Simple model of distillation Column for PICO 500

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1 Introduction

1.1 Document Purpose

This document will seek to outline how a radon distillation column will perform if integrated into PICO 500. First a rough estimate of radon contamination levels in PICO 500 will be obtained. Then the general effect of distillation column efficiency and flow rate on overall system reduction will be explained. Run cycles of distillation and detection will be presented to show their effect on average radon contamination. Then analysis of column performance will be completed using a McCabe Thiele model. Using the conditions of operation, the amount of packing material required and heating/cooling power will be calculated. This will all be done for two systems, one that has been outlined as realistic operating conditions for the column and another for highly idealized operating conditions.

1.2 Operating conditions

Idealized system:
Operating Pressure: 14.7 PSI
Operating Temperature: 237 K
Gas Density: 10.46 kg/m^3// Flow rate: 70 kg/hr
Full Gas Feed
1 % fluid loss
Other conditions specified to reach required radon reduction

Realistic Operating conditions: Operating Pressure: 200 PSI
Operating Temperature: 309 K
Gas Density: 117.20 kg/m^3// Flow rate: 12 kg/hr
Full Gas Feed
1 % fluid loss
3-5 day distill detect cycle
Cooling 1 kW

2 Calculations

2.1 Establishing estimated radon concentration

The alpha background goal for PICO 500L is that it has a radon background that is less than or equal to that of PICO-60. The alpha background of PICO-60 due to radon chain decays was evaluated to be 2.3 uBq[1]. It is reasonable to assume this is radon presence is due to emanation from the interior of the quartz tank that contains the target material. A first order approximation would be that the amount of radon emanation will scale with the tank surface area. A reasonable estimation is that the surface to volume ratio of a the tank will scale as follows, using the activity of PICO 60 and mass of PICO 60 and PICO 500.

$$A_{500} = A_{60}(\frac{M_{500}}{M_{60}})^{2/3} \tag{1}$$

Taking A_{60} = 2.3 uBq, M_{500} = 800 kg, M_{60} = 52.2 kg yields an activity level of PICO 500 of 14.2 uBq

The start and end mass concentration can then be calculated using the equation

$$\frac{m_{radon}}{m_{C3F8}} = \frac{A/\lambda_{radon}/N_A * M_{radon}}{m_{C3F8}} \tag{2}$$

where λ is the radon decay constant (2.098*10^{-6} 1/s), m = mass and M = molar mass. This yields a initial concentration of 3.12*10^{-27} and an end concentration of 5.05*10^{-28}.

2.2 Radon levels in PICO system:

The distillation column that is designed will have two primary specifications that will determine the to what level the total radon background of the distillation column can be reduced to. These are the flow rate of the system and the reduction factor of the column itself. The model used in calculating radon reduction capabilities is taken from 4.2 of [2]. The basic differential equation that this source provides is.

$$A(t) = -[\frac{\kappa}{\Lambda} - A(0)] * e^{-\Lambda t} + \frac{\kappa}{\Lambda}$$

$$\Lambda = \lambda + f(1 - R^{-1}) \tag{3}$$

$$\kappa = k_1 + k_2/R$$

Where A = activity (μBq), t=time, λ = radon decay constant, f = flowrate (1/s), R= reduction factor of column, k_1 = detector emanation rate, k_2 = column emanation rate. k_1 can be estimated as the initial radon background of the system. If the system is in a steady state radon must be emanating into the system at the same rate is decaying. As k_2 sources are less important due to them originating in the distillation column, we will treat them as 0 for simplicity.

We can now calculate the radon reduction factor for the entire system as a function of flow rate and distillation column reduction factor. These results are the radon reduction values after a long period of time (t->∞) and are a steady state. Those results are shown below.

Reduction Factor	1.5	3	5	10	25	50	100	inf
Flowrate (kg/hr)								
6	1.331	1.662	1.7944	1.8937	1.9533	1.9731	1.9831	1.993
12	1.662	2.324	2.5888	2.7874	2.9066	2.9463	2.9662	2.986
20	2.1033	3.2067	3.648	3.979	4.1776	4.2438	4.2769	4.31
40	3.2067	5.4134	6.296	6.9581	7.3553	7.4877	7.5539	7.62
60	4.31	7.6201	8.9441	9.9371	10.533	10.731	10.831	10.93
80	5.4134	9.8267	11.592	12.916	13.711	13.975	14.108	14.24
120	7.6201	14.24	16.888	18.874	20.066	20.463	20.662	20.86
200	12.033	23.067	27.48	30.79	32.776	33.438	33.769	34.1

Table 1: Radon reduction value of entire system for different column flow rates and reduction values

This table illustrates that the column flow rate plays a much larger role than the column reduction factor. After a column reduction factor of 10 is reached, further increasing the reduction factor adds little to total system reduction.

This allows us to calculate the maximum reduction capability for any flow rate. For a system processing 12 kg/hr, maximum radon reduction is ≈ 3. For 70 kg/hr the maximum radon reduction is is ≈ 11.5.

As these results are only accurate for the system at a steady state (long periods of time) it is important to also analyze what radon levels of the system would be after running for in a realistic cycle of system distillation and detection. This can be shown for a realistic system and ideal system

Realistic system:

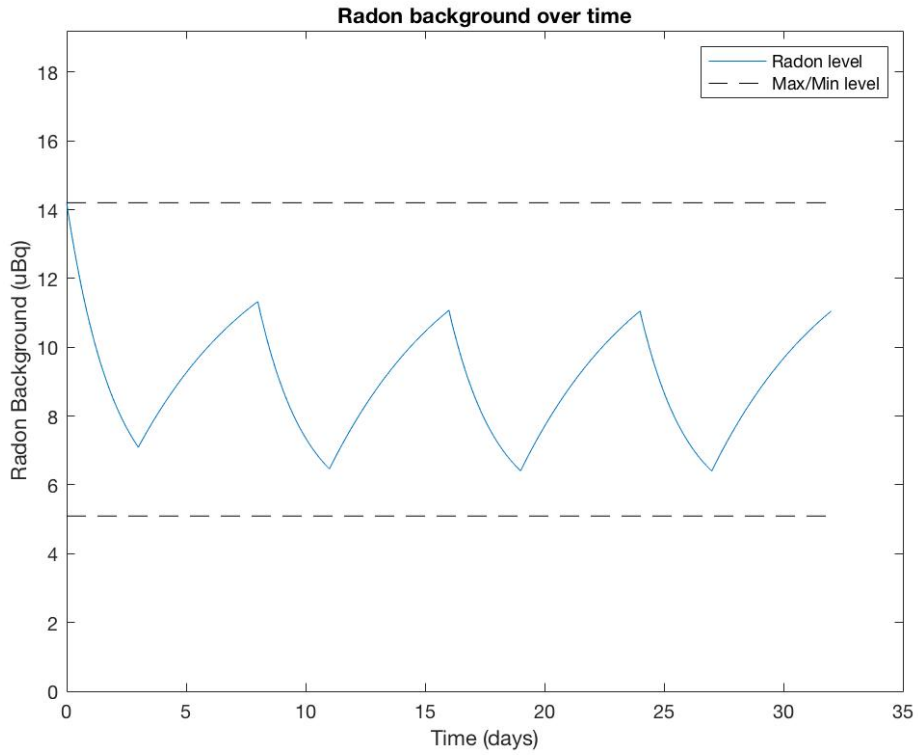

Figure 1: Radon levels for a system with f = 12 kg/hr, R=10 on a 3 day distill 5 day detect cycle, average reduction 1.56

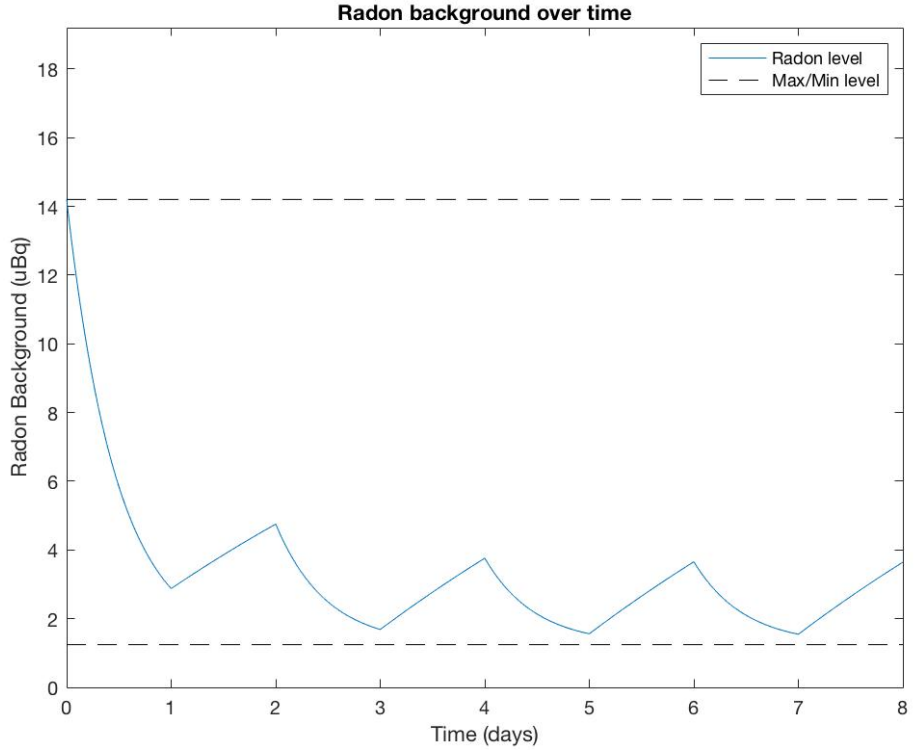

Figure 2: Radon levels for a system with f = 70 kg/hr, R=10 on a 1 day distill 1 day detect cycle, average reduction 5.40

It can be seen that a distillation column with a flow rate of 12 kg/hr has an average radon reduction of 1.56 on the 3-5 day cycle whereas the column with a flow rate of 70 kg/hr has a radon reduction of 5.40 on a 1-1 day cycle. It is worth noting that decreasing the length of the cycle increases the radon reduction power of the system. However, this includes the obvious trade off of having to switch continuously between two operational modes. Additionally, a system with a lower flow rate may have a lower power usage but will require a longer time to achieve its maximum reduction, this fact would allow one to find a flow rate which minimizes total energy usage of the column. Taking these factors into account will allow one to determine an optimal distillation/detection cycle.

The MATLAB program that produces these plots for variable inputs is available at [3].

2.3 Distillation column performance

The reduction factor of the distillation column is calculated using the McCabe Thiele method and the equations are modeled after chapter 4 of [4]. The model described in the cited thesis concerns the distillation of Krypton from Xenon for the Xenon dark matter research project. This results in a few differences in applying this model to the removal of radon from C3F8. The distillation column described in the thesis discusses the use of a distillation column for batch distillation - where the target fluid is run through the distillation column and then placed into the detector. For our system, radon is constantly emanating into the target fluid which requires a distillation column constructed in a way that it is attached to the PICO-500 detector and can be used continuously to reduce radon contamination.

A column build for the reduction of radon in C3F8 in PICO-500 will manage as high of a flow rate as possible, operate at 200 PSI and minimize the heating/cooling power while maximizing radon reduction. Additionally, the C3F8 target fluid may need to vaporized prior to distillation so that it can be passed through a particle filter.

Using a MATLAB model [5] and [3] based on the format used in the thesis previously referenced. A system that with a flow rate of 70 kg/hr, initial concentration on 14.2 uBq / 800 kg, final concentration 2.3 uBq / 800 kg, percent loss of 1 %, with a fully gaseous feed and a Reflux ratio $R=1.5R_{min}$ requires 2880 W of cooling and 4201 W of heating while running on a 1 day 1 day detect cycle. Additionally, this will require 10 theoretical stages in the distillation column, the height and material equivalent to a single stage will be calculated later.

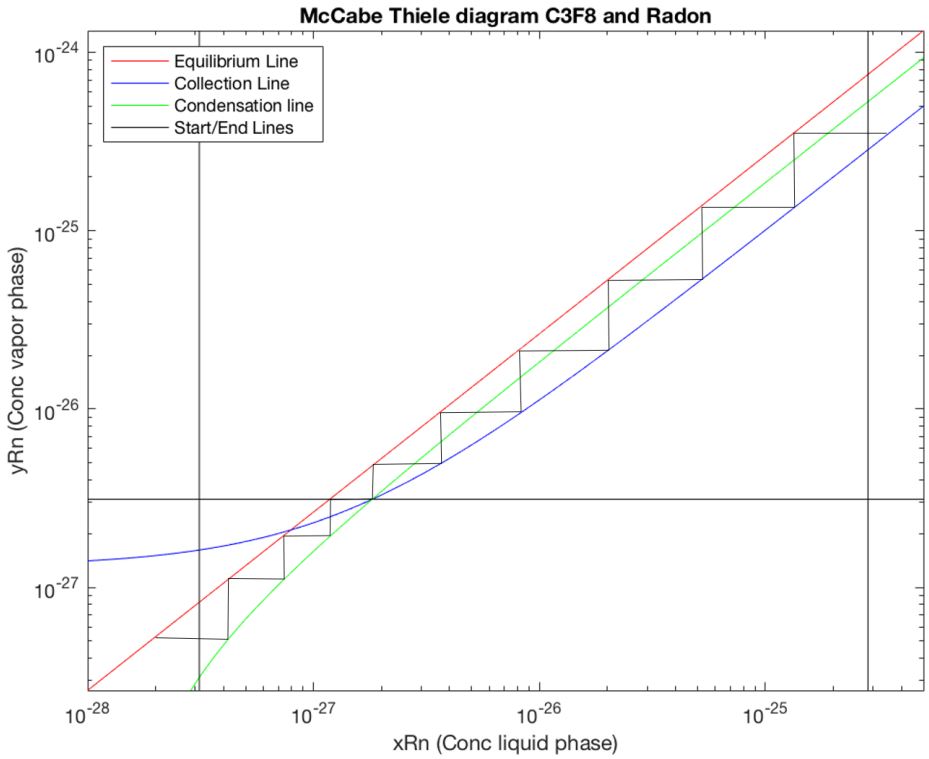

Figure 3: McCabe Thiele diagram for ideal system conditions (see section 1.2), volatility = 2.644

Creating a McCabe Thiele diagram for a realistic system outlined in section 1.2 that minimizes cooling and material costs is shown below. This system requires 961 W of cooling and 1187 W of heating.

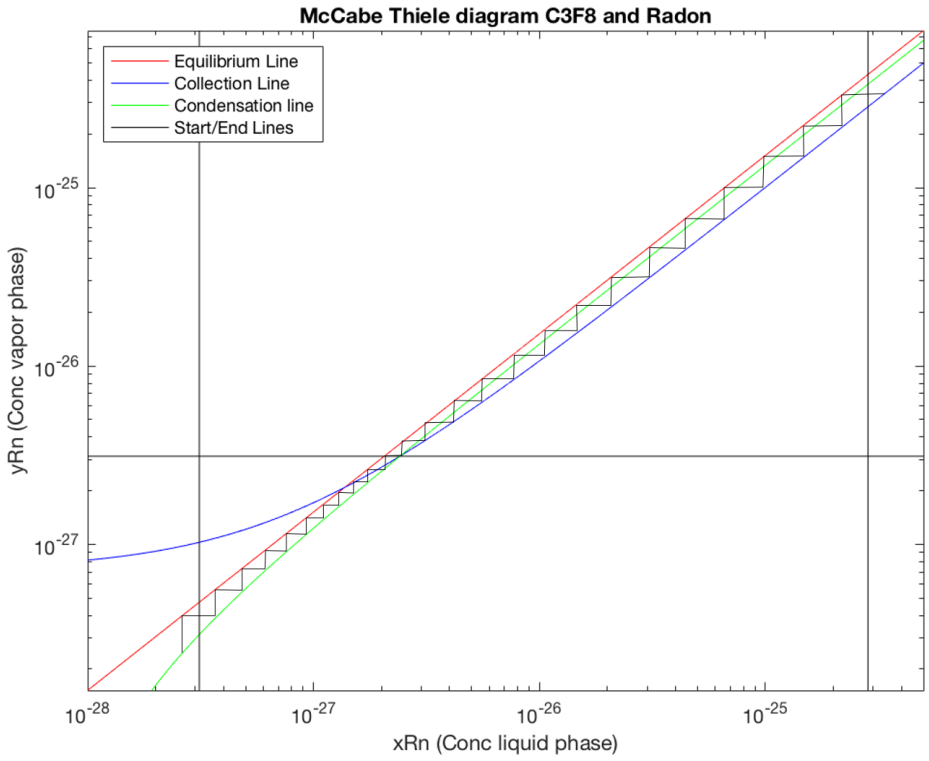

Figure 4: McCabe Thiele diagram for realistic system conditions (see section 1.2), volatility = 1.518

2.4 Distillation Column Design

To calculate the size of the column needed to achieve the stated radon reduction. The main factor for this is the HETP (Height equivalent for one theoretical plate). Companies that produce packing materials provide charts that give approximate HETP values as a function of gas load. Gas load can be calculated using the following equation.

$$F = \sqrt{\frac{4 * \dot{V}'}{\pi * \epsilon * d_c^2 * \sqrt{\rho_{GC3}}}} \tag{4}$$

Where V' is the gas flow from the stripping section, ϵ is the voidage of the packing material, d_c is the column diameter and ρ is the gas density of the column. In general a lower gas load results in a lower HETP value. Therefore, reducing stripping section gas flow and increasing gas density of the system are effective ways to reduce system size.

Packing materials considered for the distillation column can be found at [6]. The laboratory packing material offers the best HETP values and for this reason is the packing material used in estimations.

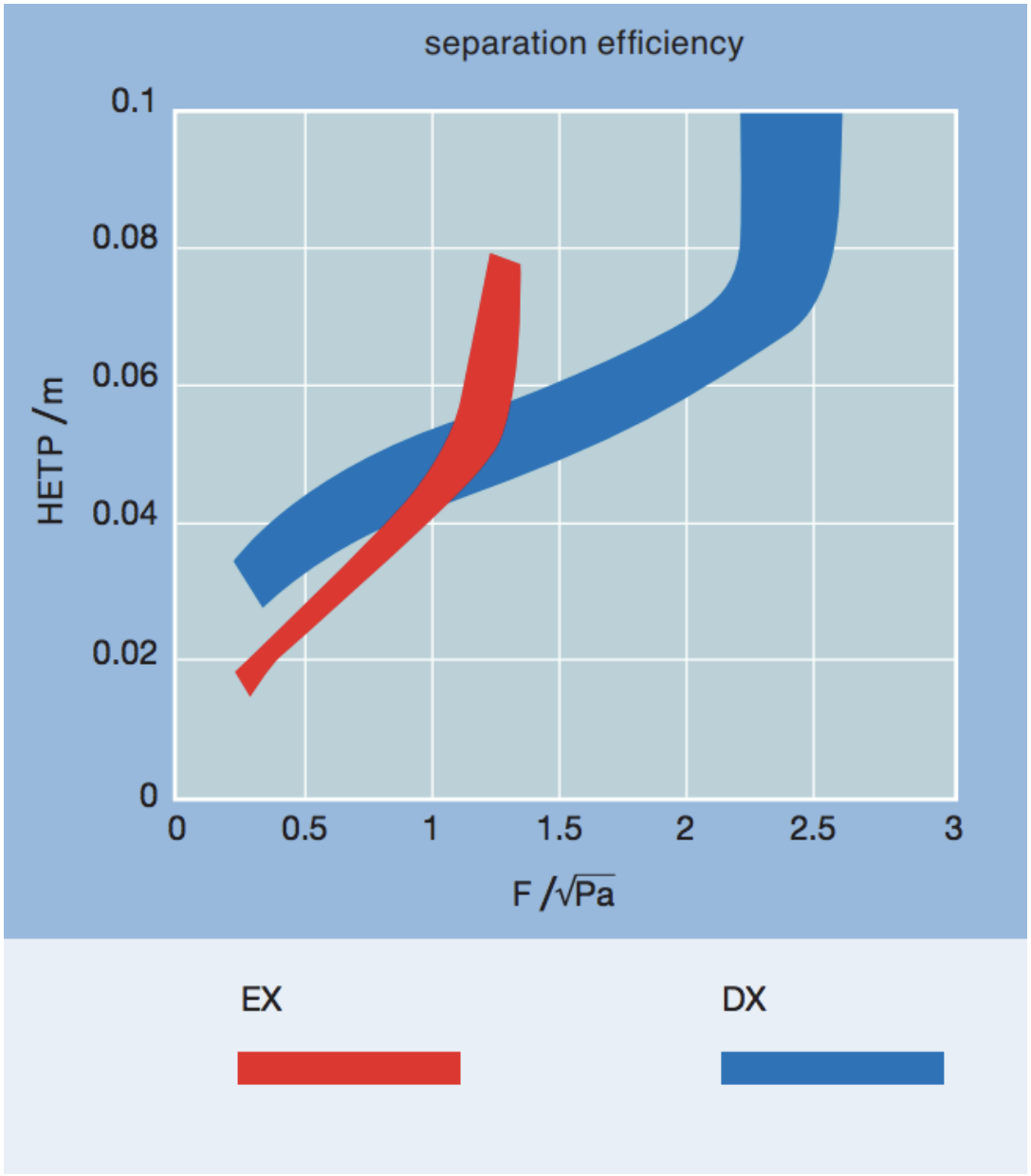

Figure 5: HETP values for gas load of labratory packing material

Realistic System: A gas load of 0.75 $Pa^{1/2}$ is used in calculating the column specifications. V' is calculated using [5] This results in a necessary column diameter of 48 mm and a HETP corresponding to 40 mm. As the number of stages required is 25 for the realistic system, the total system height is estimated to be $\approx$ 1 m. In the krypton thesis [4] they included an order of magnitude buffer for the HETP value due to the unknown performance of systems at such low concentrations. This would result in a column 10 m in height.

Ideal System: Again a gas load of 0.75 $Pa^{1/2}$ is used. This results in a column 132 mm in diameter and again a HETP corresponding to 40 mm. As the number of stages required for the idealistic system is 10, this results in a final column height of 40 cm. Applying the order of magnitude buffer would result in a system 4 m in height.

3 Model Deficiencies

Although a good first order approximation, this model is incredibly simplistic and misses a number of elements which would make this a much more exhaustive document.

1) System design:
The McCabe Thiele method describes a system in which two outputs are produced. One which would have a lower radon concentration than the input feed and one that would have a higher concentration than the input feed. In the case of our system, this higher radon output feed would be unnecessary. Radon would concentrate in the top stages of the system, but would not need to be removed, as it would decay over time. Even removing the radon and placing it in a holding tank to decay would be counter productive, as the additional lines and contact area would produce more radon. Therefore the McCabe Thiele method used in this document cannot completely accurately model the distillation column we would build.

2) System simplicity:
There a number of techniques that can be used to construct a better performing system. This basic model does not capture the details of specific packing materials, multiple feed lines, heating and cooling exchange systems that have lower power requirements etc. A system built taking these details into consideration could potentially be built smaller and more energy efficently than the one described.

3) Inherit Unknowns:
The system described concerns incredibly low levels of dissolved in C3F8. A 10^{-27} concentration would result in just a few atoms of radon dissolved in the entire system. The McCabe Thiele method is a model for a macroscopic system. The concentrations being worked with in this document are so low, the assumptions used for other systems may not completely apply in this case. There is some evidence that column distillation still works at these scales (Xenon 100 project) but there is nothing completely clear.

4 Conclusions

This document serves as a first order estimate for various factors that will determine whether or not a distillation column is a worthy investment for integration with PICO 40 or 500. As calculations/estimates are not optimized in any way, it is expected that more work will allow for the design of a system that exceeds the specifications described in this document (smaller, more efficient etc). The final system will likely have operating conditions somewhere between that of the idealized system and the realistic system. Future directions for this work involve a more thorough investigation into the mechanical design of the document and consultation with a mechanical engineer and accurately modeling of the system using chemical engineering software as well consultation with a chemical engineer to uncover any likely problems or simplifications.

References

[1] Amole, C., Ardid, M., Asner, D. M., Baxter, D., Behnke, E., Bhattacharjee, P., ... & Clark, K. (2016). Dark matter search results from the PICO-60 CF 3 I bubble chamber. Physical Review D, 93(5), 052014.

[2] Lindemann, S., Hampel, W., & Aeschbach-Hertig, W. (2013). *Intrinsic 85Kr and 222Rn backgrounds in the XENON dark matter search* (Doctoral dissertation, Ruprecht-Karls-Universität Heidelberg).

[3] $https://drive.google.com/open?id = 1RO8MXTCoTGSs\_xsiLnlbPtpdsKchME2$

[4] Murra, M. (2014). Set up and test of a cryogenic distillation column for the XENON1T experiment. Masterarbeit, WWU Münster.

[5] $https://drive.google.com/open?id = 1nJMDPnOvl9EYatiF9Se_8oo - bPOpJ5Kl$

[6] $https://www.sulzer.com/-/media/files/products/separation-technology/distillation-and-absorption/brochures/structured_packings.ashx$