simulation for decarbonization of shale gas. Industrial & Engineering Chemistry Research, 2016, 55(20): 5931-5944.

14. Zeng S, Zhang X, Bai L, et al. Ionic-liquid-based CO2 capture systems: structure, interaction and process. Chemical reviews, 2017, 117(14): 9625-9673.

15. Yu G, Dai C, Gao H, et al. Capturing condensable gases with ionic liquids. Industrial & Engineering Chemistry Research, 2018, 57(36): 12202-12214.

16. Xu R, Dai C, Mu M, et al. Highly efficient capture of odorous sulfur-based VOCs by ionic liquids. Journal of Hazardous Materials, 2021, 402: 123507.

17. Zhang X, Zhang X, Dong H, et al. Carbon capture with ionic liquids: overview and progress. Energy & Environmental Science, 2012, 5(5): 6668-6681.

18. Xie Y, Ma C, Lu X, Ji, XY. Evaluation of imidazolium-based ionic liquids for biogas upgrading. Applied Energy, 2016, 175:69-81.

19. Xie Y, Björkmalm J, Ma C, et al. Techno-economic evaluation of biogas upgrading using ionic liquids in comparison with industrially used technology in Scandinavian anaerobic digestion plants. Applied Energy, 2018, 227: 742-750.

20. Haider J, Qyyum M A, Kazmi B, et al. Simulation study of biomethane liquefaction followed by biogas upgrading using an imidazolium-based cationic ionic liquid. Journal of Cleaner Production, 2019, 231: 953-962.

21. Cho W, Lee S H, Ju W S, et al. Conversion of natural gas to hydrogen and carbon black by plasma and application of plasma carbon black. Catalysis Today, 2004, 98(4): 633-638.

22. Kim S C, Lim M S, Chun Y N. Hydrogen-rich gas production from a biomass pyrolysis gas by using a plasmatron. International journal of hydrogen energy, 2013, 38(34): 14458-14466.

23. Chen H L, Lee H M, Chen S H, et al. Review of plasma catalysis on hydrocarbon reforming for hydrogen production-interaction, integration, and prospects. Applied Catalysis B: Environmental, 2008, 85(1-2): 1-9.

24. Long Nguyen V D, Kim G S, Tran N, et al. Biogas upgrading using ionic liquid [Bmim][PF6] followed by thermal-plasma-assisted renewable hydrogen and solid carbon production. International Journal of Hydrogen Energy. Submitted.

25. Chong F K, Foo D C Y, Eljack F T, et al. Ionic liquid design for enhanced carbon dioxide capture by computer-aided molecular design approach. Clean Technologies and Environmental Policy, 2015, 17(5): 1301-1312.

26. Valencia-Marquez D, Flores-Tlacuahuac A, Vasquez-Medrano R. An optimization approach for CO2 capture using ionic liquids. Journal of Cleaner Production, 2017, 168: 1652-1667.

27. Wang J, Song Z, Cheng H, et al. Computer-aided design of ionic liquids as absorbent for gas separation exemplified by CO2 capture cases. ACS Sustainable Chemistry & Engineering, 2018, 6(9): 12025-12035.

28. Wang J, Song Z, Cheng H, et al. Multilevel screening of ionic liquid absorbents for simultaneous removal of CO2 and H2S from natural gas. Separation and Purification Technology, 2020, 248: 117053.

29. Kazakov, Andrei F., et al. Ionic Liquids Database-ILThermo (v2. 0), 2013.

30. Wang Z, Song Z, Zhou T. Machine learning for ionic liquid toxicity prediction. Processes, 2021, 9(1): 65.

31. Peng D, Kleiweg A J, Winkelman J G M, et al. A hierarchical hybrid method for screening ionic liquid solvents for extractions exemplified by the extractive desulfurization process. ACS Sustainable Chemistry & Engineering, 2021, 9(7): 2705-2716.

32. De Riva J, Ferro V R, Moreno D, et al. Aspen Plus supported conceptual design of the aromatic–aliphatic separation from low aromatic content naphtha using 4-methyl-N-butylpyridinium tetrafluoroborate ionic liquid. Fuel processing technology, 2016, 146: 29-38.

33. Song Z, Zhang C, Qi Z, et al. Computer-aided design of ionic liquids as solvents for extractive desulfurization. AIChE Journal, 2018, 64(3): 1013-1025.

34. Huang Y, Dong H, Zhang X, et al. A new fragment contribution-corresponding states method for physicochemical properties prediction of ionic liquids. AIChE Journal, 2013, 59(4): 1348-1359.

35. Sarafraz M M, Tran N N, Nguyen H, et al. Tri-fold process integration leveraging high-and low-temperature plasmas: From biomass to fertilizers with local energy and for local use. Journal of Advanced Manufacturing and Processing, 2021, 3(2): e10081.