

A Cabin CO₂ Adsorption System for a Novel Medium-range Aircraft Concept

Axel Berres^{*} and Philipp D. Niemeyer[†], Barbara Milow[‡]
German Aerospace Center

Within the ATLAS project, a concept study of a medium-range aircraft was carried out. For this purpose a technology for active management of CO₂ concentration in cabin air was investigated and evaluated for integration into the aircraft. Different adsorbents such as chitosan aerogels and zeolites were investigated in terms of specific adsorption capacity and density to realize the CO₂ management system. Chitosan aerogels offer primary amine groups on surfaces of their nanofibrillated structure. Amine groups are known to selectively and reversibly react with CO₂ via several mechanisms. Therefore chitosan aerogels were investigated as a mesoporous adsorbent made from a renewable resource. As reference material the well investigated zeolite 13X in bead form was chosen. Based on the results and insights gained, a possible system for integration into the concept of a medium-range aircraft will be presented.

Nomenclature

t	= time	λ	= heat conductivity
\dot{n}_x	= rate of adsorption	L	= length of mixed bed
\dot{m}^{Bleed}	= rate of bleed air	τ''	= dimensionless time in mixed beds
$\dot{m}^{Bleed,PAX}$	= rate of bleed air per PAX	ζ''	= dimensionless coordinate in mixed beds
m_{Ads}	= adsorbents weight	T_S	= temperature at the end of a mixed bed
X	= adsorptive capacity	T_{Des}	= desorptive temperature
α_m	= heat transfer coefficient	T_{Ads}	= adsorbents temperature

I. Introduction

The German Aerospace Center is continuously investigating new aircraft configurations within the framework of various projects. In the Advanced Technology Long-range Aircraft Concepts (ATLAS) project the task was to investigate and evaluate five different new technologies - which included CO₂ separation from cabin air - with regard to their feasibility for a medium-range aircraft. In addition to CO₂ separation the enrichment of the cabin atmosphere with oxygen was investigated in the system design for full control of CO₂ and O₂ partial pressure. In the following it is described how this technology was investigated in detail and how the Environment Control System (ECS) was adapted. The technology is then evaluated in relation to the aircraft in order to make a recommendation for possible integration into the designed aircraft.

The goal of conducting studies on new technologies is to analyze the feasibility of introducing those technologies into new aircraft designs. The keys to enabling new technologies are the reduction of the system mass as well as the consumed energy during operation. Therefore both parameters have to be analyzed.

A. Requirements on cabin air and system functions

The European Union Aviation Safety Agency (EASA) regularly publishes certification specifications (CS) containing obligations to be met when developing aircrafts for commercial use. For wide-bodied aircrafts the relevant certification specifications is CS-25.¹ The CS-25 consists of two books. Book No. 1 contains the actual certification specifications. Book No. 2 is entitled 'Acceptable Means of Compliance' (AMC). The AMC especially address developers and manufacturers of wide-bodied aircrafts to give them guidelines when new and or unusual engineer-

^{*} Scientist, Institute of Flight Systems (FT-SSY), Axel.Berres@dlr.de

[†] Scientist, Institute of Materials Research (WF-AEG), Philipp.Niemeyer@dlr.de

[‡] Professor, Institute of Materials Research (WF-AEG), Barbara.Milow@dlr.de

ing solutions demand evidence that certification specifications are met. The AMC also specify usual and malfunctioning operational states of the aircraft. The latter are commented with appropriate or minimal responses.

For systems managing cabin air chapters CS 25.831 through CS 25.841 provide specifications in terms of quantity and quality of cabin air. The latest CS-25 specifies that the cabin and crew compartments must be ventilated with at least 0.25 kg/min (0.5 lb/min) of fresh air per passenger or crew unit (PAX). Limits of gaseous contaminants as carbon monoxide, carbon dioxide and ozone are set to 50 ppm, 5000 ppm (0.5 vol.% at sea level equivalent) and 0.25 ppm respectively. The maximum cabin altitude is specified as 2438 m (8000 ft). Further information on pressure regulating valves and crew warning systems target any malfunction that lets the cabin altitude reach values above 3048 m (10,000 ft) and therefore would let the oxygen partial pressure drop below the critical value of 0.15 bar (112 mmHg) from which the saturation of hemoglobin significantly decreases.

In neither book of CS-25 the origin of 'fresh' air used for cabin ventilation purposes is clearly defined. Fresh air can be provided using 100% outside air from the external atmosphere of the aircraft at cruising altitude. Or a mixture of recycled cabin air that is diluted with any desired percentage of outside air can be used to fulfil the criteria expressed above. Common replacement rates of cabin air with outside air are around 50% per cycle resulting in approx. 20 complete exchanges per hour.

To ensure quality cabin atmosphere for passengers it should have a composition similar to that of the earth atmosphere, see Figure 1. Air is a gas mixture which contains approx. 78 vol.% nitrogen (N_2) and approx. 21 vol.% oxygen (O_2).² The 1 vol.% left is mainly argon with traces of other gases like 0.04 vol.% CO_2 . Aerosols are of no particular importance in cabin air as the fresh air is led through high efficiency particulate air filters.

Atmospheric pressure on cruising altitude is much less than cabin pressure. Therefore outside air has to be compressed before it is introduced into the air stream of the ECS. Compressed outside air can be taken either from ram or bleed air. Due to easier regulation of bleed air systems ram air is only used as redundant oxygen source. Bleed air taken from the turbofan of the engine is of several hundred degrees Celsius in temperature and of several bars in pressure. Therefore ECS include subsystems regulating temperature and pressure.

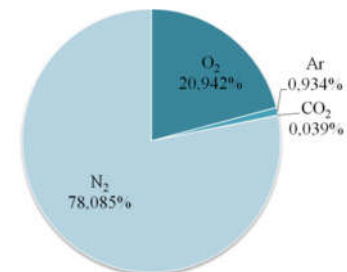


Figure 1 Cabin air composition.

B. Control of the composition of cabin air

As described in section I-A cabin air is continuously conditioned to meet required ventilation rates and low concentrations of gaseous contaminants according to CS-25. For this exchange of CO_2 -loaded air between cabin and outside atmosphere a continuous source of compressed air must be provided. With only one exception – the Boeing 787 – all wide-bodied aircrafts for civil aviation employ high energy bleed. When bleed air is extracted from the turbofan the efficiency of the engine is reduced. During a long-haul flight of an Airbus 330 with Rolls-Royce Trent 772B-60 engines more than 4% of the total fuel consumption accounts for the supply of the ECS with bleed air.³ When consequently following the idea of a more electric aircraft to improve the aircraft efficiency the load of the bleed air system has to be reduced. First and foremost we have to develop a system for cabin air revitalization, i.e. reliable CO_2 separation from cabin air and oxygen enrichment, to protect passengers.

From the state of the art different processes are known separating or concentrating specific gases from air or related gas mixtures. Examples are the *Hampson-Linde cycle*, *Membrane Separation* and *Swing Adsorption process*. Processes based on consumables like alkali oxides and alkali hydroxides are neglected since their application in civil aviation should come with certain effort to provide them in standardized cartridge form at the most prominent network points of an airline.

The *Hampson-Linde cycle* produces liquefied air. According to Venkatarathnam the cycle starts with mechanical compression of air resulting in temperature increase.⁴ A heat exchanger cools the compressed gas mixture which is then expanded. When expansion is performed below the inversion temperature of the gas mixture a temperature decrease occurs according to Joule and Thomson. Continued cycling decreases the gas temperature until liquefaction takes place. The liquefied air then has to be further separated to gain pure oxygen.

The use of the *Membrane Gas Separation process* is an energy and cost-saving alternative to the Linde process. This process enables the separation of nitrogen with a purity of 99.5%.⁵ Gas separation via membranes is based on specific solution/diffusion differences or size exclusion. One side of the membrane is supplied with the gas mixture

to be separated. Increased temperature and pressure dissolve the desired gas species in the membrane and lets it diffuse to the other side of decreased concentration (partial pressure). Since co-solvation and diffusion occur several enrichment steps are necessary for high gas purity. The absence of liquefied gases and moderate pressures let membranes appear more attractive for application in aviation. Furthermore, this membrane design has a strong influence on the lifetime and reliability of the system.⁶

The *Swing Adsorption process* is based on strong interaction of one component of the adsorptive mixture with a solid surface. Attractive interactions of adsorption reactions can be specific or non-specific. Micro- and mesoporous adsorbents may facilitate pore condensation increasing the adsorption capacity by providing not just the surface but pore volume for adsorbate concentration. Adsorption reactions that maintain the adsorbate character are reversible and specified as physisorption. Adsorption reactions that change the chemical nature of the adsorbent are specified as chemisorption.⁷ A prominent example for chemisorption is the reaction of CO₂ with amine groups bearing surfaces. Process conditions and amine type lead to different chemisorption mechanisms and combinations of those. Mild temperatures around 120°C can reverse the reaction. Separation via adsorption is achieved using at least two adsorbent beds. One adsorbent bed is loaded whereas the saturated bed is regenerated by different means (swing process). Temperature increase, pressure reduction, purging with adsorptive-free gas or combinations of those can regenerate the adsorbent. Adsorption based separation of CO₂ from air by zeolites and other sorbents is already investigated in great detail for example by Knox and Cmarik.^{8,9}

Since the Hampson-Linde process involves liquefied gases at low temperature, the energy required for this process is higher than for the other two processes. In addition, the handling and use of liquefied gases in a civil aircraft is associated with significant risks. For this reason, only membrane-gas separation and pressure swing adsorption should be further considered.

C. The evaluation of new technologies

In order to assess whether a new technology seems appropriate for integration, various system parameters such as mass, energy and the necessary installation space must be determined. Due to the integration of a new technology the system mass as well as the aircraft mass will be changed. Also those changes can have an impact on the energy consumption. Both parameters, the mass and the energy consumption, have an impact on the fuel consumption of the aircraft. The fuel consumption can be determined by the parameters block fuel and reserve fuel. If the fuel consumption can be reduced, the investigated technology has the potential to be installed in an aircraft.

For the impact assessment of a new technology, a brown paper analysis was performed at the beginning of the project. During this analysis the technologies “enrichment of cabin air with oxygen” and “extraction of CO₂ with aerogels” were considered. Experts identified the various impacts on the aircraft while the analysis was conducted. Also, parameters were identified which could impact the aircraft including whether they can have a positive or negative impact. With regards to the system mass, an increase would be considered as negative and a reduction as positive. The key parameters identified in this way were then examined in more detail during the system design.

For the impact analysis of the two new technologies first the mass of the ECS have to be estimated. Figure 2 shows that the mass of the ECS for our medium range aircraft contributes about 12.5% to the overall mass of all systems in an aircraft. By referencing Torenbeek, Raymer and Roskam it was stated by Lammering that "System models that are commonly used in early phases of aircraft design are based on statistical approaches and regression analyses" and further, "this approaches lack of correctly captured data for today's aircraft".¹⁰⁻¹³ An extension of system models for a more precise aircraft design is required and described e.g. by Koeppen.¹⁴ Both approaches use a more detailed system description to estimate system masses and power take-off. The approach is implemented in the design Tool MICADO which covers the needs of an early aircraft design.^{13,15} At the beginning of the project, the ECS mass was estimated to be about 1125 kg by using MICADO. This reference value was used for the verification of our estimations during the project. At the end of the project the mass of the ECS was estimated to be about 915 kg. This estimation deviates by only about 1% from the methods mentioned above.

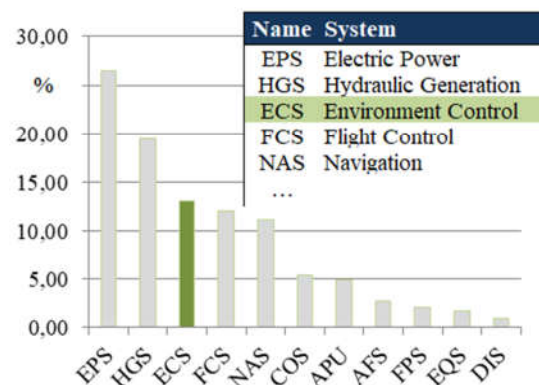


Figure 2 Impact of systems on total system mass in %.

At the beginning of the project, the ECS mass was estimated to be about 1125 kg by using MICADO. This reference value was used for the verification of our estimations during the project. At the end of the project the mass of the ECS was estimated to be about 915 kg. This estimation deviates by only about 1% from the methods mentioned above.

II. State of the art – an aircraft versus the ISS ECS system

Only systems that can be certified for aviation according to CS-25 can be used to control the cabin air. For the extraction of oxygen, various systems from the fields of medicine or aviation have been examined with regard to their possible use for a system solution.^{16,17} Afterwards the open system in an aircraft was compared with the carbon dioxide removal assembly of the ISS.

A. Aerogels as CO₂ adsorbents

Aerogels are nanostructured and highly porous materials. High specific surface areas, pore diameters in the micro- and mesoporous range together with low densities are probably the most cited properties of this material class. Uncountable proven or proposed applications brought aerogels from the laboratory of Samuel Kistler from the early 30ies of the last century not only in our hands today but even to space and back to earth again.¹⁸ Often one or a combination of multiple aerogel features enables a technical solution of a problem. In the case of adsorbent design for selective separation of CO₂ from cabin air the specific surface area and mean pore size are of special interest. When reducing the composition of air to only nitrogen as carrier gas for CO₂ three adsorptive properties are important for selective adsorption of CO₂ over nitrogen, i.e. polarizability, the ability to partake in chemical reactions with functional surface groups and saturation pressure for condensation.

Microporous aerogels e.g. made from carbon are known to adsorb substantial amounts of CO₂ at low partial pressures and ambient temperature.¹⁹ Also amine modified microporous silica aerogels are reported to adsorb CO₂ from CO₂/N₂ mixtures.²⁰ The same accounts for amine modified silica templates like MCM-41.²¹ Most of these studies neglect the condensation of CO₂ in micropores. In the ATLAS project we were interested in the CO₂ separation potential of mesoporous aerogels made from the polysaccharide chitosan naturally bearing primary amine groups. Mean pore sizes of chitosan aerogels are reported to be around 40 nm.²² According to the Young-Laplace equation, CO₂ condensation in cylindrical pores at room temperature occurs in pore diameters below 5 nm only. Therefore it is ensured that any CO₂ adsorption on chitosan aerogels is due to direct interaction with the surface and its functional groups. From the analysis of CO₂ sorption isotherms the type and quantity of adsorption mechanism can be determined.

B. Oxygen enrichment

The Körber O₂ and Oxyfly system extract the oxygen and thus achieve a concentration of about 90%.^{16,17} Oxyfly provides about 4 L/min for a flight altitude of 18,000ft and the Körber O₂ provides about 5 L/min at sea level. Oxyfly weighs about 25 kg and Körber 16 kg. In addition, both systems require electrical power for the compressors required in the system. Oxyfly requires about 400 W and Körber O₂ 280 W for operation. These values were used for a rough estimate for the later evaluation of the oxygen extraction. For the evaluation, the system was scaled to the required oxygen quantities. Savings due to a proper system design were not considered.

C. Environment Control System of an aircraft

As shown in Figure 3, the ECS has the main functions “Air Conditioning” by adaptation of cabin conditions such as pressure, temperature, gaseous contaminants and “Distributing Air” for air distribution in the aircraft. In the individual components, like the Air Conditioning Pack (ACP) are described from air quality point of view using the B767 shown in Figure 4.²³ Based on this description, the architecture of an ECS was specified.

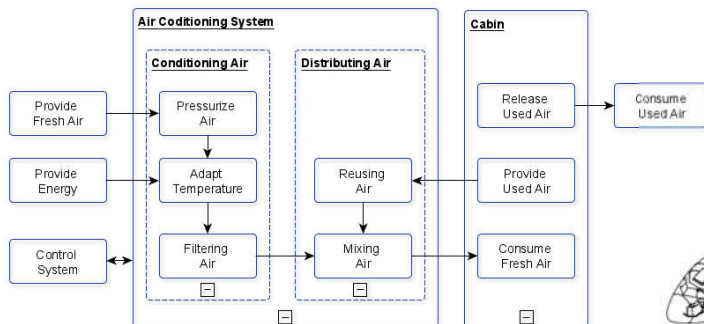


Figure 3 Functional architecture of an ECS.

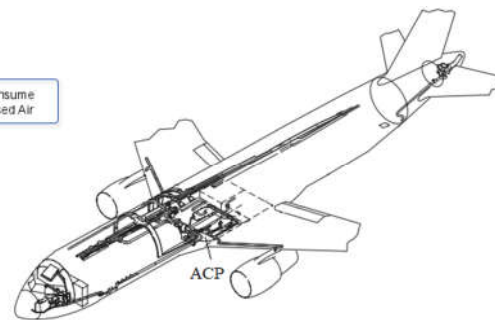


Figure 4 ECS of a B767.²³

At the start, air from the atmosphere is fed into the ACP. The ACP first regulates the pressure to the desired cabin pressure. Then the temperature is controlled to the specified value. For this purpose, energy in the form of Ram Air is supplied to the bleed air via heat exchangers. To reduce possible contamination of the cabin air, the air is filtered for particles before it is mixed with used cabin air in the mixing unit. After mixing, the processed air is fed back into the cabin. To keep the CO₂ concentration below the specified limit, used cabin air is released into the atmosphere. This leads to a regular renewal of about 50% of the cabin air.

D. The Carbon-Dioxide-Removal-Assemblies (CDRA) of the International Space Station (ISS)

During STS-111 on board the Endeavour, the first of two American systems for the selective CO₂ removal was transported to the ISS. Up to that date only the Russian system Vozdukh removed CO₂ from the ISS atmosphere. Nowadays the CO₂ removal on board the ISS is mainly performed by the two American systems. As part of the Air Revitalization System the two 4-Bed-Molecular-Sieve CDRA make a significant contribution to the quality of the ISS atmosphere. Figure 5 shows the architecture of the four-bed system.

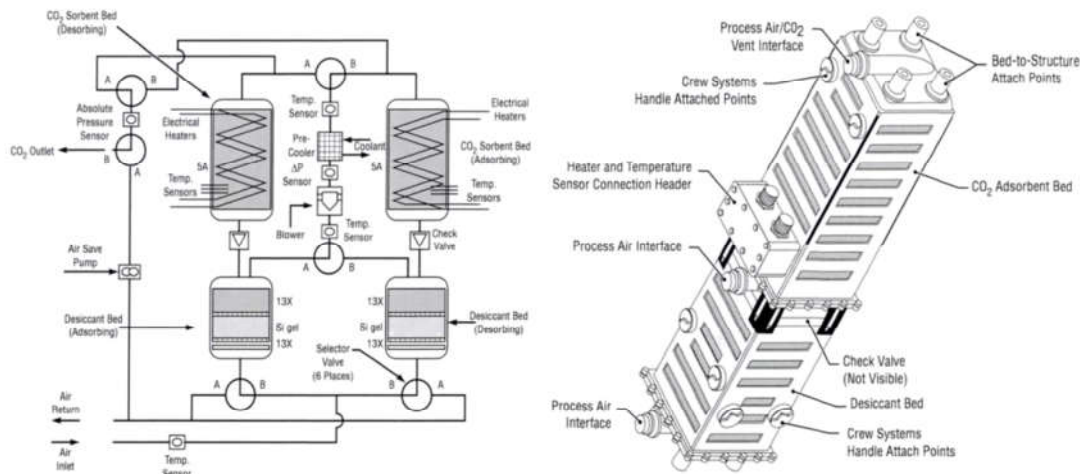


Figure 5 4-BMS CDRA architecture, Orbit Replacement Unit and CO₂ adsorbent bed.²⁴

Before CO₂ can be separated the cabin air passes through the Temperature and Humidity Control Unit (THC). After cooling to 5°C and partial dehumidification process air enters the CDRA. Within the CDRA the air passes through a desiccant bed of zeolite 13X and silica gel for further dehumidification. Thorough dehumidification to a dew point around -60°C is essential since the dedicated CO₂ adsorbent zeolite 5A is sensitive to residual moisture. The air then passes through one of the two CO₂ adsorbent beds. CO₂ is selectively removed from the gas stream via physisorption on zeolite 5A. The CO₂-depleted gas stream is then passed through the desiccant bed loaded during the previous cycle and regenerates it. Again temperature is controlled in the THC. The CO₂-free air is then fed to the atmosphere of the ISS. When a CO₂ adsorbent bed is saturated it is decoupled from the process air flow and evacuated to reduce oxygen loss. The cartridge is electrically heated up to a temperature of 204°C (400°F) and exposed to space vacuum for 104 min. CO₂ is desorbed and disposed. Subsequent cooling takes about 40 min. The regenerated and cooled cartridge then can be used for the next CO₂ adsorption cycle.

A CDRA requires an average electrical input of 497 W. It weighs 174 kg and has a CO₂ separation rate of 6 kg CO₂ per day. This separation rate is required to remove the daily amount of CO₂ emitted by a crew of six. The redundancy of the CO₂ separation is given by the simultaneous operation of two CDRA.²⁴

III. Aerogels

Chitosan of low molecular weight and high degree of deacetylation was purchased from Glentham Science[§] Glacial acetic acid and sodium hydroxide pellets were both purchased from VWR at 98% purity. Water for synthesis purposes was ion exchanged before use.

[§] Chitosan, GP7325, 100-300 cps, low molecular weight, DD ≥ 90%.

A. Development – methods and procedures

Chitosan solution was prepared from 4 wt.% chitosan dispersed in 92 wt.% water. After homogeneous dispersion with a dispersion tool 4 wt.% glacial acetic acid were added. After full homogenization the chitosan solution was set to rest until all incorporated air rose and it was clear in appearance. Beads were formed using the geniaLab JetCutter technology²⁵. Therefore, the solution was extruded through a 700 μm nozzle resulting in a stable liquid jet. Right after extrusion the liquid jet was cut into equally sized cylinders by a rotating cutting disc of 100 μm thin wires. The surface tension of chitosan solution leads to formation of perfect spheres. After an 80 cm long trajectory those spheres were collected in a regeneration bath made from 2.5 wt.% NaOH in water. By reversing the pH chitosan gel beads of approximately 1500 μm in diameter were obtained. Gel beads were washed with water until pH was neutral followed by stepwise exchange from water to absolute ethanol. Drying of ethanol exchanged beads was performed in a 60 L autoclave with CO_2 at 115 bar and 60°C under a CO_2 flow rate of 35 kg/h transforming the former alcogel beads to aerogel beads.

Static volumetric nitrogen sorption experiments at 77 K for determination of specific surface area were performed on a 3Flex from Micromeritics after pretreatment on a Smart VacPrep 067 HIVAC with a temperature ramp of 10 K/min to 120°C where samples were held under vacuum for 180 min. The equilibration interval was set to 10 s. Nitrogen gas purity was 5.0.

Static volumetric CO_2 sorption experiments were performed on a TriStar II 3020 device from Micromeritics. All samples were pretreated for 180 min at 120°C under vacuum < 0.1 mbar with a VacPrep 061 from Micromeritics. The analysis temperatures of 273 K and 298 K were controlled with an ISO Controller from Micromeritics. The equilibration interval was set to 20 s. CO_2 gas purity was 4.5. Dynamic breakthrough measurements were performed on a dynaSorb BT from Quantachrome. All chitosan samples were pretreated at 120°C under constant flow of 1 SL/min nitrogen for 60 min. For analysis at 273 K and 298 K 0.998 SL/min nitrogen mixed with 0.0025 SL/min CO_2 was used. Gas composition was controlled by mass flow controllers. For analysis of inlet/outlet gas composition a thermal conductivity sensor was employed which was calibrated to low CO_2 concentration in nitrogen.

B. Aerogel properties – evaluation of chitosan aerogels for CO_2 separation

Chitosan aerogel bead preparation with the JetCutter technology lead to aerogel beads uniform in size and shape. The final aerogel bead diameter was determined as 950 μm . Scanning electron micrographs captured a macro- and mesoporous outer shell of the aerogel beads. When dissected a homogeneous inner structure was revealed. Further magnification gave the impression of a homogeneous nanofibrillated network which is known for chitosan aerogels. Static volumetric sorption measurements with nitrogen at 77 K gave a specific surface area of 240 m^2/g when the adsorption branch was evaluated according to Brunauer, Emmett and Teller.²⁶

CO_2 sorption isotherms at 273 K and 298 K are similar in shape. Both adsorption isotherms begin a convex climb which transits into a linear incline from around 40 kPa until the end of the adsorption branch at 104 kPa. Maximum adsorbed CO_2 amounts are 1.04 mmol/g and 0.64 mmol/g at 273 K and 298 K respectively. The subsequent recorded desorption branch starts with a slight decline which decreases until the end of the desorption branch. Adsorption and desorption branch do not meet. The difference between the both branches during desorption builds up from an absolute pressure of 104 kPa to approx. 60 kPa. In the following the difference is constant at 0.22 mmol/g at 273 K and 0.11 mmol/g at 298 K until the pressure reaches 5 kPa. Sorption reactions at low absolute pressures are extremely slow and may take up to eight hours for the first/last few measurement points at a 20 s equilibrium interval.

The recorded isotherms reveal a partly irreversible type of adsorption of CO_2 on strongly heterogeneous chitosan aerogel surfaces. Four different adsorption sites are responsible for this isotherm shape. Strong and irreversible adsorption occurs via chemical reaction of CO_2 with primary amine groups according to the carbamate reaction mechanism, see Figure 6 for reaction scheme. The reaction product of that specific covalent reaction is a carbamate-ammonium salt naturally bearing ionic charges. Those ionic charges are responsible for a strong but reversible adsorption reaction with CO_2 . The negative charge of the carbamate part induces charge dislocation in CO_2 and subsequent strong physisorption, $[\text{RNHCO}_2\backslash\text{CO}_2]$. The positive charge of the ammonium part leads to an even stronger interaction with CO_2 molecules. A strong hydrogen bond complex is built up between the two oxygen atoms of the CO_2 molecules and the three protons of the protonated amine group, $[\text{RNH}_3\backslash\text{CO}_2]^+$. The shape of the linear region of the adsorption branch is determined by weaker and reversible adsorption reactions that are of non-specific dispersion. The adsorption capacities provided by dynamic break through measurements were in accordance with the values from static volumetric sorption measurements.

The reaction/adsorption rates at low absolute pressures estimated from recorded times needed for satisfaction of the equilibrium criterion lead to the conclusion that the proposed reaction mechanism occurs and strongly binds CO₂. During consumption of reactive groups and saturation of ionic reaction products with CO₂ the adsorption rates continuously increase from 0.02 mmol/g/h at 1 kPa to the plateau value of 0.17 mmol/g/h at 50 kPa for 273 K. The corresponding values for 298 K are equivalent. This sorption rate behavior indicates the transition of the predominant adsorption mechanism from strong irreversible (covalent reaction) and strong reversible (charge/adsorptive interaction) to weak reversible physisorption. These results emphasize the importance of micropores for CO₂ adsorption/condensation even when surfaces are bearing substantial concentrations of primary amine groups.

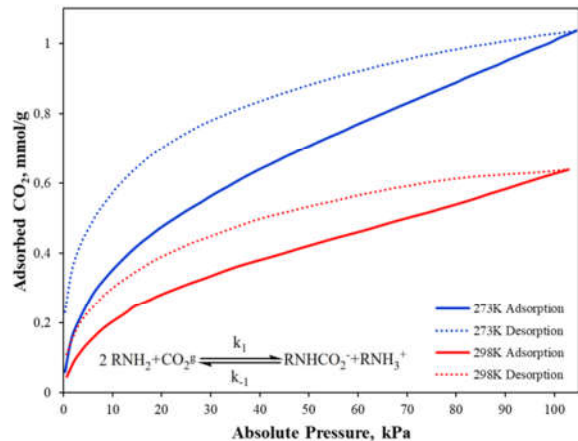


Figure 6 Chitosan/CO₂ sorption isotherms at 273 K and 298 K. The carbamate mechanism dominates the adsorption behavior at low absolute pressures.

Chitosan aerogels produced and investigated in this work are not practical for application in CO₂ separation systems that are characterized by dynamic process control. In addition to the unfavorable adsorption dynamics low tapping density of chitosan aerogel beads were measured as 80 kg/m³. When combining poor adsorption characteristics together with low tapping density a high volume of adsorbent is necessary to adsorb the expected amounts of CO₂ emitted by passengers. Therefore the well investigated alternative zeolite 13X investigated in great detail by Knox and Cmarik et al. was chosen as the adsorbent for further system development.^{8,9,30}

IV. Preliminary design and integration into the overall system

The design method PARADIGMshift (Figure 7) was used to determine the feasibility of the technologies under investigation. This method was developed especially for system analysis in early development to support the pragmatic creation of systems feasibility studies.²⁷ To separate thinking about user requirements from thinking about solutions and their trade-offs, the method consists of three parts. These parts are described hereafter

A. Problem domain

In the problem domain, the system requirements are derived from a use case and defined by system functions such as "CO₂ separation". The dependencies between functions can be modeled as material, energy and information flows and visualized by an exported diagram. This diagram describes the functional architecture of the system. In addition functions can be divided into sub functions such as "air cleaning" and further specified by additional formal requirements. In each case, the function constraints, such as the amount of CO₂ to be separated, are specified as a required parameter "maxCO2Flow = 2.65 g/s". This constraint is used to validate the value of the associated parameter in the solutions. In addition, sensitivity analyses can be done in this way to identify key parameters. For the later trade-off analysis, evaluation criteria are defined based on the identified key parameters. For each key parameter, weights or optimal values are defined to support trade-off analysis between different solution candidates.

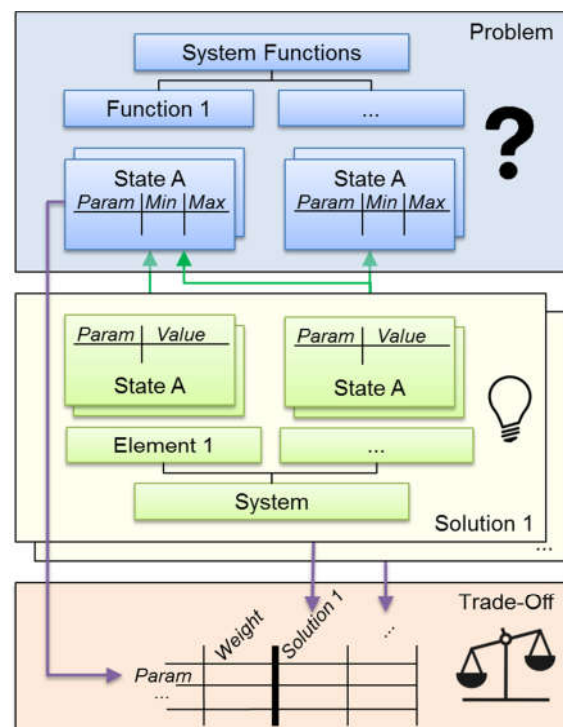


Figure 7 Overview of the PARADIGMshift method

B. Solution domain

Several possible solutions are defined in the solution domain. For each solution, the parameters of a component are assigned to the required parameters of the functions of the problem domain. This approach uncovers functions not taken into account and ensures traceability between all functions and system components of a solution. To define a solution, logical components are first identified. These components can be considered as containers for a group of components, such as a powertrain containing engine, gearbox and fuel tank components. When decomposing and describing the logical and physical components, their dependencies and connections are defined. The system architecture is result of this design step. The component behavior can be described by specifying states. A CO₂ removal system which removes carbon dioxide from the air switches from state "off" to state "on". Transitions are used to describe the change of states. To describe system properties depending on its behavior, the parameter values must be assigned to a state. Also component properties are detailed by parameters and their values. Besides to component mass and performance, also operating costs, manufacturability, maintainability, etc. are represented. The parameters can be estimated, taken from data sheets or computed by calculations using the defined system parameters. By verifying the constraints specified in the problem domain and the parameters defined in the solutions, it is possible to check whether a solution can completely fulfill the required system functionality.

C. Trade-Off-Analysis

A trade-off analysis is a pragmatic way of making decisions. It enables reproducible decisions to be made on the basis of data rather than subjective impressions. The necessary evaluation criteria were already defined during the problem description. The criteria include the key parameters, the relevance of the parameters in terms of weighting and their optimal values. Based on these criteria, a rating value is calculated, which enables a ranking of the solution candidates. Likewise, as a result of the trade-off analysis, some of the defined system functions or constructed components can be improved or specified more precisely in order to enable a meaningful assessment. In this way, one or more design iterations may be necessary for the solution candidates. At the end of this process, the trade-off analysis provides the evaluation of each solution candidate. This evaluation can then be used to decide which solution candidate will be further developed during the following phases.

D. Application

During the search for applicable physical principles and related technologies it was determined early that existing systems for O₂ enrichment need much energy. It was estimated, that the required system mass and the additional energy consumption cannot justify the effect of reducing the fuselage mass. Therefore, it was decided not to investigate this technology further in the project.

In the following it is shown how the selection of the CO₂ adsorbent was done using the PARADIGMSHIFT method. At the beginning aerogels should be examined as selective CO₂ adsorbent. Aerogels have the possibility to adsorb CO₂ as well as the property to thermally insulate. The function "Filtering Air" shown in Figure 8 is considered to be safety critical and for the implementation a robust design was chosen. For the selection of the adsorbent, the mass and volume must be calculated. The calculation is described in detail in the section IV. The essential properties of the adsorbents zeolite and chitosan aerogel (CA) together with the results of the calculation are shown in Table 1.

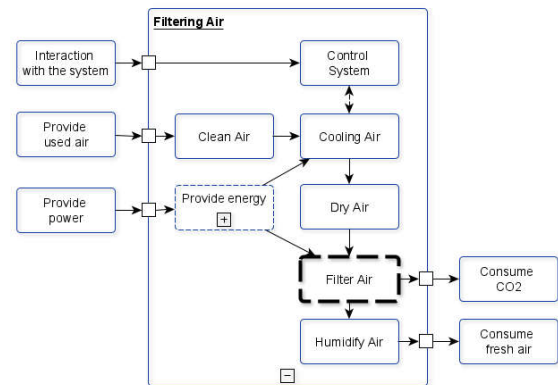


Figure 8 Problem description of separating CO₂.

Table 1 Trade-off adsorbent material

Adsorbent	Adsorption [mol/kg]	Density [kg/m ³]	Volume [m ³]	Mass [kg]
Zeolite 13X	0.900	688.5	0.044	30.1
CA	0.047	80.0	7.288	583.0

By using the PARADIGMSHIFT method an alternative selective CO₂ adsorbent was found without much effort. After the trade-off analysis, the zeolite 13X was selected as an alternative to chitosan and chitosan based aerogels. As this material is already used in the Environmental Control and Life Support System of the ISS, the system design of the ISS CO₂ removal assembly is used as a starting point.

V. From passenger (PAX) to kilogram and watt

The system impact on the aircraft can be estimated by using system parameters such as mass and required energy. Therefore, these parameters from individual components are needed as a basis. The following example of a CO₂ separation cartridge (adsorber) shows how the component mass and energy consumption can be determined.

A crowd of people in an enclosed space can be described as a consuming and emitting machine which depends on activity type and degree. It consumes nutrients and most important O₂ and water. The main emissions are CO₂, water vapor and heat. The emissions are given in Table 2 and used for adsorber the parameters estimation.^{28, 29}

Table 2 Human emissions

Average Emission	Symbol	Value
Heat	P_{Heat}	120 – 270 W
CO ₂	\dot{n}_{CO2}	7 – 12 mg/s
Water vapor (breathing)	\dot{n}_{H2O}	11 mg/s
Water vapor (transpiration)	\dot{n}_{H2O}	10 – 67 mg/s

A. Mass of the adsorber

Studies by Knox and Cmarik et al. show that zeolite 13X (SYLOBEAD MS 544^{**}) is a promising candidate for selective and reversible CO₂ adsorption.^{8,9,30} Own breakthrough curve measurements showed a CO₂ adsorption capacity up to 0.9 mmol/g at a CO₂ partial pressure of 250 Pa in nitrogen as carrier gas. Silica Gel (SYLOBEAD SG 125^{**}) with a water adsorption capacity of about 10 wt.% can be used as water adsorbent.³¹ Further assumptions are an empty tube velocity of the air of 1 m/s. The following calculations for a mixed bed adsorber are based on.³²

The required amount of adsorbent can be calculated by equation 1. The cycle time can be freely selected, in the example 20 min and optimized during the design. Here the weight is multiplied by the emission rate \dot{n}_x of the gaseous contaminant or energy with the cycle time. The emission n_x is calculated as the product of the emission rate \dot{n}_x with the number of passengers (PAX). The weight m_{13X} for an adsorber with zeolite 13X uses the value from Table 2 for the CO₂ emission rate. Similarly, the desiccant weight m_{Gel} for dehumidification with silica gel is calculated using the H₂O emission rate from Table 2.

$$m_{Ads} = \dot{n}_{CO2} * PAX * t_{cycle} / X \quad (1)$$

After completion of the 20 min separation cycle, one desiccant bed and one CO₂ adsorbent bed per system are loaded. The desiccant bed is regenerated by passing the air flow through the loaded desiccant bed after leaving the active CO₂ adsorbent bed. The regeneration of the CO₂ adsorbent bed is performed by a pressure-temperature swing cycle, heated to a temperature of 250°C to provide the desorption enthalpy and then evacuated by a pump.

B. Energy for heating and cooling of the adsorber

Based on the book from Kast, the heating and the cooling process can both be described with the aid of a breakthrough curve.³² In order to quantify the heating and cooling phases in terms of power and time, the heat transfer coefficient of the packed bed must be determined. We assume that the bed consists of uniform spheres and the heat transfer coefficient α_m can be determined by equation 2. Where $N_u(R_e, P_r)$ is the Nusselt number, R_e the Reynolds number and P_r the Prandtl number, λ the thermal conductivity and L the mixed bed length in the direction of flow. At this point, a detailed calculation of the heat transfer coefficient is omitted, it is assumed to be 95.2 W/(m²K) and reference is made to Kast for the derivation.³²

$$\alpha_m = \frac{\lambda}{L} * N_u(R_e, P_r) \quad (2)$$

$$T_S = T_{Des} - (T_{Des} - T_{Ads}) * \frac{1}{2} * erf c \left[\sqrt{\tau''} - \sqrt{\xi''} - \frac{1}{8\sqrt{\xi''}} - \frac{1}{8\sqrt{\tau''}} \right] \quad (3)$$

The change of the temperature T_S in the adsorber at location x can be described by equation 3. After a development of the Bessel function I_0 and using an approximation of Nusselt and Anzelius, the calculation of the temperature can be simplified to equation 3 with an error of less than 0.6%.³³ Here ξ'' is a dimensionless length and τ'' is a dimensionless time, each taking into account the previously determined heat coefficient α_m . Using the given equation, the temperature curve for heating and cooling is shown in Figure 9 for a fixed bed of 42 mm height.

^{**} Grace

C. Optimal number of adsorbers

During the design phase the question arose if weight could be saved by removing one adsorber. The architecture using four CO₂ adsorbers was proposed from the safety engineering perspective, to fulfill the emergency operation requirement of the ECS in case of losing the CO₂ adsorber function.

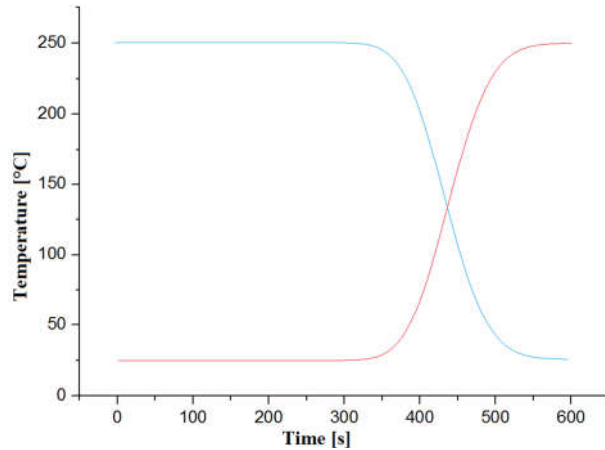


Figure 9 Adsorber temp. during heating and cooling.

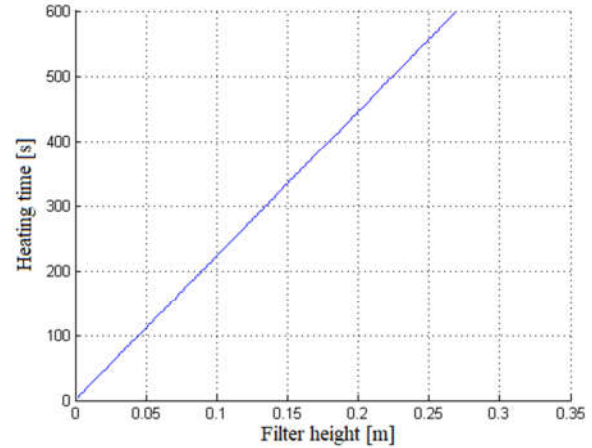


Figure 10 Heating or cooling time for a CO₂ adsorber.

For this optimization it was necessary to determine the maximum times for heating and cooling an adsorber. Based on the cycle time, the heating and cooling together must not exceed 20 min. Figure 10 shows the time required for heating or cooling an adsorber. An adsorber built with 0.25 m height, it could be heated up and cooled down within cycle time. With two adsorbers, continuous separation in alternating operation is possible. Due to the safety requirement, another adsorber should be added to provide the adsorption capacity for at least 20 min in case of failure. This time is used to take appropriate actions in the failure event without reducing the cabin air quality.

VI. Description and evaluation of the designed system

The description for the parameter estimation of individual components was necessary to improve understand regarding to the designed system. In the following, the designed system shown in Figure 11 is described. The CO₂ removal system has interfaces to the EPS, the cabin via the ECS and the bleed system to the aircraft. From the cabin the used air is fed into the system. Via the distribution system the air is sent to the drying process. In the drying process water is extracted from the air with the help of silica gel and stored. The dehumidified air is then fed into the active adsorber via the distribution system. Here CO₂ is separated from the air. The cleaned air is returned after separation to be humidified. For this purpose, the air is led into the desiccant cartridge, which should release the stored water again. The CO₂-free air is then fed to the ECS via the distribution system. After the active adsorber is saturated with CO₂ and considered "full", the separation system activates an "empty" adsorber for continuous separation. The filled adsorber can now release the CO₂ again by heating and evacuation. During this desorption phase, the released CO₂ is removed from the aircraft.

To evaluate the impact of the CO₂ separation system on the ECS, the mass and energy consumption of the components were estimated. Due to the planned integration into the ECS, further effects must be taken into account. The integration will introduce an additional resistance in the air flow into the system. The air flow is controlled by the fans in the recirculation. To counteract the additional

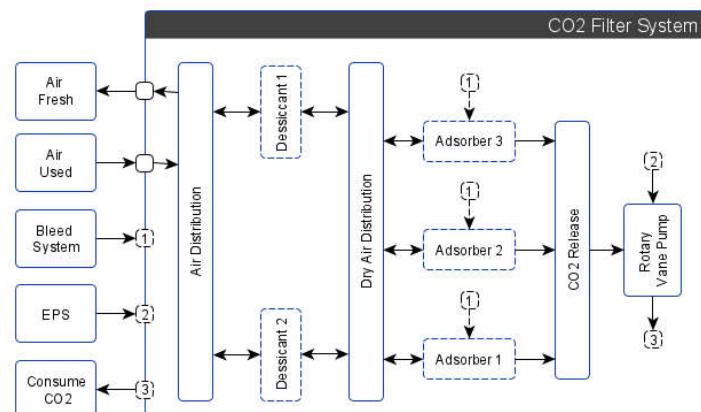


Figure 11 CO₂ Removal Systems.

resistance, the performance of the fans must be increased. Pérez-Grande and Leo describe how to optimize an ECS.³⁴ Using the described method, an existing calculation was modified in such a way that the additional resistance through the CO₂ separation system can be taken into account and the additional energy requirement calculated.

A. Results

For the CO₂ separation system, the mass and electrical power requirements of three aircraft configurations are listed in Table 3. Further, the saved bleed air was determined using equation 4 taking into account the effect on the engines. Here \dot{m}_{Bleed}^{PAX} is the prescribed fresh air rate.¹ Additionally it is considered that only 50% of the fresh air is drawn from bleed air.

$$\dot{m}_{Bleed} = \frac{\dot{m}_{Bleed,PAX}}{2} * PAX \quad (4)$$

Table 3 Determined system parameters

PAX	252 + 6 + 2	301 + 7 + 2	352 + 9 + 2
Mass [kg]	373	446	522
Electric Power [kW]	13.3	15.8	18.5
Saved bleed air [kg/s]	>0.54	>0.65	>0.75

The midrange aircraft designed in the ATLAS project could be continuously calculated by an overall calculation workflow. Then, the impact of individual systems like the ECS was determined by taking the changes of system parameters such as mass and energy consumption into account at aircraft level. The system parameters on aircraft level calculated in Table 4 were determined for configuration 3 with the maximum number of passengers.

Table 4 Impact on aircraft level

Aircraft configuration	Base	+ CO ₂ separation	[%]
Performance			
Block fuel [kg]	29418	28470	-3.2
Reserve fuel [kg]	3743	3636	-2.9
Design Masses			
MTOW	137699	136830	-0.6

As shown in Table 4, the integration of the CO₂ system has a positive effect. The engines can be operated in an optimized way by saving bleed air. As shown, this reduces fuel consumption and additionally saves weight in the engines. With this positive outcome the CO₂ separation system could be integrated into the ECS and offers advantages during operation for an operator.

VII. Conclusion

During the ATLAS project a feasibility study for a CO₂-managed cabin considering two new technologies was conducted. In the early phase, the study carried out that the enrichment of O₂ by extraction from the air introduces an additional mass and is expensive in the energy consumption. Comparing the additional mass and energy consumption the reduction of fuselage weight is not justifiable. However, there is still a lot of research to be done in order to benefit from the advantages of reducing the fuselage weight and then saving operational cost. Also, by increasing the partial pressure of O₂ the possible increasing passenger comfort is a benefit which can be paid off.

The use of currently available chitosan aerogels would lead to a higher system mass and volume compared to the use of zeolite 13X. To enable the application of aerogels the adsorption capacity needs to be increased to reduce the system mass. If a solution can be found, then beside the adsorption capability also the insulation property of aerogels can be used. Thus may save additional mass by replacing the conventional isolation of an aircraft. However, using zeolite 13X a CO₂ separation system can be integrated as an additional component into a conventional ECS. By integrating the CO₂ separation system into the recirculation the performance of the recirculation fans needs to be increased. But, due to the separation of CO₂ from cabin air, bleed air and in the consequence fuel can be saved as showed in the feasibility study. By choosing the integration into the recirculation the CO₂ separation system can be used in both newly developed and existing ECS in a retrofit. Since our design corresponds to the level of detail of a concept study, there is still potential for optimization through the detailed design.

References

- ¹ European Aviation Safety Agency, "Certification Specifications and Acceptable Means of Compliance for Large Aeroplanes CS-25," Amendment 24, 2020.
- ² Berner, E. K., and Berner, R. A., *Global Environment: Water, Air, and Geochemical Cycles*, 2nd ed., Princeton University Press, Princeton, NJ, 2012.
- ³ Sauterleute, A., "Konzeption und Entwicklung von Flugzeugklimatisierungsanlagen," Praxis-Seminar Luftfahrt, Hamburg University of Applied Sciences, Hamburg, Germany, 01.06.2006.
- ⁴ Venkatarathnam, G., *Cryogenic Mixed Refrigerant Processes*, Springer-Verlag, New York, 2008.
- ⁵ Baker, R. W., "Future Directions of Membrane Gas Separation Technology," *Industrial & Engineering Chemistry Research*, 41, 2002, pp.1393-1411.
- ⁶ Bernardo, P., Drioli, E., and Golemme, G., "Membrane Gas Separation: A Review/State of the Art," *Industrial & Engineering Chemistry Research*, 48, 2009, pp. 4638-4663.
- ⁷ Rouquerol, F., et al. , *Adsorption by Powders and Porous Solids*, Academic Press, San Diego, CA, 1999, pp. 1-26.⁸Knox, J. C., Watson, D. W., Giesy, T. J., Cmarik, G. E., and Miller, L. A., "Investigation of Desiccant and CO₂ Sorbents for Exploration Systems 2016-2017," *47th International Conference on Environmental Systems*, Charleston, SC, 2017.
- ⁹ Cmarik, G. E., and Knox, J. C., "Co-Adsorption of Carbon Dioxide on Zeolite 13X in the Presence of Preloaded Water," *48th International Conference on Environmental Systems*, Albuquerque, NM, 2018.
- ¹⁰ Torenbeek, E., *Synthesis of Subsonic Airplane Design*, Springer Science & Business Media, Dordrecht, Netherlands, 1982.
- ¹¹ Roskam, J., *Airplane Design – Part IV*, 5th ed., DARcorporation, Lawrence, KS, 2007.
- ¹² Raymer, D. P., *Airplane Design: A Conceptual Approach*, 2nd ed., AIAA Education Series, AIAA, Washington, DC, 1992.
- ¹³ Lammering, T., "Integration of aircraft systems into conceptual design synthesis," Ph.D. Dissertation, Institute of Aerospace Systems, RWTH University, Aachen, Germany, 2014.
- ¹⁴ Koeppen, C., "Methodik zur modellbasierten Prognose von Flugzeugsystemparametern im Vorentwurf von Verkehrsflugzeugen," Ph.D. Dissertation, Institute of Aircraft Systems Engineering, TU Hamburg, Hamburg, Germany, 2006.
- ¹⁵ Schültke, F., "MICADO: Aircraft Design at ILR," URL: <http://www.ilr.rwth-aachen.de/index.php?id=359> [cited 01.03.2020].
- ¹⁶ Kröber Medizintechnik, "Kröber O2," URL: https://www.kroeber.de/site/kroeber_o2_2_d.asp [cited 01.02.2020].
- ¹⁷ DÜRR TECHNIK, "Oxyfly – Oxygen Generator for Aircraft," URL: <http://www.oxyfly.com>. [cited 01.02.2020].
- ¹⁸ Kistler, S. S., "Coherent Expanded Aerogels and Jellies," *Nature*, 127, 1931, p. 741.
- ¹⁹ Guarín Romero, J. R., et al., "Kinetic and Equilibrium Study of the Adsorption of CO₂ in Ultramicropores of Resorcinol-Formaldehyde Aerogels Obtained in Acidic and Basic Medium," *Journal of Carbon Research*, 4, 2018, article 52.
- ²⁰ Wörmeyer, K., and Smirnova, I., "Breakthrough measurements of CO₂ through amino functionalised aerogel adsorbent at low partial pressure: Experiment and modeling," *Microporous and Mesoporous Materials*, 184, 2014, pp. 61-69.
- ²¹ Bacsik, Z., et al. , "Mechanisms and Kinetics for Sorption of CO₂ on Bicontinuous Mesoporous Silica Modified with *n*-Propylamine," *Langmuir*, 27, 2011, pp. 11118-11128.
- ²² Ganesan, K., Budtova, T., Ratke, L., Gurikov, P., Baudron, V., Preibisch, I., Niemeyer, P. D., Smirnova, I., and Milow, B., "Review on the Production of Polysaccharide Aerogel Particles," *Materials*, 11, 2018, pp. 2144-2181.
- ²³ Hunt, E. H., Reid, D. H., Space, D. R., and Tilton F. E., "Commercial Airliner Environmental Control System," *Aerospace Medical Association 66th Annual Scientific Meeting*, Anaheim, CA, May 1995.
- ²⁴ Wieland, P. O., "Living Together in Space: The Design and Operation of the Life Support Systems on the International Space Station," NASA TM-1998-206956/Volume I, 1998.
- ²⁵ Preibisch, I., Niemeyer, P. D., Yusufoglu, Y., Gurikov, P., Milow, B., and Smirnova, I., "Biopolymer-based Aerogel Bead Production via Jet Cutting Method," *Materials*, 11, 2018, pp.1287-1303.
- ²⁶ Brunauer, S., Emmett, P. H., and Teller, E., "Adsorption of Gases in Multimolecular Layers," *Journal of American Chemical Society*, 60, 1938, pp. 309-319.
- ²⁷ Schumann, H., Berres, A., Escher, S., and Stehr, T., "PARADIGMshift: A Method for Feasibility Studies of New Systems," *Procedia Computer Science*, 44, 2015, pp. 578-587.
- ²⁸ ASHRAE, ANSI/ASHRAE Standard 55-2010, "Thermal Environmental Conditions for Human Occupancy," *American Society of Heating, Refrigerating, and Air-Conditioning Engineers, Inc*: Atlanta, GA, 2010.
- ²⁹ ASHRAE, ANSI/ASHRAE Standard 62.1-2013, "Ventilation for Acceptable Indoor Air Quality," *American Society of Heating, Refrigerating and Air-Conditioning Engineers, Inc*: Atlanta, GA, 2013.
- ³⁰ Knox, J. C., "Development of carbon dioxide removal systems for NASA's deep space human exploration missions 2016-2017," *47th International Conference on Environmental Systems*, Charleston, SC, 2016.
- ³¹ W. R. Grace & Co.-Conn., "SYLOBEAD - Adsorbents for Process Applications," Worms, Germany, 2010.
- ³² Kast, W., *Adsorption aus der Gasphase – Ingenieurwissenschaftliche Grundlagen und technische Verfahren*, VCH Verlagsgesellschaft, Weinheim, Germany. 1988.
- ³³ Klinkenberg, A., "Heat Transfer in Cross-Flow Heat Exchangers and Packed Beds," *Industrial and Engineering Chemistry*, 46, 1954, pp. 2285-2289.
- ³⁴ Pérez-Grande, I., and Leo, T. J., "Optimization of a commercial aircraft environmental control system," *Applied Thermal Engineering*, 22, 2002, pp. 1885-1904.