Master’s Thesis – master Energy Science

Technical analysis of a simple cycle gas turbine with carbon capture storage.

GEO4-2510 - ENSM Master’s thesis Energy Science

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Abstract

Since the ratification of the Paris agreement in December 2015 large part of the world has committed to taking drastic steps towards decarbonization. The introduction of variable renewable sources causes the increase for flexible energy supply. A conventional carbon emitting flexible energy supplier is the simple cycle gas turbine.

Carbon capture technology which is appointed by the International Energy Agency as one of the key contributors towards decarbonization, has potential to decarbonize the simple cycle gas turbines. With the aim of finding cost-effective solutions this research performs a technical feasibility analysis of the carbon capture process on a simple cycle gas turbine. Post combustion carbon capture technology is selected for the framework. The post combustion carbon capture does not require major adjustments in the infrastructure opposed to oxy-fed or pre-combustion technologies.

Within the post combustion technologies, as a first step, the multiple options are screened in literature and adsorption process is selected as most suitable for the simple cycle gas turbine. As a second step the sorbents of the adsorption process are screened in literature and hydrotalcite like compounds is selected as best suited sorbent. It shows relative low regeneration energy and high cyclic stability.

The third step is finding a mathematical explanation for the sorbents sorption behaviour. Isotherm models mathematical explain the sorption behaviour of the sorbents. Multiple isotherm models are analysed and their ability to model the sorption behaviour of the sorbent is tested. The Langmuir isotherm model displayed the best fit to the sorbent and is adapted for temperature dependency.

The carbon capture set-up coupled on to the simple cycle gas turbine is temperature swing adsorption process with fixed beds. The temperature in the column is low when CO_2 enters the column and the CO_2 is adsorbed on the sorbent. The temperature is increased so that the CO_2 desorbs from the sorbent and can be separated from the flue gas. The fixed bed entails beds fixed in the column filled with the sorbent.

The fourth step is analysing the size of the set-up using the isotherm model. The adsorption and desorption processes are analysed, and the size of the column is determined. The set-up is modelled in an optimistic way, due to simplification. Flue gas is considered as a single component, where it is multi component. Also, adsorption kinetics are excluded in the modelling, moreover only one sorbent is used due to limited data availability.

Concluding the results show that the set-up is not feasible. The size of the column in the framework varies between 251 meters and 40 meters diameter with a 15 meters height. Improvement of the sorption capacity of the sorbent is suggested as best possibility for improving the feasibility of the set-up.

Preface

The gradational research ‘Technical analysis of a simple cycle gas turbine with carbon capture storage’ has been carried out for University of Utrecht. The research is part of the Energy Science program for period of a little over 6 months (February 2018 till August 2018).

The need for decarbonization has become evidently clear to me over the past 5 years studying at the University of Utrecht. During the last two years, during my master Energy Science, carbon capture and storage as an option for decarbonization peaked my interest. It became clear that Carbon capture and storage technologies is a decarbonization option with many challenges, but also a great potential.

My graduation research offered me the possibility to explore this topic in more detail. In collaboration with my supervisor, dr. Matteo Gazzani, we came up with a technical analysis of the ‘carbon capture process’ of a simple cycle gas turbine. This research is a first technical feasibility analysis on this application.

I hope you enjoy reading the research. Feel free to contact me for additional questions or remarks.

Michiel Aldenkamp
Amsterdam
Augustus 2th 2018

Acknowledgements

I would like to thank my supervisor dr. Matteo Gazzani of the Copernicus Institute of the University of Utrecht, for all his time and effort. As the topic of this thesis has a more technical nature than ‘regular’ Energy Science topics, additional supervision was offered by Matteo, for which I would like to show my appreciation. Secondly, I would like to thank my farther dr. Freek Aldenkamp in the final stage of the thesis he provided me with crucial and critical feedback. For all his time and effort, I would like to thank him.

Contents

List of abbreviations

CCR	Carbon capture rate
CCS	Carbon capture and storage
GHG	Greenhouse gasses
HTC	Hydrotalcite like compounds
PCC	Post combustion capture
PV	Photovoltaic
RES	Renewable energy source
SC-GT	Simple cycle gas turbine
VRES	Variable renewable energy source

Chapter 1 Introduction

Since the ratification by the United nations of the Paris agreement in December 2015 the world has taken drastic steps towards the decarbonisation of the global energy system (United Nations, 2015). The Paris agreement sets out an action plan for all the 195 participating countries to decrease their greenhouse gas (GHG) emissions in order to limit the global warming to below a 2 °C increase as compared to pre-industrial levels (COP, 2015). The Intergovernmental panel on climate change (IPCC) has constructed different scenarios related to the emissions of the GHG in order to explore possible pathways towards this stabilization of the global climate (Nakicenovic & Swart, 2000). The pathway corresponding with achieving climate stabilization shows that drastic measures in decreasing carbon emissions needs to be taken (Morita, Nakićenović, & Robinson, 2000). The International energy agency (IEA) suggests multiple measures in different technology areas in order to reach the goal (IEA, 2017a). The scenario from the IEA, corresponding with limiting the temperature increase to 2 °C, is the 2DS scenario (Ibid). The main changes, in comparison to the current system, are an increase in energy efficiency, an increase in renewable energy sources (RES), increase in nuclear energy, fuel switching and carbon capture storage (CCS) (Ibid). Figure 1 shows a visual representation of the IEA scenario 2DS with corresponding CO_2 reduction per technology area (Ibid).

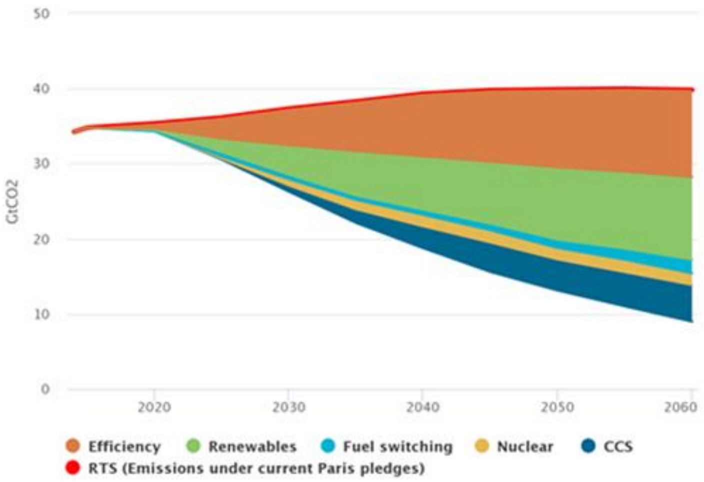
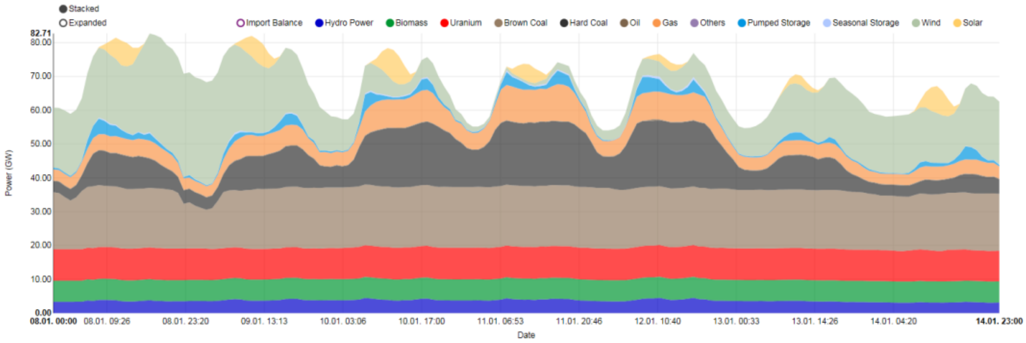


Figure 1: 2DS scenario International Energy Agency *source: IEA, 2017a*

Most of these changes have a large influence on the supply side of the energy sector, which in turns will trigger changes on the demand side as well. On a daily basis the demand differs every hour of the day (U.S. Energy Information Administration, 2018). Figure 2 shows the energy production in Germany in the period of the eight of January 2017 to the fourteenth of January 2017 (Fraunhofer ise, 2018).



Net generation of power plants for public power supply.
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Figure 2: Energy demand Germany 08-02-2017 until 14-2-2017 *source: Fraunhofer ise, 2018*

The energy production reflects the energy demand. The demand of energy differs during the hours of the day and during the days of the week due to the daily demand pattern of people (Richardson, Thomson, Infield, & Clifford, 2010). Moreover, a seasonal variation is also present because of the different needs throughout the year. Two demand peaks which are important to note in figure 2 are the morning peak and the evening peak. These peaks occur during time periods of the day when there is little to no irradiance and thus little to no Photovoltaics (PV) energy production. Notably, the expected increase in non-dispatchable RES (i.e. wind and PV), needed to meet the Paris agreement, will result in an increase in these peaks (Denholm, O'Connell, Brinkman, & Jorgenson, 2015). California is another example where this already has happened to some extent. Figure 3 shows the development of the net load in California and the expected development in the future (ISO, 2012). Besides the time dependency of the PV, other renewables also show variability in their production (VRES) (Chandler, 2008). This results in an increasing demand for flexible energy production, which is currently covered by fossil sources (Lo, 2017; van Meerwijk, Benders, Davila-Martinez, & Laugs, 2016).

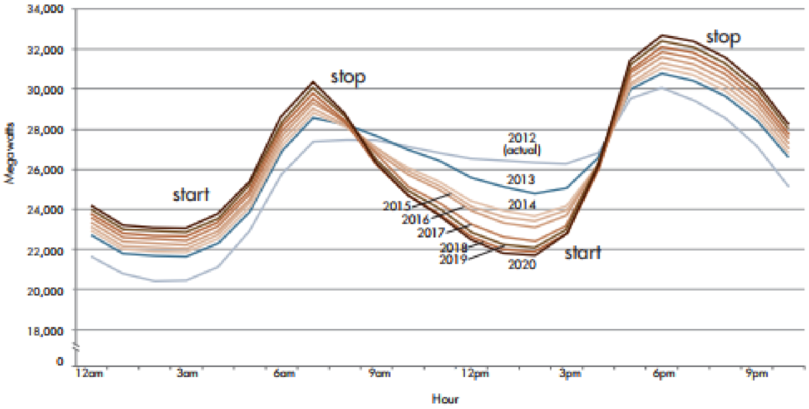

Figure 3: Net load in California on 11 January 2017 *source: ISO, 2012*

There are a number of different approaches in dealing with this need for flexibility in the system; supply side solutions, demand side solutions, energy storage solutions, network solutions and system solutions (Papaefthymiou, Grave, & Dragoon, 2014) . The short-term flexibility suppliers are defined as being able to balance the market in up to one hour, which is needed for the demand peaks show in figure 2 and figure 3. A research by Ecofys (2014) compares these options and shows that one of the promising solutions for short term flexibility is a simple cycle natural gas turbine (SC-GT). The SC-GT can ramp up and down within this short time frame. An example of a SC-GT is the LM6000 from General Electrics which can ramp up to full load of 57 MW within 5 minutes (Corporation, 2010). However due to the high price of operation (high price of natural gas coupled with limited efficiency), these gas turbines mainly operate during peak demands of the day. This means they operate infrequent and for short periods of time (Global CCS Institute, 2012). Although natural gas burns as one of the cleanest fossil fuels, GHG are still emitted, which is not in line with the Paris agreement (International Energy Agency, 2012).

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To handle the issue of the CO_2 emissions of the natural gas turbines a new solution, being suggested by IEA, is using carbon capture storage (see box 1) as one of the key players for achieving the 2DS scenario (Global CCS Institute, 2012; IEA, 2017a).

Box 1: Carbon capture and storage

CCS builds upon a group of technologies and techniques which enable the capture of CO_2 from fuel combustion or industrial process; after the capture the CO_2 it is transported and stored (Samantha McCulloch, Simon Keeling, Raimund Malischek, Tristan Stanley, 2016). There are three main routes recognized in the field of CCS; post-combustion, pre-combustion and oxy-fuel combustion (Gibbins & Chalmers, 2008). In post-combustion the carbon is removed after the fuel is burned, before the carbon rich flue gasses are vented into the atmosphere. Pre-combustion uses a reforming or gasification process where the carbon is removed out of the fuel before the combustion of the fuel. This produces a syngas which than can be combusted in a carbon free manner. In oxy-fuel combustion the combustion takes place with pure oxygen instead of air. This results in a flue gas that mainly consist of water and carbon dioxide which are relatively easily separated. Figure 4 gives a visual representation of the three routes.

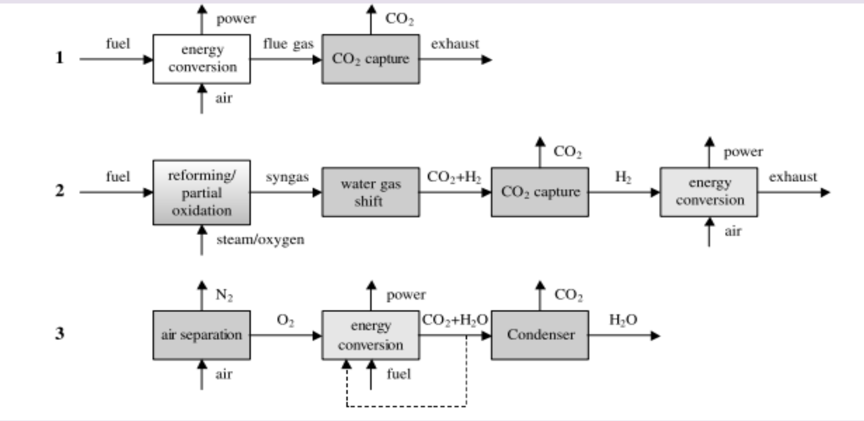

Figure 4: Three main routes of carbon capture storage (1) Post-combustion capture (2) pre-combustion capture (3) oxyfuel combustion source: Damen, Troost, Faaij, & Turkenburg, 2006

CO_2 removal from syngas/flue gas has been used in different industries for many years, but is only recently gaining more and more attention in the energy-related sector (RVO, 2017). Besides gaining more attention in the energy sector, more novel materials for carbon capture are being researched (Boot-Handford et al., 2014). Different processes for carbon capture storage within the three main routes are researched (Figueroa, Fout, Plasynski, McIlvried, & Srivastava, 2008), also in combination with different set-ups with a gas turbine (Kvamsdal, Jordal, & Bolland, 2007). Furthermore, 21% of the world energy mix was covered by natural gas in 2017 (Enerdata, 2018; IEA, 2017c). Using this existing energy mix and adding the CCS units to this existing infrastructure, reduces the need for major investments for adaptions in the infrastructure by either costly or immature alternatives (Global CCS Institute, 2012).

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There is an evident mismatch between the conditions of the flue gas from SC-GT (e.g. high Temperature of flue gasses), especially when used for peaking applications, and the carbon capture preferred characteristics (e.g. low temperature flue gasses) (Mason, Sumida, Herm, Krishna, & Long, 2011). Due to this there are no, up to now, well-established processes for carbon capture applied to SC-GT. This research makes a first step in filling this gap and has the following main research question.

What is a technical feasible set-up for post combustion carbon capture applied to a simple cycle natural gas-fed gas turbine?

This main research question will be answered via the following sub-questions:

1. What kind of existing capture technologies are better suited for a simple cycle natural gas turbine?
2. What kind of sorbent medium is better suited for the previous selected capture technology?
3. What mathematical description should be adopted or developed to simulate the process and to calculate the resulting performance?
4. For the most promising solution, how should we adapt the capture process to meet the requirements of the application of interest?
5. What are the key operating parameters of the process? How do they affect the technical feasibility of the system?

Looking at the three main technological CCS routes, and keeping in mind the cost-effective solution, two of the three routes can already be excluded. In fact, both pre-combustion and oxy-fuel combustion share features, as complex plants for pre-combustion and major technology modifications for oxy-fed GT, that make them unsuitable for this framework application(Samanta, Zhao, Shimizu, Sarkar, & Gupta, 2012). In this project framework, the compression and the storage steps of the CCS are both excluded as these are well established research fields. This research will continue with the explanation of the methodology for the research. After the methodology a chapter on the technology screening and selection, followed by a chapter on sorption medium screening and selection. After the selection of the sorption medium, a chapter on isotherm model fitting followed by the results on the set-up sizing. The final two chapter are the discussion and conclusion of the research.

Chapter 2 Methodology

The method chapter is divided in the following research steps. First an identification of the framework. Second an explanation of how the literature review on appropriate carbon capture technologies is conducted and how the most suited technology for the SC-GT is selected. The technologies generally make use of sorbents for the CO_2 to be captured in. Therefore, third an explanation of how the literature review on the sorbent is conducted and how the appropriate sorbent is selected. Fourth an explanation which mathematical models are used to test the technology and sorbent in the SC-GT framework, followed by an explanation how the models are adapted for the research. Finally, the methodology on the sizing of the set-up to indicate the feasibility of the set-up.

2.1 Identification of the framework

The identification of the framework is done to specify what type of SC-GT is used in this research, what the operating characteristics are of the SC-GT and how the SC-GT is operated. The identification of the framework is divided into two steps, first an explanation of the selection criteria of the SC-GT and the selection of the SC-GT. Second the explanation of the constructing and the construction of the dispatch profile for the selected SC-GT. The dispatch profile is the number of start-up's the SC-GT makes and the duration of operation after the start-up.

Simple cycle gas turbine selection criteria

The selection of the SC-GT is based on three criteria. The first criterion is the start-up time of the SC-GT. The SC-GT has to start-up within a period of a maximum of 5 minutes to fit the function of supplying energy for the short-term flexibility (Papaefthymiou et al., 2014). The second criterion is the capacity of the SC-GT. The SC-GT only needs to supply peak demand as temporary addition to the baseload. Therefore, the capacity can be limited between a range of 25 MW to 70 MW. The third criterion is the age of the SC-GT, only new models not older than 5 years (2013) are considered. These have a longer lifetime remaining (30 years), are more efficient and are therefore a cost-effective solution (Carlsson, 2014).

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Using these three criteria a desk research is conducted constructing a list of SC-GT. The main brands in the handbook of gas turbines are included in the desk research; General electrics, Iskra Energetika, Kawasaki Heavy Industries, MAN, MAPNA group, Mitsubishi Hitachi power system, Mitsul Engineering & Shipbuilding, Motor Sich, MTU Friedrichshafen, NK engines, OPRA, Orenda, PW Power system, Rolls-Royce, Siemens, Vericor and Zorya-Mashproekt (Soares, 2015). From the list of the desk research a single SC-GT is selected for the research that fits the criteria best.

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From the selected SC-GT the following operating characteristics are of importance to the carbon capture process. The temperature of the flue gasses (T_f), flue gas mass flow and the weight content of the CO_2 in the flue gasses.

Selection of the Simple cycle gas turbine.

From the selection criteria mentioned above table 1 is constructed. Although not all have a suitable start-up time, all manufacturers refer to these types of SC-GT as designed for flexible operation.

Table 1: List of Simple cycle gas turbines, based on simple cycle gas turbine selection criteria.

Brand	Type	Year	Capacity (kW)	Start-up time)	efficiency (%)	mass flow (Kg/sec)	exhaust Temp T_f (^0C)	CO_2 content (wt.%)	Source
General Electric	LM 6000	2016	57479	5	40.8	146	487	6	(Corporation, 2010)
Siemens	SGT-750	2012	37031	<10	39.5	114.21	459	6	(Siemens AG, 2016)
MHPS	H-25 (42)	2014	42030	22	37.2	110.67	556	6	(Mitsubishi Hitachi power system, 2014)
Kawasaki	L30A	2012	30120	?	40.1	88.72	470	7	(Kawasaki Heavy Industries, 2010)

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The simple cycle gas turbine that meets the criteria the best, including the start-up time criterion, is the LM 6000 from General Electric. This is therefore the SC-GT selected in this research as the turbine for the framework.

Dispatch profile construction

To calculate the amount of CO_2 that is produced by the SC-GT a daily dispatch profile is constructed. The dispatch profile in this research is the number of start-ups the SC-GT must make each day and the time the SC-GT is operational after the start-up. This research looks at the peak demand during the day, in which two big peak demands occur (morning peak and evening peak see figure 3). The number of start-ups daily is therefore assumed to be two for this research. Using the capacity factor of SC-GT's, the number of hours it is operational after the start up is calculated. The capacity factor is the average power generated (MW) divided by the maximum capacity (MW) of the SC-GT (IEA, 2017b). The number of hours is multiplied by the flue gas per hour when operational, to calculate the total amount of flue gas that needs to be processed after each start-up. The capacity factor used in this research for the SC-GT is the average capacity factor of all the SC-GTs in the U.S.. Since the SC-GT is used as a peak demand supplier it operates as a marginal cost operator and therefore operates at full capacity. The average capacity factor of the SC-GT per month in the U.S. is shown in figure 5. The average capacity factor over the year is 9.4% which means the SC-GT on average operates for 2.25 hours per day (e.i.a. , 2017). The number of start-ups per day is assumed to be two, which means operation of 1.125 hours after each start-up. Which corresponds with the peak load demand of the world energy model of the IEA (IEA, 2017b).

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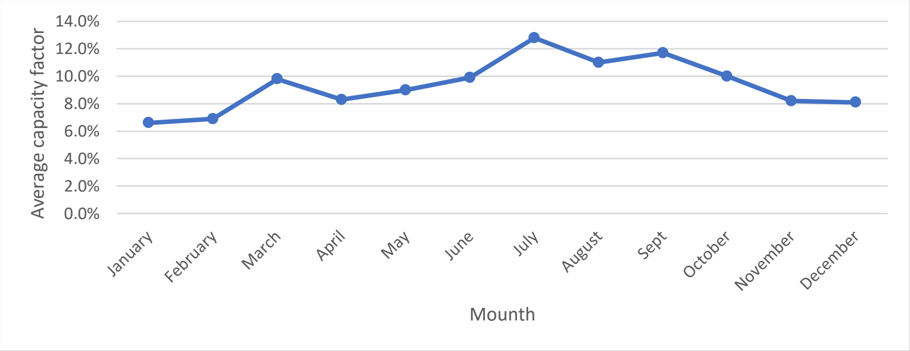

Figure 5: Average capacity factor SC-GT in the U.S. monthly. *Source: e.i.a., 2017*

2.2 Technology screening and selection

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To identify the most suitable post combustion carbon capture technique for the framework, a literature review is conducted. The literature is screened on technologies and the most suitable technology is selected on five criteria which are important to the framework.

The first criterion is a suitable working condition. The working conditions include the temperature and pressure in which the technology can operate. These should match or be in the range of the temperature and pressure of the SC-GT selected. The second criterion is the dynamic performance of the technology. Since the framework in which the set-up should work in, is a peak demand supplier, the technology should be able to handle flexible operations. The third criterion is the energy requirements of the CCS set-up. The aim of the SC-GT is to generate energy and therefore, the energy penalty on the SC-GT of the carbon capture process should be limited. The fourth criterion is the productivity of the sorbent. This entails the amount of sorbent needed to capture the CO_2. To have a feasible set-up it needs to be as compact as possible, thus limiting the size of the equipment and therefore limiting the amount of sorbent product needed. The fifth criterion is the separation performance, which is the purity of the recovered CO_2 and the amount removed CO_2 from the flue gasses. The purity is needed for the storage, after the capture step. The amount removed should be maximized, as the aim of the CCS set-up is to prevent the emission of the CO_2. The selection criteria and corresponding parameters are listed in table 2.

Table 2: performance criteria and parameters

Criterion	**Parameters**	**Typical range**
Suitable working condition	Pressure and temperature	Near ambient pressure T>300 ^{0}C
Dynamic Performance	flexibility operating points	Able to handle the flexibility
Energy requirements	Energy penalty inflicted	Minimalized
Productivity	Moles of CO_2/kg of sorbent	As high as possible
Separation performance	Purity and recovery CO_2	As high as possible

The literature review will be performed using the most powerful academic search engines, e.g. Google Scholar and ScienceDirect selecting relevant articles.

2.3 Screening and selection of the sorption medium

After the technology is selected a literature review is conducted on the sorbents (sorption medium) available in the selected technology. The sorbent is selected on the criteria listed in table 3, after table 3 an explanation of the selection criterion follows.

Table 3: selection criteria for sorbents

Criterion	**Parameter**	**Typical range**
Sorption capacity	Moles of CO_2/kg of sorbent	High as possible
Cyclic capacity	Stable sorption capacity in cycles operation	Cycles $\geq$10
Regeneration energy	Regeneration energy	As low as possible
Data availability	Available adsorption capacity q_{ix} at a CO_2 partial pressure P_{ix} range	-

First high cyclic stability since the sorbent must be used multiple times in high temperatures in the framework. Second lowest regeneration energy to avoid high energy penalties on the SC-GT. This research makes use of isotherm models which will be further explained in chapter 2.4 therefore, the third criterion is the availability of isotherms data, this is necessary for the selected sorbent. The isotherm data consist of the sorption capacity of the sorbent, at different CO_2 partial pressures with a minimum of two different temperatures.

2.4 Process synthesis.

The process synthesis is analysing the performance of the sorbent in the framework. To analyse the performance, this research uses isotherm models. Isotherm models are a mathematical approach in predicting the sorbents sorption behaviour (X. Chen, 2015). The isotherm models explain the sorption behaviour at framework pressure and temperature. The available isotherm models in literature are explained, followed by selecting the best model for the sorbent. After selecting the best available model for the sorbent, it is adapted to a temperature dependent model to adapt the sorption behaviour of the sorbent to the framework.

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Isotherm model fitting.

The sorbent isotherm data retrieved from the literature shows data points for the sorption capacity (q_{ix}) of the sorbent at a certain temperature (T) and partial pressure of the CO_2 (P_{ix}). The isotherm data is fitted to different isotherm models found in literature. The data is fitted to the models using the lsqcurvefit function in MATLAB which is a non-linear curve-fitting solver (see box2).

After fitting the data, the isotherm models are plotted with the sorbent isotherm data. The fit of the models to the data is tested using the R-Squared value (denoted as R^2). The R^2 value is a measure for the goodness of fit of the estimations of the different isotherm models and the sorbent data (The Pennsylvania State Univercity, 2018). The R^2 value has a value between 0 and 1 where 1 is a perfect fit, the isotherm model predicts all the data points for all the variations. For a R^2 value of 0 there is no fit at all, the corresponding isotherm model predicts for none of the data points. The R^2 is calculated with the following formula;

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$$(1)\ R^2 = 1 - \frac{SEE}{SST}$$

Where the SSE is the error sum of squares, the SSE quantifies the variation of the sorbent sorption capacity data points y_i around the estimation of the isotherm model sorption capacity y_{pi}. The SSE is calculated in the following manner;

$$(2)\ SEE = \sum_{i=1}^{n}(y_i - y_{pi})^2$$

The SST is the total sum of squares, The SST quantifies the variation of the sorbent sorption capacity data points y_i around their mean $\bar{y}$. The SST is calculated in the following manner;

$$(3)\ SST = \sum_{i=1}^{n}(y_i - \bar{y})^2$$

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The isotherm equation with the highest R-squared value predicts the sorption behaviour of the sorbent best and is used for the sorbent for the following step.

Box 2: Description and Syntax of the lsqcurvefit function in MATLAB

Description:

The lsqcurvefit is a solver for nonlinear curve-fitting problems in a least-squares sense. The solver finds the coefficients x which solves the problem;

$$\frac{min}{x} \parallel F(x, xdata) - ydata \parallel \frac{2}{2} = \frac{min}{x} \sum_i (F(x, xdata_i) - ydata_i)^2$$

Where the xdata is the input data and ydata is the observed output data. The F(x,xdata) is a user-defined function that computes a matrix with the same size as the ydata.

Syntax:

x = lsqcurvefit(fun,xo,xdata,ydata)
Where;
x= output matrix with fitted coefficients
fun = user-defined function that fits the x-coefficients using the xdata to the observed ydata.
x0=initial x guesses.
xdata=input data.
ydata=observed output data.

Temperature dependence model fitting

The isotherm models in the previous step explain the sorption capacity of the sorbent at different P_i at a certain fixed temperature. To predict the sorption capacity in the framework temperature, the model with the highest R^2 value, which is the best model, is made temperature dependent.

After adapting the model, the sorbent isotherm data is fitted using the fmincon function in MATLAB (see box 3). In this fitting step multiple isotherms from different temperatures are used, in contrast to the previous step where only one temperature isotherm is fitted.

Box 3: Description and syntax of the Fmincon function in MATLAB

Description:
The fmincon function is a nonlinear programming solver. The solver finds the minimum of a problem which is specified by;

$$\frac{min}{x} f(x) such\ that \begin{cases} c(x) \leq 0 \\ ceq(x) = 0 \\ A * x \leq b \\ Aeq * x = beq \\ lb \leq x \leq ub \end{cases}$$

Syntax:
[x,fval,exitflag,output] = fmincon(fun,xo,A,b,Aeq,beq,lb,ub,nonlcon,options)

Where;

x= output matrix with fitted coefficients.
Fval = returns the value of the objective function at the solution x
Exitflag = describes the exit condition of fmincon
Output = information about the optimization process.
fun = user-defined function that fits the x-coefficients.
x0=starting point for the x coefficients.
A= linear inequalities input A*x ≤ b.
b= linear inequalities input A*x ≤ b.
Aeq= linear equalities input Aeq*x ≤ beq.
Beq= linear equalities input A*x ≤ beq.
Lb= lower bound constraint for x so that lb≤x .
Ub= upper bound constraint for x so that ub≥x.
Nonlcon= defines the nonlinear inequalities c(x) or equalities ceq(x), c(x)≤0 and ceq(x)=0.
Options= specification of the minimization options.
If there is no linear inequality, linear equalities, upper and lower bound or nonlinear inequality set the corresponding matrix to [].

The Fmincon-function is a function that minimalizes the objective by changing the parameters x with the objective;

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$$(4)\ objective = \frac{\min}{x} \sum_{i=1}^{n} \left(\frac{y_{pi} - y_i}{y_i}\right)^2$$

Where;

y_{pi} = predicted sorption capacity with corresponding temperature and P_i of the temperature dependant model.

y_i = retrieved sorption capacity data (q_{ix}) from literature with corresponding temperature (T) and CO_2 partial pressure (P_{ix}).

X = the temperature dependent parameters of the adapted model.

By minimizing the objective, the difference between the predicted sorption capacity of the model and the sorption capacity of the sorbent data are minimized.

Set-up sizing

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What I investigate
- -CCR
- -Operating time

Key paramters.

The last step in analysing the set-up is testing the feasibility of the set-up. The feasibility of the set-up in this research is dependent on the size of the set-up, where the objective is minimizing the size of the set-up. The set-up is coupled to the LM-6000 SC-GT which operates for 1.125 hours per start-up. Assumed is that the amount of CO_2 emitted in this period is processed by the set-up before the next start-up. The initial requirements of the set-up are a minimum carbon capture rate of 0.9 meaning 90% of the CO_2 in flue gasses should be captured with a purity of the captured CO_2 of 95%. After the initial sizing two parameters are altered, the operation hours and the CCR.

As explained in the introduction the energy demand can vary through the year, month and day. Furthermore, the increasing flexibility demand in the future could influence the dispatch profile. A key parameter in the process is thus the operation hour. Therefore, the influence of a variating operation hours, from 0.5 hours per start-up to 3 hours per start up, on the sizing of the set-up is analysed.

The CCR has an obvious direct influence on the size of the set-up, as it defines the amount of CO_2 captured. To analyse the influence on the feasibility, the CCR is varied from a 1 CCR to 0.1 CCR.

Chapter 3 Technology Screening and selection

This chapter is divided into two parts. The first part is the screening of the different post combustion carbon capture techniques. This screening consists of an explanation of the fundamentals of the technology. Based on the selection criteria in table 2, in the second part, the technology most suited for the framework is selected.

3.1 Technology screening

The literature is screened for post-combustion carbon capture technologies. Three main technologies are identified; absorption, membranes and adsorption (Horn & Zbacnik, 2015). The fundamentals of each of the technologies are explained separately.

Commented [MA18]: Reference?

Absorption

The post combustion carbon capture absorption can be split up into physical absorption and chemical absorption of CO_2. The physical adsorption is based on 'Henry's law', where CO_2 is physically absorbed into a sorbent (Wang, Lawal, Stephenson, Sidders, & Ramshaw, 2011) . Henry's law states that the solubility of a gas into the sorbent is directly proportional to the partial pressure of the gas. The gas is pressurized and solved into the sorbent. In chemical absorption the CO_2 forms a weakly bounded intermediate compound by chemically reacting with the solvent (Ibid). The resulting equilibrium between CO_2 and solvent is dependent on temperature. The solvent can be regenerated by heat application dissolving the CO_2 from the sorbent into a stream of CO_2 and leaving the sorbent (Ibid). Figure 6 shows a typical set up for post combustion CO_2 capture using chemical absorption.

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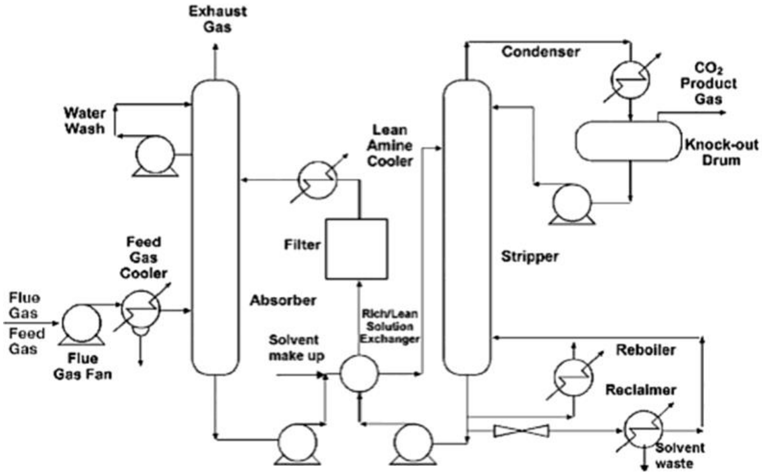

Figure 6: Typical configuration of an absorbent based post-combustion carbon capture process. Source: Wang et al., 2011

Membranes

Membranes are a porous material that can filter CO_2 from the flue gas. The membrane depends on the selectivity and permeability. The selectivity is the quality of filtering one component out of the flue gas over other components. The permeability is the amount of a substance can pass through the membrane at a certain pressure (Bhown & Freeman, 2011). Permeability has a direct influence on the membrane surface needed for a certain amount of flue gas. Doping the membranes with sorbents is an option to enhance the performance of the membranes (Zhao et al., 2016). The gas can either be pushed though the membrane by pressurizing the flue gas, or pulled through the membrane by creating a vacuum on the other side of the membrane (Horn & Zbacnik, 2015). Figure 7 gives a visual representation of the mass transfer trough a gas-liquid membrane.

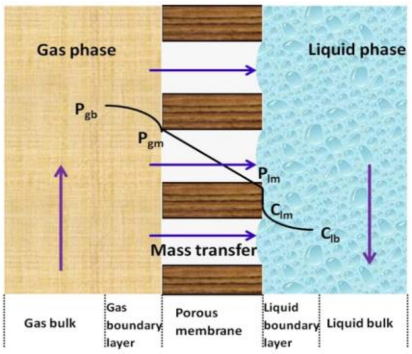

Figure 7: Mass transfer through a gas-liquid membrane for CO_2 capture. Source: (Zhao et al., 2016)

Adsorption

Adsorption relies on the adsorption of the CO_2 onto the surface of a solid sorbent. This can rely on either a covalent bound called chemisorption or on a weaker bound based on 'van der Waals' forces called physisorption. The CO_2 is directed into a column where it is adsorbed onto the sorbent, after which the CO_2 is regenerated by changing the pressure (pressure-swing) and/or temperature (temperature-swing) of the column or switching to another column with a different pressure and/or temperature. The switch in pressure and/or temperature liberates the CO_2 from the sorbent inducing a CO_2 stream out of the column (Bhown & Freeman, 2011). Figure 8 shows a representation of a Temperature swing adsorption process.

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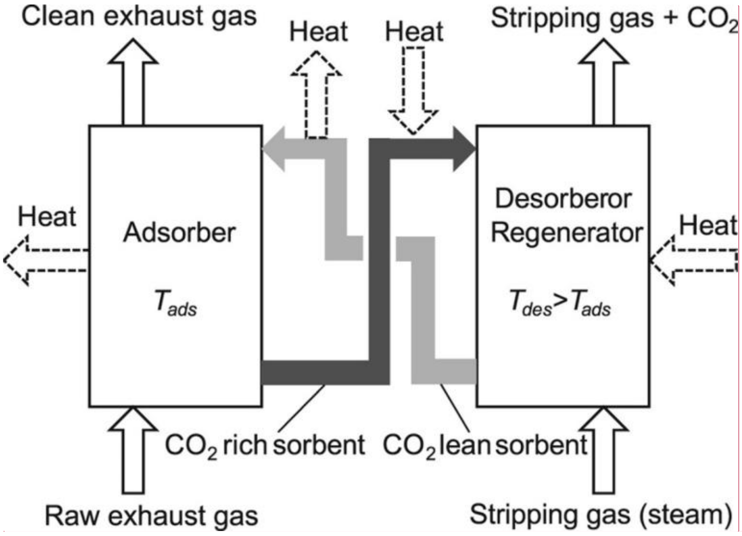

Figure 8: Representation of a temperature swing adsorption process source: (Pröll, Schöny, Sprachmann, & Hofbauer, 2016)

Commented [MA24]: Introduction and evaluation of a double loop staged fluidized bed system for post-combustion CO_2 capture using solid sorbents in a continuous temperature swing adsorption process

3.2 Technology selection

Based on the performance criteria from table 2, adsorption is selected as the only suitable technology for the framework. Table 4 shows a summary of the different technologies and their score on the performance criteria. After table 4 the three technologies and their score on the performance criteria is explained.

Table 4: Technology selection based on criteria from table 2. Green score: technology well suited for the framework Orange score: technology able to operate in framework, but not preferred Red score: Technology not able to work in the framework.

	Suitable working conditions	Dynamic performance	Energy requirements	Productivity	Separation performance
Absorption	🟥	🟩	🟩	🟩	🟩
Membranes	🟥	🟨	🟥	🟩	🟥
Adsorption	🟩	🟩	🟨	🟨	🟩

Absorption

Suitable working conditions; Absorption for both chemical and physical scores red on suitable working conditions. for both the physical and chemical absorption the sorbents in the absorption process show high volatility and degradation at elevated temperatures. Typical temperature ranges for absorption are between 40 ^{0}C to 60 ^{0}C (Davis & Rochelle, 2009) . The pressure range in which the absorption process operates in is slightly above atmospheric pressure 1.5-2 atm (Ibid).

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Dynamic performance; absorption scores green on dynamic performance. The design of a cyclic set-up the absorption can achieve good dynamic performance (Peeters, Faaij, & Turkenburg, 2007).

Energy requirements; for physical absorption the energy requirements scores red. In physical absorption the energy penalty relatively high, due to the high heat/power requirements for solvent regeneration and the requirement of pressurization of the feed(Wang et al., 2011). In low CO_2 partial pressure streams (<15%) the physical absorption process is deemed not economical due to the pressurization requirements (Ibid). For Chemical absorption, the absorption scores green because it shows a high selectivity for CO_2 and therefore no pressurization is needed of the feed gas. This reduces the energy penalty significantly (Ibid).

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Productivity; for physical absorption the productivity scores red it shows low selectivity for CO_2 and thus a relatively large amount of sorbent is needed(Wang et al., 2011). Chemical sorbents score green, it shows a high selectivity for CO_2, a relative small amount of sorbent is needed for the chemical absorption process (Ibid).

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Separation performance; Absorption scores green in separation performance in general, however the sensitivity of the solvents to losses in chemical purity/quality due to infiltrations from other by-products (e.g. SOx, NOx) in the flue gas streams, which leads to reduction in efficiencies of purity and recovery(Wang et al., 2011).

Membranes

Suitable working conditions; Membranes score red on the suitable working conditions. The thermal stability of the membranes is low, they depend on the glass transition temperature (T_g) and the melting temperature (T_m). The Polyether ether ketone (PEEK) shows the highest thermal stability with a Tg of 145 ^{0}C and a Tm of 335 ^{0}C (Zhao et al., 2016). The Membranes can operate in the required pressure of the framework (Ibid).

Commented [MA29]: status and progress of membrance contractors in post-combustion carbon capture: a state of the art review of new developments.

Dynamic performance; The membranes score green on the dynamic performance. The membranes show good dynamic performance, as they can be modular added to the plant. An experimental example is the Polyamidoamine dendrimer and MEA-tube side(Zhao et al., 2016).

Energy requirements; The membranes score red on energy requirements. The mass transfer increases with an increased partial pressure in the gas. Pressurization of the flue gasses above the ambient pressure to P>1Mpa is necessary for an efficient mass transfer. The pressurization of the flue gasses is an energy intensive process (Zhao et al., 2016).

Commented [MA30]: https://chem.libretexts.org/Textbook_Maps/Physical_and_Theoretical_Chemistry_Textbook_Maps/Supplemental_Modules_(Physical_and_Theoretical_Chemistry)/Physical_Properties_of_Matter/Solutions_and_Mixtures/Ideal_Solutions/Dissolving_Gases_In_Liquids%2C_Henry's_Law

Productivity; the membranes score green on productivity. The membranes act as barriers non-dispersive contacting system to separate two phases, this set-up has a large contact area for mass transfer (Zhao et al., 2016). Therefore, the size of the set-up and amount of sorbent needed can be limited, thus showing good productivity (Ibid).

Separation performance; The separation performance scores red for the membranes. The separation performance is depending on the pressure difference between the sides of the membrane. Pressurization of CO_2 partial pressure of above 20% is preferred for good separation performance (Wang et al., 2011).

Adsorption

Suitable working conditions; Adsorption scores green on suitable working conditions. The working conditions of the adsorption show high temperatures, this is caused by the non-volatility nature of the sorbents (Joss, Gazzani, & Mazzotti, 2017). The temperatures range between 300 ^{0}C and 900 ^{0}C for the adsorption step. The pressure typical for adsorption process is around ambient pressure (Shokrollahi Yancheshmeh, Radfarnia, & Iliuta, 2016).

Commented [MA31]: rational design of temperature swing adsorption cycles for post-combustion CO_2 capture.

Commented [MA32]: Sources from table

Dynamic performance; Adsorption scores green on dynamic performance. Similar to absorption, in adsorption cyclic set-ups are able to achieve good dynamic performance (Reynolds, Ebner, & Ritter, 2006).

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Energy requirements; adsorption scores orange on energy requirements. The energy requirements for the adsorbents is relatively high, since the regeneration is done by either compressing or heating to high temperature. Especially calcium looping and ceramics requires high regeneration temperatures and thus high energy requirements (Shokrollahi Yancheshmeh et al., 2016).

Productivity; adsorption scores orange on productivity. Adsorbents in general suffer from a low selectivity for CO_2 compared to the other technologies. The adsorbents also show a relative large decrease in productivity when the adsorption temperature increases (Samanta et al., 2012).

Commented [MA34]: Post combustion CO_2 capture using solid sorbents: a Review

Separation performance; adsorption scores green on separation performance. The separation performance of the adsorption process show that purities of above 95% are reached with recovery also above 60% (Shokrollahi Yancheshmeh et al., 2016).

Chapter 4 Sorbent screening and selection

The sorbent screening and selection is divided into two pats. First a screening section where the fundamentals of the sorbents are explained. Followed by the selection of the appropriate sorbent for the framework based on the selection criteria from table 3.

4.1 Sorbent screening

The sorbent screening identifies three main adsorption sorbents available; Calcium, ceramics and Hydrotalcite like compounds (HTC) (Halabi, De Croon, Van Der Schaaf, Cobden, & Schouten, 2012). The fundamentals of each sorbent are explained separately.

Commented [MA35]: High potassium-promoted hydrotalcite for CO_2 caputer in H_2 production

Calcium Looping

The CaO is known as one of the most famous natural CO_2 sorbents in the form of limestone and dolomite (Samanta et al., 2012). The basic adsorption and desorption reaction of the CaO looping is given by;

$$(5)\ CaO(s) + CO_2(g) \leftrightarrow CaCO_3(s)$$

The regeneration of the CO_2 from the formed $CaCO_3$ is done by heat application (Samanta et al., 2012).

Ceramics

Ceramics are presented as an alternative to the CaO looping for CO_2 adsorption (Shokrollahi Yancheshmeh et al., 2016). A well investigated example is the Li_4SiO_4, with the following adsorption and desorption reaction:

Commented [MA36]: High temperature co_2 sorbents and their application for hydrogen production by sorption enhanced steam reforming process.

$$(6)\ Li_4SiO_4(s) + CO_2(g) \leftrightarrow Li_2CO_3(s) + Li_2SiO_3(s)$$

The ceramics are considered due to their ability to retain good sorption capacity at high temperatures in contrast to the CaO (Shokrollahi Yancheshmeh et al., 2016). Regeneration of CO_2 is like the CaO done by heat application to break the strong chemical bounds (Ibid).

Hydrotalcite like compounds (HTC)

Hydrotalcite like compounds have been researched as a CO_2 adsorbent for more than a decade(Bhatta, Subramanyam, Chengala, Olivera, & Venkatesh, 2015). The HTC belongs to the anionic basic clays and are also known as the layered double hydroxides (Ibid). The structure of the HTC is a positively charged brucite-like layer and a negatively charged interlayer. A general formula for the structure of the HTC can be represented as; $[M^{2+}_{1-x}M^{3+}_{x}(OH)_2]^{x+}(A^{n-}_{\frac{x}{n}})\cdot mH_2O$ where the M^{+2} can be any of the following elements Mg, Cu, Ni, Mn, Zn; and M^{3+} any of the following elements Al, Fe, Cr, V; A^{n-} is the interlayer anion and can be any of the following ions CO_3^{2-}, CL^-, NO_3^-, SO_4^{2-}. The x can be within the range of 0.1 and 0.33.

Commented [MA37]: Progress in hydrotalcite like compounds and metal-based oxides for CO_2 caputer: a review.

4.2 sorbent selection

Table 5 shows a summary of the scores of the sorbent based on the selection criteria of table 3. The hydrotalcite like compounds is selected as the only sorbent suited for the framework. After table 5 the scores of the sorbents are explained separately. After each of the explanations a table with additional consulted articles is presented. After the explanation the characteristics of the specific Hydrotalcite like compounds selected for the next step are shown in table 9.

Table 5: Sorbent medium selection based on selection criteria from section 2.3. Green score: sorbent well suited for the framework Orange score: sorbent able to operate in framework, but not preferred Red score: sorbent not able to work in the framework.

	Sorption capacity	Cyclic stability	Regeneration Energy	Data availability
Calcium looping	🟩	🟨	🟨	🟥
Ceramics	🟩	🟨	🟨	🟥
HTC	🟨	🟩	🟩	🟩

Calcium looping

Calcium looping scores green on sorption capacity; the theoretical CO_2 uptake of the CaO is high, as high as 17.8 mol CO_2 per kg of sorbent. With adsorption temperatures well above 600 ^{0}C (Shokrollahi Yancheshmeh et al., 2016).The regeneration energy scores red for calcium looping; the regeneration temperatures are high for CaO looping due to the thermodynamically unfavourable desorption reaching temperatures at minimum of 700 ^{0}C (Halabi et al., 2012). The cyclic stability scores yellow for calcium looping, due to sintering and build-up of irreversible $CaCO_3$ (Ibid). Producing CaO from various calcium precursors or pre-treating the sorbent with the aim of high thermal and cyclic stability has been studied (Ibid). The results show an increase of cyclic stability (up to 100 cycles) however a decrease in the sorption capacity (0.38 mole CO_2/kg sorbent), still high regeneration temperatures (850^{0}C) (Ibid). Table 6 shows additional articles consulted on calcium looping experimental data.

Commented [MA38]: To select the medium for this framework a literature review for the different mediums is conducted. The medium is selected based on the adsorption temperature, adsorption pressure, adsorption capacity and cyclic capacity. The adsorption temperature is the temperature at which the medium is still able to operate in, this temperature needs to be as high as possible. The adsorption pressure is the pressure at which the medium adsorbs in, the adsorption pressure should be as close to the ambient pressure as possible. Adsorption capacity is the moles of CO_2 the medium is able to adsorb per kg of medium. The cyclic capacity is the capacity of the medium to operate multiple times with a stable adsorption capacity.

Commented [MA39]: High capacity potassium-promoted hydrotalcite for CO_2 capture in H_2 production.

Commented [MA40]: High capacity potassium-promoted hydrotalcite for CO_2 capture in H_2 production.

Table 6: additional consulted articles for Calcium looping. The sorbent base, sorbent support, adsorption temperature of described experiment, adsorption pressure of described experiment, sorption capacity and additional information.

Calcium Looping						
Sorbent base	**Sorbent support**	**Temperature**	**Pressure**	**Capacity (mol CO_2/kg sorbent)**	**Additional information**	**Reference**
CaO	-	-	-	1.77	Long term sintering problem	(Shokrollahi Yancheshmeh et al., 2016)
Organomatallic precursors	-	-	-	-	Sintering problem	
Strassburg limestone CaO	CaCo3	850 C	atmospheric	-	Extreme decrease in CO2 sorption in number of runs	(Sun, Jim Lim, & Grace, 2008)
CaO	Ca12AL14O33	650 C	-	0.99	No Sintering after 30 cycles.	(Liu, Li, Liu, & Li, 2013)
CaO (nano)	MgO	700 C	-	0.45	calcination in N2 at 730 C. Also Calcination with CO2 with an increase in sintering!	(Lan & Wu, 2014)
CaO sol-gel-derived	ZrO2	650 C	-	0.77	-	(Broda & Müller, 2014)
CaO	hydration during carbonation	-	-	-	Very small impact and diverse results in literature	(Shokrollahi Yancheshmeh et al., 2016)
CaO	hydration after regeneration		-		ittrition, sintering and costly	(Shokrollahi Yancheshmeh et al., 2016)
CaO (limestone)	Heat-pretreated	650 C	-	0.2	Energy penalty?	(Valverde, Sanchez-Jimenez, & Perez-Maqueda, 2014)
CaO	Chemical pretreatment	650 C	-	0.2	Cost of concern	(Valverde et al., 2014)
CaO (limestone)	Chemical pretreatment	650 C	-	1.47	With pellets which increase the cost dramatically	(H. Chen, Zhao, & Yang, 2013)

Ceramics

Ceramics score green for sorption capacity, because it shows a high sorption capacity (up to 59 mol CO_2/kg sorbent). Ceramics scores yellow for cyclic stability, it shows improved cyclic stability compared to the CaO based sorbents (up to 100 cycles)(Halabi et al., 2012). however, ceramics show a strong chemical bounding with the CO_2 resulting in a high energy need for regeneration (>700 ^{0}C) (Ibid). Therefore, the ceramics scores red on regeneration energy. The ceramic sorbents are also experimental and are only tested in small scale laboratory-based experiments. Besides only being tested in laboratory-based experiments, the kinetic models explaining the adsorption and desorption process are still being investigated (Ibid). Table 7 shows additional articles consulted with on ceramics experimental data.

Commented [MA41]: High capacity potassium-promoted hydrotalcite for CO_2 capture in H_2 production.

Table 7: additional consulted articles for Ceramics. The sorbent base, sorbent support, adsorption temperature of described experiment, adsorption pressure of described experiment, sorption capacity and additional information.

Ceramics						
Base	**Support**	**Temperature**	**Pressure**	**sorbent capacity**	**Additional information**	**Reference**
Li2ZrO3	Prepared by spray drying	575 C	?	0,24 g CO2/ g sorbent	regeneration in an Ar environment at 650 C	(Ochoa-Fernandez, Ronning, Grande, & Chen, 2006)
Li4SiSO4	K	580 C	atmospheric pressure of flow	0,15 g CO2/ g sorbent	Regeneration in N2 at 700 C	(Seggiani, Puccini, & Vitolo, 2013)
Na2ZrO3		575 C	?	0,15 g CO2/ g sorbent	Unfavorable regeneration kinetics. Regeneration at 680C in Ar	(Shokrollahi Yancheshmeh et al., 2016)
Other ceramics					Highly experimental and theoretical	(Shokrollahi Yancheshmeh et al., 2016)

Hydrotalcite like compounds

The HTC scores yellow on sorption capacity because it shows relative low adsorption capacity compared to calcium looping and ceramics (0.3-0.9 mol CO_2/kg sobent)(Halabi et al., 2012; Selow, Cobden, Verbraeken, Hufton, & Brink, 2009). HTC scores green on cyclic stability; dispersing the HTC of a large surface, shows good cyclic capacity and improved adsorption capacity. The cyclic stability shows a 5-10% loss of capacity after up to thousand cycles(Bhatta et al., 2015). The regeneration energy requirements of the HTC relatively low compared to the other sorbents due to the lower heat of adsorption(Iruretagoyena, Shaffer, & Chadwick, 2014). Table 8 shows additional articles consulted on hydrotalcite like compounds.

Commented [MA42]: Adsorption of carbon dioxide on graphene oxide supported layered double oxides.

Commented [MA43]: Process in hydrotalcite like compounds and matal-based oxides for CO_2 capture: a review

Commented [MA44]: Adsorption of carbon dioxide on graphene oxide supported layered double oxides.

Table 8: additional consulted articles for Hydrotalcite like compounds. The sorbent base, sorbent support, adsorption temperature of described experiment, adsorption pressure of described experiment, sorption capacity and additional information.

HTC						
Sorbent (basis)	**support**	**Temperature ^{0}C**	**Pressure (bar)**	**Capacity q_i (molCO_2 /kg sorbent)**	**Other**	**Reference**
HT	GO	300 C	1 bar absolute	0.30	multicycle isotherms are fitted after stabilization of the capacity	(Iruretagoyena et al., 2014)
AL HTLc	K-promoted Mg	400 C	Pressure swing from 3,5-1 bar	0,89		(Halabi et al., 2012)
HTlc	k2CO3 promoted	400 C	28 bar feed pressure	0,29	Stable after the multiple cycles.	(Selow et al., 2009)
HTLc	K2 CO3 promoted	400 C	2 bar	0,77		(Oliveira, Grande, & Rodrigues, 2008)

Table 9: Sorbents selected based on availability of isotherm data set.

** Size of LDO1, LDO2 and LDO3 was not available, size was set to 800 by default.*

Name	Base	support	Wt% support	Size kg/m^3	Source
LDO1	$Mg_{0.6}Al_{0.3}(OH)_2(CO_3)_{0.15}\cdot nH_2O$	No	0	800*	(Iruretagoyena et al., 2014)
LDO2	$Mg_{0.6}Al_{0.3}(OH)_2(CO_3)_{0.15}\cdot nH_2O$	GO	20/1	800*	(Iruretagoyena et al., 2014)
LDO3	$Mg_{0.6}Al_{0.3}(OH)_2(CO_3)_{0.15}\cdot nH_2O$	GO	3/1	800*	(Iruretagoyena et al., 2014)
HTC1	$MgO:Al_2O_3$	K_2CO_3	22	748.6	(Halabi et al., 2012)
HTC2	$MgO:Al_2O_3$	K_2CO_3	22	748.6	(Halabi et al., 2012)

Table 9 describes the characteristics of the HTC sorbents selected for the research. These sorbents are selected because of the availability of isotherm data, the isotherm data is shown in table 17 in Appendix A.

Chapter 5 Isotherm-model fitting

As explained in chapter 2.4, to test the performance of the different sorbents in the framework this study uses isotherm models. There are many different isotherm models described in the literature, the isotherm models used in this report are listed in table 10. This chapter starts with a description of the isotherm models used. Followed by fitting the models to the isotherm data of the selected sorbents. At the end of the fitting section the best model for each of the sorbent is shown.

5.1 isotherm model selection

The first model described is the Langmuir model, which originates from 1918 (Do, 1998). The Langmuir model describes the adsorption on a monolayer ideal surface(Ibid). The model has two parameters, the first parameter is n_i^∞ which is the saturation capacity of the surface and the second parameter k_i which is a constant. The second isotherm model is the Freundlich equation (1932), which is the first empirically used model (Ibid). In this model the adsorption capacity is dependent on two temperature dependent parameters K and n. The parameter n is to account for the non-linearity in the adsorption capacity with respect to the pressure(Ibid). The third model is the Sips (Langmuir-Freundlich) model (1948) which shows the same parameters as the Langmuir model where, it adds one extra parameter c_i accounting for the inhomogeneity in the surface (non-ideal surface) (Ibid). The Freundlich equation shows low validity in the low and high end of the pressure range, where the Sips equation shows low validity in the low range of the pressure range(Ibid). Both equations do not provide the correct Henry law type behaviour (Ibid). Therefore, a fourth isotherm model is included; the Toth model. The C_{us} is the saturation capacity, the b and the t describe the heterogeneity in the system and are specific for the sorbent and the component (Ibid). This three-parameter equation can describe many adsorption data well (Ibid).

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Pure and binary adsorption of CO_2, H_2 and N2 on activated carbon.

Commented [MA46]: . Meaning the (page 33).

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Table 10: Isotherm model used in this research.

Isotherm type	Equation	Source?
Langmuir	$(7)\ q_i(P_i) = \frac{n_i^\infty * k_i * P_i}{1 + k_i * P_i}$	(Do, 1998)
Freundlich	$(8)\ q_i(P_i) == K * P_i^{\frac{1}{n}}$	(Do, 1998)
Sips	$(9)\ q_i(P_i) = n_i^\infty * \frac{k_i * P_i^{c_i}}{1 + (k_i * P_i)^{c_i}}$	(Do, 1998).
Toth	$(10)\ q_i(P_i) == C_{us} * \frac{b * p}{(1 + (b * p)^t)^{\frac{1}{t}}}$	(Do, 1998)

5.2 Isotherm model fitting

The retrieved sorbent isotherm data points from literature for the sorbents selected in chapter 3 (table 17 in appendix A) are fitted to the isotherm models from table 10 using the lsqcurvefit function in MATLAB (see box 2). As input for the lsqcurve fit for the different models the matrix x0 is set as default to 1. The xdata is the partial pressure data from the literature (P_{ix}), the ydata is the adsorption capacity data (q_{ix}). For all the sorbents the lsqcurvefit function is run, the resulting parameters for the different models shown in table 11. The R^2 values are calculated using equations (1), (2) and (3) and resulting R^2 values are shown in table 12. The parameter output is plotted in figures 9 to figure 15.

Table 11: Lsqcurvefit function parameter output for isotherm models parameters of table 6.

	Langmuir		Freundlich		Sips			Toth		
	n_i^{∞}	k_i	K	n	n_i^{∞}	k_i	c_i	q_s	b	t
$LDO1_{low}$	0,194	27,38	0.2000	5,563	0.296	5.709	2.476	14.88	0.189	1.449
$LDO1_{high}$	0,168	14,9	0,1693	3,893	0.238	4.554	1.834	10.75	0.160	1.351
$LDO2_{low}$	0,255	21,00	0,2579	4,868	0.384	4.905	2.222	15.67	0.250	1.211
$LDO2_{high}$	0.203	17.38	0.2075	4.233	0.312	3.809	2.125	12.54	0.206	1.098
LDO3	0,297	20,41	0,3073	4,499	0.573	1.355	2.748	20.65	0.330	0.785
HTC1	1,28	2,368	1,009	1.796	4.616	0.108	1.600	1.444	12.45	0.254
HTC2	1,19	3,740	1.009	2.300	5.258	0.051	2.035	18.21	27.11	0.151

Table 12: R^2-value for the fitted isotherm models to the sorbent data. The green highlights show the highest R^2 value for each of the models per sorbent. Subscript low = 300^0C, high=350^0C

	Langmuir	Freundlich	Sips	Toth
$LDO1_{low}$	0,961	0,810	0,880	0,926
$LDO1_{high}$	0.997	0.884	0.952	0.994
$LDO2_{low}$	0,994	0,856	0,925	0,988
$LDO2_{high}$	0.951	0.910	0.950	0.937
LDO3	0,906	0,980	0,990	0,923
HTC1	0,873	0,927	0,920	0,914
HTC2	0,843	0,944	0,936	0,932

The green highlights in table 12 show the highest R-squared values for the isotherm equations of the different sorbents. As can be seen in figure 9, figure 10, figure 11 and figure 12 the $LDO1_{low}$, $LDO1_{high}$, $LDO2_{low}$ and $LDO2_{high}$ are best described by the Langmuir and the Toth model. The Langmuir model shows a slightly higher R^2 value than the Toth model, therefore the Langmuir model is adopted for $LDO1_{low}$, $LDO1_{high}$, $LDO2_{low}$ and $LDO2_{high}$ sorbents. LDO3 shown in figure 13 shows that the R^2 value are highest for the Freundlich and the Sips equations. The Sips model has a R^2 value of 0.990 which is 0.01 higher than the Freundlich and is therefore adopted for the LDO3. HTC1 and HTC2 shown in figure 14 and 15 show that Freundlich and the Sips model describe these sorbents best. HTC1 and HTC2 have a R^2 value of 0.927 and 0.944 respectively for the Freundlich model, which are the highest R^2 values. The Freundlich model is therefore adopted for the HTC1 and HTC2 sorbents.

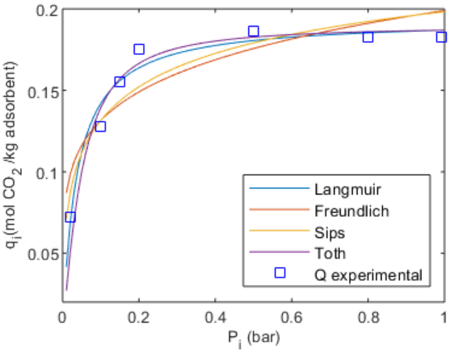

Figure 9: LDO1$_{low}$ isotherm model plots with sorption

Capacity Q$_{experimental}$ retrieved from literature T = 300 ^{0}C

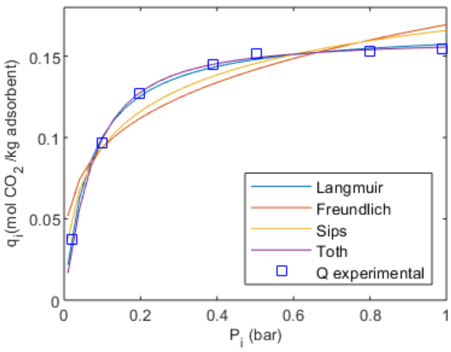

Figure 10: LDO1$_{high}$ isotherm model plots with sorption

Capacity Q$_{experimental}$ retrieved from literature T = 350 ^{0}C

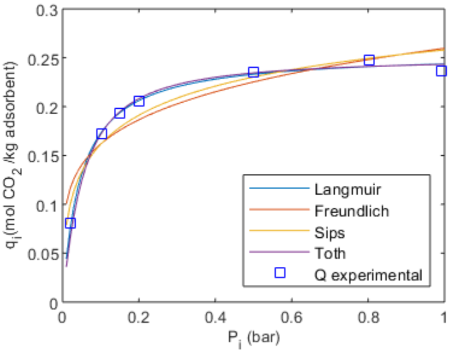

Figure 11: LDO1$_{low}$ isotherm model plots with sorption

Capacity Q$_{experimental}$ retrieved from literature T = 300 ^{0}C

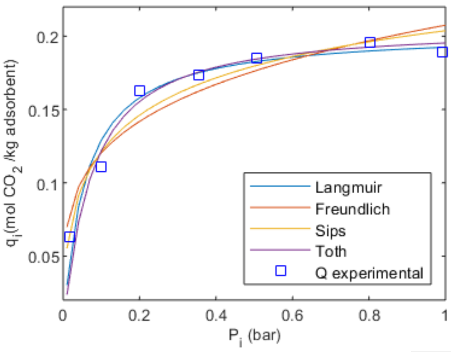

Figure 12: LDO2$_{high}$ isotherm model plots with sorption

Capacity Q$_{experimental}$ retrieved from literature T = 350 ^{0}C

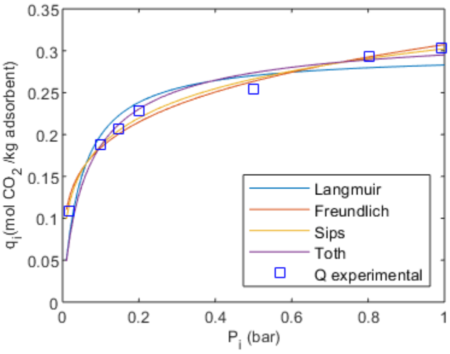

Figure 13: LDO3 isotherm model plots with sorption

Capacity Q$_{experimental}$ retrieved from literature T = 300 ^{0}C

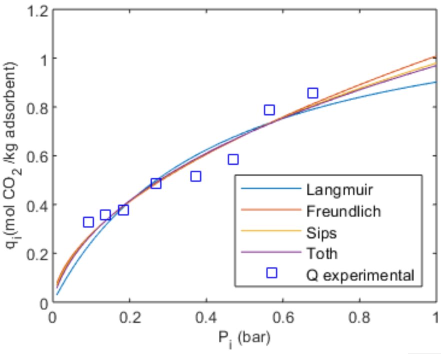

Figure 14: HTC1 isotherm model plots with sorption

Capacity Q$_{experimental}$ retrieved from literature T = 400 ^{0}C

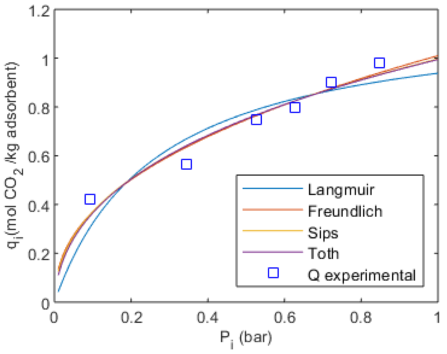

Figure 15: HTC2 isotherm model plots with sorption

Capacity $Q_{experimental}$ retrieved from literature $T = 400\ ^0C$

6 Temperature dependent isotherm model

The isotherm models described and fitted in the previous chapter describe the sorption behaviour of the sorbents for different CO_2 partial pressure. To describe the sorption behaviour for the working temperature of the selected framework, the models need to be adapted to temperature dependent models. This chapter starts with an explanation of how the model is made temperature dependent, followed by the fitting of the new temperature dependent model to the sorbent data.

To adapt the model to a temperature dependent model, it is fitted to multiple isotherms of different temperatures. Only for LDO1 and LDO2 isotherm data at multiple temperatures is available. LDO2 outperformed LDO1 on sorption capacity as can be seen in figure 9, figure 10, figure 11 and figure 12. Based on the available data and the better performance of the sorbent, it was decided to test the temperature dependent model on the sorbent LDO2. Moreover, LDO2 is the sorbent used for the final set-up sizing.

Commented [FA48]: Ik weet niet of mijn toevoeging een juiste weergave is?

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6.1 Temperature dependent model adaption

The Langmuir isotherm model describes the sorption behaviour best for LDO2. Therefore, the Langmuir model is adapted and made temperature dependent. The Langmuir isotherm model contains two parameters; n_i^∞ the sorption capacity and the constant k_i. The adaption of the temperature dependency of the two parameters is done using Arrhenius-type equations (13) and (14) (Schell, Casas, Pini, & Mazzotti, 2012). The equations adapt the temperature independent parameters to temperature dependent parameters, with temperature independent parameters a_i , b_i, A_i and B_i respectively;

$$(11)\ n_i^\infty = a_i \exp(\frac{-b_i}{R*T})$$

$$(12)\ k_i = A_i \exp(\frac{-B_i}{R*T})$$

Which results in the following temperature dependent description of the Langmuir model equation;

$$(13)\ q_i(P_i,T) = \frac{a_i \exp(\frac{-b_i}{R*T})*A_i \exp(\frac{-B_i}{R*T})*P_i}{1+A_i \exp(\frac{-B_i}{R*T})*P_i}$$

6.2 temperature dependent model fitting

Both the 300 ^{0}C and the 350 ^{0}C isotherms data of LDO2 is fitted simultaneously to equation (15) by using the fmincon function in MATLAB (see box 3). The fmincon function generates the unknown parameters a_i, b_i, A_i and B_i. The input for the bounds, the non-linear constraint and starting values for the fmincon in MATLAB is shown in table 13. Lb is the lower bound of the parameters and Ub is the upper bound of the parameters. The bounds will range between a minimum and a maximum based on an educated guess. The nonlcon is set so that the $q_i(p)$ cannot be higher than the maximum of the isotherm equation solution of the non-temperature dependent isotherm equation solution (see figure11). This is done so that the fmincon solver does not find a local minimum above these maximum values. The X0 is set by default within the range of the lb and the ub. Additional inputs for fmincon, not mentioned in table 13, are the objective, the linear equalities, linear inequalities and the options. The objective is set to minimize the difference between the sorbent isotherm sorption capacity data y_i and the temperature dependent isotherm model data y_{pi}. The fmincon function minimizes the objective by changing the parameter x which are the temperature independent parameters a_i, b_i, A_i and B_i.

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$$(14)\ objective = \frac{\min}{x} \sum_{i=1}^{n} (\frac{y_{pi}-y_i}{y_i})^2$$

Commented [MA51]: Formula (4)

There are no linear equalities and no linear inequalities in the optimization problem, therefore;

A = [] b = [] Aeq = [] beq = []

The Fmincon minimizes the objective within the bounds. It finds local minimums which are not necessary the optimal solutions for the optimization. Therefore, Fval is used in the optimization of the isotherm model equation. The bounds with the lowest Fval show the lowest minimalization of the objective and are therefore the best solution of the minimization. The options are used to select the appropriate algorithm. The SQP algorithm is selected, this algorithm shows strict feasibility with respect to bounds.

The resulting parameters for the temperature dependent Langmuir isotherm model are shown in table 14. The Langmuir model is plot with the sorbent isotherm data is shown in figure 16. As can be seen in figure 16, for the lower temperature of 300 ^{0}C the adapted model describes the sorption behaviour well. The model reacts to the decrease of the last sorbent data point, which decreases again in sorption capacity. Therefore, the model does not predict the two data points in the mid pressure range. For the higher temperature of 350 ^{0}C the model shows an adequate fit to the sorbent isotherm data. Especially in the lower pressure region, the model does not fit to the sorbent isotherm data. This is most likely due to the small data availability of the sorbent. Overall the new temperature dependent Langmuir isotherm model equation (15) is adopted as an appropriate model equation describing sorption behaviour of LDO2 for different temperatures and CO_2 partial pressures.

Table 13: fmincon lower bound (lb), upper bound (ub), non-linear constraint (Nonlcon) and initial starting points (X0) s input for MATLAB for LDO2 sorbent.

lb range								ub range								Nonlcon	X0			
ai		bi		Ai		Bi		ai		bi		Ai		Bi						
low	high	low	high	low	high	low	high	low	high	low	high	low	high	low	high		ai	bi	Ai	Bi
0.01	0.1	-10000	-8000	0.01	0.1	-10000	-8000	0.18	0.4	-8000	-6000	0.2	5	-8000	-6000	0.22	0.1	-10000	0.2	-10000

Table 14: fmincon parameter output for the temperature dependent Langmuir isotherm model and the fval value for the adsorbent LDO2

	a_i	b_i	A_i	B_i	Fval
LDO1	0.05	-7500	5	-7500	9.3740

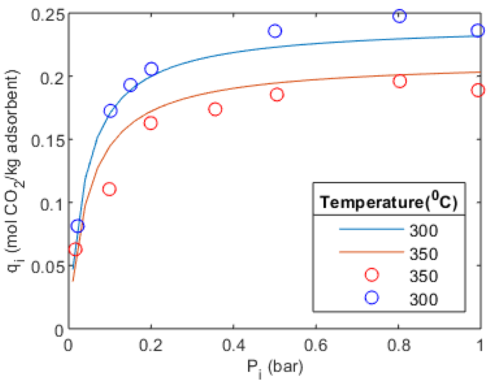

Figure 16: LDO2 plot, with temperature dependent parameters and adsorption data.

Chapter 7 Set-up sizing

In this chapter the initial sizing of the set-up is explained. The chapter starts with an explanation of the kind of set-up that is being optimized, followed by the results of the set-up sizing.

7.1 Set-up characterization

For the adsorption fundamentals and a background in set-up configurations see box 4. For this research simple set-up is considered of a commonly used temperature swing adsorption process in a single column fixed bed (Hedin, Andersson, Bergström, & Yan, 2013).

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Box 4: Adsorption fundamentals and background.

The equilibria revers to the mechanism of the sorbent having different abilities to accommodate different components (Do, 1998). Different sorbents have different preferences to adsorb to certain component, the equilibrium characteristics describes the preference of the sorbent to adsorb a certain component (e.g. CO_2) (Ibid). The kinetics are based on the different rates of diffusion into the pores of the sorbent (Ibid). The higher the rate of diffusion into the pores of the sorbent the faster the component is adsorbed onto the sorbent(Ibid). Both high equilibrium and high kinetics are preferred in a sorbent to adsorb as much and as fast as possible onto the sorbent.

The regeneration of the component out of the sorbent is done using pressure and/or temperature swing approaches. When changing pressure, temperature or both temperature and pressure the component is forced out of the sorbent and can be captured. The regeneration characteristics (i.g. Temperature and pressure) are specific for the sorbent.

Cyclic adsorption process is an adsorption process which has been studied extensively in recent years. In cyclic adsorption processes the process is a process in which multiple columns/beds are connected (Hedin et al., 2013). Different conditions (i.g. Temperature and Pressure) are present in the columns, the feed undergoes the columns in succession recovering the CO_2 out of the feed (Ibid). The process conditions, meaning the number of columns and column conditions are used to optimize the CCS-process (Ibid).

The target is the minimization of the single column bed volume. The bed volume is filled with the LDO2, therefore the amount of LDO2 (kg) and the density (kg/m^3) of the LDO2 is needed. To calculate the amount of LDO2 needed the adsorption and desorption cycle is modelled, containing the following steps; first the feed introduction in the column and adsorption of the CO_2, second a heating step where the target amount of CO_2 is desorbed at target purity. Last a cooling step, where the column is returned to the original conditions.

In the feed introduction step, the flue gasses from the SC-GT are introduced into the column and closed. The CO_2 is adsorbed in the column by the LDO2, the temperature of the column is set to 300 ^{0}C which is the minimum temperature where the LDO2 is still able to operate. This is done to optimize the adsorption capacity of the LDO2. The pressure is kept constant at ambient pressure during the feed introduction. This research assumes instant equilibrium within the column after the introduction of the flue gasses. The adsorption in the column is single component adsorption of CO_2. Single component adsorption simplifies the adsorption process in the adsorption of a single pure component CO_2 (Do, 1998).

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Second the column is opened and heated so that the CO_2 desorbs from the LDO2 at the required purity level. For this process the target temperature (T_{target}) is calculated. The target temperature is calculated by keeping the adsorption capacity at a constant level, while increasing the temperature where the CO_2 partial pressure reaches 0.95 or 95% purity level. Increasing the temperature to the target temperature is calculated using equation 15 based on equation 13.

$$(15)\ q_i(P_{0.06}, T_f) = \frac{a_i \exp\left(\frac{-b_i}{R*T_f}\right)*A_i \exp\left(\frac{-B_i}{R*T_f}\right)*P_i}{1+A_i \exp\left(\frac{-B_i}{R*T_f}\right)*P_i} = \frac{a_i \exp\left(\frac{-b_i}{R*T_{target}}\right)*A_i \exp\left(\frac{-B_i}{R*T_{target}}\right)*P_i}{1+A_i \exp\left(\frac{-B_i}{R*T_{target}}\right)*P_i} =$$

$$q_i(P_{0.95}, T_{target})$$

After reaching the target temperature the temperature is increased further so that the CO_2 desorbs from the LDO2 and can be caught from the column. There is a trade-off between the amount of sorbent needed and the increase in temperature, a higher temperature leads to more desorption in the column per kg of adsorbent. The Δq_i is calculated to see the desorption capacity (mole CO_2/kg sorbent) which is the sorption capacity at required purity level at a specific temperature subtracted from adsorption temperature and adsorption P_i.

The Δq_i and temperature ratio (θ) are calculated to calculate the amount of sorbent needed. The Δq_i and θ are calculated in the following manner;

$$(16)\ \Delta \mathrm{qi} = q_i(0.04\ , 300) - q_i(0.95\ , T_{hot})$$

Where;

T_{hot} = temperature range from desorption temperature (T_{target}) (^{0}C) to twice T_{target}

$$(17)\ |\theta| = \frac{T_{cold} - T_{hot}}{T_{cold}}$$

Where;

T_{cold} = adsorption temperature (^{0}C)

T_{hot} = Desorption temperature (^{0}C)

The amount of CO_2 that needs to be processed after each start-up is calculated in the following manner;

$$(18)\ m_{CO_2} = y_{CO_2} *\ m_{fg}$$

Where;

m_{co2} = the mass stream of CO_2 in kg/sec

Y_{co2} = the mass fraction CO_2 in the flue gasses

m_{fg} = the total mass stream of the flue gasses

Using the dispatch profile, the amount of CO_2 is calculated in the following manner;

$$(19)\ M_{CO_2} = m_{CO_2} * t_{op} * CCR$$

Where;

M_{CO2} = is the total amount of CO_2 captured after each dispatch time (kg)

t_{op} = operation time in each dispatch (sec)

CCR = Carbon capture rate

The amount of sorbent is calculated in the following manner;

$$(20)\ M_{sb} = \frac{M_{CO_2}/MW_{CO_2}}{\Delta q_i} * 1000\ mol/kmol$$

Where;

M_{sb} = the amount of sorbent needed in millions of kg.

MW_{CO2} =Molar weight of CO_2

Δqi = sorption capacity change at temperature ratio θ

The volume needed for the sorbent is calculated by;

$$(21)\ V_{sb} = \frac{M_{sb}}{\rho_{sb}}$$

Where;

V_{sb}= the volume of the sorbent in m^3

ρ_{sb} = the density of the sorbent in kg/m^3

With the volume of the sorbent the volume of the column can be calculated. The height of the column is set to 15 meters by default, calculating the diameter in the following manner;

$$(22)\ D_{column} = \sqrt{\frac{4*M_{sb}}{\rho_{sb}*\pi*H_{collumn}}}$$

where;

D_{column} = the diameter of the column in (m)

H_{column} = the height of the column in (m)

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7.2 Set-up sizing results

The target temperature is calculated using equation 15 for the LDO2, the resulting target temperature corresponding to a 95% purity is 684 ^{0}C. A visual representation of the process of the temperature increase to the target temperature is shown in figure 17. From this point the Δqi is calculated, to calculate the desorption capacity subject to the temperature ratio θ. The temperature ratio is calculated with equation (17) where T_{hot} starts from 684 ^{0}C and goes up to 1368 ^{0}C. A visual representation of the desorption capacity is shown in figure 18. The relation between the desorption capacity and the temperature increase in figure 18 shows that initial increase in temperature increases the desorption capacity more than further down the θ.

From the Δqi the relation between θ and the column diameter D_{column} is calculated using equations (18), (19), (20), (21) and (22). The visual representation of the relation between θ and D_{column} is shown in figure 19 for standard framework conditions where; t_{op} = 4050 (1.125 hours) seconds and CCR = 0.9. The relation shows the inverse of figure 18, D_{column} decreases fast at the low θ region and from a θ = 1 the decrease of D_{column} stabilizes to an incremental decrease. The D_{column} varies between 251 meters to 40 meters for θ of 0.69 and 2.33 respectively.

Figure 20 shows the relation between the D_{column} and the θ with variating the t_{op} from 10800 seconds (3 hours) to 1800 seconds (0.5 hours) and CCR=0.9. The relation between the D_{column} and θ show the same relation as for the standard framework. Table 15 shows the D_{column} at minimum θ and maximum θ for the different t_{op}.

Table 15: Minimum and maximum column diameter(m) for varying t_{op} (hours) for minimum and maximum ϑ.

t_{op} (hours)	D_{column} (meter) for θ=0.69	D_{column} (meter) for θ=2.33
0.5	167	27
1	237	38
1.5	290	47
2	334	54
2.5	374	60
3	410	66

Figure 21 shows the relation between the D_{column} and the θ with variating CCR from 1 to 0.1 and t_{op}=1.125 hours. The relation between the D_{column} and θ show the same relation as for the standard conditions of the framework. Table 16 shows the D_{column} at minimum θ and maximum θ for the range of CCR.

Table 16: Minimum and maximum column diameter(m) for varying CCR for minimum and maximum ϑ

CCR	D_{column} (meter) for θ=0.69	D_{column} (meter) for θ=2.33
0.1	84	13
0.2	118	19
0.3	145	23
0.4	167	27
0.5	187	30
0.6	205	33
0.7	221	36
0.8	237	38
0.9	251	40
1	265	42

Figure 17: Determination target temperature using equation ***(15)****. Target temperature reached at 684* ^{0}C

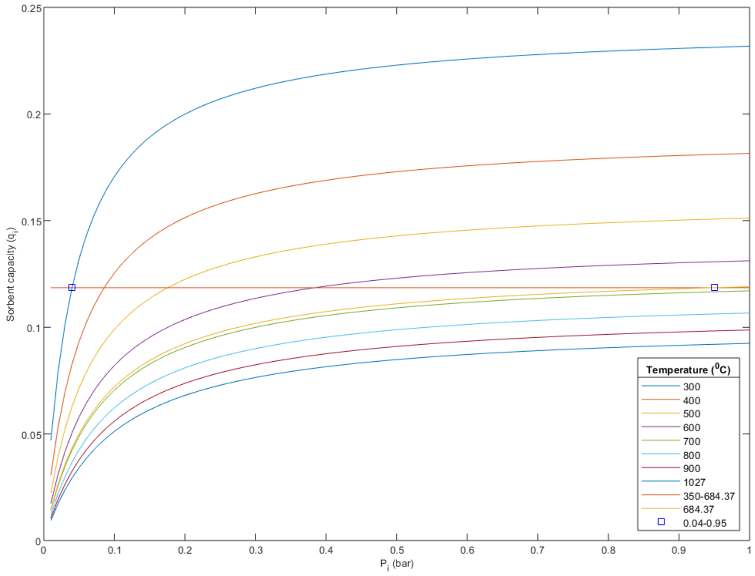


Figure 18: desorption capacity Δq_i *vs temperature ratio* ϑ

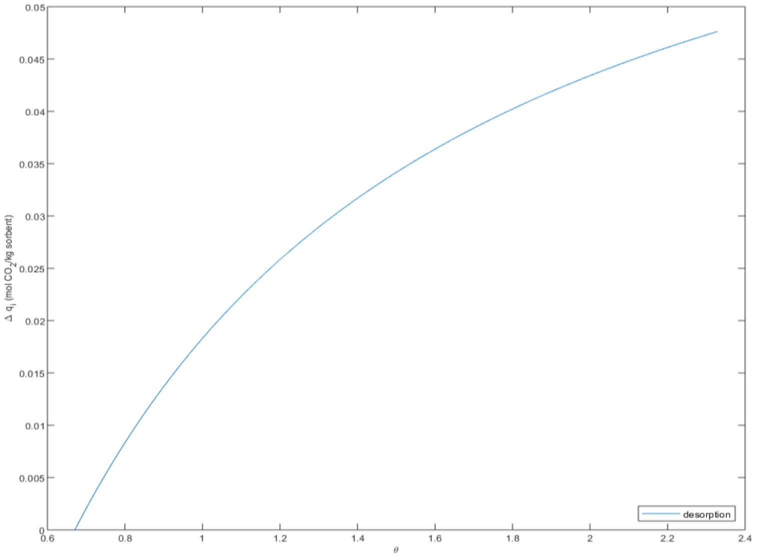


Figure 19: Diameter column (m) at framework conditions t_{op}= 1.25 hours CCR = 0.9

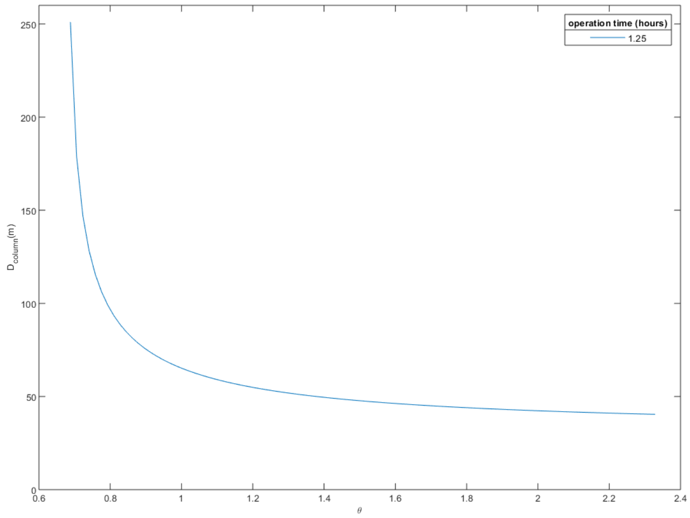


Figure 20: D_{column} on temperature ratio ϑ with variation on t_{op} with CCR=0.9

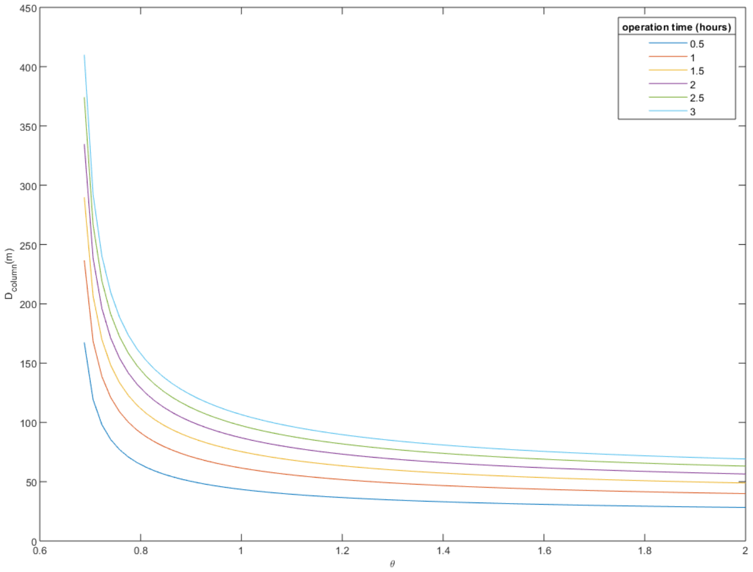
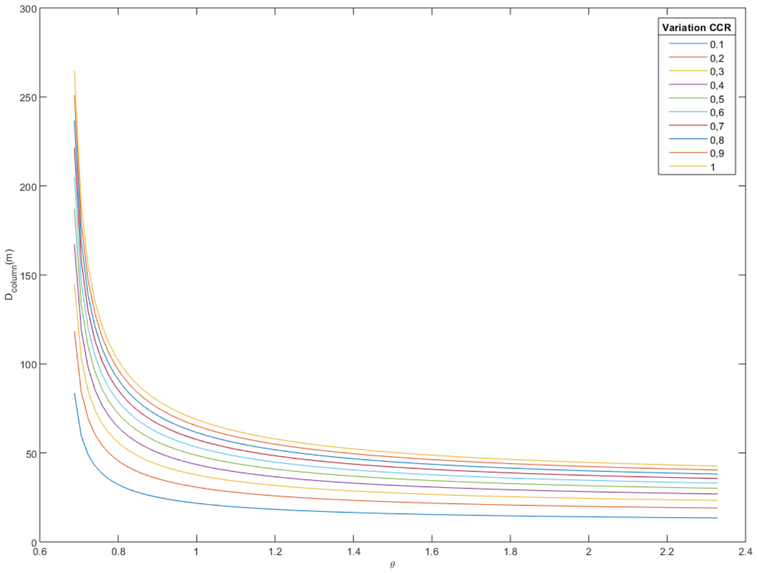


Figure 21: D_{column} on temperature ratio ϑ with variation on CCR with t_{op}=1.125 hours



Chapter 8 Discussion

The technical feasibility analysis in the research is a simplification of the actual process. The simplifications of the research limit the results to some extent, the limitations are discussed here. After the limitations the theoretical and policy implication of the research are discussed.

Limitations

The adsorption process is simplified to single component adsorption, which neglects the competition between other components in the flue gas for adsorption on the sorbent. The sorption capacity could therefore be lower than indicated in this research (Do, 1998). However, using the single component adsorption is useful to analyse a specific application of a sorbent as presented in this research (Schell et al., 2012) . The sorbent used (LDO2), was the only sorbent found applicable for the research based on data availability. Despite communication with authors of different articles the isotherm data sets seem to be lacking. Different sorbents could have different behaviour in the framework conditions, thus altering the results (Yong & Rodrigues, 2002). Therefore, more research in isotherm data of different sorbents is required. Besides presenting a sizing of the set-up the research also shows a model how this sizing for different sorbents could be performed. Different sorbents, when available, could be analysed using this model. The column where the CO_2 is adsorbed and desorbed is simplified. The adsorption kinetics are neglected with instant equilibrium in the column and no column evolution. This limitation could limit the sorption capacity of the LDO2 further and could affect the applicability for using it in consecutive times in short time periods (Joss et al., 2017; Schell et al., 2012). The function of the SC-GT is generation of electricity, which after the sorbent selection is not analysed anymore. The energy penalty inflicted by the CCS process is an important next step to research as the energy penalty can be high (Hedin et al., 2013). Incorporation of energy requirements in the model and optimizing for size and energy requirements could be a future prospect for the model.

Implications

The theoretical implication of the research is a validation of the adaption of the Langmuir model to a temperature dependent model. For future research the other isotherm model (e.g. Freundlich, Sips etc.) could be adapted in a similar manner and used to analyse other sorbents.

Furthermore, the research presented a first preliminary analysis of high temperature adsorption process for post combustion carbon capture on a realistic framework of a SC-GT for demand peak supply. The framework for the analysis and the supporting MATLAB scripts, could be adapted for different frameworks e.g. other energy suppliers or other dispatch profiles. Furthermore, adding to the framework to limit the simplifications mentioned above the framework could serve as a solid basis for in-depth analysis of post combustion CCS adsorption. Also expanding the set-up in the model for multicolumn adsorption and desorption could limit the size of the set-up (Reynolds et al., 2006).

Besides limiting the simplifications, economic parameters could be added for an economic feasibility analysis. The economic feasibility could be used to compare the set-up to alternative peak demand suppliers. This model is focused on temperature-swing adsorption, looking into other adsorption-desorption processes such as pressure swing adsorption, hybrid pressure and temperature swing or steam reforming would be an interesting alternative for reducing the size of the set-up.

Since carbon capture and storage technologies is appointed by the IEA as one of the contributors for the decarbonization, policy makers need frameworks to analyse this opportunity. This research offers such a framework and is applied to a simple cycle gas turbine as validation for the framework.

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Rational design of temperature swing adsorption cycles for post-combustion CO_2 capture.

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Additional data needed.

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Chapter 9 Conclusion

The possibility of using carbon capture on a simple cycle gas turbine was explored by performing a technical feasibility analysis. The simple cycle gas turbine analysed was a LM 6000 from general electric used for demand peak supply.

What is a technical feasible set-up for carbon capture storage applied to a simple cycle natural gas-fed gas turbine?

The aim of retrofitting to the existing infrastructure led to the choice of post-combustion capture technologies and the exclusion of both oxy-fed and pre-combustion capture technologies. Adsorption was selected as best suited post combustion technology and absorption and membranes where excluded based on literature review. Both absorption and membranes were not able to operate in high temperature flue gasses. Membranes also showed high energy requirements and bad separation performance. Within the adsorption technology, calcium loopin, ceramics and hydrotalcite like compounds were considered as sorbents in the adsorption process. Based on literature review hydrotalcite like compounds was selected as most suitable due to the high cyclic stability and low regeneration energy requirements compared to the alternatives. Due to the limited data availability, as discussed in the discussion, the selected hydrotalcite like compound used in the framework was LDO2.

The Langmuir isotherm model used to model the sorption behavior of the sorbent showed good fit (R^2 value of 0.997) to the LDO2 data retrieved from literature. The adaption of the model to temperature a temperature dependent model using Arrhenius type equations generated good results. Sorption behavior dependent on both CO_2 partial pressure and temperature was modeled. Both the selection of appropriate isotherm model and model adaptation are thus appropriate steps when modeling sorption behavior of sorbents in a specific framework.

The framework used the volume of the sorbent needed for the sizing of the column of the carbon capture set-up. The set-up consists of a commonly used fixed bed column, with temperature swing adsorption and desorption. The height of the column was set by default to 15 meters and the diameter was analyzed for the size. Due to the limitations, discussed in the discussion, one should note that the model produces optimistic results. The results show that the size of the set-up is very big for a simple cycle gas turbine. Within the framework conditions (t_{op}=1.125 hours, CCR=0.9) a range of the diameter of the column from 251 meters to 40 meters is generated by the model. The simple cycle gas turbine is a relative small (peak only) energy supplier, thus even for the smallest set up of 40 meters this is considered not feasible. When variating key parameters, the operation time and CCR, the set-up size variates proportional to the parameters. The set-up is still not considered feasible, as for the lowest operation time and lowest CCR the set-up still has a diameter of 27 and 13 meter respectively.

An improvement for the set-up is necessary when considering post combustion carbon capture on simple cycle gas turbine for demand peak supply. In this framework the sorbent is not adequate to adsorb enough CO_2 and thus improvement of the sorbent is suggested. However, the method used in the research showed good results as a preliminary technical feasibility analysis for the framework.

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Appendix A

Table 17: Isotherm data for sorbents selected in table 8. Isotherm data consist of CO_2 partial pressure P_{ix} with corresponding sorption capacity q_{ix} in mol CO_2/kg sorbent at a fixed temperature.

LDO1$_{@300 C}$		LDO1$_{@ 350}$		LDO2$_{@300 C}$		LDO2$_{@ 350}$		LDO3$_{@300}$		HTC1$_{@400}$		HTC2$_{@400}$	
P_{ix} (bar)	q_{ix} (mol CO_2/kg sorbent)	P_{ix} (bar)	q_{ix} (mol CO_2/kg sorbent)	P_{ix} (bar)	q_{ix} (mol CO_2/kg sorbent)	P_{ix} (bar)	q_{ix} (mol CO_2/kg sorbent)	P_{ix} (bar)	q_{ix} (mol CO_2/kg sorbent)	P_{ix} (bar)	q_{ix} (mol CO_2/kg sorbent)	P_{ix} (bar)	q_{ix} (mol CO_2/kg sorbent)
0,0193704600484262	0,0723404255319149	0,0191145867998030	0,0377008686922903	0,0217654171704958	0,0813016049824551	0,0163616495638771	0,0628485176933462	0,0163341609724648	0,108951218369573	0,0929368029739777	0,328897338403042	0,0915645207285774	0,420326168290358
0,0992736077481841	0,127659574468085	0,0990724453354114	0,0969115598064709	0,101571946795647	0,172537625710214	0,0985944521793883	0,110508507269175	0,0985626741444197	0,187828350767295	0,137546468401487	0,355513307984791	0,345594095725104	0,563394665581226
0,148910411622276	0,155319148936170	0,196546226627467	0,127079181070076	0,149939540507860	0,192954510320467	0,198990596555517	0,162820242502298	0,147540617896190	0,207015747451831	0,184634448574969	0,378326996197718	0,525320574535865	0,750048137974403
0,199757869249395	0,175177304964539	0,389166750002717	0,144594165675169	0,200725513905683	0,205670698005366	0,355752028775979	0,173823054912303	0,200194974825047	0,228394937793215	0,268897149938042	0,484790874524715	0,627945861231016	0,797771760192454
0,500000000000000	0,186524822695035	0,501922950688882	0,151430359999845	0,500604594921403	0,235722983289462	0,505344065954878	0,185376417767419	0,501033991206055	0,254289557692694	0,371747211895911	0,515209125475285	0,722949505092876	0,900613972443143
0,800242130750605	0,182269503546099	0,799124894584490	0,152987305413464	0,802902055622733	0,247566690737521	0,803739317843321	0,196041133704221	0,801928778418027	0,293870339510511	0,470879801734820	0,583650190114068	0,848690768964534	0,978799792336435
0,99152	0,182978	0,98924	0,154511	0,99274	0,236056	0,99331	0,188853	0,99267	0,303281	0,56505	0,787072		

5423728813	723404255	9438661550	650174733	4860943168	728156759	8684364872	624339166	6174477930	332610543	5762081785	243346007		
										0,676579925650558	0,855513307984791		