Flexible operation of an IGCC plant coproducing power and H$_2$ with CO$_2$ capture through novel PSA-based process configurations

Luca Riboldi$^{a,*}$, Olav Bolland$^a$

$^a$Energy and Process Engineering Department, the Norwegian University of Science and Technology, NO-7491 Trondheim, Norway

**Abstract**

The coproduction of power and H$_2$ in an integrated gasification combined cycle (IGCC) plant with CO$_2$ capture demonstrated to entail interesting potentials in terms of flexible operations. The possibility to shift between the two energy products allows operating the plant in a load-following mode, where the reduction in net power output is counterbalanced by an increased H$_2$ throughput. Within this framework, pressure swing adsorption (PSA) as gas separation technology showed to offer advantages in comparison to the common process layout involving an absorption process for capturing CO$_2$. Two novel PSA-based process configurations are presented in this sense (i.e. Two-train PSA and One-train PSA) and their performance reported. The objective of this paper is to investigate the degree of flexibility achievable by the two novel process configurations. Some limitations arose in the capability of the One-train PSA process configuration to meet the ultrapure H$_2$ specifications (99.999% vol. purity) in the different cases tested. The flexibility can be realized if more relaxed purity specifications apply. Process simulations of the Two-train PSA process configuration demonstrated the plant capability to significantly reduce its load (about 31% reduction), while processing a constant coal feed. At the different plant loads tested, the H$_2$ specifications were met and the plant efficiency was only slightly decreasing, thus the flexibility was realized. The simulation of similar loads reduction in a reference IGCC plant for power generation with CO$_2$ capture, showed a more significant decrease in efficiency, confirming the effectiveness of the novel process configuration proposed.

© 2017 The Authors. Published by Elsevier Ltd. This is an open access article under the CC BY-NC-ND license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

Peer-review under responsibility of the organizing committee of GHGT-13.

**Keywords:** Integrated gasification combined cycle; CO$_2$ capture; power and hydrogen; pressure swing adsorption; flexibility.

* Corresponding author. Tel.: +47-73593559.

_E-mail address:_ luca.riboldi@ntnu.no

13th International Conference on Greenhouse Gas Control Technologies, GHGT-13, 14-18 November 2016, Lausanne, Switzerland
1. Introduction

Global warming mitigation has been widely accepted as one of the major challenges of our time, implying the necessity of a strong and immediate commitment [1]. The energy sector is responsible for a large fraction of anthropogenic greenhouse gas emissions and needs to be at the forefront of this commitment. In order to reduce the carbon footprint of the energy system, two strategies are a massive deployment of renewable energy sources and the utilization of carbon capture and storage (CCS). The progressive penetration of intermittent renewable energy sources is substantially changing the energy system. Fossil fuel based power plants are more and more often requested to operate in a load-following mode, while they are expected to capture a large fraction of the CO\textsubscript{2} formed [2,3]. These requirements introduce significant challenges to efficient power plants operations and their ability to adapt to this new context is extremely important to the long-term economics [4]. A possible way to deal with the issue is to differentiate the energy products and, for instance, coproduce power and H\textsubscript{2} [5]. An enhancement of flexibility is achieved when a varying power-to-hydrogen output ratio can be obtained, allowing the plant to follow to some extent the fluctuations in power demand. When the power demand is low, the H\textsubscript{2} throughput can increase, while the efficiency of the plant remains on good levels. Vice versa when there is a high power demand. An underlying assumption at the basis of this concept is that a H\textsubscript{2} market will develop in the near future [6].

This paper deal with the coproduction of power and ultrapure H\textsubscript{2} (99.99+% vol.) in an integrated gasification combined cycle (IGCC) plant with CO\textsubscript{2} capture. The common coproduction layout involves an absorption unit for removing CO\textsubscript{2} from a shifted syngas followed by a pressure swing adsorption (PSA) unit for purifying a part of the resulting H\textsubscript{2}-rich gas stream [7–9]. A previous paper presented two novel process configurations, relying solely on PSA as gas separation technology [10]. The utilization of PSA demonstrated to entail interesting process integration opportunities, which may result in increased plant efficiency. The aim of this paper is to further investigate the degree of flexibility achievable by the PSA-based process configurations. In this context, the term flexibility has been intended as the plant capability to efficiently shift between the two different energy products (i.e. electricity and H\textsubscript{2}), while processing a constant coal input. If the overall plant efficiency is not compromised at the different modes of operation, the flexibility is realized.

The paper first describes the methodology and modelling assumptions at the basis of the work. In a second section, the PSA-based process configurations of the IGCC plant are shortly presented and their performances reported. In the last part of the paper, the flexible operations of these systems are assessed. Proper PSA process designs were defined, able to handle a wide range of operating conditions and to shift easily between the two energy products. Such PSA processes were integrated into the IGCC plant in order to increase its flexibility. The obtained performances are analysed and discussed.

2. Modeling and simulation of the plant

The results presented in the paper are obtained from process simulations of the system analyzed. A composite model was developed, including a dynamic model of the PSA process and a steady-state model of the IGCC plant. The mathematical model for dynamic simulation of PSA relies on material, energy and momentum balances. The kinetic of the mass transfer process is accounted for the linear driving force (LDF) approximation, while the nonlinear multicomponent adsorption equilibrium isotherms make use of appropriate models, according to the adsorbent under consideration (whether an activated carbon or a zeolite 5A). The complete set of equations constituting the PSA process model can be found in [10], together with a more complete overview of the modelling assumptions used. The model was implemented in gPROMS (Process System Enterprise) [11].

The IGCC model is based on the set of fundamental assumptions recommended in the European Benchmarking Task Force (EBTF) [12]. The model of the IGCC plant was developed in THERMOFLEX (Thermoflow Inc.) [13]. Figure 1 shows the general flowsheet of the IGCC plant considered. It is possible to list five main sections of the plant: (i) air separation unit (ASU); (ii) gasification and syngas treatment section; (iii) CO\textsubscript{2} separation and ultrapure H\textsubscript{2} production unit; (iv) CO\textsubscript{2} compression and flash separation unit; (v) power island.
A short description of the overall system is presented, in order to outline the main processes. For a more detailed description of the IGCC plant and of the design parameters selected, reference should be made to [10]. A cryogenic ASU separates the gas components of an incoming compressed air stream. Pure O₂ is produced and fed to the gasifier. Also pure N₂ is available, which is used as fuel transport gas for coal and as dilution gas in the gas turbine. 50% of the compressed air entering the ASU is taken from the compressor of the gas turbine. A Shell-type gasifier converts the bituminous coal into syngas. The high-temperature syngas leaving the gasifier is cooled down in a convective syngas cooler and partially recirculated into the gasifier. The cooled syngas is following processed to remove particles into a wet scrubber before undergoing a shift process. A sour water-gas shift (WGS) process converts CO and H₂O into CO₂ and H₂ to a large extent. The shifted syngas, now rich in H₂ and CO₂, is further cooled down to undergo the gas cleaning processes operating at low temperature. During this cooling step, a large fraction of water present in the shifted syngas condenses and is knocked out of the syngas stream. H₂S is removed from the shifted syngas by means of an acid gas removal (AGR) unit, which involves a single stage absorption process. The sulfur-free syngas is then routed to the PSA unit for CO₂ separation and H₂ purification. The PSA unit can include one or more PSA stages. The configurations proposed are defined in the next section. The CO₂-rich gas stream leaving the PSA unit is sent to the CO₂ compression and flash separation section. The power island is responsible for syngas energy conversion into electricity. A combined cycle is adopted for the purpose, consisting of a gas turbine and a steam bottoming cycle. The gas stream fueling the gas turbine is composed by the H₂-rich gas stream leaving the PSA unit plus the additional H₂ recovered in the flash processes. A dilution with N₂ coming from the ASU is included for NOₓ formation control. The gas turbine (GT) considered is a Siemens SGT5-4000F, a large-scale “F class” gas turbine. The exhaust gas from the turbine is used to produce steam at three pressure levels by means of a heat recovery steam generator (HRSG). The steam produced by the HRSG is expanded in a steam turbine, providing an additional power output. A certain heat integration is designed within the system. Steam is extracted from the steam turbine to meet process heat requirements of the plant. At the same time, steam is produced by some processes and sent to steam turbine for expansion.
3. Performance parameters definition and gas specifications

The performance parameters used in the paper are defined in this section.

Given the two different energy products, proper indicators had to be defined in order to evaluate the energy performance of the system. The net electric efficiency ($\eta_{el}$) and the hydrogen efficiency ($\eta_{H2}$) give a first indication of the coal energy input fraction converted into electricity and H$_2$, respectively. They were defined as following:

$$\eta_{el} = \frac{\text{Net electric power output}}{\text{Coal energy input}_{LHV}}$$  \hfill (1)

$$\eta_{H2} = \frac{\text{Ultrapure H$_2$ energy}_{LHV}}{\text{Coal energy input}_{LHV}}$$  \hfill (2)

The two energy outputs of the system (i.e. electricity and ultrapure H$_2$) are not thermodynamically equal. A direct comparison of them would be misleading. In order to deal with the issue and define an overall efficiency term which allows an immediate comparison of different systems performances, the H$_2$ energy content has been weighted through proper factors. A first approach applies a factor of 0.6 beforehand the comparison with electricity. This value has been chosen referring to a previous work [14] and can be thought to represent the efficiency of a combined cycle for electricity production. Accordingly, a first cumulative energy efficiency ($\eta_{tot.60}$) was defined:

$$\eta_{tot.60} = \eta_{el} + 0.6 \cdot \eta_{H2}$$  \hfill (3)

A second approach discounts the H$_2$ energy content with a factor termed power production efficiency ($\eta_{el,prod}$):

$$\eta_{el,prod} = \frac{\text{Gross electric power output}}{\text{Syngas energy input to the gas turbine}_{LHV}}$$  \hfill (4)

This factor wants to estimate the additional amount of power that could be obtained if the ultrapure H$_2$ was sent to the power island of the IGCC plant. The underlying assumption is that the combined cycle efficiency would remain constant if all the H$_2$ was burned in the GT. This is an approximation but helps to obtain reasonable estimations. A second cumulative energy efficiency ($\eta^*_{tot}$) was then defined:

$$\eta^*_{tot} = \eta_{el} + \eta_{el,prod} \cdot \eta_{H2}$$  \hfill (5)

The effectiveness of the gas separation processes in the plant is evaluated through commonly used parameters. The CO$_2$ purity ($Y_{CO2}$) measures the volumetric concentration of the specific component into the product gas stream, likewise for the H$_2$ purity ($Y_{H2}$). The CO$_2$ recovery ($R_{CO2}$) measures the overall fraction of the formed CO$_2$ which is captured and subsequently transported for final storage. The CO$_2$ formed may originate from various form of carbon in the fuel. Similarly, the H$_2$ recovery ($R_{H2}$) is the ratio between the H$_2$ produced, either as fuel gas or as pure gas, and the total H$_2$ formed. The H$_2$ formed may originate from the gasification and shift processes.

The specifications applying to the different gas streams have been defined in accordance with recommendations from the literature [6,15]. The CO$_2$-rich gas stream is requested to have a CO$_2$ volumetric concentration above 95%. Stringent specifications commonly apply for the production of ultrapure H$_2$. In the paper, the target value for H$_2$ purity has been set to 99.99+% vol., in order to comply with PEM fuel cell requirements.
4. Novel PSA-based process configurations

The novel process configurations proposed are based on PSA as only gas separation technology. Previous studies focusing on IGCC plants coproducing power and H$_2$ with CO$_2$ capture, relied on both absorption and PSA. Absorption is known to perform better for CO$_2$ separation [16,17], while PSA is the benchmark technology for H$_2$ purification [18]. The reason for investigating these new process configurations was that the utilization of a single technology could potentially entail integration opportunities.

The first novel configuration proposed relies on two PSA trains in series (Two-train PSA). A first PSA stage process the shifted syngas in order to separate the CO$_2$. The CO$_2$-rich product gas stream is sent to the compression and further purification unit. While a fraction of the outlet H$_2$-rich product gas stream is sent to the GT as fuel, the remaining part is processed by the second PSA stage. The obtained ultrapure H$_2$ can be stored and, possibly, marketed. A by-product of the second PSA stage is a PSA tail gas stream. Given the significant content of H$_2$, this gas stream is normally compressed and combusted in the GT. Even though the additional power contribution, this process is made less attractive by the significant power consumption associated with the tail gas compression. The Two-train PSA process configuration avoids the tail gas compression by recycling the PSA tail gas stream to the first PSA.

The second process configuration proposed succeeds to carry out both CO$_2$ separation and H$_2$ purification within a single PSA train (One-train PSA). The inlet shifted syngas is processed in order to obtain three different product gas streams: (i) a CO$_2$-rich gas stream; (ii) an ultrapure H$_2$ gas stream; (iii) and a fuel-grade H$_2$-rich gas stream. The presence of a single gas separation unit instead of two has an obvious advantage in terms of volume and footprint of the equipment, which can, possibly, translates in lower capital costs. Further, this layout avoids as well the PSA tail gas compression process.

Simple block-flow diagrams of the two novel process configurations are shown in Figure 2 and Figure 3. The common process configuration is also shown in Figure 4. A more detailed insight on the characteristics of the two process configurations can be found in [10].
5. Performance of the novel PSA-based process configurations

A set of performances is reported (see Table 1), referring to different layouts of an IGCC plant coproducing power and ultrapure H₂ with CO₂ capture. As basis for comparison, also the performance of IGGC plants producing only power is reported, whether capturing CO₂ by absorption (i.e. *Only power absorption*) or by PSA (i.e. *Only power PSA*). Some results taken from the literature are additionally reported, in order to complete the picture by showing the performance of plants using absorption for CO₂ separation, either with (i.e. *Coproduction absorption & PSA*) or without (i.e. *Only power absorption 2*) H₂ coproduction. This comparative analysis gives an overview of the status for the coproduction concept and paves the ground for further considerations on flexibility. The systems analyzed comply with a defined operational framework, which includes assumptions with regard to the energy product outputs (i.e. net power output ≈ 350 MW and H₂ output LHV ≈ 100 MW) and specifications (i.e. H₂ purity 99.99+% vol.).

Table 1. Performance of power generation IGCC plants implementing CO₂ capture with or without ultrapure H₂ as secondary energy product.

<table>
<thead>
<tr>
<th>Energy products</th>
<th>Coal input MW</th>
<th>CO₂ capture technology</th>
<th>R_{CO₂}</th>
<th>Y_{H₂}</th>
<th>η_{H₂}</th>
<th>η_{el}</th>
<th>η_{el prod}</th>
<th>η_{tot}</th>
<th>η_{tot60}</th>
<th>η_{tot60}^*</th>
</tr>
</thead>
<tbody>
<tr>
<td>Only power absorption</td>
<td>Power</td>
<td>961</td>
<td>Selexol</td>
<td>90.9</td>
<td>-</td>
<td>-</td>
<td>36.8</td>
<td>-</td>
<td>36.8</td>
<td>36.8</td>
</tr>
<tr>
<td>Only power PSA</td>
<td>Power</td>
<td>971</td>
<td>PSA</td>
<td>84.6</td>
<td>-</td>
<td>-</td>
<td>36.2</td>
<td>-</td>
<td>36.2</td>
<td>36.2</td>
</tr>
<tr>
<td>Two-train PSA</td>
<td>Power &amp; H₂</td>
<td>1095</td>
<td>PSA</td>
<td>84.7</td>
<td>99.991</td>
<td>8.86</td>
<td>31.5</td>
<td>64.8</td>
<td>36.9</td>
<td>37.3</td>
</tr>
<tr>
<td>One-train PSA</td>
<td>Power &amp; H₂</td>
<td>1088</td>
<td>PSA</td>
<td>85.7</td>
<td>99.983</td>
<td>8.84</td>
<td>31.3</td>
<td>64.9</td>
<td>36.6</td>
<td>37.0</td>
</tr>
<tr>
<td>Only power absorption 2 [9]</td>
<td>Power</td>
<td>1167</td>
<td>Selexol</td>
<td>92.4</td>
<td>-</td>
<td>-</td>
<td>36.0</td>
<td>-</td>
<td>36.0</td>
<td>36.0</td>
</tr>
<tr>
<td>Coproduction abs. &amp; PSA [9]</td>
<td>Power &amp; H₂</td>
<td>1167</td>
<td>Selexol</td>
<td>92.4</td>
<td>99.950</td>
<td>8.57</td>
<td>31.1</td>
<td>-</td>
<td>36.2</td>
<td>-</td>
</tr>
</tbody>
</table>

With regard to the coproduction layout, PSA-based configurations seem to outperform the absorption-based counterpart, in accordance with the defined energy performance indicator defined (i.e. cumulative energy efficiency). The *Two-train PSA* configuration achieved the highest performance in terms of energy efficiency (36.9%) and H₂ purity (99.991%). The *One-train PSA* configuration returned a slightly lower performance (36.6% and 99.983%) but still better than the absorption-based case (36.2% and 99.950%).

6. Flexible operations of the coproduction layout

In accordance with the main objective of this paper, the maximum flexibility of the novel process configurations proposed was investigated. Within the *One-Train PSA* configuration, a high degree of flexibility in the energy products is hindered by strict purity specifications on the ultrapure H₂. Assuming that 99.99+ % vol. H₂ purity is requested, the
plant load cannot be significantly modified [10]. More relaxed constraints on H₂ purity would change the picture but have not been considered in this work. Therefore, the following analyses focuses on the Two-train PSA configuration.

In comparison to the first assessment of this process configuration [10], some modifications needed to be introduced in order to guarantee a larger margin of possible operations. Many of those modifications have the disadvantage of negatively impacting the productivity of the system. However, this is a price-to-pay in order to seek for an increased flexibility. The main parameter controlling the share between the energy products (i.e. power and ultrapure H₂) is the fraction of H₂-rich gas stream, leaving the first PSA stage, sent to the second PSA stage and not to the power island. Therefore, the possibility to process a wide range of inlet flow rates in the second PSA stage was desired. For the purpose, the column diameter in the second PSA train works was increased, with respect to the first design, from 2.8 to 4.0 meters. This gives an ampler room for maneuver to handle different operating conditions, thus the possibility to obtain a variety of H₂ throughputs and, consequently, of power outputs. On the other hand, when the inlet flow rate in the second PSA stage is low, a large fraction of the column remains unused, with a correspondent low productivity. Other modifications introduced dealt mainly with the scheduling of the cycle. The different PSA outlet gas streams have to fulfil requirements, in terms of recovery and purity. An additional degree of complexity comes from the integration between the two PSA trains, as the tail gas of the second train is the purge gas of the first train. Therefore, any changes in the operating conditions needed to be properly counterbalanced through adjustments in the PSA cycle, in order to meet the requirements. In appendix A, the scheduling of the PSA cycles used for the different cases is shown in Table 2 and the rationale behind the modifications introduced is briefly outlined.

The cases simulated were named after the ratio of net power output and ultrapure H₂ energy output (PW/H₂). The design case was selected to be the one with the highest power output and, consequently, the lowest H₂ throughput (i.e. case PW/H₂ 2.96). Since the aim of this case was to obtain a large power output, a large fraction of the H₂-rich outlet gas from the first PSA train is sent to the gas turbine, which is accordingly running close to full load. The off-design cases entail a growing fraction of the H₂-rich gas sent to the second PSA train for producing pure H₂. Accordingly, the PW/H₂ ratio decreases. It is worth stressing that the coproduction layout entails the processes upstream the gas separation unit – such as air separation, gasification and syngas treatment – to be basically unaffected by the modification in the PW/H₂ ratio since the coal input to the plant is kept constant. Thus, those units can work efficiently at their design conditions in all cases, meeting a first objective in order to realize plant flexibility. A second objective involves the capability to retain the overall plant efficiency at good levels, while substantially reducing the PW/H₂ ratio. Figure 5 shows the results obtained.

Figure 5. Share of energy products at different plant loads. The different cases are named after the ratio of net power output and ultrapure H₂ energy output (PW/H₂). The performance of the Two-train PSA process configuration is also reported in terms of cumulative efficiency (η*\text{tot}), together with the performance of a reference IGCC plant for power generation implementing CO₂ capture through absorption and without any H₂ production (η*\text{tot ref}).
The net power output could be significantly reduced within the framework studied. If the plant shows a net power output of 335MW at design case (i.e. PW/H₂=2.96), a proper modification of the PSA processes allowed to decrease it down to 232MW (i.e. PW/H₂ 0.92), a relative plant load reduction of 31%. Such control of the load would be ineffective if the plant efficiency was substantially decreased. Figure 5 shows a gradual decline of η*tot. This trend can be explained by an efficiency decrease of the combined cycle, which needs to operate at conditions progressively farther from design, and by a slight increase in the auxiliary power consumptions. However, the performance reduction is not drastic and good levels of η*tot are still achieved at the lower load tested. In this sense, it is interesting to compare the results with those of a reference IGCC plant with CO₂ capture (i.e. Only power absorption), which are shown also in Figure 5. The recommendations of EBTF [12] were used to define such plant, where CO₂ capture is carried out through a Selexol-based absorption process and where there is no ultrapure H₂ production. This plant was chosen as basis for comparison because it represents the benchmark in the context investigated. A comparative analysis is proposed to evaluate possible improvements in terms of plant flexibility coming along with a coproduction layout, aware of the approximations introduced by comparing outputs from two different plant configurations. The net power output of the reference IGCC plant was decreased by means of coal input reductions. The results reported represent the cumulative energy efficiency (which is equal to η₄ₑ₄ given that there is no H₂ output) for similar relative decreases of net power output as those achieved by the coproduction plant under investigation. If, for example, η*tot at PW/H₂=1.43 represents the efficiency of the coproduction plant with a load reduction of about 17%, the η*tot is equal to η₄ₑ₄ given that there is no H₂ output) for similar relative decreases of net power output as those achieved by the coproduction plant under investigation. If, for example, η*tot at PW/H₂=1.43 represents the efficiency of the coproduction plant with a load reduction of about 17%, the η*tot represents the efficiency of the reference IGCC plant for power generation with approximately the same load reduction. Whilst initially the trend is comparable, for larger reductions of net power output the off-design performance of the coproduction layout is clearly better than that of the reference IGCC plant (e.g. for a load reduction of about 31%, η*tot is equal to 35.8% while η*tot is equal to 33.3%). The larger efficiency drop can be explained by the high energy demand from ancillary plant, which is not decreasing proportionally to the reduced coal input. This comparative analysis demonstrates the effectiveness of a coproduction layout to enhance plant flexibility.

The framework tested demonstrated the capability to reduce the net power output of approximately 31% while processing a constant coal input to the plant and retaining a good efficiency. The maximum flexibility can be increased even more but that would involve correspondent further decreases in the productivity of the PSA processes. For example, the second PSA stage can be designed as a multi-train process. This would allow to vary to a larger extent the fraction of H₂-rich gas stream to be purified, while meeting the ultrapure H₂ specifications. Summing up, there is a trade-off between maximum degree of flexibility and productivity of the gas separation process.

7. Conclusions

Two novel PSA-based process configurations of an IGCC plant coproducing power and H₂ with CO₂ capture are presented. A first one, termed Two-train PSA, involves two PSA stages in order to separate CO₂ from a shifted syngas and purify H₂, respectively. The second one, termed One-train PSA, involves a single PSA stage to accomplish both gas separation processes. A comparative analysis of the performance of the systems based on these process configurations demonstrated the potential advantages in comparison to the common coproduction layout relying on an absorption process for capturing CO₂. Among the different layouts, the Two-train PSA configuration achieved the best results, in terms of energy efficiency and H₂ purity. The One-train PSA configuration returned a slightly lower performance. The core of the paper was then to investigate the degree of plant flexibility achievable by the two PSA-based systems. Proper designs were defined in order to increase the capability of the PSA processes to perform efficiently at various operating conditions. Such PSA processes were integrated into the IGCC plant and plant load reductions simulated. The One-train PSA process configuration could not meet ultrapure H₂ specifications (99.99+% vol. purity) at the different cases simulated. This issue limits the plant flexibility, unless more relaxed constraints on the H₂ purity are considered. The Two-train PSA process configuration enabled a reduction of the plant load down to 31%. While testing the different operating conditions, the coal feed was maintained constant so that the processes upstream the gas separation unit were unaffected and could perform efficiently at design conditions. The ultrapure H₂ specifications were met in all cases and the cumulative energy efficiency showed only a limited decline (i.e. from 37.2% to 35.8%). In order to evaluate the effectiveness of the proposed coproduction concept, a comparison with a reference IGCC plant for power generation with CO₂ capture was carried out. When similar reductions of plant load
were simulated, the reference plant showed a more significant decrease of efficiency (i.e. from 36.8% to 33.3%). Therefore, the novel PSA-based process configuration demonstrated an increased ability to work in load-following mode.

Acknowledgements

The authors gratefully acknowledge the financial support provided through the Norwegian University of Science and Technology (NTNU).

Appendix A. Characteristics and scheduling of PSA cycles for flexible operations

In order to deal with different operating conditions while meeting the gas product specifications, the PSA cycles of the Two-train PSA process configuration were properly modified. A first challenge was to retain an acceptable CO2 recovery in the cases characterized by low ultrapure H2 throughput. The second PSA stage of such cases process a fairly low inlet gas stream and, thus, also the amount of the available tail gas to purge columns of the first PSA stage is small. A measure to partially address this issue was to increase the time of the purge step in the first PSA cycle, with a correspondent decrease of the time of the blowdown step. Conversely, the time of the blowdown step was following increased to keep under control the increase of CO2 recovery when more gas is sent to the second PSA stage. Another effect that needed to be controlled was the expected decrease of H2 purity in the second PSA stage when a larger gas flow rate is processed. The two main strategies to deal with it were to reduce the cycle time and to increase the purge-to-feed mole flow rate ratio. Table 2 shows the resulting characteristics and scheduling of PSA cycles used for allowing flexible operations.

Table 2. Characteristics and scheduling of the PSA cycles for the different cases simulated.

<table>
<thead>
<tr>
<th>Step time (s)</th>
<th>Mole flow rate (mol/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>A</td>
</tr>
<tr>
<td>PW/H2 2.96</td>
<td>PSA 1</td>
</tr>
<tr>
<td></td>
<td>PSA 2</td>
</tr>
<tr>
<td>PW/H2 2.51</td>
<td>PSA 1</td>
</tr>
<tr>
<td></td>
<td>PSA 2</td>
</tr>
<tr>
<td>PW/H2 1.91</td>
<td>PSA 1</td>
</tr>
<tr>
<td></td>
<td>PSA 2</td>
</tr>
<tr>
<td>PW/H2 1.43</td>
<td>PSA 1</td>
</tr>
<tr>
<td></td>
<td>PSA 2</td>
</tr>
<tr>
<td>PW/H2 1.18</td>
<td>PSA 1</td>
</tr>
<tr>
<td></td>
<td>PSA 2</td>
</tr>
<tr>
<td>PW/H2 0.92</td>
<td>PSA 1</td>
</tr>
<tr>
<td></td>
<td>PSA 2</td>
</tr>
</tbody>
</table>

References