Supporting Information B

Report – Optimization of an Oxygen Concentrator via Parameter Manipulation

Knowledge Transfer in Support of the Development of Oxygen Concentrators in Emergency Settings During the COVID-19 Pandemic

Urs B. Lustenberger[§], Alexandra Krestnikova[§], Olivier G. Gröninger, Robert N. Grass, and Wendelin J. Stark *

ETH Zurich, Vladimir-Prelog-Weg 1, 8093 Zurich, Switzerland

§ U.L. and A.K. share co-first authorship and contributed equally to this paper

**wendelin.stark@chem.ethz.ch*

B1. Introduction

This document aims to support the reader in operating and optimizing the oxygen concentrator for the given set-up. For information regarding the construction and functionality of the DIY oxygen concentrator, please refer to the Manual*.* This work encompasses a summary of the set-up as seen in the manual, an explanation of the adjustable parameters and the analysis of parameter manipulation, based on the experiments conducted in our lab.

In the case of the given oxygen generator PSA (Pressure Swing Adsorption) was used, which is a technology that exploits different affinities of gases to a specific adsorbent used to separate a gas from a gas mixture. Here, air is pumped into the system, where it first gets purified/dried in a container filled with silica gel. The silica gel is a porous form of silica (silicon dioxide), whose pores can take up liquids or vapours, acting as a desiccant. Through a solenoid valve, the dry air enters the zeolite column. Zeolites are microporous minerals that, under pressure, trap the nitrogen and let the oxygen pass, hence separating the two gases. The oxygen reaches a buffer tank via a check needle valve, which is responsible that only a little oxygen leaves the buffer when the column is depressurized, and nitrogen leaves the system. This small amount of oxygen also helps clean the column from any remaining nitrogen. The dry nitrogen passing through the drying container restores the silica gel by taking up the humidity, making it reusable for a certain amount of time. A constant oxygen stream can be then accessed from the buffer tank through a needle valve. Additionally, this system is more efficient once a second zeolite column and drying container are added, as an antiparallel operation can be performed resulting in a continuous process. This process requires a switch of positions in the solenoid valve controlled by a timer. The full set-up can be seen in Figure SB.1.

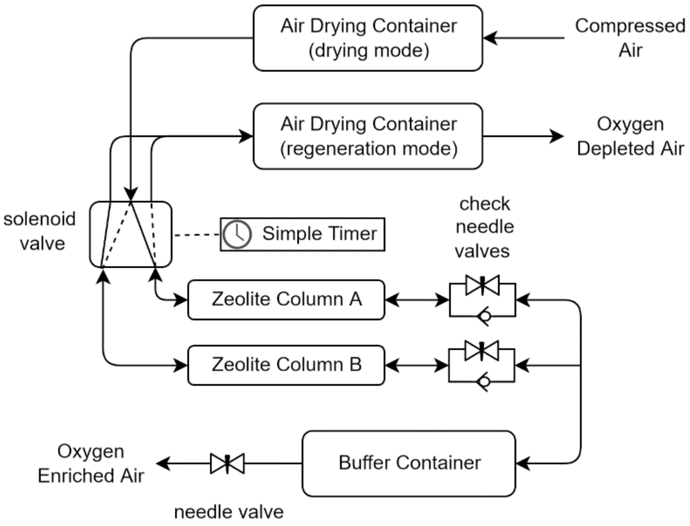

Figure S.B1: Two column set-up of the oxygen concentrator.

The adjustable parameters are the input air pressure, the switch time, the setting of the check needle valve (CNV) and setting of the needle valve (NV). To evaluate the oxygen concentrator the input air flow rate, the output oxygen flow rate and the oxygen concentration were determined in the experiments. From those, the most important properties of the oxygen concentrator can be acquired such as the oxygen recovery *R*, the purity *P*, the productivity *PR*, and the bed size factor *BSF*, which can be described by the following formulas respectively.

$$R = \frac{O_2conc. \in O_2enrichedair[\%] * flowrateofO_2enrichedair\left[\frac{normalL}{min}\right]}{O_2conc. \in air[\%] * flowrateofair\left[\frac{normalL}{min}\right]}$$

$$P = O_2conc. \in O_2enrichedair[\%]$$

$$PR = \frac{O_2conc. \in O_2enrichedair[\%] * flowrateofO_2enrichedair\left[\frac{normalL}{min}\right]}{100}$$

$$BSF = \frac{O_2conc. \in O_2enrichedair[\%] * flowrateofO_2enrichedair\left[\frac{normalL}{min}\right]}{100 * mass\ of\ Zeolite\ [kg]}$$

While it is obvious why purity and productivity are important properties, as purity gives the quality and productivity the quantity of oxygen, the relevance of oxygen recovery and the bed size factor should be explained. The feed air flow rate for the process is inversely proportional to R, so it can be used to estimate how much air has to be compressed, ideally recovery should be maximized. The BSF can be seen as the productivity per amount of zeolite. As the total amount of adsorbent in the system is inversely proportional to the BSF, it should also be maximized. For a given system, there is usually a trade-off between oxygen purity and oxygen recovery.[1]

In commercial devices the manufacturer presets the system to the optimal operating conditions, while the DIY oxygen concentrator needs to be optimized manually. This process is crucial, but also time-consuming, which is why we have already established optimal working conditions for the system through meticulous testing.

Nonetheless, adjustments in the valve settings for the needle valves (NV), the check needle valves (CNV), inlet pressure as well as cycle time can be made, to optimize the concentrator further to a specific requirement. Therefore, a set of experiments was conducted, where those 4 parameters were varied independently from one another and the input flowrate, output flowrate and the oxygen concentration were measured.

B2. Experimental

Four experiments were conducted, where the inlet pressure, the switch time and the settings of the valves were adjusted. For all the experiments the input air flow rate, the output oxygen flow rate and the oxygen concentration were measured. The setting of the valves was quantified by the number of rotations opening the valve. A base case of settings was determined prior to the experiments and the response of the device when deviating from 3 bar relative to atmospheric pressure, a switch time of 4.5 seconds and valve settings of 4 rotations to open the CNV and 0.75 rotations for the NV was studied.

In the first experiment, the feed pressure was varied between 2 and 4 bar in steps of 0.5 bar, with a fixed cycle time of 4.5 s and valve settings of 0.75 NV rotations and 4 CNV rotations.

In the second experiment the switch time was changed every second between 2 and 7 seconds, under a pressure of 3 bar and valve settings as chosen in experiment 1.

For the study of the check needle valve setting the rotations were varied between 2.5 and 5.5 rotations in steps of half rotations. The pressure was set to 3 bar and the cycle time was 4.5 s.

In the fourth study, in case of the needle valve, the rotations ranged from 0.25 to 1.25 rotations in steps of quarter rotations. The pressure was set to 3 bar and the cycle time was 4.5 s as well.

While this procedure and these intervals worked for this specific oxygen generator, that does not mean that the same line of action will lead to optimal results in every other case. A thorough testing can be time consuming but is crucial for obtaining good results and must be conducted for every specific concentrator using a procedure tailored to the device. Thus, the presented results may be helpful as a reference point.

B3. Results and Discussion

B3.1. Inlet Pressure

Figure SB.2 presents the results of the first experiment considering the input and output flow rate respectively. The blue points show an increase, meaning that with rising inlet pressure the flow rates of both air and oxygen streams can be increased. This result is not surprising as with more pressure more gas can be transported and as the volume of the system remains the same as before, the rate of gas flow increases following mass conservation. Note that the flow rate of the outlet, while also increasing, is much smaller than that of the inlet. This is due to the trapping of nitrogen, so that less gas is further transported into the buffer container resulting in a smaller flowrate of the oxygen stream.

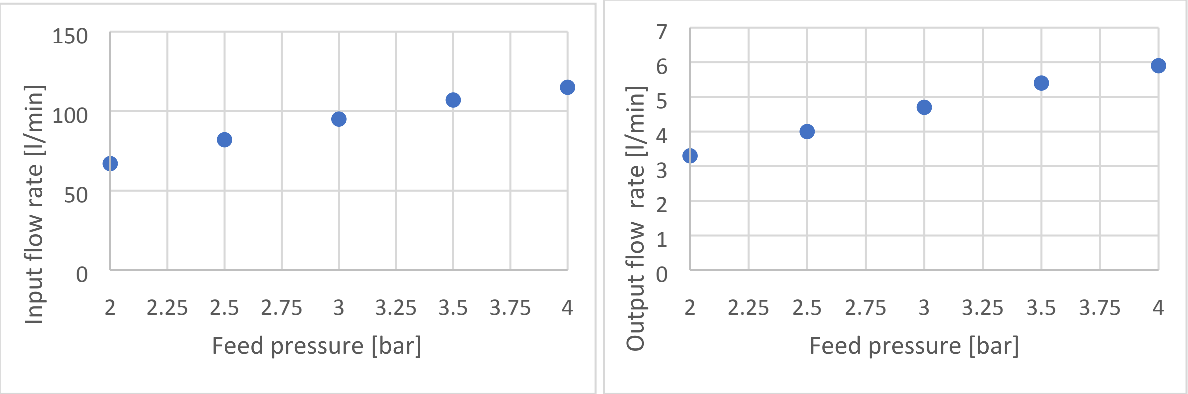

Figure SB.2. Right: The input flow rate vs the feed pressure. Left: The output flow rate vs the feed pressure. The blue dots show that with more pressure a higher flow rate can be achieved.

Figure SB.3 shows the oxygen concentration in relation to the inlet pressure. It is evident that the concentration doesn’t change between 2 and 3.5 bar, remaining at its maximum, but it decreases at 4 bar. In order to choose the inlet pressure correctly to assure pure oxygen, one has to take care of two important things. First, the zeolite columns have to be pressurized enough for them to work efficiently, as zeolites need a certain pressure to adsorb nitrogen. With an inlet pressure lower than 2.5 bar, the concentrator struggles to build enough pressure in our experience or requires longer cycles. Second, too much pressure can also lead to loss of efficiency. As the zeolite can adsorb only a finite amount of nitrogen increasing the pressure and hence the flow rate leads to more nitrogen passing through instead of being adsorbed and decreasing the oxygen concentration.

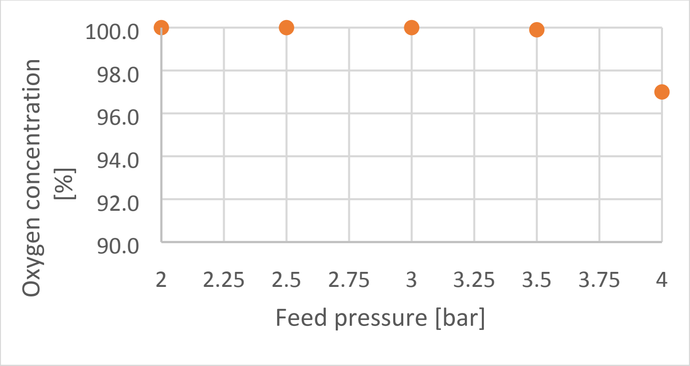

Figure SB.3: The oxygen concentration vs the feed pressure. While between 2 and 3.5 bars there is no change

Table SB.1 describes the results of the important system variables, calculated with the measured data. The purity, as described above, decreases with more pressure. For the productivity and the bed size factor one notes a steady increase, as more gas is compressed in general. Though, if the pressure were to be further increased it could lead to a severe decrease of purity, resulting in a decrease of productivity. Also note that under too much pressure the zeolite could crush and produce dust, which clogs the valves. For an optimal efficiency of the current oxygen generator a pressure of 3 bar was chosen.

Table SB.1. Results oft he pressure variation experiments

Pressure [bar]	Recovery [%]	Purity [%]	Productivity [L/min]	BSF [L/min/kg]
2.0	23.5	100.0	3.3	4.9
2.5	23.2	100.0	4.0	5.9
3.0	23.6	100.0	4.7	6.9
3.5	24.0	99.9	5.4	7.9
4.0	23.7	97.0	5.7	8.4

B3.2. Cycle time

Figure SB.4 shows the input and outlet flow rate in dependence of the cycle time. The longer the switching time, the smaller is the input flow rate of the air. On the other hand, with increased cycles times the oxygen flow also increases, as more pressure is built up.

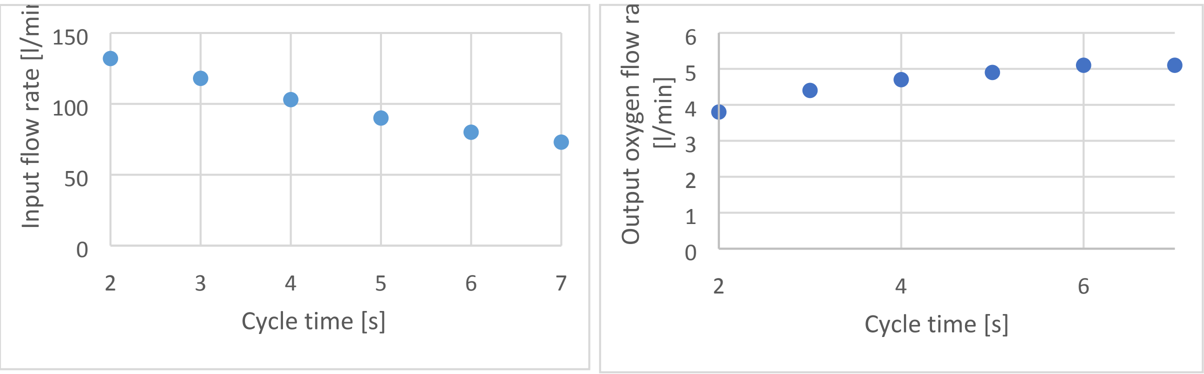

Figure SB.4. Right: The input flow rate vs. the cycle time. Left: The output flow rate vs. cycle time. The blue dots show that more time, results in a lower flow rate and a higher flow rate out.

Figure SB.5 shows how the oxygen concentration changes with the switching times. As the values first increase and then decrease, one can easily see that the cycle time should not be too short or too long. If the cycle is too short there is not enough time to build pressure in the column, so the zeolite does not adsorb nitrogen properly and the purity is impaired. With long switch times arises the problem, that after a while the input air just flows through, as the zeolite can only adsorb so much nitrogen. If you increase the feed flow rate, you will need to reduce the cycle times.

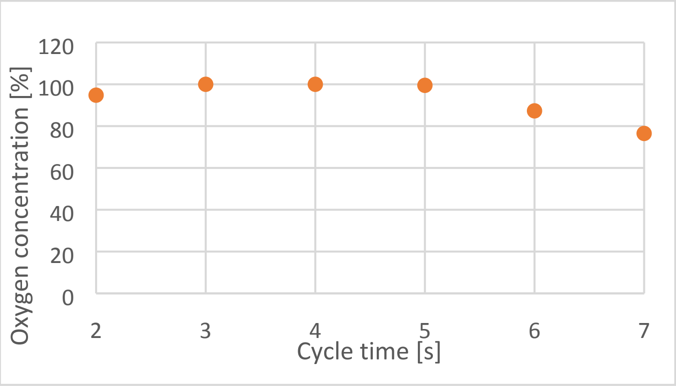

Figure SB.5. The oxygen concentration vs the cycle time. The purity is lower if there is not enough pressurization time or too much nitrogen enters the column.

As seen in Table SB.2, the best combination of high recovery, high purity, high productivity, and low bed size factor could be achieved with a cycle time of 4 seconds. Generally, productivity and BSF decrease with slower cycles and one could argue that in case of very small cycle times the system is not pressurized enough, which impairs the efficiency.

Table SB.2. Results of the cycle time variation experiments

Cycle time [s]	Recovery [%]	Purity [%]	Productivity [L/min]	BSF [L/min/kg]
2	13.0	94.8	3.6	5.3
3	17.8	10.0	4.4	6.5
4	21.7	100.0	4.7	6.9
5	25.8	99.5	4.9	7.2
6	26.5	87.3	4.5	6.5
7	25.5	76.5	3.9	5.7

B3.3. Check needle valve setting

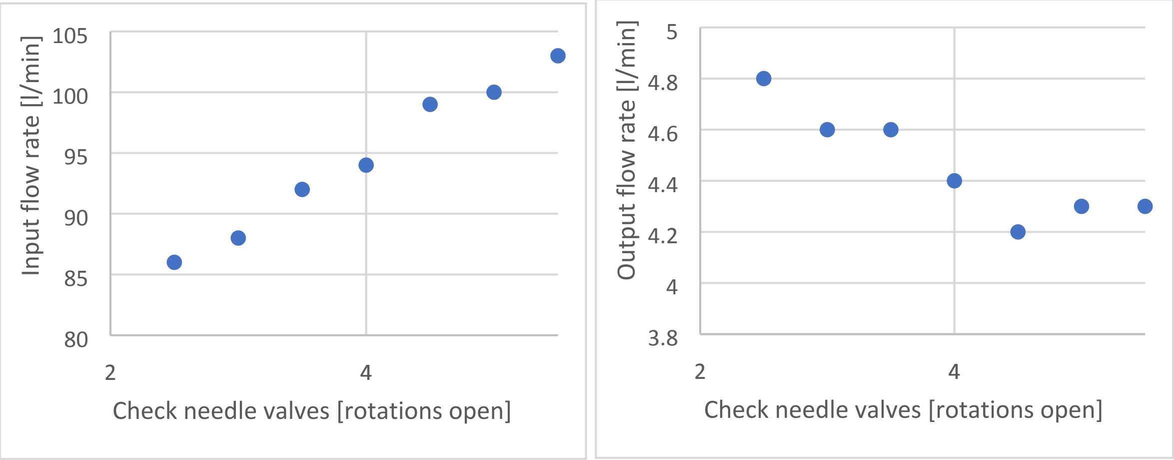

Figure SB.6. Right: The input flow rate vs the rotations of the CNV. Left: The output flow rate vs the rotations of the CNV. The blue dots show that more rotations, result in a higher flow rate and a lower flow rate out.

Figure SB.6 shows that the more the CNV is opened the higher is the input flow. Meanwhile the oxygen flow decreases, as more of the produced oxygen streams from the buffer tank, though the column and drying container out of the system. Also, the pressure starts to fluctuate more, and the overall pressure drop is bigger.

Figure SB.7 also shows that opening the valve further decreases the oxygen concentration. This is again due to increased amount of oxygen leaving the system. Furthermore, one can observe that if the valve is closed too tightly, the purity also is lower. This occurs because there is almost no oxygen to re-enter the column when it is being depressurized. Hence the column is not being cleaned from the remaining nitrogen, which impairs the oxygen purity. Additionally, opening the CNV wide may result in difficulty to pressurize the column, which leads to efficiency loss.

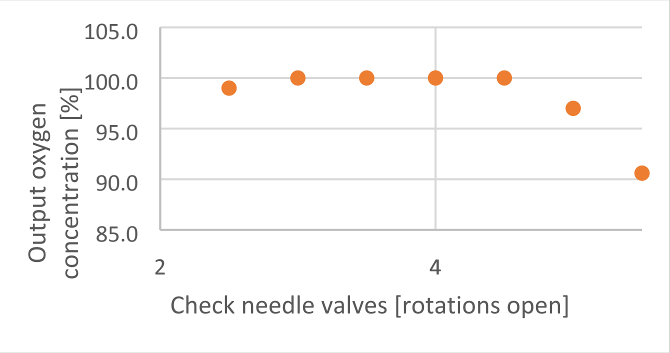

Figure SB.7. The oxygen concentration vs the rotations of the CNV. The purity is lower if too much nitrogen can pass the CNV or no oxygen can purge the column.

As recovery, purity, productivity as well as bed size factor have the best values at very few rotations, as seen in Table SB.3, one should choose to keep the CNV not very widely open, while still allowing some oxygen to flow back and purge the columns.

Table SB.3. Results of the CNV rotation variation experiments.

CNV [rot.]	Recovery [%]	Purity [%]	Productivity [L/min]	BSF [L/min/kg]
2.5	26.3	99.0	4.8	7.0
3.0	24.9	1000	4.6	6.8
3.5	23.8	100.0	4.6	6.8
4.0	22.3	100.0	4.4	6.5
4.5	20.2	100.0	4.2	6.2
5.0	19.9	97.0	4.2	6.1
5.5	18.0	90.6	3.9	5.7

B3.4. Needle valve setting

The more the needle valve at the end of the buffer tank is opened the more oxygen flows out. Hence the output flow rate is increased, while the input flow rate is not strongly affected, as seen in Figure SB.8.

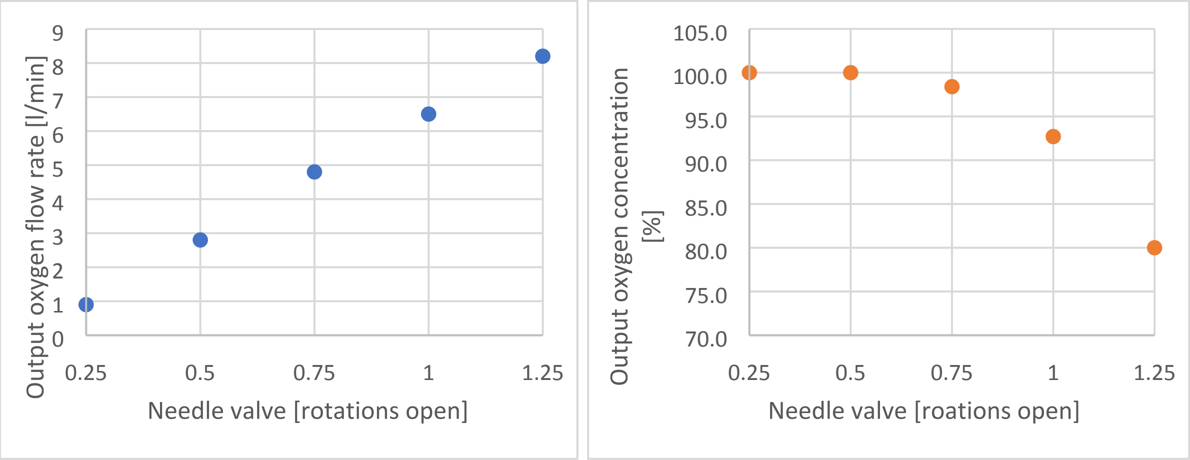

Figure SB.8. Right: The put flow rate vs the rotations of the NV. Left: The oxygen concentration vs the rotations of the NV. One can see that more rotations, result in a lower higher oxygen flow rate and a lower purity. The graphic for the inlet flow rate can be seen in the appendix.

Additionally, the oxygen concentration decreases with more NV rotations, as also nitrogen has a higher chance to leave the system through the buffer tank. Summarizing, opening the NV increases the oxygens flow rate and hence its recovery, productivity and BSF, while decreasing its purity, as seen in Table SB.4.

Table SB.4. Results of the CNV rotation variation experiments.

NV [rot.]	Recovery [%]	Purity [%]	Productivity [L/min]	BSF [L/min/kg]
0.25	4.4	100.0	0.9	1.3

0.50	14.2	100.0	2.8	4.1
0.75	23.9	98.4	4.7	6.9
1.00	30.2	92.7	6.0	8.9
1.25	32.5	80.0	6.6	9.6

B3.5. Zeolite particle size and column size

While this document does not show any data on how the performance is affected by other parameters, we still would like to give some notes on that matter.

Another parameter that can be changed is the length (L) to diameter (D) ratio of the column. While a shorter column, hence low L/D ratio, can reduce the pressure drop over the column, a ratio that is too small can lead to complications, such as insufficient gas distribution, deficient contact between gas and solid particles or channelling, where the air finds a way to pass directly through the zeolite without any mass transfer. In our setup we use for the zeolite columns with 5 cm diameter and 28 cm length, so the length/diameter ratio is 5-6. One also has to consider, when changing the length or diameter of the columns, the volume will change as well. This means fully pressurizing the columns might take a different amount of time. Hence switch times, and or pressure must be adjusted accordingly to find a suitable air flow rate.

Finally, particle size of the zeolite plays a big role. Generally, one seeks higher ratio of reaction (here: adsorption) surface to particle volume, so as to increase the efficiency. But a very small particle size can lead to agglomerations or clumps and a big pressure drop, hence interfering with the mass transfer and doing more harm than good.

B3.6. Optimization towards a certain goal

It was investigated how the adjustment of different settings of the oxygen concentrator influence its performance. Here we present how to use these findings to improve the process towards a needed goal. It was found that the oxygen concentrator with the given set-up operated best at 3 bar, a switch time of 4.5 seconds and valve settings of 4 rotations to open the CNV and 0.75 rotations for the NV. With these values it was possible to achieve oxygen concentration of up to 100% as well as a flow rate of around 5 l/min. 100% purity is very unlikely and may be traced back to an error of the sensor, as the measurement was carried out at high flowrates, which could build pressure on the sensor and distort the result. Also, the guaranteed lifetime of the sensor is only one year, which might have put additional strain on the sensor. Nonetheless, these settings were chosen as a base case, starting from which the oxygen concentrator can be further optimized towards specific requirements, as energy consumption or the size of the adsorbent bed. The detailed data can be found in the supporting material.

In order to minimize the energy demand of the device, the pressure can be lowered. As the flowrates depend directly on the pressure, lowering the energy consumption leads to a lower productivity of the oxygen concentrator. Furthermore, the inlet pressure cannot be chosen arbitrarily small, as the adsorbent needs a certain pressure to adsorb the nitrogen.[2] Should the energy demand be disregarded, and the pressure increased, the productivity will not increase indefinitely, as the purity will decrease once the adsorbent is saturated with nitrogen.

To reduce the size of the adsorbent columns, the bed size factor needs to be considered. To maximize the BSF, one should operate at low cycle times, and hence high pressures and fast flow, as fast cycles enable a more frequent usage of the adsorbent.[3] Note that a very short cycle time might not be sufficient to fully pressurize the column, which then leads to efficiency loss and requires more zeolite again. Further opening the CNV decreases the purity, as more air is allowed to pass through, which needs to be compensated with more adsorbent. Hence, the CNV should be closed just tight enough to still allow some oxygen back for the purge. Same goes for the goal of maximized productivity of oxygen as the BSF is proportional to the productivity.

B4. Conclusion

All in all, the oxygen concentrator with the given set-up operated best at 3 bar relative to atmospherical pressure, a switch time of 4.5 seconds and valve settings of 4 rotations to open the CNV and 0.75 rotations for the NV. With these values we were able to achieve an oxygen concentration of over 95% as well as a flow rate of around 5 l/min.

Pressure should be chosen, as high that the system can sustain it and the columns can be sufficiently pressurized, while avoiding too much nitrogen for the zeolites in the columns. With cycle times a similar approach should be applied, as there should be enough time for the column to be pressurized but not so much that the column is filled with too much air again. The check needle valve should not be kept widely open, as purity and the oxygen flow rate will suffer, but oxygen must be allowed to stream back into the column to clean it. Finally, there is a trade-off with the needle valve, as opening it means increasing the oxygen flow rate on the one hand and decreasing purity on the other.

Please note, that while the presented parameters are optimized for the given set-up it does not guarantee that every other oxygen generator will operate in a most efficient way under the same settings. As every individual set-up can vary and conditions or material may differ, the concentrator must be optimized differently. In conclusion the acquired parameters should be used as a starting point, as it takes a lot of time to find the correct setting, but proper adjustments must be made individually.

Literature

[1] Chai, Siew Wah, Mayuresh V. Kothare, and Shivaji Sircar. "Rapid pressure swing adsorption for reduction of bed size factor of a medical oxygen concentrator." Industrial & Engineering chemistry research 50.14 (2011): 8703-8710.

[2] M. W. Ackley, “Medical oxygen concentrators: a review of progress in air separation technology,” Adsorption, vol. 25, no. 8. Springer New York LLC, pp. 1437–1474, Nov. 01, 2019. doi: 10.1007/s10450-019-00155-w.

[3] K. R. Ward, G. S. Huvard, M. McHugh, R. R. Mallepally, and R. Imbruce, “Chemical oxygen generation,” in Respiratory Care, Jan. 2013, vol. 58, no. 1, pp. 184–194. doi: 10.4187/respcare.01983.