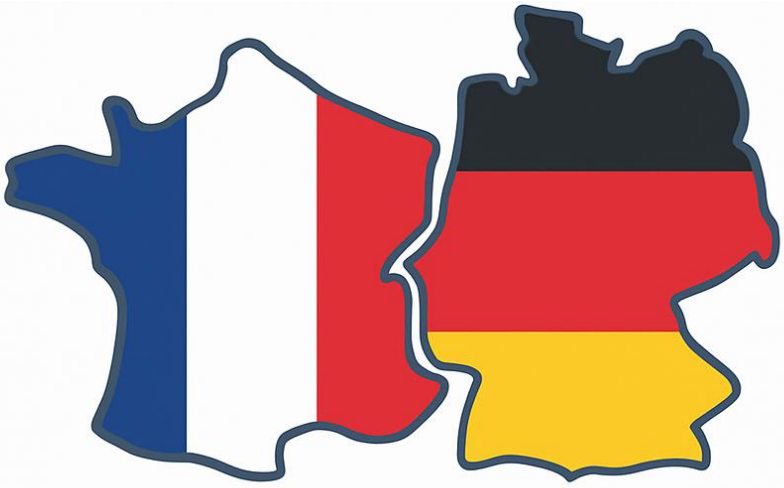

FRENCH-GERMAN ADSORPTION INITIATIVE

SCIENTIFIC PROGRAM

Duisburg,

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March 2026

Welcome

The 2nd Adsorption Conference organized by the “French-German Adsorption Initiative” will be held in Duisburg (Germany) between March 24th and 26th, 2026. The conference is supported by the German Adsorption Group (DECHEMA) and the French “Association Francaise de l’Adsorption (AFA)”. The aim of the conference is to bring together and foster collaboration between scientists from these two communities. However, we see this joint initiative as a platform that could be extended to all European countries in the very near future. Therefore, we are open for presentations from France, Germany and neighboring countries.

Adsorption phenomena play a crucial role in many processes, with applications ranging from catalysis to treatment of waste streams. Current research ranges from the development of innovative adsorbent materials to using molecular modeling tools to predict adsorption behavior. The scope of adsorption research is also expanding into new fields, including energy systems, environmental protection, and the life sciences.

As we want to cover the whole bandwidth from basic research to applied technology, we invite people both from academia and industry to present their topics. This creates an excellent environment for the exchange of ideas and knowledge between scientists and practitioners in the field.

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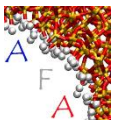

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Investigations on the influence of process conditions in chemisorptive CO_2-capture from industrial gas streams

Philipp Keil[a]
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CO_2 capture from industrial emission gas streams and subsequent storage are essential technologies for effectively achieving emission reductions for climate change actions, particularly for industries with hard to abate emissions like waste incineration plants or cement works. Adsorptive CO_2 capture by PSA and TSA processes have attracted increasing interest in recent years as an alternative to absorption processes. Despite decades of industrial experience in the adsorptive removal of CO_2 from process gas streams like synthesis and natural gas, there is still need for extensive research to develop new innovative processes and optimized adsorbents for the specific requirements of CO_2 capture from emission gas streams. Among many other aspects, the influence of moisture plays a significant role under dynamic process conditions. It is well known that many common physisorbents used for CO_2 adsorption, e.g. zeolite 13X, quickly deplete in CO_2 capacity in the presence of water due to competitive adsorption. Therefore, chemisorbents that enable non-competitive adsorption of CO_2 and water are of great interest, as they simplify selective CO2 removal from moist gas streams using TSA processes without water removal. [1,2].

This contribution presents selected results from current research on the experimental characterization of commercial and newly developed chemisorbents in the course of scaling up a CO_2 capture TSA from flue gases. Systematic measurements of breakthrough curves on lab scale with the commercially available amine-functionalized polymer adsorbent Lewatit® VP OC 1065 as model adsorbent reveal, that both humidity of the gas stream as well as the water loading of the adsorbent have a relevant influence under dynamic process conditions [3]. Experimental results on long-term stability under dynamic conditions reveal, that aside of temperature, humidity and gas composition during regeneration is significant, too. The findings are discussed combined together with equilibrium data with respect to process design. For scaleup and process optimization, a dynamic, non-isothermal adsorption model has been implemented, which is based on static-volumetrically measured isotherm data, and contains also adapted models for considering the influence of water in gas and adsorbent on CO_2 capacity and thermal properties [4]. A containerized pilot plant has been designed together with an industrial partner, which will be operated by latter onsite with real flue gas streams for adsorbent testing, process optimization and to provide data for model validation for further development and scaleup in the outlook.

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Stability of Amine-Functionalized Sorbents for Direct Air Capture in the presence of O_2, CO_2, and H_2O at high temperature

T. Aztiria [a], *A. Marberger* [a], *D. Albani* [a];
[a] *Climeworks AG, Zürich, Switzerland*

Direct Air Capture (DAC) is a critical technology for climate change mitigation that removes CO_2 from the atmosphere. Despite its key role in climate goals, few studies address the stability of amine-functionalized sorbents under process relevant conditions. Most stability studies are limited to O_2/N_2 exposures in dry or humid conditions, with little consideration given to the potential role of CO_2 and H_2O on the degradation of the sorbent, despite their variable concentrations within the DAC process. Available research on the effect of H_2O has primarily focused on aminopolymers supported on silica or alumina, showing that H_2O vapor can suppress or accelerate degradation depending on the support and amine structure [1-3]. Similarly, research on the effect of the simultaneous presence of CO_2, O_2, and H_2O at elevated temperatures has focused primarily on polyethylenimine (PEI) supported on silica and alumina, showing on one side that high concentrations of CO_2 can protect the amine groups against oxidation [1,4], while low concentrations of CO_2 can accelerate the degradation of the material [5,6].

In this study, we focus on degradation tests that are relevant to Climeworks' DAC process by performing accelerated degradation experiments with variable O_2, CO_2, and H_2O vapor concentrations at moderate and elevated temperatures. We demonstrate that the presence of H_2O and CO_2 can impact the effects of O_2 on amine-functionalized sorbents, depending on their concentration in the gas phase. Through characterization of the degraded samples, we track the effects on the amine functionalities to uncover possible variations in the oxidative degradation mode due to the presence of H_2O and CO_2. These results highlight the importance of extending the stability assessment of sorbents for DAC to conditions that are more relevant to the process, allowing to unveil potential synergistic effects of the different components that will impact the lifetime of the material.

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Capture and separation of CO_2 from N_2 using activated carbons prepared from N-rich precursors

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As CO_2 is one of the main greenhouse gases, the increase in its concentration in the atmosphere leads to global warming. For this reason, numerous researches are presently focused on CO_2 separation from industrial gases in the post-combustion process. In this work, nitrogen-enriched Activated Carbons (ACs) with nitrogen content up to 10 wt.% were synthesized in two successive steps in the same furnace. The first step was a pyrolysis (10 $K.min^{-1}$, 1173 K, N_2 flow rate: 200 $mL.min^{-1}$) of nitrogen-rich precursors: lyophilized millimetric beads and powder of chitosan (7 wt.% N), coffee grounds (3 wt.% N) and polyacrylonitrile powder (26 wt.% N). The second step was a gasification activation with an NH_3/H_2O mixture (90 wt.% NH_3, NH_3 flow rate: 30-36 $mg.min^{-1}$) at 1173 K using N_2 as carrier gas (activation time: 15-120 min).

The physisorption isotherms at 77 K of N_2 and H_2 indicate that the synthesized ACs are mainly microporous. The BET surface areas vary in the range: 325-1390 $m^2.g^{-1}$. Adsorption isotherms of CO_2 and N_2 on ACs were studied at $P \leq 1$ bar, at three different temperatures: 273 K, 298 K and 323 K. The amount of CO_2 physisorbed at 1 bar ranges from 1.79 to 2.98 $mmol.g^{-1}$ at 298 K. The CO_2 isosteric adsorption heats were determined from the isotherms network. To assess the ability of ACs to select CO_2 over N_2, the CO_2/N_2 selectivities were calculated for a mixture containing 15% vol. of CO_2, using the Ideal Adsorbed Solution Theory (IAST) model applied to the adsorption isotherms of the pure gases.

The dependence of CO_2 isosteric adsorption heat on coverage is typical of heterogeneous surfaces, reflecting a distribution of various pore sizes. At 298 K, the CO_2/N_2 selectivity value of the ACs ranges from 24 to 110. The highest selectivity is obtained for the AC from coffee grounds activated for 120 min at 298 K. To better understand this behavior, statistical methods such as Principal Component Analysis (PCA) and Partial Least Squares regression (PLS regression) were applied. They demonstrate that the impurity content in ACs affects the CO_2/N_2 selectivity at 298 K. This is corroborated by SEM coupled to EDS, that has revealed the presence of mineral impurities containing Ca, K, Mg and P, which are likely to affect selectivity at $T > 298$ K.

Acknowledgments: National French Agency and France2030 supporting CATALPA ANR-22-PESP-0007 project (Spleen).

Direct Air Capture of CO_2 Using Amine-appended Metal-Organic Frameworks

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The continuous rise in atmospheric CO_2 is driving the urgent need for efficient carbon capture technologies. Among them, direct air capture (DAC) offers a promising approach by extracting CO_2 directly from ambient air. Conventional liquid amine-based sorbents, though effective, face challenges related to high regeneration energy, corrosion, chemical degradation, and operational costs. These drawbacks have motivated the exploration of solid-state alternatives such as metal–organic frameworks (MOFs), whose modular structures and tunable chemistry offer exceptional potential for DAC[1].

Amine-functionalized MOFs, particularly polyamine-grafted systems like mmen-Mg_2(dobpdc) [2] and amino acid-modified frameworks (e.g., lysine@MOF-808(Zr)) [3], have recently emerged as high-performance materials. In this work, we explore a greener post-synthetic grafting route to incorporate amine-containing moieties onto MOFs, aiming to enhance CO_2 affinity and chemical robustness of the adsorbent. Notably, the monoamine-grafted system exhibits a remarkable CO_2 uptake of ~0.5 mmol g^{-1} at 0.4 mbar with a heat of adsorption around –70 kJ mol^{-1}, confirming the effectiveness of the single amine group in capturing low-pressure CO_2 (Figure 1).

This presentation will detail our amine grafting strategy, initial single-component gas adsorption results, and stability under humid conditions. The influence of moisture on performance, as well as preliminary breakthrough studies under $CO_2/H_2O/N_2$ gas mixture, will also be discussed. Finally, we will outline how extending this strategy toward polyamine grafting could further enhance CO_2 sorption capacity under realistic DAC environments.

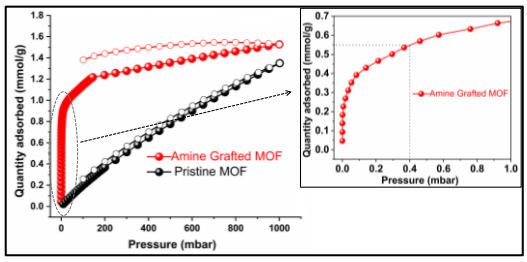

Figure. 1. *CO_2 adsorption isotherm at 25 °C yielded a CO_2 uptake 0.5 mmol g^{-1} at 0.4 mbar.*

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Experimental screening of zeolites for application in an industrial sorption tumble dryer

Henri Schmit [a], Tobias Schubert [a], Eberhard Lävemann [a], Stefan Hiebler [a]
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Open adsorption systems based on water adsorption and desorption on zeolites can be used for heating, cooling, and thermal energy storage. Within an ongoing project, the integration of such a sorption system into an industrial gas-fired tumble dryer is being investigated, aiming to reduce the energy demand by up to 30%. Typical industrial tumble dryers operate with drying times of about 20 min and temperatures up to 210 °C. The target conditions for zeolite desorption in this application are 300 °C and a dew point of 80 °C.

Four commercial binder-free zeolites from Chemiewerke Bad Köstritz (CWK) were investigated (3ABFK, 4ABFK, 5ABFK and NaYBFK) as well as one standard zeolite with binder (4AK) and an ion-exchanged sample, Mg-4ABF (32% exchange rate). The volumetric water uptake and hydrothermal stability were investigated to identify the most suitable zeolite for industrial tumble dryer conditions.

Characteristic curves were determined using equilibrium water uptake data obtained from a simultaneous thermal analysis (STA) device operated in thermogravimetric analysis (TGA) mode with a coupled humidity generator. Adsorption conditions ranged between 80–100 °C (temperature) and 40–60 °C (dew point temperature), while desorption was fixed at 300 °C and 80 °C dew point temperature. Under these conditions, NaYBFK exhibited the highest volumetric water uptake (0.207–0.270 $cm^3\ g^{-1}$), followed by Mg-4ABF (0.203–0.253 $cm^3\ g^{-1}$). Among the A-type zeolites, 4ABFK showed the largest range (0.175–0.205 $cm^3\ g^{-1}$).

Hydrothermal stability was assessed using 16 combinations of temperature (200–300 °C) and dew point (30–70 °C) over a 10-day period, followed by reference adsorption cycles to quantify ageing. Hydrothermal ageing results revealed only a marginal decrease (~1%) in water uptake for 4ABFK, within the measurement uncertainty. The binder-containing 4AK had a maximum decrease of 3.3% for 200 °C and 70 °C dew point temperature. Mg-4ABF showed a maximum loss of ~7.5% under 200–233 °C and 60–70 °C dew point temperature. Tests for the remaining zeolites under target conditions are ongoing.

Influence of cation Exchange on Low-Pressure Adsorption of CH_4, CO_2, N_2 and Ar in 13X Faujasites.

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[b]*Université de Strasbourg, France*

Gas phase adsorption process

In this study, the influence of charge-compensation cations on adsorption at low-pressure of CH_4, CO_2, N_2 and Ar was investigated using 13X faujasite. First, charge-compensation cations Na+ of the13X faujasite was exchanged with alkali and alkaline-earth cations (Li^+, K^+, Mg^{2+}, Ca^{2+} & Sr^{2+}) in order to identify the most versatile adsorbent. Ca-exchanged faujasite exhibited promising results, particularly for CH_4 and N_2 adsorption, while Sr-exchanged faujasite showed enhanced performance for CO_2 (Figure 1.A). Second, sodium cations were replaced by calcium, followed by partial introduction of divalent transition-metal cations (Co^{2+}, Ni^{2+} & Cu^{2+}) at relatively low exchange levels. The adsorption performance strongly depends on the nature of the exchanged cation. Calcium/copper exchanged faujasites show promising selectivity for CH_4 and Ar adsorption, while calcium/cobalt exchanged samples demonstrate versatile adsorption behavior towards studied gases (Figure 1.B). These findings highlight the crucial role of charge-compensation cation composition in tailoring adsorption properties, with potential applications in gas trapping under low-pressures environments.

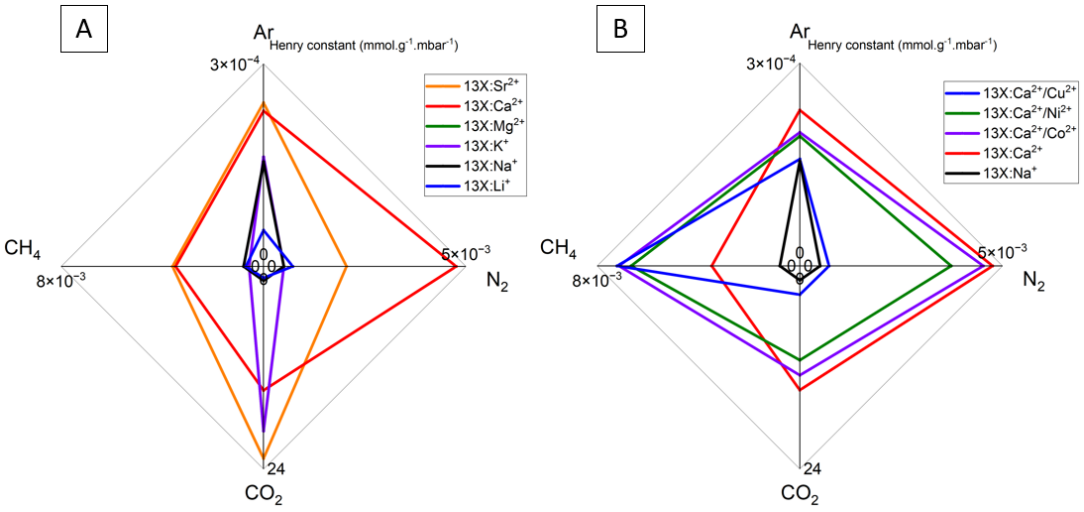

Figure 1: Henry's constant determined for the adsorption of CH_4, CO_2, N_2 & Ar at 20°C on faujasites exchanged with (a) alkali & alkaline-earth cation or (b) divalent transition-metal cations.

Insights into Krypton Sequestration Mechanism in a Tailored LTA Zeolite

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Krypton is a rare noble gas with various industrial applications, including lighting, insulation, and medical imaging. While krypton is currently stored in high-pressure cylinders, alternative storage methods could offer advantages for specific applications requiring controlled release or ambient pressure handling. Adsorptive storage in microporous solids represents a promising approach for rare gas capture and retention under mild conditions. The objective of this work is to investigate zeolites capable of strongly capturing krypton with limited desorption, thereby exploring a novel storage approach for this gas.

Through a systematic screening of bicationic **LTA** zeolites, we identified a specific composition, $K_{4.2}Ca_{3.9}$-LTA, which exhibits distinctive krypton adsorption-desorption isotherms. While K-LTA shows negligible adsorption and Ca-LTA displays fully reversible adsorption, $K_{4.2}Ca_{3.9}$-LTA demonstrates pronounced hysteresis, indicating potential for long-term storage (**Fig. 1.a**). This hysteresis diminishes with increasing adsorption temperature. Desorption kinetics were assessed through manometric experiments, revealing that krypton can be effectively trapped within this specific zeolite, with minimal release under ambient T and P.

Synchrotron PXRD studies were conducted, providing structural insights, especially regarding the cation distribution. The results reveal a specific arrangement of K^+ and Ca^{2+} cations that simultaneously provides accessible adsorption sites while maintaining pore-blocking cations. **(Fig. 1.b)** The effect of temperature was also investigated to correlate the non-monotonic temperature dependence observed in adsorption with cationic mobility.

This study demonstrates the potential of specifically tailored zeolites for gas storage at ambient pressure and temperature.

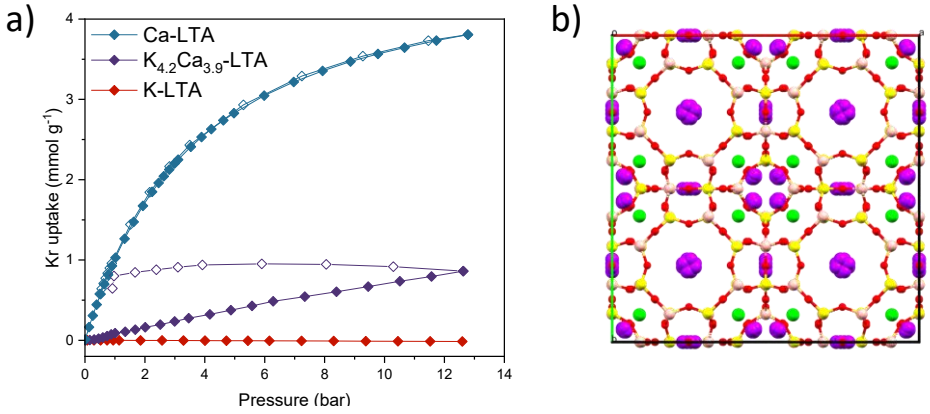

Fig. 1 a) Kr adsorption isotherms on cation-exchanged LTA zeolites at 298 K. b) View of the crystal structure of the KCa LTA, K^+ positions are represented in purple, Ca^{2+} positions in green.

D_2/H_2 separation on zeolites under cryogenic conditions: revealing the mass transfer mechanism through breakthrough curves analysis

Claire Coutier [a b], *Clément Cabaud* [b], *Igor Bezverkhyy* [a]

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Separation of hydrogen isotopes is an important technological issue due to numerous applications of deuterium and tritium in research and industry. Microporous sorbents of different nature (zeolites, MOFs and activated carbons) have been shown to be selective towards heavier isotopes during adsorption under cryogenic conditions (< 77 K). This selectivity is due to the "quantum sieving" effect observed in micropores when the pore size is similar to the size of H_2 molecules (~ 3 Å). An important research effort has been developed in this field and it has been recently shown that D_2/H_2 selectivity of magnitude higher than 20 can be achieved at 40 K in CHA zeolites and in some MOFs.

The high values of D_2/H_2 selectivity in microporous materials were obtained under *equilibrium* conditions. It is not clear however if a high separation efficiency can be maintained under *dynamic* conditions used in industry since the information on the diffusion of D_2 and H_2 in microporous solids at low temperature is lacking. To fill this gap, we realized a detailed kinetic study of D_2/H_2 mixture separation at 40 K using the breakthrough curves technique. The mass transfer characteristics were obtained through analysis of the breakthrough curves measured in a laboratory scale setup (~ 1 g of sorbent) for several shaped zeolites of FAU and LTA structure. For some materials the breakthrough curves were also measured using an industrial pilot column (~ 200 g of sorbent).

Before analysing the kinetic parameters, the axial dispersion coefficients were determined from the series of measurements for different flowrates. This data was used to subtract accurately the contribution of the axial dispersion and to obtain the characteristic time corresponding only to the mass transfer in zeolite particles. Also, it was shown that the adsorption isotherms of D_2 in the presence of H_2 are linear for all materials. This finding allowed to represent the overall diffusion time obtained from the breakthrough curves as a linear combination of the characteristic times of different steps involved in the adsorption process (film transfer, macropore and micropore diffusion). By realizing measurements for different particle sizes (300 – 700 µm) we determined the values of macropore and micropore diffusion coefficients in the studied zeolites and identified the most performant sorbent.

Sub topic – Thermodynamics and kinetics of adsorption

Small-Angle Scattering Insights into the Equilibrium or Metastable Nature of Capillary Condensation

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[a] *Dep. Chemical Engineering, University of Liège, Belgium*
[b] *Polymer Chemistry and Materials, KULeuven, Belgium*

Sub topic – Characterization of porous materials

Questions about the origin of the adsorption/desorption hysteresis are as old as sorption experiments themselves. Most existing methods to extract pore size distributions from sorption data assume that adsorption is a metastable process and that desorption takes place at thermodynamic equilibrium. Here we report on nitrogen and argon sorption on a series of fourteen SBA-15 ordered mesoporous silicas, and we use small-angle X-ray scattering (SAXS) to independently determine their pore sizes. We find that capillary condensation systematically occurs close to thermodynamic equilibrium according to a Derjaguin−Broekhoff−de Boer calculation [1]. Our analysis suggests that many earlier works have significantly underestimated the actual pore size in SBA-15 materials. It also highlights the critical role of the reference isotherm used to calibrate the fluid−solid interaction in the models.

The presentation of these new results will also be an occasion for a more general discussion of capillary condensation in a broader historical perspective. Although the phenomenon was first described more than 150 years ago by Lord Kelvin, ordered mesoporous materials have only been available for about 30 years. Testing theories of capillary condensation on these types of materials is a difficult process, for two distinctly different reasons. First their structure is more complicated than initially acknowledged, and understanding the effect of geometrical non-idealities (pore constriction, corrugation, etc.) on sorption is still an active subject of research. The second difficulty pertains to the dual status of capillary condensation/evaporation as both a research topic and a characterization method. In that situation, it is occasionally difficult to discriminate theories that are truly validated from others that are merely self-consistent. Independent characterization methods, such as small-angle scattering, have an important role to play in that process [2].

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Adsorption Potential Theory and strong confinement effects on CO_2/H_2O competition in CALF-20.

P. Grisanti [a]; *Y. Magnin*[b]; *B. Coasne*[a,c]; *S. Gravelle*[a].

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To limit global warming in the coming decades, capturing CO_2 from industrial emissions using nanoporous materials is a promising approach. Among them, Metal–Organic Frameworks (MOFs) show great potential due to their versatile structures and tunable properties. However, humidity in flue gases often hinders CO_2 capture by competing for adsorption sites. A deeper understanding of these interactions is thus crucial for selecting suitable MOFs and guiding the design of next-generation sorbents. In this context, atomistic numerical simulations provide a microscopic understanding of the thermodynamic properties and interactions of CO_2 in these materials.

In this work, Grand Canonical Monte Carlo (GCMC) simulations of CO_2 and water mixtures were performed in CALF-20, a recently reported structure by Shimizu *et al*. with promising capture properties. To understand what distinguishes this material from others, the century-old Polanyi's Adsorption Potential Theory (APT), was tested to compare both species. While the theory describes water adsorption well, unexpected behavior was observed for CO_2, highlighting the need for corrections in the subnanoporous regime. With our proposed correction, we show that this theory is capable of predicting isotherms even in this highly confined system, as shown in the figure where dots correspond to simulations and dashed lines to predictions. To better understand the difference between water and CO_2, their structural and energetic interactions were compared to explore their competitive adsorption behavior.

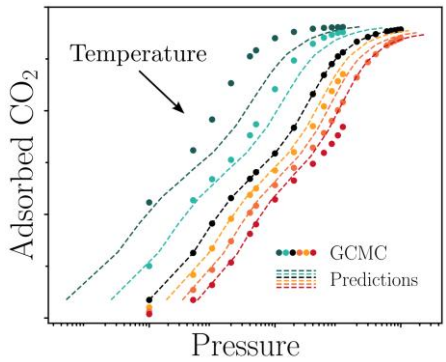

Figure: Simulated adsorption isotherms (dots) and model predictions (lines) at different temperatures.

A non-local Density Functional Theory for water adsorbed in nanoporous materials of arbitrary geometry

Antoine Barthes [a]; *David Grégoire* [a]; *Christelle Miqueu* [a]
[a] *Universite de Pau et des Pays de l'Adour, CNRS, LFCR, Anglet, France.*

Water confined in nanoporous materials has focused many attentions due to its vast number of technical applications and scientific fields [1]. Indeed, confinement of water in nanopores affects its thermodynamic properties such as its density, its freezing temperature, the crystal structure, *etc*. For some years now, porosimeter manufacturers have been integrating the ability to perform high-precision measurements of adsorption of vapors at low pressure, including water. In parallel, thermoporosimetry appears to be a good alternative - or at least a good complementary technique - to gas porosimetry and mercury intrusion, especially for the investigation of the samples that can be destroyed in drying process [2]. The common features between water vapor sorption analysis and thermoporosimetry is that a reliable model of water adsorption inside nanopores is necessary to interpret the experimental data and try to obtain structural information of the porous materials from these measurements. In this work, we present a new NLDFT framework for confined water based on the general formulation of Wertheim's thermodynamic perturbation theory [3] and the statistical associating fluid theory [4]. The resulting model can be employed to determine the microscopic structure of inhomogeneous water in pores of arbitrary 3D geometry. It is first used to evaluate the phase behavior of water confined in carbon slit pores over a wide range of pore sizes and thermodynamic conditions, thanks to the low computational cost of the method. Then, the focus is done on the thin water film confined between an ice crystal and a graphitic surface, as it is assumed that the pressure exerted by the latter could initiate mechanical damage in nanoporous materials.

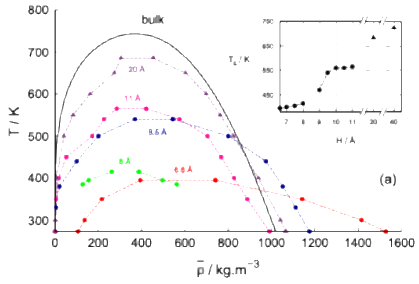

Figure 1 : liquid-vapour phase diagram of water confined in graphitic pores by SAFT-NLDFT

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Resource and Sustainability Considerations in the Activated Carbon Industry

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The global market for activated carbon is experiencing strong growth. In recent years, demand has risen sharply, driven by stricter environmental protection measures and emission control regulations. Germany's demand has more than doubled since 2010 and now exceeds 80,000 tonnes annually, highlighting both the rapid market expansion and the need for a secure and sustainable raw material supply.

At the same time, an analysis of current resource base reveals growing constraints on traditional feedstocks such as lignite, whose availability is rapidly declining, and hard coal, which depends on long international supply chains. This dependency results in price instability, potential impacts from coal phase-out policies, shipping issues, and limited sustainability due to long transport routes and extraction-related emissions. Against this backdrop, resource efficiency and sustainability have become key priorities.

The presentation provides an outlook on how innovative solutions can be used to counteract the impending shortage of raw materials. For example, the regeneration and reuse of spent activated carbon that has already been used in exhaust gas purification processes offer a practical and environmentally friendly alternative to primary production. It shows that it is possible to significantly reduce resource consumption and CO_2 emissions while maintaining product quality. This presents an effective solution for reducing dependence on new raw materials and promoting the circular economy within the industry.

Looking ahead, Carbon Service & Consulting is already implementing the principles that will define the future of the activated carbon sector. The presentation will highlight ways in which the activated carbon industry can combine sustainability with reliability through closed regeneration cycles, regional raw materials, and process optimizations to improve energy efficiency and reduce emissions. These measures ensure long-term raw material security, economic stability, and a significant reduction in environmental impact — and show that the transition toward a circular, low-emission, and sustainable activated carbon industry has already begun in practice.

Advanced textural characterization of Carbon Molecular Sieves complementing the development of material structure and process performance correlations

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As a consequence of the tailored pore structure, carbon molecular sieves (CMS) enable separations of industrially relevant gas mixtures, including O_2/N_2, CO_2/CH_4, N_2/CH_4, or CO_2/N_2 by exploiting a significant difference in mass transfer rates among adsorptives. Thus, PSA/VSA techniques utilize primarily that effect for the efficient production of purified gas streams. The proper design of kinetic-based separation processes requires an extended, application-performance-oriented information about the selected adsorbent, as adsorption capacity, mass transfer kinetics, selectivity, or regenerability. However, as these material characteristics result from the adsorbent structural properties, specifically surface-topology and surface-chemistry, acquiring that structure-oriented information shall not be omitted, as it is fundamentally in control of PSA/VSA performance.

The reliable textural characterization of CMS materials remains challenging due to their complex pore network, consisting of macropores and ultramicropores connected by very narrow necks. Physisorption of argon and nitrogen at 87 K and 77 K, respectively, remains one of the most widely applied techniques within this context, however, it does not allow for an accurate and comprehensive characterization of CMS, given substantial diffusion limitations within the narrow neck at cryogenic temperatures. Thus, a selection of suitable probe molecules – considering their size, shape, and polarity – as well as the choice of appropriate testing conditions given available validated mathematical solutions, is not trivial. Moreover, an additional complexity dimension to the stated problem lies within the lack of standardized characterization protocols to determine the specific CMS structure-oriented properties beyond the simple assessment of their pore size distribution, as the distribution of neck sizes including their distinct geometry, specific location/orientation of deposited pyrocarbon layers forming the neck, or type/quantity/location/orientation of surface functional groups as well as associated charge distribution, especially around the entrance of ultramicropores.

To address these challenges, we have developed a novel methodology targeted towards a comprehensive and detailed textural and surface-chemistry characterization of CMS materials, based on the combination of gas and vapor physisorption of proper adsorptives at unique testing conditions, coupled with advanced data reduction methods. We demonstrate the unique correlations among different material assessment strategies, namely textural-based and process-based methods, particularly to highlight the importance of diverse complementary techniques towards a holistic understanding of CMS structure-performance association.

Challenges and opportunities in the industrial reactivation of PFAS-laden granular activated carbon

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Per- and polyfluoroalkyl substances (PFAS) represent a class of synthetic compounds with a high potential to pose risks to both animal and human health. These substances are widely used in medical products, cosmetics, coatings, lubricants, and firefighting foams. The use of PFAS in such applications is primarily due to their high stability and resistance to chemical and thermal degradation. However, intentional or unintentional release, results in the continuous accumulation of these substances throughout the biosphere, since the mineralization of PFAS into CO_2 and HF does not occur under environmental conditions. To address these challenges, the use and circulation of PFAS is to be regulated through national and international legislation. Frameworks such as drinking water ordinances and the EU-wide POP Regulation (Persistent Organic Pollutants) define limit values for an increasing number of PFAS. Existing environmental contamination is to be reduced through adsorptive processes, for example as a part of industrial soil washing, drinking and or wastewater treatment. In that sense, activated carbons (AC) have proven to be effective adsorbents for a broad range of PFAS. The resulting PFAS-laden AC must, depending on their loading, be landfilled, incinerated, or thermally reactivated. Successful thermal reactivation though, requires the mineralization of all PFAS contaminants to prevent the release of secondary or decomposition products.

In this contribution we present results from the thermal reactivation of PFAS-laden granular activated carbon (GAC) with the aim of the complete removal and mineralization of PFAS on an industrial scale. For this purpose, PFAS-laden GAC from soil wash and wastewater treatment plants were collected and characterized in terms of their PFAS content and distribution by a combination of basic methanole extraction and HPLC-MS/MS method. The thermal reactivation was carried in two different rotary kiln setups (one direct fired, the other one indirectly) under systematically varied operational conditions. To overview the potential release of secondary PFAS or decomposition products the kiln output, cooling water, exhaust gasses prior and after thermal oxidizer as well as the reactivated GAC were continuously analyzed for their PFAS content. The determined loadings have shown that the tested AC are efficient adsorbents for medium to short-chain PFAS. Furthermore, characterization by Ar-physisorption at 87 K revealed an influence of the pore-structure on their removal capacity. From the collected data a mass balance, proving the complete mineralization of PFAS compounds, was obtained. The results therefore indicate that AC will continue to play an important role in the remediation of PFAS contaminated environments and proves that the thermal reactivation of PFAS-laden GAC represents a safe route for the successful elimination of PFAS contaminants.

Gas Separation via Flexible MOFs

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Metal-Organic Frameworks have received considerable attention in recent years and the Nobel Prize in Chemistry in 2025. Flexibility is a unique feature of a limited number of MOFs. They open their pores selectively for specific gases excluding others that cannot open the pores. This feature leads to outstanding separation selectivity in specific cases. However, their degree of flexibility is systematically affected by their particle size and morphology. This feature enables systematic tuning of selectivity and provides a deeper understanding of the role of flexibility on separation selectivity.

We outline the understanding and performance of flexible MOFs focusing on a well established model system. DUT-8 (DUT= Dresden University of technology) is a gate pressure MOF belonging to the class of pillared-layer systems [1]. Particles with a size below 500 nm are typically rigid, while larger particles (> 2 μm) show pronounced flexibility. We compare the single and multi-component adsorption isotherms to highlight the impact of flexibility on separation selectivity. As prototypical examples, we focus on CH_4/CO_2 and H_2/D_2 separation studies. In particular the flexible form of DUT-8 shows high selectivity for D_2 vs. H_2 [2] and CO_2 vs. CH_4. In situ NMR and diffraction studies are used to deeper investigate the mechanisms behind these phenomena. Finally, we discuss insights from Xe NMR [3] in regard to noble gas separations and outline open questions in the field of gas separation regarding flexible MOFs for gases and vapors.

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Temperature-Dependent CO_2 and N_2 Adsorption on 2D Hofmann Clathrates Exhibiting Spin-Crossover Properties

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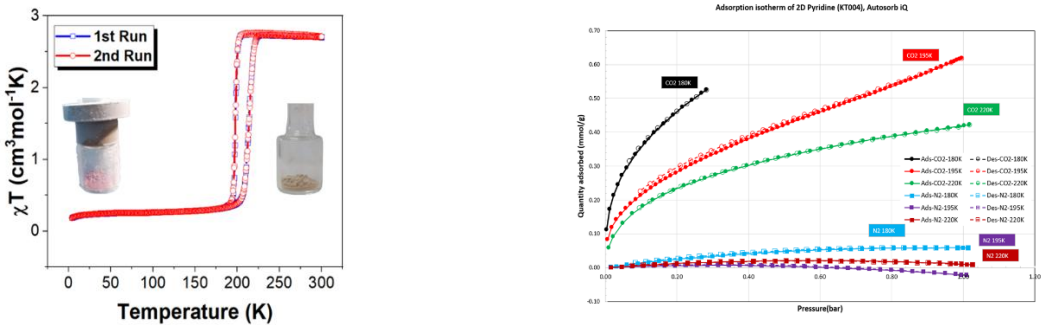
The discovery of the first Hofmann clathrate with spin-crossover (SCO) properties, $[Fe(pyridine)_2Ni(CN)_4]$, by Kitazawa and co-workers in 1996 marked a significant milestone in the development of switchable coordination materials[1]. In this compound, Fe(II) centers reversibly switch between low-spin and high-spin states under external stimuli such as temperature or pressure[2,3]. The material forms a two-dimensional interdigitated framework, offering a model platform for investigating the interplay between spin-state transitions, framework flexibility, and selective gas adsorption. In this study, we investigate the temperature-dependent adsorption of CO_2 and N_2 on $[Fe(pyridine)_2Ni(CN)_4]$ across a wide temperature range. Gas porosimetry with N_2 and Ar at cryogenic conditions revealed only minimal uptake, indicating a predominantly closed framework under these conditions. Magnetic susceptibility measurements confirmed a sharp SCO transition at ~195 K, accompanied by a visible color change (see Fig. 1). CO_2 adsorption showed significantly higher uptake compared to N_2 supporting both selective interactions with the framework and gate-opening (see Fig. 1). Moreover, steep initial slopes in the CO_2 isotherms suggest subtle structural flexibility or gate-opening behavior. The effects of mechanical processing (grinding and pelletization) on gas uptake were also evaluated, showing measurable variations in adsorption capacity.



(a) (b)

Figure 1: (a) $Fe(pyridine)_2Ni(CN)_4$ at high spin (Left) and low spin (Right), (b) Adsorption isotherms of CO_2 and N_2 at 180 K, 195 K, and 220 K.

Ligand-substitution (e.g. Phenyl-4-pyridylimine) was then performed to tune cavity size and adsorption behaviour and a custom coupled manometric–vibrational spectroscopy (Raman/IR) setup was designed to investigate structural changes and framework flexibility during CO_2 adsorption, and to correlate adsorption behavior with vibrational signatures of the host framework.

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Exploring adsorptive window effects: Unusual adsorption and diffusion patterns for CHA and AEI zeolites

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The Henry constants K_H for the adsorption of linear alkanes in zeolites are often found to increase exponentially with carbon chain length[1]. However, a limited number of studies with small-pore CHA-type zeolites have indicated an unusual variation in K_H with carbon number N_c.[2,3] This behaviour is known as a *cage effect* occurring when the alkane molecule approaches and exceeds the size of the zeolite's structural cages. Recently[4], similar effects were observed on AEI zeolite, where the K_H shows a remarkable minimum for *n*-octane.

In this presentation we revisit and explore these unusual adsorption effects, before expanding into a the associated unusual diffusion coefficient (D) trend. Using inverse gas chromatography, *n*-alkanes and 1-alkanes C_1-C_{12} were injected on various CHA and AEI zeolites, with different Si/Al ratios. For AEI and CHA, respectively, K_H rises up to C_5 and C_6, then drops to a minimum at C_8 and C_9 before rising again. The unusual non-monotonic trend is contrasted with that of a ZSM-5 zeolite, which shows a linear trend of $\ln(K_H)$ with N_c. Similar trends where observed for 1-alkenes with a shift in local minima and maxima for N_c.

By monitoring the second moments, information on the adsorption kinetics can be obtained. The AEI and CHA-alkane systems were studied using two pellets sizes and two different carrier gasses, indicating micropore diffusion as a key mass transfer resistance. Typically, a lower diffusion coefficient with increasing N_c is expected, as experimentally confirmed for ZSM-5. The AEI zeolite showed a remarkable trend. From C_5–C_8, D rises by nearly two orders and for N_c larger than 8 it drops again. The trends are confirmed at 200, 245 and 290°C, and reveal activation energies between 40-80 kJ/mol. These unusual trends can be rationalized based on computational simulation work[5] on *window effects*.

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Development of a novel swing-adsorption gas separation technique using force-responsive carbons

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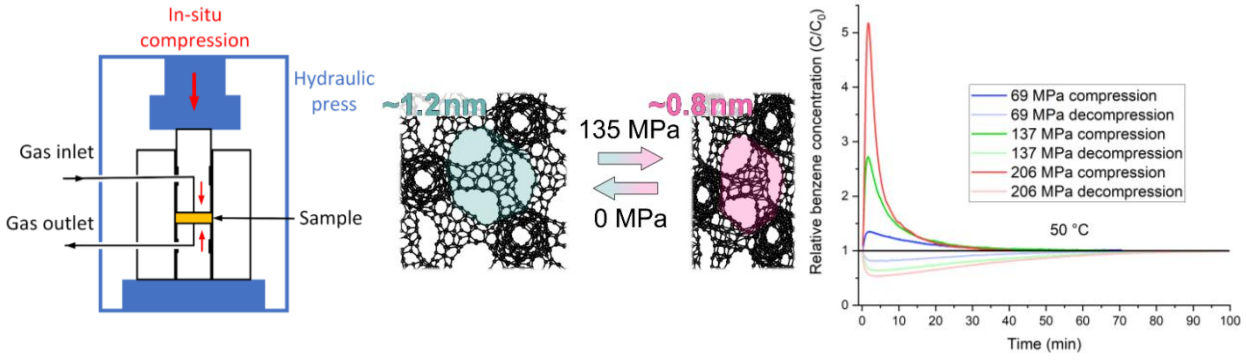
[a] *Eindhoven University of Technology, Eindhoven, Netherlands*

Gas separation is one of the most energy-intensive steps in the chemical industry. To improve the sustainability of this industry, much research has been done on advancing existing processes, e.g. pressure and temperature swing adsorption. However, these techniques still require a lot of energy due to the harsh swing conditions (high/low temperatures and pressures) required to complete the separation. To decrease the energy costs of these separations, it may be necessary to develop novel gas separation methods.

By applying a mechanical force to zeolite templated carbons (ZTC), the pore size has been shown to reversibly decrease. ZTCs are 3D-ordered nanoporous (0.6 – 1.2 nm) frameworks composed of curved graphene fragments that can act as nanosponges. When ZTC is mechanically compressed at 200 MPa, its adsorption capacity for 1-hexene is decreased by over 20%. By oscillating the degree of compression, two products streams are created: one with a high concentration, and one with a low concentration of adsorbate. Based on this, we propose a novel gas separation method utilizing the force-responsive behaviour of these flexible porous materials – compression-swing adsorption. Furthermore, the permeance through ZTC particles can be also strongly modulated upon compression, turning it promising for fabrication of force-responsive molecule sieving membranes.



Predictive breakthrough curve model for methyl iodide adsorption by activated carbons employed in the nuclear context

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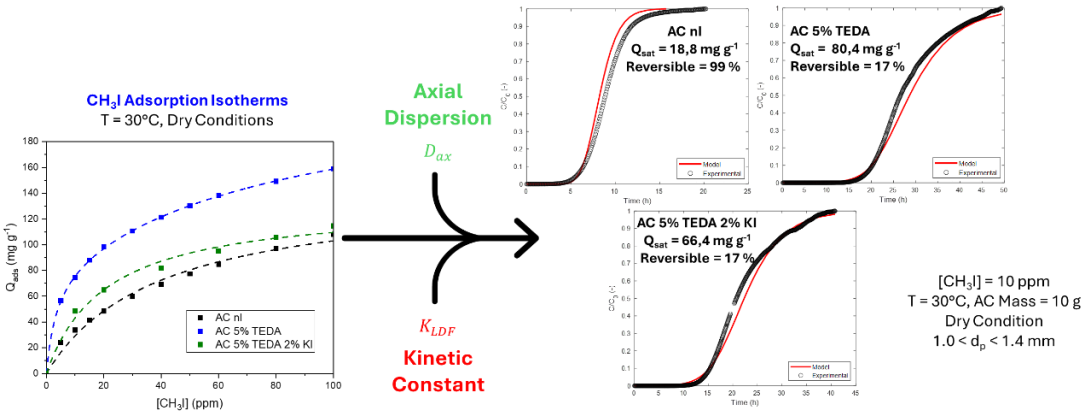
Iodine traps (IT) are widely used in nuclear facilities to mitigate the release of volatile radioactive iodine species. These systems are composed of highly microporous activated carbons (AC), with three capture mechanisms: physisorption, chemisorption with triethylenediamine (TEDA) and isotopic exchange with potassium iodide (KI). The focus of this work is modeling the adsorbent performance under different conditions while accounting for all involved mechanisms. The simulation pairs adsorption isotherms, which characterize equilibrium behavior, with a kinetic model based on the Linear Driving Force (LDF). This methodology, successfully applied in our previous work on H_2O in AC [1], the primary poison in IT, was extended here to CH_3I adsorption.

Three AC samples representative of nuclear applications were investigated in a progressive manner. First, a model adsorbent (AC nI) was studied, followed by a singly impregnated material (AC 5% TEDA), and finally a material representative of the nuclear context (AC 5%TEDA 2%KI). Adsorption isotherms were measured (T = 30°C, dry condition) using a microbalance with high precision at low CH_3I concentrations (5 - 200 ppm). The adsorption affinity parameter in the Langmuir model increased as expected with the addition of TEDA (0.026 ppm^{-1} to 0.071 ppm^{-1}), while the maximum adsorbed quantity stayed around 150 mg g^{-1} for all materials. However, to best describe the TEDA-impregnated adsorbents, it is necessary to decouple physisorption and chemisorption using a Langmuir dual-site adsorption. The simulation showed good agreement for the three investigated materials. Additional results are shown below:



As a perspective, the isotopic exchange reaction towards radioactive CH_3I will be implemented for a model AC with KI [2], before describing it in TEDA/KI co-impregnated AC under varying operational conditions.

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Investigation of the different functionalities of inhalation anesthetics on adsorption

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Halogenated ethers, especially fluranes, are used as inhalation anesthetics during medical treatment of humans and animals. Due to their chemical properties, they pose significant health risks to medical personnel with prolonged exposure and contribute to long-term environmental pollution, which requires their removal from hospital exhaust air. Adsorption processes are applied for this removal. The characteristic structure of flurane molecules, in addition to the carbon backbone, includes functional groups such as halogens and ether bridges, which significantly influence the adsorption properties. However, the molecular mechanisms of the relevant functional groups on adsorption are not well studied, and a mechanistic understanding is lacking.

In order to examine the influence of the individual functionalities on the adsorption properties, a study on the adsorption of propane, perfluoropropane, dimethyl ether, iso-pentane, iso- and sevoflurane was carried out. As adsorbents, FAU-type zeolites and activated carbons were selected. The research setup includes magnetic suspension balances, a fixed-bed adsorber, and a gas-phase IR spectrometer, allowing the adsorptives to be studied simultaneously both gravimetrically and spectrometrically. To systematically investigate and mechanistically understand the interactions in multi-component adsorption, pure substance and multi-component isotherms are measured in the temperature range from -20 to +25 °C.

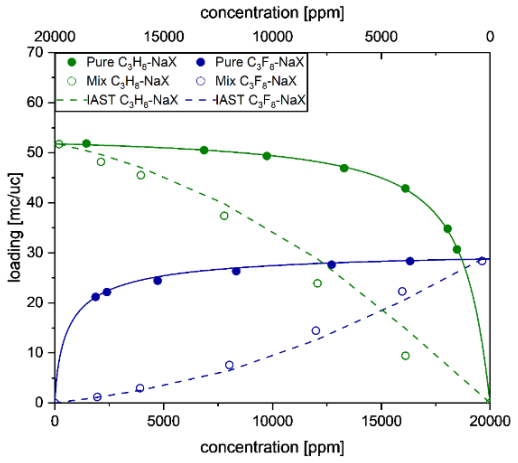

Fig. 1: Pure substance and mixture isotherms, as well as IAST predictions for propane (C_3H_8) and perfluoropropane (C_3F_8) on 13XBF at -20 °C.

Additionally, mixture adsorption isotherms are predicted using the Ideal Adsorbed Solution Theory (IAST). Exemplary pure substance and mixture isotherms, as well as IAST calculations at -20 °C for propane and perfluoropropane on the FAU-type zeolite 13XBF are shown in Fig. 1. The mixture isotherms of propane and perfluoropropane show significant deviations from the pure substance isotherms. This indicates that strong competition is present. The influence of type of interaction, molecular size, as well as number and type of cations on adsorption and displacement mechanisms will be presented and discussed in the presentation based on selected results.

Metal-organic frameworks for waste anesthetic emissions: data-driven discovery and material testing

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Nitrous oxide (N_2O) usage is ubiquitous in anaesthesia (e.g. as a carrier gas) and analgesia applications (e.g. as a sedative in dentistry and childbirth).[1] However, over 95% of the inhaled N_2O is not metabolised by the patient, contributing to accumulation of N_2O in hospitals and in the atmosphere.[2] N_2O is an ozone-depleting greenhouse gas with a global warming potential almost 300 times that of CO_2 and its buildup in hospitals poses a risk to hospital staff. Currently, there is no universal technology for abating the emissions; proposed solutions for several global healthcare sectors are limited to inefficient activated carbon filters and scavenging systems, and alternatives to inhalational anaesthesia.[1] Here, we utilise high-throughput computational tools[3] to identify top metal-organic framework (MOF) candidates for high-volume capture of N_2O from waste emissions. Successful MOF structures were evaluated under real-world operating conditions, namely temperature, humidity and clinically relevant partial pressures. Practical considerations for widescale roll-out of MOF technology for abating the emissions will be presented, alongside their performance in real-world simulated conditions using breakthrough analysis (BTA).

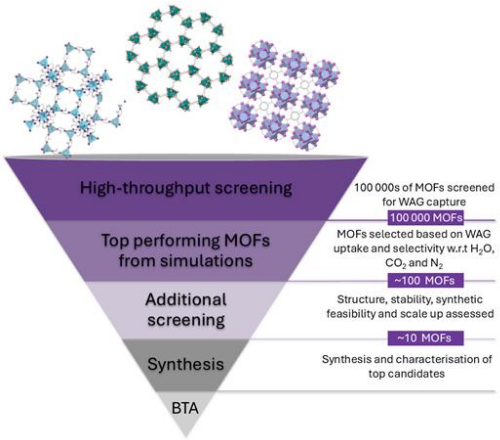

Figure 1: Schematic showing the computer-aided selection of MOFs for N_2O capture from waste emissions.

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New method for quantitative thermal gravimetric analysis per compound applied to adsorption of organochlorines on faujasite

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Subtopic - Thermodynamics and kinetics of adsorption

Organochlorine compounds (OClCs), a class of persistent organic pollutants (POPs), pose serious environmental and health risks due to their toxicity, long-term stability, and bioaccumulation. They are widely used in industrial applications and are unintentionally released from waste incineration plants. The challenge is to efficiently remove these pollutants from contaminated environments. Faujasite X zeolite emerges as a good adsorbent for capturing OClCs pollutants regarding its pore opening which matches the size of the molecule, typically around 7.4 Å [1, 2]. The aim of this study is to better understand the sorption of OClCs into FAU X (Si/Al=1.3, extraframework cation: Na^+) using experimental approaches and DFT simulations [3, 4]. The selected OClCs are toluene, chlorobenzene and bis chlorinated aromatics with different Cl positions to better understand the role of aromatic rings and Cl atoms (number and position) on the adsorption properties. Solution depletion method is used to determine the kinetics and isotherms of adsorption at 298 K by using isooctane as a solvent. Enthalpy of adsorption is determined by calorimetry. The temperatures of desorption of the molecules, which depends on the energies of interaction between the molecules and the different sites of adsorption of FAU X, are determined by thermal gravimetric analysis (TGA) coupled to mass spectrometry analysis (MS). We propose a new mathematical method described in [5] that does not require calibration of the evolved gases to determine the true quantity value and the desorption temperature distribution of each desorbed compound [6]. The amount desorbed is compared to the amount adsorbed to validate the method. This new approach is particularly powerful to better understand the thermodynamic of adsorption when combined with other techniques like calorimetry and molecular-scale simulations as done in this study.

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Understanding the adsorption mechanisms of LiCl extraction on LiAl-LDH

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The lithium market is currently being disrupted by the high demand for electric batteries and is considered a strategic metal in the world. As a consequence, large R&D efforts concentrate on the development of low-cost and/or high-yield lithium extraction technologies. Direct Lithium Extraction (DLE) technique using selective adsorbents is promising since it allows Li extraction from brines (saline solutions) in an environmentally sustainable way. The main challenge lies in the development of a performing adsorbent which can recover Li at low concentration (100-500 ppm) from a highly saline solution (>1mol/L). LiAl-LDH, Aluminium-based Layered Double Hydroxide, is a good candidate thanks to the presence of the cationic vacancies fitting the size of Li.[1] It can adsorb up to 35 mg/g. However, breakthrough curves obtained experimentally show that the effective adsorption capacity remains low, not exceeding 4–8 mg/g.

The objective of this study is to understand the mechanism and model the kinetic of Li adsorption process on LiAl-LDH sorbent synthesized at Saint-Gobain by an innovative process.

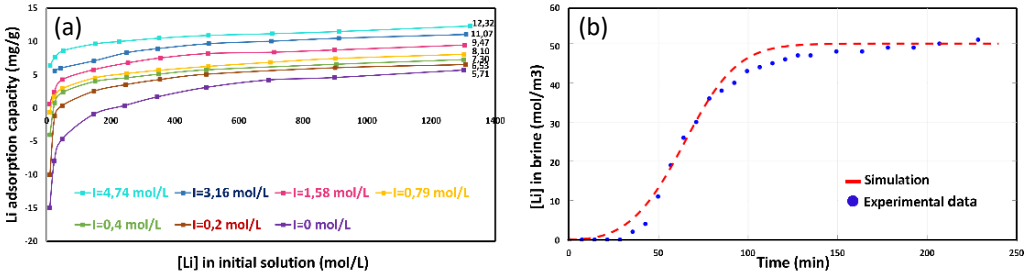

Figure 1: (a) Adsorption isotherms at different ionic strengths (I) obtained from batch tests using the powder material; (b) Experimental and modeled breakthrough curves for the fixed-bed extraction test using the shaped material (beads)

The thermodynamic studies of Li ion exchanges were performed for LiAl-LDH material via the measurement of adsorption isotherms in batch tests. The investigation of isotherms considered not only variations in lithium concentration but also evaluated the effect of the concentrations of other salts present in the solution (Figure 1(a)). Surprisingly, we found that the driving force of the adsorption process is mainly governed by the solution's ionic strength whereas the Li concentration plays a second role. To identify the limiting steps of the overall Li adsorption process a dynamic model was developed basing on this experimental data and coupling hydrodynamic and adsorption/desorption phenomena (Figure 1(b)). We set a thermodynamic model of adsorption derived from the Langmuir concept incorporating the effect of ionic strength.

This careful thermodynamic study allows us to conclude that the working capacity is limited by the stability of the material at the desorption step.

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Nanoparticle Organic Frameworks (NOF): A Breakthrough Technology for the Selective Recovery of Critical Metals from WEEE

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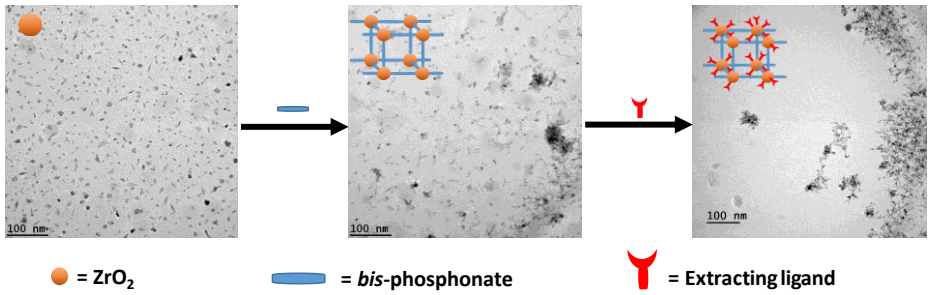
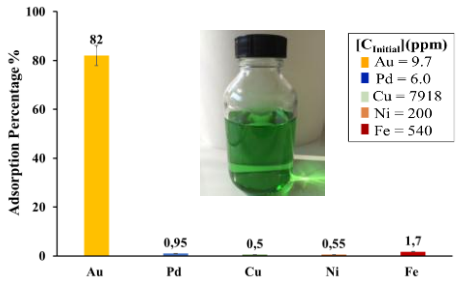
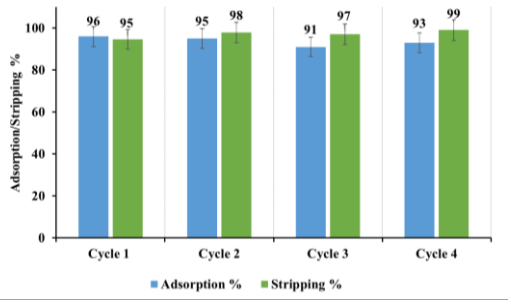
The secure supply of critical metals is a major challenge for the energy transition and the circular economy. Platinum group elements, lithium, cobalt, and rare earths are indispensable for electronics, renewable energy, and e-mobility, yet conventional mining remains environmentally harmful and economically fragile. Urban mining, based on the valorization of Waste Electrical and Electronic Equipment (WEEE), provides a sustainable alternative but is hindered by the inefficient recovery of trace metals from hydrometallurgical streams **[1]**.
We present an innovative solution based on Nanoparticle Organic Frameworks (NOFs), a new class of self-assembled hybrid materials **[2]**. Our NOFs are built from zirconia nanoparticles linked by bis-phosphonate ligands, yielding highly stable, large-surface architectures. Further functionalization with selective ligands enables the targeted capture of precious metals, such as gold, even at ultra-low concentrations (< 100 ppm) within complex mixtures (Figure below).



Experimental validation demonstrates adsorption capacities of ~20 mg Au/g material, remarkable selectivity, and, crucially, exceptional recyclability without washing steps (Figures below) - a breakthrough compared to conventional adsorbents. This innovation addresses both economic and environmental bottlenecks of metal recovery and opens the way to scalable industrial applications.





[1] S. Asaad et al., *Molecules* **2023**, 28, 2219 **[2]** S. Asaad et al., Patent FR2411116

Adsorption/desorption properties of chitosan-based passive samplers for the analysis of norovirus in different types of water

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Human noroviruses are the main cause of acute gastroenteritis in humans worldwide. The aim of this work is to design passive samplers based on chitosan for the concentration and the analysis of norovirus in various aqueous media. The viruses' desorption by elution allows their quantification through RNA analysis.

Two types of hydrogel beads were synthesized: chitosan porous beads (CS) and copper-imprinted chitosan non-porous beads (CS-IMP). Hydrogels were characterized by zetametry, and after freeze-drying by sorptometry (N_2 at 77 K) and scanning electron microscopy. They were tested for the adsorption of murine noroviruses (MNV-1, a non-pathogenic model virus for human norovirus) in spiked saline water (NaCl 0.1 mol.L^{-1}), tap water (Montbonnot, France) and wastewater from the outlet of a WWTP (Chambéry, France). The elution of MNVs adsorbed on the hydrogels was studied using solutions of different ionic strengths (NaCl 0.1-4 mol.L^{-1}), pH (7-9), surfactant concentration (Tween-20 0.005-0.5%), temperature (25-60°C), time (0.5-4 h) and adsorbent mass (0.1-1.0 g). RNA extraction of the desorbed MNV-1 was achieved by lysis and washing steps prior to RT-qPCR analysis for virus quantification.

The adsorption kinetic studies of MNV-1 revealed a quasi-equilibrium after 6 h. CS beads (S_{BET} ~ 70 $m^2.g^{-1}$) and CS-IMP beads (S_{BET} ~ 4 $m^2.g^{-1}$) adsorbed respectively ~ 80% and ~ 30 % of the spiked viruses within 2 h. Using the determined optimal desorption conditions, a maximum desorption efficiency of ~ 82% and ~ 31% was achieved for CS and CS-IMP beads, respectively. Desorption was shown to be facilitated by large pore sizes (in the meso/macro scale). In spiked tap water, both types of beads adsorbed more than 75% of the viruses, with desorption efficiencies of ~ 60%. In spiked wastewater, less than 1% of the viruses were adsorbed, indicating an interaction with the other components of the wastewater. An automatic sampler using CS beads as sampling materials was developed in our laboratory. This device was tested for the daily monitoring of an outlet municipal WWTP water, and a 24h-integrated sample was collected for comparison. Using the concentrations measured in the integrated sample as reference, about 10% of the autochthonous viruses were adsorbed, against 50% if a prior filtration at 63 µm was carried out. Even if a temporal variability was observed, the daily concentrations of autochthonous viruses measured directly in the outlet WWTP water followed the same trend as those determined by automatic passive sampling.

Acknowledgment : Auvergne-Rhône-Alpes Region (France) for supporting the "VIROCAPTUR" Pack Ambition Recherche Project.

Adsorption thermodynamics and kinetics of simple and complex fluids: Effect of surface saturation, reservoir depletion and lateral interactions

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Adsorption-based remediation techniques are very promising for the removal of emerging pollutants from water. In particular, numerous detection and remediation tools have been developed in recent years for emerging pollutants such as per- and polyfluoroalkyl substances (PFAS), and pharmaceutical and personal care products (PPCP). However, because of their complex behavior near solid surfaces, the adsorption mechanisms of these emerging compounds raise unprecedented challenges. They often exhibit unusual adsorption isotherms arising from cooperative effects driven by lateral interactions. Typically, depending on the water matrix, the adsorbing surface, and the concentration range of the adsorbate, the observed adsorption isotherm may display one or more inflection points – a behavior that severely challenge existing theoretical frameworks for surface adsorption. In this context, we develop a thermodynamic framework that accounts for two- and three-body lateral interactions, recovering complex adsorption isotherms with zero, one or two inflection points. When fitted with experimental adsorption isotherms, this model provides valuable insights on the underlying adsorption mechanisms. Additionally, this model can predict adsorption isotherms shape over a wide concentration range, using only a limited experimental dataset. Moreover, unusual adsorption kinetics adsorption have been reported for both simple (non-interacting) and complex (interacting) molecules. This behavior stems from cooperative mechanisms as well as reservoir depletion effects that cannot be avoided at very low bulk concentrations. Consequently, we build a kinetic model to investigate the role of surface saturation, reservoir depletion and lateral interactions. In particular, the instantaneous bulk concentration is found to strongly impact the adsorption kinetics through its coupling with surface saturation – leading to unusual mixed-order kinetics.

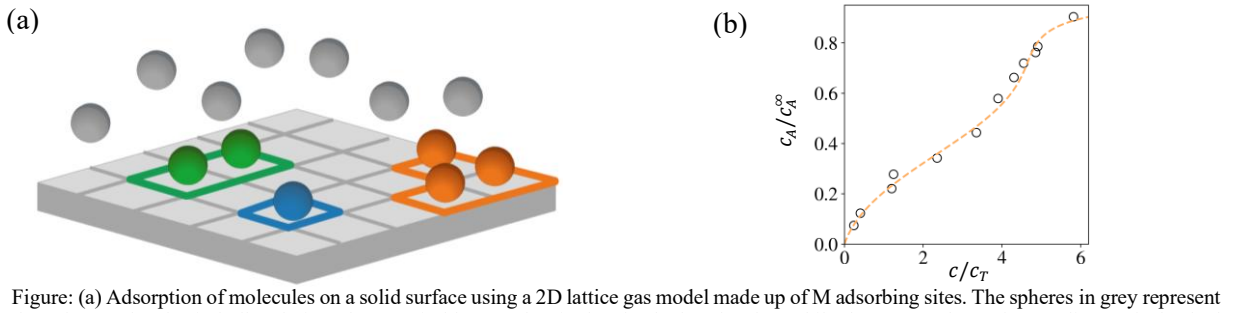

Figure: (a) Adsorption of molecules on a solid surface using a 2D lattice gas model made up of M adsorbing sites. The spheres in grey represent the solute molecules in bulk solution, the ones in blue are the single adsorbed molecules, while the green spheres form a dimer of adsorbed moelcules and the orange ones form a trimer of adsorbed molecules. (b) Adsorption isotherm of ciprofloxacin on magnetic nanosorbents. The cirlces are the experimental datapoints while the dashed line is the fit with the mean-field model including two- and three-body lateral interactions.

A temperature-induced desorption approach for the measurement of multicomponent isotherms in nanoporous materials

Nicolas Chanut[a], Robbe Van Loenhout[a], Cesar Parra Cabrera[a], Masaya Sugihara[a], João Fernandes[a], Margot Verstreken[a], Leen Boullart[a], Rob Ameloot[a]

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Equilibrium single-component measurements are routinely performed using volumetric or gravimetric techniques. However, because industrial processes deal with mixtures and different molecules compete for the same adsorption sites, single-component isotherms are of **limited use in designing a separation process**. Researchers have long tried to predict mixture adsorption based on single-component isotherms (*e.g.*, ideal adsorbed solution theory), but non-ideal behavior remains challenging to forecast without actual mixture adsorption experiments. Unfortunately, **measuring multicomponent adsorption is complex and time-consuming**. A range of methods has been developed, yet none combines ease of operation, straightforward data analysis, and fast measurements. Breakthrough methods, by far the most common approach, illustrate this trade-off. While it provides robust multicomponent adsorption data, each data point requires a few hours to one day due to the relatively large adsorbent mass (> 100 mg) and the reactivation of the adsorbent between each measurement, making this approach time-consuming for the collection of full multicomponent isotherms.

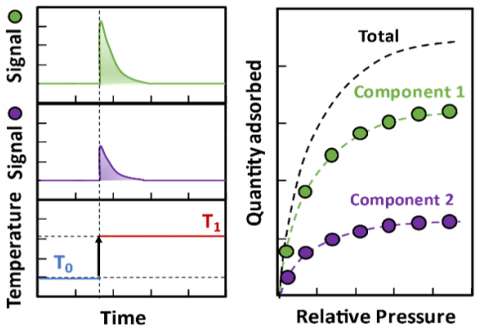

***Figure 1: Multicomponent isotherm measurement approach**. A heat pulse is applied to desorb all guest molecules, which are quantified using MS. Each desorption pulse yields one point on the multicomponent isotherm, i.e., one uptake value for each component for a given mixture composition.*

In this presentation, we will present a new methodology for the rapid measurement of reliable multicomponent adsorption isotherms. Instead of a concentration change in the atmosphere surrounding the adsorbent, a **sudden temperature change of the adsorbent is used** to induce full desorption after equilibration at every partial pressure. The desorbed fraction is quantified downstream using a mass spectrometer, by integration of the signal in excess of its baseline. Because of the use of downstream MS analysis, the method can be readily extended to multicomponent measurements (Figure 1). Results of multicomponent adsorption measurements on industrially relevant adsorbents and their interpretation will be further detailed in the presentation.

Fluid Transport in Nanoporous Materials and at their Interface: Intermittent Brownian Motion and Surface Resistance

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Nanoporous solids, like metal-organic frameworks and zeolites, are promising candidates for fluid transport mechanisms, in complex separation processes. The entry-exit of penetrants across surface boundaries is still not a well studied dynamical process, and our understanding is only at a nascent stage. Using molecular simulations (grand canonical Monte Carlo, and all-atom molecular dynamics) of CO_2 in zeolite (MFI-type silica) we study the intermittency of gases diffusing across the host solid surface. In this work, we will present how the effective surface experienced by fluids may grow both inwards or outwards from the geometrical edge. We study the relations between gas diffusivity, width of the interface, and the fractional occupancy by considering the zeolite to be in series or parallel to the dynamics. The intermittency at the surface motivates us to study surface residence and relocation times, and then proceed to understand their statistics based on physical laws. We quantify the intermittency based on survival probabilities, rate of transition, and compare the analytical spectral density against computationally obtained results.

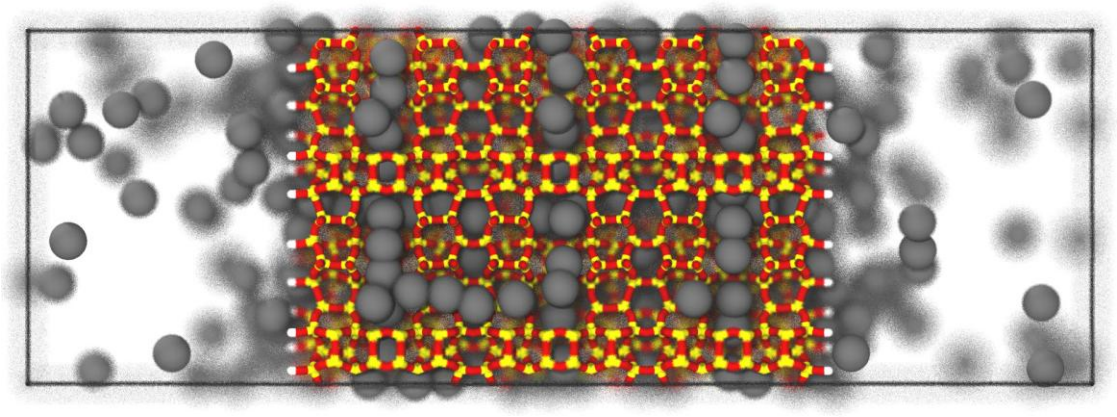

Fig. 1. Simulation setup of CO_2 molecules across an MFI-IZA type silica interface. The CO_2 molecules at interfaces experience intermittent exchanges between adsorbed and bulk phases, creating resitence towards diffusion.

Pore Size Analysis by Advanced NMR Relaxometry and Gas Adsorption

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During the last decades, major progress has been made in the synthesis of nanoporous materials, allowing the tailoring of nanoporous materials for targeted applications in various fields such as separation, catalysis, gas and energy storage. To increase the efficiency of these processes, it is necessary to tune the selectivity of the porous material to certain compounds of interest. Textural properties, such as the specific surface area and pore size may affect the process efficiency. Therefore, valid textural characterization methodologies are essential for both surface area assessment and pore size analysis. In this context, gas adsorption is widely used; however, its application is limited to dry materials, i.e., gas adsorption cannot determine effective textural properties of wet porous materials utilized in liquid phase processes such as chromatography and catalysis. Hence, novel methodologies for textural characterization of solvated porous materials are required. Within this context, we have recently shown that NMR relaxometry is promising for surface area assessment of solvated nonporous and nanoporous silica and carbon [1]. Within this work, we expand the applicability of NMR relaxometry for reliable pore size analysis.

Pore size analysis by NMR relaxometry is based on the fact that different liquid regimes may exhibit different relaxation times if diffusion is slower than their relaxation resulting in relaxation time distributions. Deciphering the exponential magnetization decay curve measured from a low-field 1H NMR spin-spin relaxation measurement into a reliable relaxation time distribution remains one of the challenges. This requires a trustworthy solution of the Fredholm integral of the first kind with Tikhonov regularization.

Using the Two-Fraction-Fast-Exchange model developed by Brownstein and Tarr [2], one can convert a relaxation distribution to a pore size distribution. The application of NMR relaxometry for pore size analysis was pioneered in the 80s and 90s by Smith and co-workers [3]. However, a rigorous validation of NMR relaxometry for pore size analysis was not possible at that time due to a lack of well-defined model materials as well as limitations in adsorption characterization. This study therefore presents a systematic study to investigate the effect of confinement on the NMR relaxation behaviour using nanoporous model materials with well-defined pore structure. The NMR relaxometry results are compared with benchmark pore size and surface area data determined with Ar 87 K adsorption [1,4].

This work represents a first step towards the development of NMR relaxometry for reliable pore size analysis. The experimental investigations were complemented by molecular dynamics simulations, which are further used to study the effect of confinement on NMR relaxation. Our

results strongly indicate the potential of NMR relaxometry for advancing liquid phase textural characterization.

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Characterization of Porous Materials Using Quasi-Equilibrated Temperature-Programmed Desorption and Adsorption (QE-TPDA) of Volatile Compounds

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Quasi equilibrated temperature programmed desorption and adsorption (QE-TPDA) of volatile compounds is an experimental method dedicated for characteization of porous solids, proposed in 2007. It has been extensively used in studies on zeolites, mesoporous silicas, and metal-organic frameworks (MOFs). The aim of this contribution is to present recent advances in this approach, covering both new experimental solutions and applications, including studies on the adsorption of water and the alcohols in MOFs and characterization of their hydrothermal stability.

Thermodesorption of vapors may be studied under quasi-equilibrium conditions in a flow system equipped with a thermal conductivity detector (TCD), using helium with small admixture of the adsorptive as a carrier gas. The QE-TPDA experiments are performed by controlled cyclic heating and cooling of the sample. The QE-TPDA profiles, consisting of desorption maxima and adsorption minima, may be easily converted into approximate adsorption isobars. Based on the QE-TPDA data one may calculate micro- and mesopore volume, mesopore size distribution as well as the enthalpy and entropy of adsorption.

Recently, two new experimental solutions have been successfully used in the QE-TPDA experiments. A flow-through non-dispersive infra-red sensor (NDIR) was applied in studies on sorption of alcohols in MOFs. The combined thermal conductivity/humidity sensor was adapted to QE-TPDA measurements of water or nonane. Both sensors did not require the use of expensive helium. For both sensors, QE-TPDA measurements at much larger concentration range of the adsorptive could be performed compared to those with the use of TCD.

Based on the QE-TPDA profiles of water and alcohols, two different types of adsorption-desorption mechanisms were distinguished: one related to the pore-filling scheme and another, indicating a phase transition triggered by adsorption or desorption. For the latter one, some fragments of the desorption maxima and desorption minima were independent of the heating or cooling rate. Such fragments present in the QE-TPDA profiles of water for CAU-10 confirmed occurrence of a reversible adsorption-induced phase transition. Their analysis according to the Van't-Hoff equation yielded reasonable values of the adsorption enthalpy.

The QE-TPDA measurements were also applied to probe the hydrothermal stability of MOFs. The sample was placed in the flow of carrier gas saturated with water vapor and subjected to a complex cyclic temperature change program. In each cycle, apart from being slowly heated in the low temperature range for the purpose of recording the desorption profile, the sample was hydrothermally treated by being heated at a high temperature. After 3 cycles, the temperature of hydrothermal treatment was increased. The results of such experiments show that CAU-10 retained its stable sorption capacity for water after hydrothermal treatment at temperatures up to 400°C.

Using calorimetry of H_2 adsorption to identify nature of Pt in a novel non-reduced Pt/Al_2O_3 catalyst for H_2 combustion at room temperature

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To solve the problem of catalyzing the reaction of hydrogen combustion (CHC) at T_{room}, we previously synthesized a novel non-reduced Pt/Al_2O_3 catalyst from Bayerite [1]. Detected by XPS, highly dispersed Pt^{4+} species on its surface are capable to initiate the CHC reaction at T_{room} (Fig. 1) via uncertain up today mechanism. We use calorimetry of H_2 adsorption in attempt to understand the role of Pt nature for hydrogen activation at low temperatures.

H_2 adsorption on the catalysts' surface at 30°C was studied by calorimetry using a Calvet calorimeter coupled with volumetric equipment. The differential heats of H_2 adsorption were measured when successive small increasing amounts of H_2 introduced in a cell containing the catalyst, preliminary pretreated under secondary vacuum at high temperature.

Recorded exothermic peaks (Fig. 1) indicate that the novel catalyst adsorbs/activates H_2 at 30°C, while the reference catalyst doesn't. The peaks intensity and the corresponding calculated differential heat evolve unregularly during H_2 injections indicating most likely the evolution of the surface of the novel catalyst under H_2. High values of the differential heats released during H_2 adsorption on the surface of the non-reduced novel catalyst (up to 346 kJ/mol H_2) exceed those obtained on the reduced $Pt°/Al_2O_3$ catalyst (110 – 25 kJ/mol H_2). This suggests that H_2 is possibly activated and most likely oxidised at 30°C when contacting the non-reduced catalyst with the reduction of the superficial ionic Pt^{4+} species. We propose that on Pt^{4+} species, H_2 activates differently than H_2 homolytic cleavage which takes place on Pt° – heterolytic cleavage of H_2 molecule on Pt^{4+} species with hydride attraction and proton released is proposed.

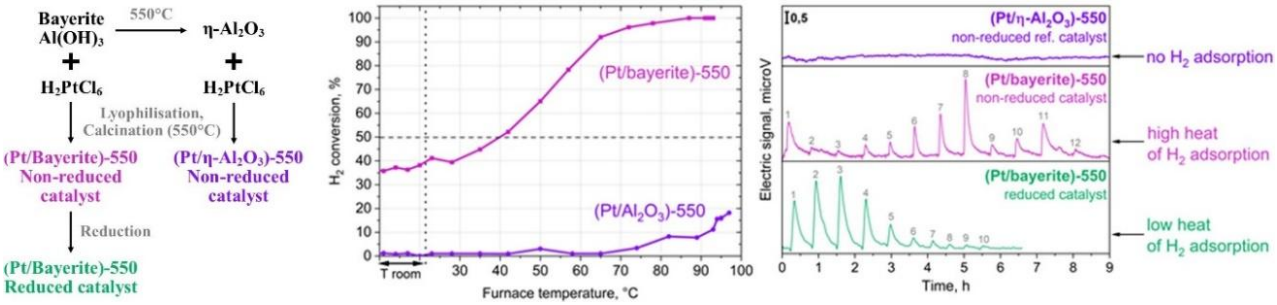

Fig. 1. Schematic illustration for catalysts' synthesis and corresponding results of the catalytic hydrogen combustion test and calorimetry of H_2 adsorption

[1] N. Abel. and al. *Energy & Fuels 2025*, 39, 11898.

The authors acknowledge Produits Berger for their financial support.

Hengst's Modular Pre-Filter System for Direct Air Capture (DAC)

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Direct Air Capture (DAC) is a cutting-edge technology that removes carbon dioxide (CO_2) directly from the atmosphere. One of the biggest challenges in scaling DAC is reducing the cost per ton of captured CO_2. This includes extending the service life of DAC components while minimizing operational risks.

One of many challenges in this realm is acidic gases such as SO_2 and NO_2, which are commonly found in ambient air due to sources like combustion emissions, metal smelting, and volcanic activity. Typical concentrations are in the range of 1-50 ppb (SO_2) and 10-500 ppb (NO_2). Due to their chemical similarity to CO2, these gases readily adsorb onto the active sites of sorbent materials. To put this into perspective: an atmospheric air volume flow of 50 000 m³/h carries approximately 5.2 kg of SO_2 (at 5 ppb) and 22.6 kg of NO_2 (at 30 ppb) per year. Without proper filtration, these pollutants can significantly impair DAC system performance. Competitive adsorption with amine-sites of common DAC adsorbents reduces the number of available sites for CO2, thereby lowering the overall capture capacity of the DAC system. That is where Hengst's modular pre-filter steps in to make a difference. Designed to protect DAC units from particulate matter, harmful gases, extreme temperatures, and more, Hengst modular DAC pre-filters can be tailored to specific environmental and system needs – significantly reducing operational cost (OpEx) of DAC modules

Having controlled the threats and costs from particulate matter and noxious gases, reducing the cost per ton of captured CO_2 further by applying well-tailored DAC adsorbents and cleverly designed DAC filter elements in optimized DAC processes is indispensable. Each of the three is accomplished by Hengst's development teams and chemical laboratory, who characterize and develop adsorbent-specific DAC processes for clients, investigate climatic influences on CO_2 productivity and energy requirements, propose process adjustments in dependency of location or weather and more. The Hengst DAC demonstrator, capable of removing up to three tons CO_2 per year from the atmosphere, is a complementary tool to apply temperature-vacuum-swing adsorption (TVSA) methods, validate laboratory findings from static volumetric isotherm measurements or dynamic breakthrough tests, test filter elements and develop TVSA processes for/with clients.

While DAC operations are evolving and have well been proven to be feasible on a relevant scale, many challenges still need to be addressed regarding adsorption: screening and finding of new and better adsorbents, application-oriented cycling tests, shaping of adsorbents and filter integration, adsorption process developments and optimizations, including predictions of key performance indicators (KPIs) of DAC like cycle times, minimum energy demand, maximum CO_2 productivity, filter lifetime – ultimately enabling to predict and minimize OpEx for DAC systems.

NMR relaxometry applied to drying and wetting properties of Ion Exchanged Resins used in Direct Air Capture

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Direct Air Capture (DAC) is a fast-growing field dedicated to removing CO_2 directly from the atmosphere. Adsorption processes using solid amine sorbents are at the forefront of the many different technological options currently being developed for DAC. For adsorption-based DAC, it is crucial to know the amount and the localisation of water within the sorbent because it influences the equilibrium (coadsorption) and kinetics of CO_2 adsorption.

NMR relaxometry is a non-invasive and non-destructive method that relies on the property that the time constant describing the relaxation of the component of the nuclear spin magnetization perpendicular to the magnetic field (T2) is significantly different for molecules in contact with a solid interface and molecules in the liquid bulk. This technique is used here to quantify the wetting and drying dynamics of Ion Exchanged Resins used in DAC (Figure 1).

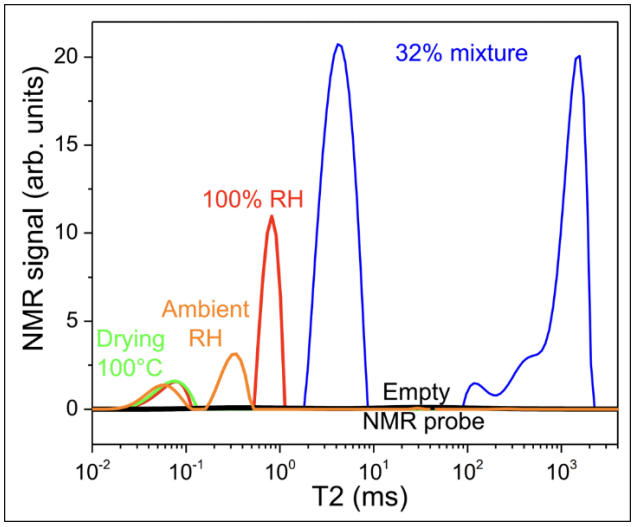

Figure 1 - T2 time distribution obtained for different amount of water: 32% solid content (blue), material in equilibrium with 100% RH (red) or ambient RH (orange), material dried at 100°C

Influence of water and porous carrier on the CO_2 capture mechanism of amine- and carbonate-based solid sorbents

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The combined influence of water vapor and porous carrier structure plays a decisive role in defining the adsorption mechanism, kinetics, and long-term stability of solid sorbents for CO_2 capture. Despite substantial progress in sorbent development, systematic comparisons between amine- and carbonate-based materials under identical, humidity-controlled conditions remain limited.

In this work, two representative classes of chemisorbents were synthesized and evaluated: amine-functionalized materials incorporating choline- and glycine-derived ionic liquids, and K_2CO_3-impregnated composites, both supported on silica gel and activated carbon. Breakthrough experiments were conducted across a temperature range of 20–100 °C and relative humidities from 0–100 % to determine how water and carrier morphology influence CO_2 adsorption efficiency, mass-transfer resistance, and thermal behavior.

Under dry conditions, the amine sorbents exhibit rapid CO_2 uptake characteristic of strong chemisorptive interactions, whereas carbonate materials remain largely inactive. With increasing humidity, both systems display enhanced adsorption capacity and altered breakthrough profiles, indicating the formation of water-assisted reactive domains within the pore structure. The magnitude of improvement is governed by the polarity and hydrophilicity of the carrier: silica provides greater water retention and promotes faster adsorption kinetics, while activated carbon restricts hydration.

To ensure reproducibility and mechanistic comparability, all samples were prepared using a controlled impregnation procedure based on the pore volume of the support, followed by drying and activation under inert gas. Long-term cyclic testing will assess structural and functional stability, while FTIR spectroscopy and equilibrium CO_2 isotherms will be used to monitor changes in chemical and sorptive behavior. Together, these experiments provide a unified understanding of how water and carrier polarity govern reactivity, diffusion, and stability in amine- and carbonate-based sorbents, offering new design guidelines for robust, regenerable materials suitable for realistic flue-gas applications.

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Computational tuning of zeolite chemical composition for CO_2 capture

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The CO_2 adsorption performances of zeolites significantly depend on their chemical composition and in particular on the chemical nature, concentration and localization of charge-compensating cations. Monte Carlo (MC) simulation is a well suited computational tool for both, determining the cationic distribution [1] even in bi-cationic zeolites, which remains a challenging task for experimental techniques (especially in presence of mixed occupancies in crystallographic sites), and studying the adsorption properties of carbon dioxide (CO_2) in zeolites.

In the present study, we applied the MC scheme to NaX faujasites, exchanged with Ca^{2+} cations, to exchange rates of [0; 20; 40; 60; 80; 100%] and we have validated the obtained cationic distributions through accessible experimental data. Based on such established realistic microscopic models, we achieved the Grand Canonical Monte Carlo simulations of the CO_2 adsorption. Our outcomes have evidenced an enhancement of CO_2 affinity at low pressure when substituting Na^+ cations with Ca^{2+} up to 60% exchange rate (Figure 1a). Surprisingly, beyond this exchange rate the adsorption performances drop. From the microscopic point of view, this trend is associated to a cooperative adsorption mode, when both Ca^{2+} cation and Na^+ cation interact simultaneously with a single CO_2 molecule (Figure 1b), allowing an optimal scenario for an effective CO_2 capture.

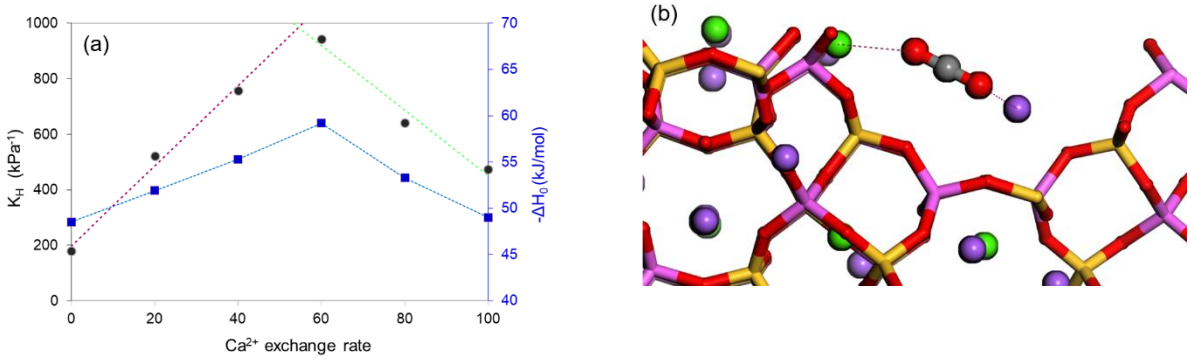

Figure1: (a) Evolution of Henry constant and adsorption enthalpy as function of Ca^{2+} exchange rate, (b) CO_2 dual cation adsorption mechanism.

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Reliable KPI Measurement in PSA Pilot and Commercial Plants

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The technology of pressure swing adsorption (PSA) was initially developed in 1960 for the separation of industrial gases. Subsequently, it has become a well-established technology in numerous industrial sectors and an important product. As part of the final acceptance test (FAT) of commercial PSA plants, it is essential to determine the key performance indicators (KPIs) in a reliable manner in order to demonstrate the functionality of the plant to the customer. Similarly, in PSA pilot plants used for R&D purposes, the reliability of performance measurement is of great importance to study new process schemes or new adsorbent materials.

The two principal key performance indicators (KPIs) of a PSA are the recovery of the product component and the capacity, which is defined as the maximum feed flow that can be routed to the PSA while ensuring that the product requirements, for example maximum 10 ppm of carbon monoxide (CO), are met. In theory, both KPIs can be determined with relative ease. However, the resulting KPIs may be significantly flawed due to the reliance on the quality of the flow measurements and the precision of the gas analysis. Consequently, when evaluating the performance of a PSA under operating conditions, it is crucial to consider the potential for inaccuracies in the flow measurements or the analysis.

The objective is to present an approach that introduces additional evaluation criteria with the purpose of initially assessing the quality of the measurements. Subsequently, the reliability of the KPIs can be evaluated based on the quality of the measurements. The evaluation of measurement quality is based on total and component-wise mass balances, enrichment factors and independent methods for calculating the recovery of the product component.

The approach has been successfully deployed in both pilot plants and commercial PSAs. In the context of pilot plants, the additional evaluation criteria facilitate improvements in measurement quality. In the case of commercial PSAs, they provide a robust foundation for performance discussions with customers.

Dynamic Cycle Control in Adsorptive Separation Processes for Enhanced Energy Efficiency in Air Separation Units

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Technical gases are essential to a wide range of industrial applications, including metal processing, electronics manufacturing to medical technology. Ensuring their reliable and energy-efficient supply is therefore of both economic and ecological significance. In addition to other processes, adsorptive separation processes are used to produce and extract these gases, either as temperature swing adsorption (TSA), (vacuum) pressure swing adsorption ((V)PSA), or combined processes. In times of rising energy prices and growing sustainability requirements, energy efficiency of gas production processes has become a critical objective.

One approach to increasing efficiency lies in optimizing adsorption processes, such as those used in the Front-end of air separation plants to remove CO_2 and H_2O. These components must be eliminated to prevent freezing and subsequent plugging in downstream cryogenic equipment. The design and operation of these adsorption systems are based on worst-case scenarios, incorporating conservative safety margins to ensure reliability under all possible operating conditions. While this approach guarantees robustness, it often leads to significant underutilization of adsorption bed capacity during normal operation, resulting in unnecessary energy consumption and increased mechanical wear due to frequent cycle transitions.

To address these inefficiencies, this work proposes the implementation of a dynamic cycle control strategy that adapts the duration of adsorption cycles to real-time process conditions. By utilizing existing instrumentation together with live calculation of thermodynamic data and resultant bed utilization, the cycle times under favorable conditions can be significantly extended, thus reducing the number of cycles and the total energy consumption for the air pre-treatment. This new control strategy was implemented in a full-scale production plant, with a resultant reduction in specific energy consumption of air purification in the order of up to 36%.

Applications of Artificial Intelligence tools on N_2-PSA Plants

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The integration of Machine Learning (ML) and Artificial Intelligence (AI) tools into chemical engineering is leading to new perspectives for the optimisation of industrial processes [1, 2]. These technologies facilitate the identification of complex, non-linear relationships that would necessitate significant modelling effort using conventional mathematical methods [3]. The N_2-PSA process, which efficiently generates pure nitrogen from compressed air, presents design and control challenges due to the multivariable interactions between the ambient condition, the demand situation, and process variables [4]. In this context, AI represents a promising resource.

As the compressor is the dominant power consumer in these plants, the authors present a neuro-probabilistic model for the prediction of the air demand and the quantification of its uncertainty. They demonstrated that data point estimators, such as the Gradient Boosting Regressor (GBR), the Random Forest Regressor (RFR) and the Multi-Layer Perceptron (MLP), trained under the assumption of homoscedasticity, can achieve high performance according to statistical evaluation metrics. However, the analysis of the scatter plots and the residuals distribution revealed the process's heteroscedasticity, making the deterministic predictions ineffective. To address this issue, a Probabilistic Neural Network (PNN) was developed, whose output consists of two parameters (the mean and the standard deviation) that parametrise a normal distribution. This approach enables not only the estimation of air demand, but also the associated uncertainty. Consequently, the neuro-probabilistic approach offers significant advantages over traditional data point estimators, making it a valuable tool for surrogate modelling in scientific ML, especially in the perspective of process optimisation.

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Optimization of a VPSA CO_2 pre-concentration unit using 13X/MOFs for cryogenic CO_2 capture

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Vacuum Pressure Swing Adsorption (VPSA) technology plays an important role in hybrid carbon capture systems, particularly for pre-concentrating CO_2 from low-concentration flue gas streams (5–20% CO_2). This study investigates a hybrid system combining a VPSA unit with a cryogenic purification unit (CPU) to treat 70,000 Nm^3/h of flue gas, e.g. equivalent to 1,000 t/day of clinker production. The VPSA acts as a pre-concentration stage, increasing CO_2 purity above 50% while maximizing recovery, before the CPU further purifies the stream to over 99.999%. The CPU waste stream is recycled to the VPSA inlet to minimize CO_2 loss [1].

The VPSA cycle initially used is the Skarstrom cycle with pressure equalization [2], using zeolite 13X for its commercial availability and CO_2/N_2 separation performance. The system is optimized by varying cycle times, reflux flow rates, pressure levels, and bed volumes. Surrogate modeling and Aspen Adsorption V14 simulations enable rapid evaluation of CO_2 recovery, purity and energy consumption. Results show that the VPSA unit can reach purity higher than 50% for flue gas higher than 10% CO_2, but failed to treat lower concentration. An alternative 3-bed 6-step VPSA cycle [3] was evaluated to treat diluted flue gas (5% CO_2) allowing to reach higher purity while maintaining a high recovery (>90%). Comparison between energy consumption and cost was performed for the two cycle configurations for its integration with a cryogenic unit.

Further optimization explores advanced adsorbents like MIL-160(Al) and MIL-120(Al) metal-organic frameworks (MOFs), which offer high CO_2 capacity and selectivity, potentially reducing operational and capital costs. Energy consumption can be drastically reduced with these materials compared to zeolite 13X showing their potential for this application. Nevertheless, the high price of MOFs makes the economical optimum between 13X and MOFs dependent on the inlet CO_2 concentration and the target recovery of the unit.

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MIL-160: A Green and High-Performance Adsorbent for Water Harvesting and Chillers

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MIL-160, a robust and readily scalable MOF, demonstrates significant advantages over current commercial sorbents for water adsorption and desorption processes. Comparable to the benchmark FAM-Z02 commonly used in chiller and water harvesting systems,[1] MIL-160 displays similar adsorption profiles, with both materials exhibiting water uptake at close relative pressures. Nevertheless, MIL-160 achieves a 70% higher working capacity of 170 mg g^{-1} compared to 100 mg g^{-1} for FAM-Z02, making it more effective for cooling applications.

Dynamic adsorption experiments reveal similar S-shaped breakthrough curves for both materials but confirm the superior uptake of MIL-160. Its key advantage lies in desorption performance during cycling: at 60 °C, the waste heat temperature level, MIL-160 releases 80% of its adsorbed water, enabling a cycling sorption capacity of 16.2 mmol g^{-1} with stability over repeated cycles. In contrast, FAM-Z02 desorbs only 60% of its adsorbed water, corresponding to 9.5 mmol g^{-1}. Increasing the regeneration temperature to 80 °C enhances the cycling performance of FAM-Z02 to 76% (12 mmol g^{-1}), yet this remains lower than the capacity of MIL-160 at 60 °C. Furthermore, the composition of MIL-160, based on abundant and low-toxic aluminum, available and biosourced FDCA linker, combined with a green synthesis route, makes it highly suitable for large-scale production.[2] The combination of enhanced adsorption capacity, efficient regeneration, and a green synthesis route highlights the strong potential of MIL-160 for water harvesting technologies.

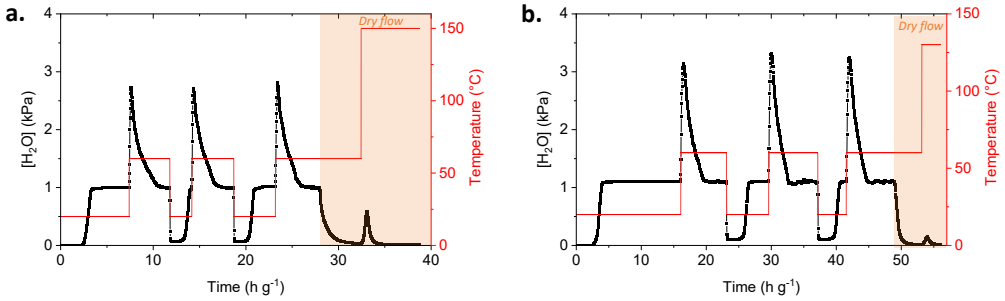

Figure 1: Breakthrough curve of water at 20 °C followed by a desorption at 60 °C on FAM-Z02 (a) and MIL-160 (b).

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Putting ZIF-8 in Shape: ZIF-8 / Polymer Extrudates for Gas Phase Alcohol/Water Separations

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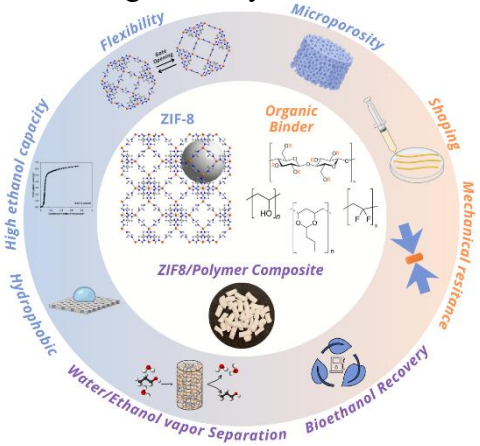
ZIF-8 is one of the benchmark MOFs for alcohol/water separations owing to its high hydrophobicity and sigmoidal alcohol adsorption isotherm. The gate-opening flexibility of the framework enables molecules such as ethanol (kinetic diameter ≈ 4.3 Å) to penetrate its pores, despite the smaller size of its six-membered ring apertures (≈ 3.4 Å).[1] Since bioethanol is typically produced via energy-intensive distillation (80% of the production cost), ZIF-8 represents a promising alternative adsorbent for ethanol recovery. For practical use, ZIF-8 powder must be formulated with binder to yield mechanically robust and abrasion-resistant structures.[2] Yet, shaping ZIF-8 remains particularly challenging, as the process must preserve all the intrinsic properties of the initial powdered MOF (structural integrity, flexibility, adsorption properties), while the incorporation of binders can profoundly influence, or even compromise, them.

In this work, we developed millimeter-sized ZIF-8 extrudates while preserving their intrinsic framework flexibility. Different binders were screened, using polymeric organic binders (polyvinyl butyral and polyvinylidene fluoride) and cellulose-based binders (methylcellulose, hydroxypropyl cellulose, and carboxymethylcellulose). The shaped materials retained the textural properties and structural flexibility of ZIF-8, as confirmed by nitrogen sorption (77K) and PXRD analyses. As in one of the rare cases in open literature, the mechanical strength of the extrudates was quantified, showing crushing strengths comparable to commercial zeolite pellets and highlighting the strong influence of the binder nature on the mechanical behavior of the composites. Thermogravimetric analysis showed that the formulation process modifies the heat transfer properties of the formulated materials. Selectivity for ethanol over water, based on IAST calculations, showed that, while hydrophobic binders preserved the ethanol-water separation performance of ZIF-8 (with PVDF exhibiting the highest selectivity, α=1 473), hydrophilic binders drastically reduced the selectivity, in some cases reducing it to almost negligible levels. This work highlights how shaping MOFs with organic binders can alter their structural flexibility and, depending on the binder chemical nature, significantly influence their adsorption properties.



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H_2O and CO_2 adsorption in different MOFs: experimental isotherms, heats of adsorption and their modeling

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Carbon capture from flue gas or air presents unique challenges, as it is often accompanied by significant amounts of water. Amongst many adsorbents considered for capturing CO_2, MOFs are regarded as potential candidates. This family of adsorbents presents a wide range of water adsorption behavior [1] which can be very complex to predict numerically and can more or less compete with CO_2. Because water plays a critical role in the process, accurately representing its isotherms is essential to simulate CO_2 capture properly. For that, an understanding of underlying adsorption mechanisms is crucial, and the measurement of adsorption enthalpy – as done in this work thanks to a home-made calorimetric/manometric setup – brings important information. As a typical example, our methodology is applied to Al-Fumarate which presents the so-called "S" shaped water isotherm (see Fig. 1), and high adsorption enthalpies at low loading followed by a plateau. It is shown that the modified Do and Do model [2,3] initially developed for water adsorption on activated carbons to account for the successive water adsorption mechanisms - strong interaction of the first water molecules adsorbed with specific sites followed by cluster formation – allows a good and temperature-consistent water adsorption modeling. Additionally, modeling of CO_2 adsorption was also performed on Al-Fumarate in good agreement with calorimetric experiments and the methodology was transferred to other MOFs such as CALF20.

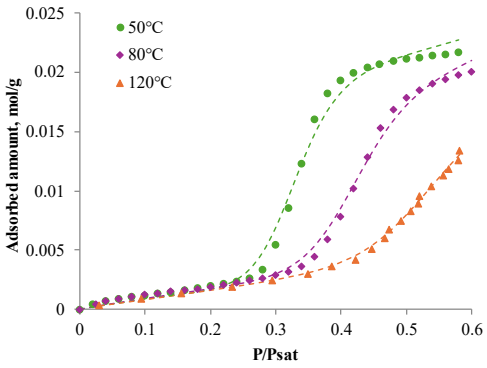

Fig. 1: Water isotherms of Al-Fumarate and corresponding modeling (dashed lines)

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Advancing MOF Simulations with Machine-Learned Potentials

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Machine-learned potentials (MLPs) are transforming materials science by enabling accurate and efficient modeling of complex materials, such as metal-organic frameworks (MOFs). These data-driven approaches overcome the limitations of traditional methods like density functional theory (DFT), which are computationally prohibitive for large-scale simulations. MLPs offer a hybrid alternative by learning the potential energy surfaces from quantum mechanical data, thereby providing rapid and precise predictions of material properties across extended length and time scales. One area where MLPs prove especially valuable is in the modeling of flexible MOFs, which can exhibit phase transitions and mechanical deformations in response to external conditions (thermal, mechanical pressure). Using MLPs, we explore the MOF CALF-20's phase space with unprecedented efficiency, revealing distinct two-step elastic deformation and high fracture strain, which are critical for potential applications in flexible electronics and sensors. Furthermore, MLPs extend their utility to adsorption simulations, particularly for MOFs with open metal sites (OMS), where strong host-guest interactions are challenging for classical force fields to describe accurately. We demonstrate this by developing an MLP for H_2 adsorption in Al-soc-MOF-1d, an OMS-containing framework. The MLP accurately models H_2 binding and diffusion, offering insights into adsorption performance that can guide the design of MOFs for hydrogen storage applications. MLP is also a key feature to describe the guest-assisted local dynamics of narrow pore MOFs like MIL-120(Al). These examples illustrate the potential of ML-based approaches to advance the computational modeling of MOFs.

Optimal stratification improves efficiency in fixed-bed separation

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Motivation and method

Several studies have demonstrated the advantages of gradients in the stationary phase of fixed-bed separation columns. For this reason, we developed a model-based optimal control approach that determines optimal stratification [1]. To investigate the effectiveness of this approach, we executed experiments with optimally stratified activated carbon adsorption columns for the removal of phenol from water [2]. We conducted two different case studies. In both case studies, the goal is to achieve the sharpest possible breakthrough curve by optimal stratification.

Results

Optimal stratification improves the sharpness of the breakthrough curve by 48.26 % in the first case study and by 51.87 % in the second case study. Here, the results of the first case study are presented. Fig. 1 plots the particle diameter over the axial position for the homogeneous column, the optimal stratification, and the optimal layers. Optimal stratification refers to the theoretical results derived from the optimal control approach. Since this continuous stratification is difficult to produce, discrete layers were fitted to the optimal stratification and built for the experimental runs. Fig. 2 shows the experimental breakthrough curves for the homogeneous column and the optimal layers. The separation curve produced by the optimal layers is distinctly sharper compared to the homogeneous column.

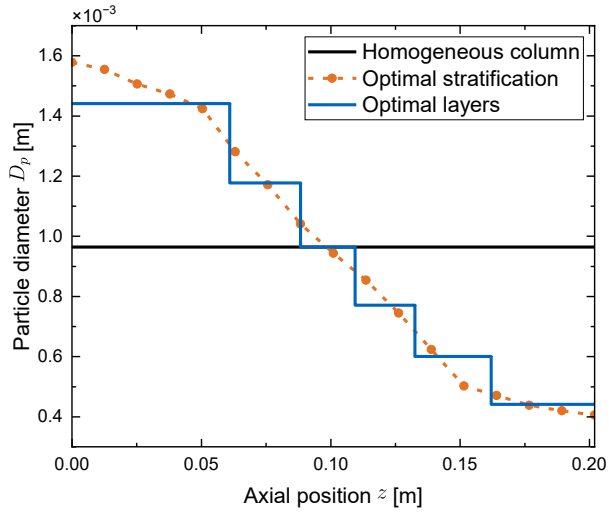

Fig. 1: Stratification of all columns.

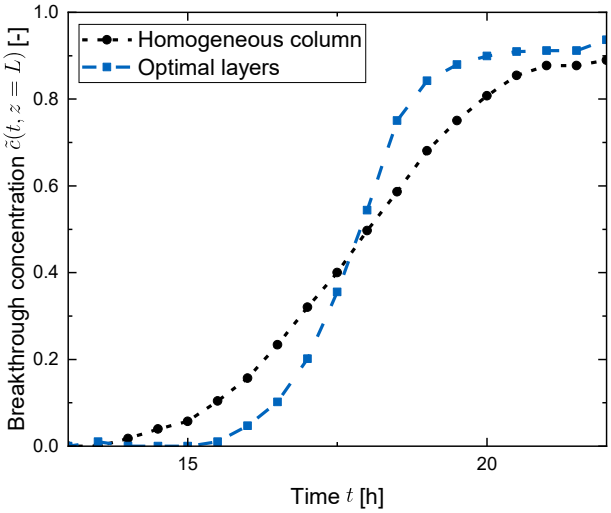

Fig. 2: Experimental breakthrough curves.

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Adsorption phenomena on Activated Carbons in Bioprocesses

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A key pathway toward a circular economy is the biotechnological conversion of renewable feedstocks into platform chemicals such as carboxylic acids [1]. By employing *in situ* adsorption to selectively and continuously remove the target carboxylic acid during fermentation, product inhibition, which is a typical limitation of bioprocesses, can be mitigated, thereby improving the viability and competitiveness of bio-based products relative to fossil-derived alternatives [2-5]. In this study, we select activated carbons as adsorbents owing to their high specific surface areas and their derivation from sustainable precursor materials.

Adsorption thermodynamics and kinetics for the target molecule, as well as for co-solutes (e.g., salt ions), are strongly governed by the carbon's pore structure and surface functional groups. These properties depend on both the precursor and the activation method and therefore vary among activated carbons [6]. Consequently, the selection of the activated carbon is crucial for achieving optimal process performance. Moreover, pH exerts a great influence on ion adsorption: surface functional groups protonate or deprotonate as a function of pH, thereby attracting or repelling ions according to the surface charge. This results in complex system of coupled acid–base dissociation and adsorption equilibria [7,8]. Building on these considerations, we present current research results regarding the adsorption behavior of the described system by providing a systematic comparison of activated carbons and revealing structure–performance relationships.

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Mixture breakthrough curve analysis to parameterize a modified multi-component BET isotherm model

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The design and optimization of adsorption-based separation processes, such as preparative chromatography, rely on accurate quantitative knowledge of competitive adsorption isotherms. Measuring and analyzing breakthrough curves (BTCs) is an established technique for determining adsorption equilibria in single-component systems. Parameters of single-component isotherms obtained from dedicated experiments can be applied in multi-component isotherm models; however, validation using competitive equilibrium data is recommended [1,2]. Lee *et al*. [3] introduced a multi-component BET isotherm model and applied it to the case of an infinite number of adsorbed layers. In this work, a modified multi-component BET model is proposed, which considers a finite number of N adsorbed layers.

In this study, the adsorption equilibria of three benzene derivatives with different aliphatic carbon chains (*tert*-butylbenzene (tBB), *sec*-butylbenzene (sBB), and *n*-butylbenzene (nBB)) were investigated based on measured BTCs using C18-bonded silica as the adsorbent. Single- and multi-component BTC experiments were performed under varying acetonitrile (ACN)/water compositions in the fluid (mobile) phase (60–90 vol.% ACN). Analysis of the single-component BTCs revealed that, with increasing ACN content, the shapes of the adsorption isotherms gradually transitioned from convex to concave. The multi-component BTCs exhibited complex front propagation behavior (anti-Langmuirian, Langmuirian, or mixed adsorption behavior), depending on the specific ACN concentration in the mobile phase.

Numerous single-component BTCs measured for different mobile phase compositions were well described using the proposed BET isotherm model. However, applying the estimated single-component isotherm parameters in the proposed multi-component BET model resulted in limited accuracy in describing binary and ternary BTCs. An improved agreement with these experimental mixture data was achieved by modifying, for each component, a specific parameter quantifying competition in layers 2 to N, which does not alter the description of the single-component isotherms. The best overall agreement was obtained by analyzing the mixture and single-component BTCs jointly. The parameters of the modified BET model enabled reliable prediction of both single- and multi-component equilibria for all solvent compositions.

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Investigation of the temperature dependence of adsorption enthalpy

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The heat of adsorption represents a crucial design parameter for industrial adsorption processes, as the temperature has a considerable impact on adsorption capacity and process kinetics. The temperature dependence of the heat of adsorption is of particular importance in the context of TSA (temperature swing adsorption) processes, which are characterized by pronounced temperature shifts between adsorption and desorption. Accordingly, an understanding of the load- and temperature-dependent behavior of the heat of adsorption offers potential for process optimization. The heat of adsorption, as a process variable, is obtained by adding an RT-term (R: universal gas constant, T: temperature) to the adsorption enthalpy, which is a variable of state. The adsorption enthalpy provides a measure of the strength of interactions between the adsorbent surface and adsorptive molecules and thus allows conclusions regarding the adsorption mechanisms.

In experimental investigations, pure substance adsorption isotherms and load-dependent adsorption enthalpies are measured simultaneously between -40°C and +40°C using a sensor gas calorimeter. The investigation comprises systems of different adsorbents, including zeolites, silica gels and activated carbons, and a variety of adsorptives, such as hydrocarbons, ammonia and water. Depending on the combination of adsorbent and adsorptive, different interaction types are formed.

The experimental results demonstrate a quantifiable variation in the adsorption enthalpies with temperature, indicating alterations in the strength of interactions formed between the adsorbent surface and adsorptive molecules. The load-dependent adsorption enthalpies, measured directly at different temperatures, are compared with isosteric adsorption enthalpies, calculated from the corresponding adsorption isotherms using the Clausius-Clapeyron equation (see Fig. 1). This comparison indicates that in some cases the isosteric adsorption enthalpy does not adequately reflect the experimental data. The data can be used to identify the limitations of the isosteric method and derive recommendations for its application. In the presentation, selected results of adsorption experiments will be shown and discussed.

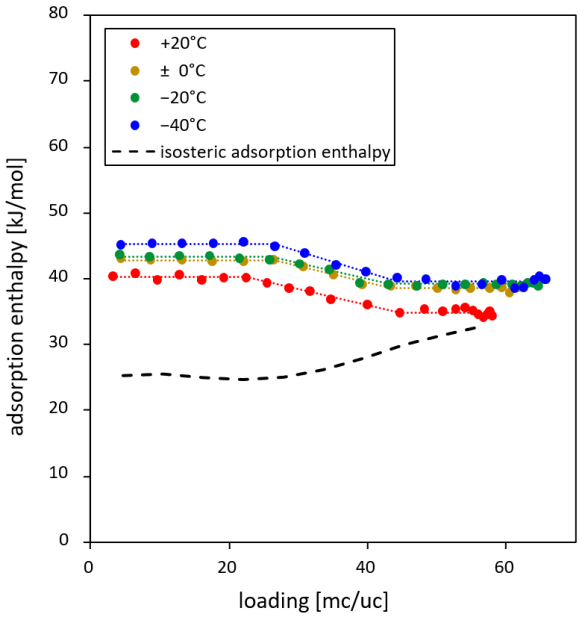

Figure 1: Calorimetric and isosteric adsorption enthalpies of ethylene on FAU type X zeolite

Carbon Filters for the analysis of stratospheric organic aerosols from weather balloon flights in France

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Stratospheric aerosol particles are a critical component to both the ozone layer and the Earth's radiative balance, resulting in ozone destruction, stratospheric warming and net surface cooling[1]. Their burden is largely controlled by well-established natural emissions of sulfur-gas precursors, which can be dramatically enhanced by sporadic volcanic eruptions as inferred from satellite observations[2]. Also, the last decade has been particularly affected by episodes of intense wildfires certainly resulting the increasing frequency and severity of fire weather, driven by anthropogenic, meteorological and climatic factors[3]. The extent to which wildfires and anthropogenic sources contribute to the stratospheric organic aerosol load and composition remains largely uncertain. Furthermore, the chemical composition and mixing state of organic aerosols in the stratosphere remains a scarcely documented aspect. These knowledge gaps hinder our ability to evaluate the impact of wildfire events and human-induced disturbances on stratospheric organic aerosols, and consequently, on the ozone layer and climate. In this work we present a unique offline analysis of organics collected from the ground to the stratosphere with ultimate sensitivity using a sampling technique based on carbon filters with modulated properties deployed on weather balloons[4]. Porous carbon fabrics have been applied to adsorb chemical compounds in gaseous and aerosol form during various flight campaigns in France. Coupled with ultra-high-resolution mass spectrometry, this has allowed the detection of thousands of organic compounds, and highlighted high-carbon-number organics, indicating oligomerization in long-lived tropical stratospheric air masses. This approach has demonstrated that large stratospheric sulfate aerosols from volcanic eruptions play a crucial role in the formation of secondary aerosols with higher carbon numbers.

Acknowledgements. The authors thank the funding of Region Centre Val de Loire (ACTAM) and ANR (ORACLE).

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Assessing Thermodynamic Equilibrium and Corrective approach for VOCs Adsorption on Microporous Activated Carbon

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Advances in air purification increasingly rely on high-performing adsorbents for volatile organic compounds (VOC) removal, with material innovations in microporous and mesoporous frameworks[1]. However, accurately characterizing adsorbent affinity for VOCs at low concentration remains challenging due to extremely slow adsorption kinetics in highly confining ultramicroporous solids. In this context, accurately determining the Henry constant K_H for VOC adsorption in microporous solids at low pressures is limited by difficulties in reaching thermodynamic equilibrium in standard experimental methods.

Here, a thermodynamically grounded three-step methodology is introduced for reliable estimation of the Henry constant in such diffusion-limited systems. In practice, this strategy is illustrated by considering cyclohexane adsorption on commercial activated carbon (AC). The approach involves (1) measuring adsorption isotherms at elevated temperatures (which ensure that thermodynamic equilibrium is reached), (2) extrapolating to the target temperature via Polanyi's adsorption potential theory[2], and (3) finally deriving K_H from the recalculated low-pressure region.

This method allows reconstructing the adsorption isotherm. This strategy, which is validated by showing that the adsorption isotherms match those obtained from independent breakthrough experiments, reveals systematic underestimation of adsorption at low pressure with standard protocols (up to a 15-fold difference in K_H). This study demonstrates how corrections based on Polanyi's adsorption potential theory allow overcoming equilibrium limitations, outperforming both measurements and kinetic-based protocols alone.

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YoungFluidSeps
Early Career Fluid Dynamics and Separation Engineers

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We are the early career group of the DECHEMA/VDI "Fluid Dynamics and Separation Technology" section. Our mission is to promote the professional exchange and networking of new members within the section. We aim to lay the foundations for a dynamic community and create opportunities for young talents to grow and develop their careers.

Target group

The term “young” does not refer specifically to age. Our activities are intended for junior group leaders, doctoral candidates, and early career professionals in the field of fluid dynamics and separation technology. We aim to provide a platform that connects active members with interested young professionals from both industry and academia.

Activities

We organise both online and in-person activities to encourage professional exchange and networking. These include gatherings and more (e.g., poster prizes) at the annual expert meetings within our DECHEMA section, virtual workshops, and a yearly field trip. To stay updated on our latest news, we invite you to visit our website and subscribe to our newsletter. If you have suggestions for upcoming activities, please feel free to reach out to us. We welcome active supporters to help us organise engaging events. Further information about the YoungFluidSeps group and our planned activities for 2026 can be found on our poster.

YOUNG FLUID SEPS
Early career fluid dynamics and separation engineers

Adsorption measurements and modeling in the context of high-pressure natural gas dehydration

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Adsorption is regarded as a key technology for gas separations. Dynamic adsorption processes such as TSA and PSA are commonly used for water vapor capture applications like air drying and natural gas dehydration. To assess the natural gas dehydration performance, this study focuses on adsorption equilibrium of water as well as some alkanes that are commonly present in natural gas such as methane, propane and butane. An activated carbon is used as a desiccant for water vapor capture in presence of light hydrocarbons. Adsorption isotherms at three different temperatures of the four pure gas components were measured using gravimetric systems.

The Heterogeneous Do & Do model that has been developed to describe water adsorption mechanisms on activated carbon materials [1] is used to fit water adsorption isotherms. And Toth model is used to fit the adsorption isotherms of methane, propane and butane. The good dependency of all parameters with temperature allowed to assess the consistency of the models used and thus to predict adsorption isotherms at other temperatures. These findings would facilitate quantifying adsorption equilibrium at various temperature conditions by reducing the need for extensive experimental campaigns.

Finally, co-adsorption of water with methane, propane and butane is predicted using the Ideal Adsorbed Solution Theory (IAST).

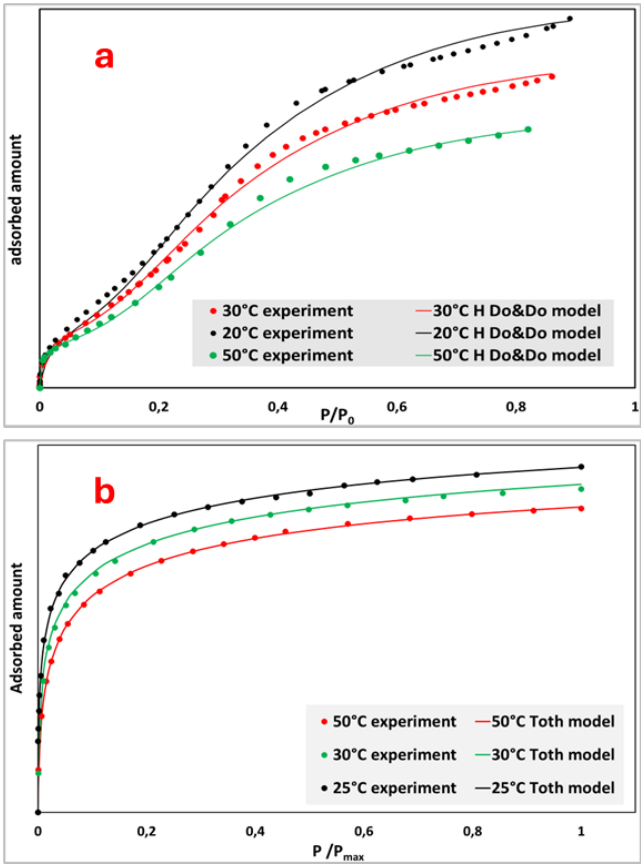

Figure 1 Adsorption isotherms on activated carbon for water (a) and propane (b).

References:
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Co-Adsorption of Water and Carbon Dioxide on a Commercial Material for Direct Air Capture (DAC)

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Introduction

Direct Air Capture (DAC) of CO_2 is considered as a key technology to mitigate the consequences of the anthropogenic climate change. The high dilution of CO_2 in the atmosphere, along with the presence of humidity, places stringent demands on any capture material. A typically employed material class for DAC are polymeric amines supported on different materials. Amine-based materials offer the advantage that humidity – to a certain extent – supports the adsorption of CO_2, rather than competing with CO_2 as on many other materials. A frequently used commercialized amine-based benchmark material is Lewatit VP OC 1065. This work aims to give insight into the cooperative and competitive adsorption behaviour of CO_2 and H_2O on Lewatit.

Experimental setup/Methodology

As a first step, pure CO_2 and H_2O adsorption isotherms were measured. To gain deeper insights into the co-adsorption of CO_2 and H_2O, dynamic gravimetric (Surface Measurement Systems DVS Vacuum) and breakthrough measurements (3P Instruments mixsorb SHP) were performed at DAC (400 ppm CO_2) and flue gas (15% CO_2) conditions at 25°C.

Results

At flue gas conditions, the presence of H_2O does not improve the adsorption of CO_2 and can even hinder it. It could be shown, however, that the presence of CO_2 increases the adsorption capacity of H_2O. In contrast, at Direct Air Capture conditions, humidity drastically improves the adsorption capacity of CO_2 and vice-versa. Consequently, the combined adsorption capacity of CO_2 and H_2O is higher than the sum of their pure component capacities. The dynamic gravimetric method and the breakthrough analysis provide consistent results.

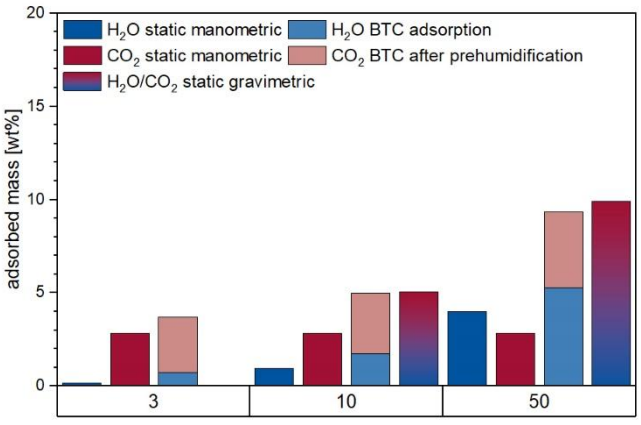

Figure 1. Gravimetric uptake of CO_2/H_2O at DAC conditions (400 ppm CO_2) and different relative humidities (3, 10 and 50%) at 25 °C.

Overall, this work provides valuable insights on the co-adsorption of CO_2 and H_2O, from a methodological as well as from a mechanistic perspective.

Temperature and moisture dependent adsorption kinetics of polyethylenimine (PEI) coated carbon nanofibers

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In the last decade, polyethylenimine (PEI) has gained much attention in Direct Air Capture (DAC) applications due to its high amine group density which enables high CO_2 chemisorption. In combination with suitable backbone materials, such as carbon nanofibers (CNFs), adsorbents with high CO_2 uptake, selectivity and fast kinetics can be tailored for a wide range of process conditions. In order to understand how to design novel materials, a look into the adsorbent-adsorbate interaction during various process conditions is needed.

In this study, PEI coated CNFs are investigated in respect of their general CO_2 uptake and kinetics at various humidities and temperatures. A well-established way to analyze these properties are breakthrough experiments. By tracking the movement of a gas or vapor stream through a column filled with adsorbent, information about the adsorption rate and capacity can be drawn. For the experiments of this study, a gas mixture, containing He as a carrier gas , N_2 and CO_2, was directed over PEI coated CNFs at different temperatures and humidities, with a flow rate of 50 mL/min (45 mL/min He, 4.98 mL/min N_2, 0.02 mL/min CO_2) at 1 bar.

The aim of this study is to illustrate how the change of several parameters at the same time strongly influences the CO_2 adsorption behavior and therefore the screening of novel adsorption materials. The kinetics for the CO_2 uptake under atmospheric conditions (400 ppm in air), strongly depend on the relative humidity. As can be seen in Figure 1, the breakthrough flattens with more moisture present in the gas stream. Additionally, the amount of adsorbed CO_2 increases with humidity. A raise of the temperature from 25 °C to 40 °C leads to a later breakthrough. If humidity and temperature are increased simultaneously, less amount of moisture is adsorbed, compared to 25 °C.

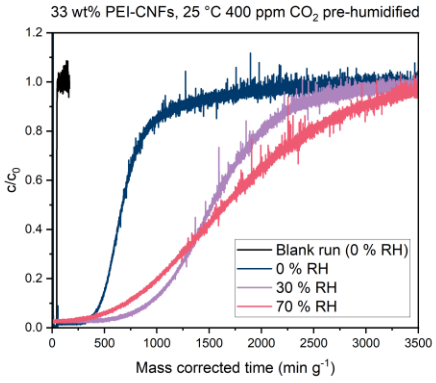

Figure 1: Breakthrough curves of CO2 on PEI coated CNFs. The shape of the curves depends on the humidity.

It can be learned from this study that moisture has a cooperative effect on the CO_2 adsorption. Temperature on the other side fastens the kinetics for dry CO_2 streams but also decreases the amount of moisture uptake.

Model-Based Optimization of Phosphate Recovery From Municipal Wastewater Using Iron Hydroxide Fixed-Bed Adsorption

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Phosphorus is an essential but finite resource, indispensable for agriculture and industry, and listed by the European Union as a critical raw material. Its growing demand motivates recovery from secondary sources like municipal wastewater. While conventional methods involve chemical precipitation or enhanced biological phosphorus removal, adsorption is particularly attractive when the goal is direct phosphate recovery from the liquid phase. However, fixed-bed adsorption is only viable if the process is energy- and resource-efficient and operable at scale.

This study investigates a coupled adsorption-desorption process for phosphate recovery from municipal wastewater using parallel fixed-bed columns packed with iron hydroxide particles. Iron hydroxide is an attractive adsorbent due to its low cost and high availability. Phosphate-rich wastewater is periodically fed through the beds, which selectively separate phosphate, yielding phosphate-lean water. A saturated bed is regenerated via pH-swing, producing a concentrated aqueous phosphate solution suitable for subsequent salt precipitation. Optimizing this complex process is challenging due to the large variety of operating and design parameters.

Therefore, a model-based approach was chosen to efficiently screen large parameter spaces and identify optimal conditions. A linear driving force model was employed to describe both the adsorber breakthrough and the pH-swing regeneration. Model parameters were determined using batch kinetic experiments and adsorption isotherms. Kinetic studies confirmed that intraparticle diffusion is the rate-limiting step, which guided the selection of an optimal particle size balancing fast mass transfer against an acceptable pressure drop. Column hydrodynamics were also characterized via residence-time distribution measurements.

Our simulation results demonstrate that desorption performed in the same flow direction as the preceding adsorption step yields a significantly higher overall regeneration efficiency than counter-current operation. This benefit stems from a more favorable alignment of concentration and loading gradients, leading to more uniform bed utilization and improved phosphate recovery across cycles. The results confirm that our model-based approach facilitates swift and effective process optimization for sustainable phosphorus recovery.

Lattice Boltzmann Method for the adsorption and transport of complex pollutants in bimodal porous media

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Modeling the transport and adsorption of emerging pollutants in double porosity media (i.e., systems exhibiting both micro- and macroporous phases corresponding to small and large pore sizes, respectively) is essential for the design of efficient adsorption-based remediation techniques (e.g., porous filters) and for characterizing pollutants uptake in natural porous media such as soils and sediments. In this context, the Lattice Boltzmann method (LBM) is an efficient highly parallelizable technique for solving the fundamental flow and transport equations in complex geometries as well as in large systems. In this study, we investigate the impact of both the adsorbable tracer and the adsorbing surface properties (e.g. adsorption kinetics, porosity, permeability) on the transport of the tracers through a porous disk. First, the Darcy-Brinkman equation describing the flow field in a double porosity media is solved using a two-relaxation-time (TRT) operator. Then, the advection-diffusion equation (ADE), coupled with a newly developed adsorption kinetic equation for complex pollutants, is again solved with a TRT operator. The study explores the combined impact of microporosity and flow rate, along with the role of adsorption kinetics – including surface saturation and lateral interactions between adsorbed species – on the overall transport and retention behavior of pollutants in double-porosity systems.

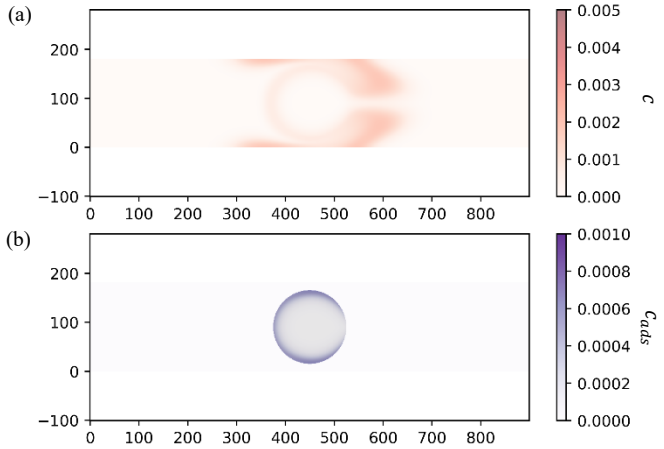

Figure: Transport of adsorbable tracers through a porous disk. (a) Bulk concentration of free tracers and (b) adsorbed concentration in the porous disk.

Isothermal vs. adiabatic process investigations of CO_2/H_2O co-adsorption effects on amine-based adsorbents under flue gas conditions

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Amine-based adsorbents are known to be lucrative for post-combustion CO_2 capture [1-3]. Flue gas is inherently humid, with H_2O quantities equal to or greater than CO_2, making co-adsorption central to process design. Following on our latest findings on humidity-enhancing CO_2 uptake on benchmark Lewatit VP OC 1065®, we note that humidity also influences temperature rise in non-isothermal fixed beds via co-adsorption kinetics, potentially affecting adsorbent cycle productivity; adiabatic temperature swing adsorption (TSA) thus deviates from isothermal predictions [4]. This study aims to compare CO_2/H_2O co-adsorption dynamics on amine adsorbents in TSA operated isothermally vs. adiabatically under defined relative humidity using model-assisted fixed-bed breakthrough experiments. Hence, this work provides information on axial *T*-profiles and flue gas transport phenomena under fluctuating, dynamic process conditions.

Dynamic sorption cycle measurements were carried out on a fixed-bed adsorber reactor (L = 40 cm) using an evaporation system to saturate the flue gas. The adsorber was equipped with a thermostated double-jacket for isothermal and vacuum isolated for quasi-adiabatic operation. Temperatures in the bed were measured at distinct distances in axial flow direction. Amine adsorbents were investigated under a wide process window (RH = 0-90%, $T_{ads/des}$ = 293-378 K, $p_{ads/des}$ = 1-3 bara). Dynamic TSA breakthrough curve simulations were performed using a 1D PFTR adsorber model developed in MATLAB®. Co-adsorption dynamics of CO_2/H_2O and adsorber *T*-profiles were modeled numerically over coupled mass and energy balance using central difference method with time-efficient ode15s solver and validated against experimental data.

Our model-assisted axial temperature investigations on adiabatic adsorption show clear ΔT peaks related to the humidity of the feed gas stream, which resulted in losses to CO_2 working capacity and thus productivity of the amine adsorbents. This data revealed the need for considering CO_2/H_2O co-adsorption kinetics in adiabatic TSA. Therefore, with our extended adsorber model, we demonstrate dynamic process modeling of fluctuating TSA cycles, which enables error quantification of the isothermal assumption of breakthrough curves under humidity influence.

Joint project H2-Reallabor Burghausen/ChemDelta Bavaria, BMFTR, grant code: 03SF0705D.

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Radon Adsorption in Cation-Exchanged Ferrierite: A Combined molecular simulation – experimental study

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The sensitivity of low-background detectors used in rare-event physics is often limited by trace radioactive impurities, with radon (^{222}Rn) being one of the most persistent sources. Mitigating this background requires materials capable of selectively trapping radon under ultra-clean conditions. Zeolites have shown an interesting potential for this application [1] and a preliminary Grand Canonical Monte Carlo (GCMC) simulation study predicted as optimal zeolite topology the ferrierite (FER) (Figure 1a), with high charge compensating cations content.

In this study, we have combined molecular simulation techniques in order to predict the Rn adsorption performances and guide the successive experiment. The initial modeling stage allowed us to assess the aluminum distribution along the T-sites of the FER framework and the nature and location of extra-framework cations (Ag^+, Ni^{2+}, Cu^{2+}). Furthermore, we determined the influence of those parameters on the Rn adsorption performances (Figure 1b). GCMC simulations showed that Ag– and Ni–exchanged FER possess the highest radon adsorption capacity in the low-pressure region, corresponding to the trace partial pressures encountered in low-background detectors. Finally, the FER samples (Si/Al = 10) exchanged accordingly to the simulation outcomes have shown high radon adsorption performances, experimentally corroborating the simulated prediction.

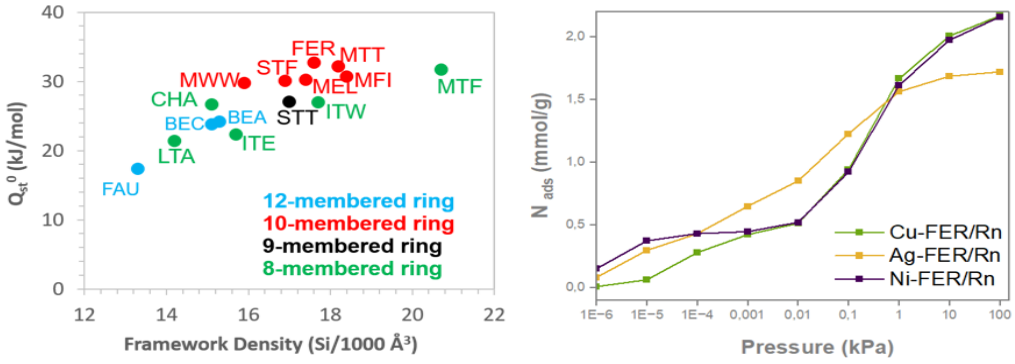

Figure1: Comparative adsorption performance of silica zeolites with varying pore apertures (8-, 10-, 12 MR) **(a)**; Adsorption isotherms of Rn on cation-exchanged FER **(b).**

[1] Veselska, O. *et al. Prog. Theor. Exp. Phys.* **2024**, *023C01*.

CO_2 Capture using porous silica-based materials at multiscale porosity

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[b] Centre de Recherche Paul Pascal (CRPP), Université de Bordeaux, Pessac, France

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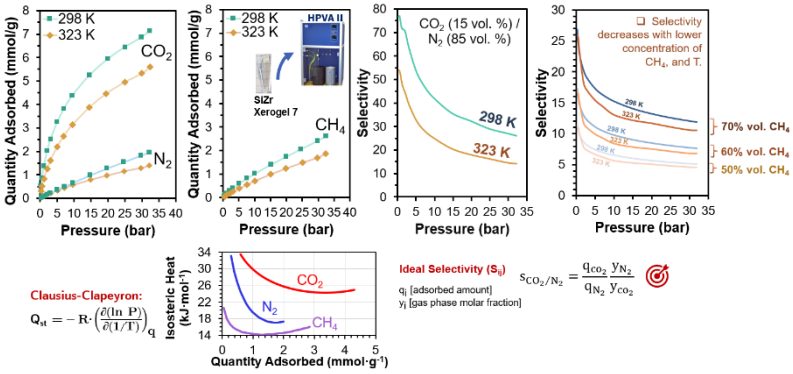
[d] Institut Jean Lamour (IJL), Université de Lorraine, Epinal, France

Industrial flue gases and raw biogas require sorbents that combine high CO_2 uptake, strong selectivity, fast kinetics, and regeneration using low-grade heat [1,2]. We present a family of hierarchical porous silicas (HPS) synthesized via a simple sol–gel route, coupled with either supercritical CO_2 drying (aerogels), ambient evaporation (xerogels), or high-internal-phase emulsion (HIPE) templating (macrocellular foams), followed by thermal treatments [3,4]. By tuning the precursor pH and Zr/Al doping, we adjust the fractions of macro-, meso-, and micropores. N_2 sorption yields specific surface areas > 1000 $m^2 \cdot g^{-1}$; SAXS confirms a mass-fractal network; TGA shows < 12% mass loss up to 600 °C, indicating cycling stability.



At 273 K and 1 bar, Si–Zr xerogels adsorb 2.7 mmol·g^{-1} of CO_2, while ultralight foams reach 2.0 mmol·g^{-1}. The volumetric capacity for xerogel SiZr-7 rises to 240 kg·m^{-3} at 30 bar / 298 K, exceeding that of other porous silicas and more sophisticated materials under identical or comparable conditions. Ideal selectivity exceeds 75 (CO_2/N_2, 0.15 bar) and 20 (CO_2/CH_4, 1 bar); isosteric heats remain < 35 kJ·mol^{-1}, ensuring low-energy regeneration. Conversely, pre-loaded humidity (≤ 20% RH) reduces the CO_2 adsorption capacity at 323 K by ≤ 60% for all our silicas, according to gravimetric CO_2/H_2O co-adsorption tests. Given the high affinity for water, amine grafting by CVD (chemical vapor deposition) was implemented for APTES/DEAPTES to increase selectivity and humidity tolerance.

These preliminary results position HPS as an alternative to amine scrubbing, warranting further studies to contribute to the development of new CCS technologies. Remaining tasks include mixed-gas selectivity measurements (IAST/breakthrough) and PSA cycling tests, to validate stability and regenerability under industrial conditions.

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VPSA Process For Capturing CO_2 From Industrial Flue Gas at Post-Combustion Conditions Using Experimental and Simulation Procedures

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The persistent greenhouse gas emissions from the Industrial Revolution have driven global warming and environmental change. One of the most prominent greenhouse gas emissions in Earth's atmosphere is carbon dioxide, which accounts for over 60% of global warming. CO_2 is typically emitted by energy-intensive industries such as power plants, cement kilns, steel mills, and lime kilns. To address the detrimental effects of continuous CO_2 emissions, global energy supplies reliant on fossil fuels must be managed through efficient, cost-effective solutions. In this regard, post-combustion carbon capture has emerged as a more convenient retrofit option for existing industries. The conventional post-combustion CO_2 capture processes, such as absorption, are energy-intensive. Therefore, there is a growing and significant need to develop more sustainable and efficient CO_2 capture alternative techniques. As a result, adsorption has been quantitatively studied as a promising technology for capturing CO_2 from flue gases, potentially overcoming the energy penalty associated with amine-based processes and offering lower costs and environmental impacts. The vacuum pressure swing adsorption (VPSA) process is one of the adsorption processes that offers several practical advantages for post-combustion CO_2 capture, including lower energy consumption, reduced investment costs, minimal environmental impacts, and ease of achieving automated operation. Nevertheless, fine-tuning adsorption materials (adsorbents), process configurations, and operating conditions is essential to promote an efficient carbon capture process. Thus, testing different VPSA cycles like three-bed, six-step, and Two-unit, five-step with operating conditions (2 bar adsorption pressure, 0.1 bar vacuum pressure, and feed flow rate of 1 Nm^3/h for a mixture of 15% CO_2/85% N_2), along with adsorbents (MOF/MIL-120 (Al) and zeolite 13X), has been conducted experimentally on a lab-scale VPSA pilot [1], and via ASPEN Adsorption software V14 simulation to maximize CO_2 purity and recovery in the product stream and minimize energy consumption. The best experimental results for the three-bed, six-step using MIL-120 (Al) showed a CO_2 purity of 94.1% and a recovery of 90.13%, while zeolite 13X achieved a CO_2 purity of 94.5% and a recovery of 64.5%. On the other hand, the optimal simulation results for the two-unit, five-step VPSA process using zeolite 13X yielded a CO_2 purity of 95.1%, a recovery of 90.95%, a unit productivity of 45.68 $kgCO_2/(m^3$ adsorbent. Hour), and a total electrical energy consumption of 0.339 $kWh/kgCO_2$.

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New adsorption database containing 1000+ experimental datasets for vapor and gas adsorption on zeolites and other porous solids

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The experimental adsorption databases play a crucial role in the development of the field. From the practical point of view, they may give guidelines for the choice of sorbents. Their importance is even greater for the understanding of the adsorption mechanisms and establishing general structure – property relationships. In the recent years the importance of such experimental databases has further increased due to advent of machine learning approaches for predicting adsorption properties.

The team ASP ("Adsorption sur Solides Poreux" or "Adsorption on Porous Solids") located in Université Bourgogne Europe (Dijon) has been working for more than 40 years in the field of adsorption. To respond to the growing demand of experimental data in the field of adsorption studies, we decided to gather the measurements of different types realized in the team and to provide a free access to this data for the adsorption community.

The current version of the ASP database contains 1079 entries containing both published and unpublished high-quality data. According to the data type, the major part are the adsorption isotherms (845). The database contains also the isobars (124) and the differential adsorption enthalpy as a function of loading (110). The main type of the sorbents are the zeolites (652 datasets) of FAU, MFI, BEA and CHA structure. Other porous solids well represented in the database are silica-based materials (MCM41 and SBA15) (167), active carbons (86) and MOFs (67). Among the sorbates water vapor is the most represented case (394) followed by aromatic hydrocarbons, mostly toluene (217). It should be noticed that the ASP database contains substantial amount of data for chloro-organic (121) and sulphur-containing species (50).

Sub topic – Thermodynamics and kinetics of adsorption

Advanced characterization of nanoporous materials using a novel *in-situ* vapor sorption calorimetry method

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Porous materials play a key role in separation and catalysis processes. Ongoing advances in material science lead to new emerging nanoporous materials, that offer great potential for optimizing applications in many areas, including separation, catalysis, as well as gas- and energy storage. Within this context, a reliable and comprehensive textural and surface characterization of these materials is essential to understand their properties and to identify key structure-property-performance relationships. In addition to the assessment of textural properties—such as surface area, pore size/volume distribution, and pore network characteristics—a reliable determination of surface properties, including the hydrophilicity and hydrophobicity, is crucial here.

To address these challenges, we developed a novel high-precision manometric *in-situ* vapor adsorption calorimetry apparatus, which is based on a combination of a high-precision 3D-Calvet calorimeter paired with a novel vapor sorption apparatus capable of high, homogenous manifold temperatures. Depending on the chosen adsorptive (vapor), the manifold can be heated up to > 100 °C to completely prevent any vapor (e.g., water) adsorption on the manifold tubing [1], which ensures both highly accurate water adsorption and heat data. It enables our setup to accurately and simultaneously measure the adsorbed amount and the resulting, corresponding heat of adsorption for each adsorption isotherm data point (for a given pressure). We have successfully validated our system by performing water adsorption experiments (at 308 K) using a well-known microporous carbon reference material (BAM-P109), which was utilized in an international round robin to obtain a water adsorption reference isotherm [2,3]. Furthermore, the obtained adsorption heat data showed good agreement with published literature data [4].

The obtained heat of adsorption as a function of coverage yields information on surface heterogeneity, surface chemistry and site energy distribution. Moreover, we demonstrate that by coupling *in-situ* adsorption heat data with the results of an advanced textural characterization (based on argon adsorption at 87 K coupled with methods of statistical mechanics such as density functional theory), it is possible to assess pore surface characteristics and wetting behavior of adsorptives on the pore walls and correlate this information with the underlying pore size distribution of the adsorbent.

We present results obtained from water adsorption experiments utilizing pristine mesoporous silica materials with well-defined pore structures such as SBA-15, controlled pore glass (CPG) and functionalized silicas (SBA-15 and CPG) with varying degrees of TMS (trimethylsilanol) and C_{18} groups. Such adsorbents have potential applications as stationary phase materials in liquid chromatography.

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TSA Plant Design: Optimizing Regeneration Conditions

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Thermally regenerated adsorption systems are most frequently used for drying different gas streams. An exemplary application is the drying of a stream upstream of a cold box to protect it from icing. For the design of adsorbers and the optimization of operating conditions, mathematical models are indispensable. These models require adsorption isotherms and single-component breakthrough curves as a basis. In order to validate the models under application-related conditions, experimental investigations in pilot plants are also essential.

In this contribution, a approach for designing adsorption plants is presented. For the experimental validation of the models, a multipurpose pilot plant has been set up that allows for the investigation of various application cases. The plant consists of three adsorbers, allowing different operating modes to be considered. The feed gas is compressed to up to 40 bar by a membrane compressor. Different gas flows can be used to regenerate the adsorbers, which are heated at the inlet of the adsorbers. The experimentally determined process data from the various applications as well as the simulations are used to optimize the regeneration conditions of TSA system.

Combining Induction Heating and 2-D Modeling to Investigate Heat and Mass Transfer Phenomena in Fixed-Bed Adsorption

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Understanding coupled heat and mass transfer in fixed-bed adsorption systems is critical for scaling up adsorption-based gas separation technologies. In this work, induction heating is introduced as a novel diagnostic approach to probe heat transfer dynamics in a lab-scale fixed-bed adsorption unit (Fig. 1). The experiments reveal a strong radial heat transfer dominance, challenging the validity of conventional one-dimensional modeling approaches. Complementary CO_2/N_2 breakthrough measurements further confirm radial temperature gradients developing within the bed.

To interpret these phenomena, a two-dimensional heterogeneous heat and mass transfer model was developed and validated across lab-scale (ID: 16 mm) (Fig 2). The model captures pronounced spatial variations: in the lab-scale bed, a quadratic temperature profile forms at the adsorption front (Fig 3), while the gas-phase concentration rapidly equilibrates. At pilot scale (ID: 30 cm)[1], significant radial gradients in both temperature and concentration form near the wall region. These insights establish a robust framework for accurately modeling and scaling thermally coupled adsorption processes.

This work introduces induction heating as a novel diagnostic method for adsorption beds and demonstrates, through 2-D modeling, how radial heat and mass transfer fundamentally affect the breakthrough curve.

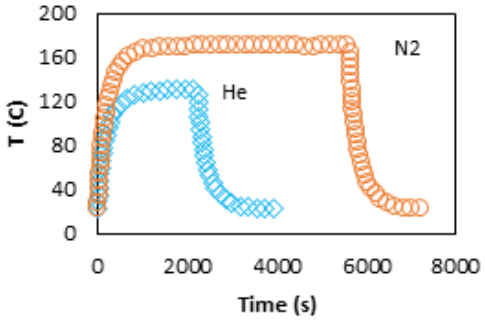

Fig 1: Temperature at the bed core under induction heating rate of 0.8 W/g, 30 Nml/min flow of N_2 and He

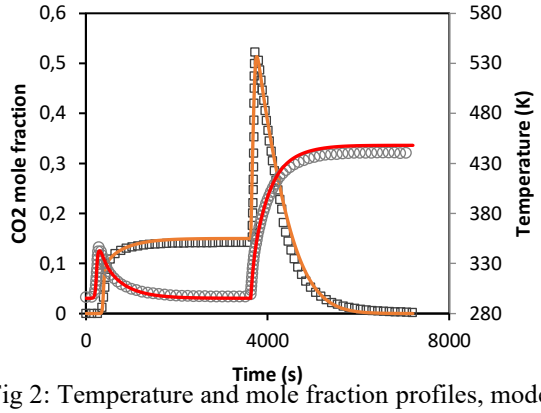

Fig 2: Temperature and mole fraction profiles, model predictions versus experimental data

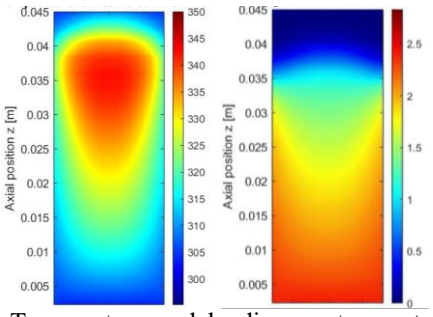

Fig 3: Temperature and loading contours at a specific time during adsorption, Column ID: 16 mm

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Effect of the Regeneration Method on the Characterization of Platinum Nanoparticles using H_2 Chemisorption

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Introduction

With H_2 being a promising energy carrier for the future, the importance of large-scale PEM electrolyzers increases. To characterize and analyze the degradation of the platinum catalyst in the membrane electrode assembly (MEA) of a PEM, H_2 chemisorption can be applied. A prerequisite for accurate measurements is a surface free of adsorbed gases. However, since the platinum layer of electrolyzer MEAs is exposed to hydrogen during operation, it is necessary to properly pretreat the material before the measurement. The standard pretreatment procedure for Pt surfaces characterization with hydrogen according to DIN 66136-2 includes temperatures of 350 °C over 3 h. Usually, Pt catalysts are supported for example on silica or carbon while MEAs use support-free Pt catalysts. Here, elevated temperatures can cause damage to the support-free catalyst, for example by sintering. Therefore, a modified pretreatment procedure is required.

Methodology

To evaluate the effect of different pretreatments on the structure and adsorption properties of the sample, several methods for the preparation and regeneration of the Pt nanoparticles with diameters of 20 nm have been applied. These regeneration methods vary from more gentle approaches like vacuum treatments at 25 °C with different durations to more harsh conditions like at elevated temperatures. Additionally, a combination of O_2 exposure at different temperatures and a following vacuum treatment were tested as well. Before and after each treatment, H_2 chemisorption and titration measurements at 25 °C were carried out. Furthermore, BET measurements were performed.

Results

The regeneration according to the established DIN 66136-2 method proves to be ineffective on unsupported Pt nanoparticles. Each regeneration reduces the accessible surface area of the platinum sample. Our investigation showed that vacuum up to 100 °C only results in incomplete desorption of hydrogen. During additional tests the sample was regenerated under a diluted O_2 in He stream followed by a vacuum treatment. This treatment proved to be a significant improvement of the regeneration without the need for elevated temperatures. Increasing the temperature during the O_2/He stream to 100 °C further increases the effectiveness of the regeneration. The H_2 uptake of the nanoparticles pretreated under these optimized conditions is identical to the uptake of the pristine nanoparticles. The developed regeneration method provides a valuable tool towards the characterization of Pt layers on PEM electrolyser MEAs using H_2 chemisorption.

Adsorption of Np(V) and U(VI) onto zirconia (ZrO_2): a batch, spectroscopic, and modeling study

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The safety of high-level radioactive waste repositories requires an understanding on how radionuclides interact with corrosion products in the vicinity of a given repository. In this context, zirconia (ZrO_2) – a corrosion product of the zircaloy cladding on nuclear fuel rods – constitutes an important initial barrier against radionuclide release.

Multiple methods were used to comprehensively investigate how Np(V) and U(VI) adsorb at the water–zirconia interface in the absence of ambient CO_2(g). pH-dependent batch sorption experiments (varying ionic strength, Np(V)/U(VI) concentration, and solid-to-liquid ratio), as well as sorption isotherms experiments (pH 4.5 and 6.0 for Np(V); pH 3.5 and 4.3 for U(VI)) were performed at constant ionic strength. The uptake of Np(V) and U(VI) increased with pH, starting at pH 3 with a maximum at pH 6 and above. Np(V) and U(VI) uptake was independent of ionic strength, suggesting the predominance of Np(V) and U(VI) inner-sphere complexes on the zirconia surface. Concomitantly, electrokinetic measurements showed that the isoelectric point of neat ZrO_2 shifted to higher pH values in the presence of Np(V) and U(VI). The adsorption edges of Np(V) and U(VI) shifted to lower pH with higher solid-to-liquid ratio, suggesting the presence of both strong and weak sorption sites, which was also supported by the shape of the sorption isotherms.

In situ attenuated total reflection Fourier-transform infrared spectroscopy and extended X-ray absorption fine structure spectroscopy confirmed the presence of a Np(V) bidentate inner-sphere surface complex in the weak sorption site regime. For U(VI), an inner-sphere mononuclear U(VI) bidentate surface complex was predominant at acidic pH. As the pH increased, a polynuclear U(VI) hydrolysis surface species became predominant. Laser-induced luminescence spectroscopy at alkaline pH suggested the formation of another mononuclear U(VI) hydrolysis surface species.

Macroscopic and molecular data were used to parameterize a charge distribution multi-site complexation model, yielding thermodynamic constants that improve predictions of the environmental fate of Np(V) and U(VI) in nuclear waste repository assessments and aid in evaluating safety scenarios for extended interim spent nuclear fuel storage [1].

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Selective radon adsorption on carbon materials

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Xenon (Xe) is an attractive candidate for detectors searching for neutrinoless double beta decay (from 136Xe) and direct dark matter. Xe has no troublesome long-lived radioactive isotopes, produces scintillation light and is easy to purify. However, the presence of ^{222}Rn represents a particularly important constraint when the detection medium is Xe. Xe and Rn have very similar atomic radii, 130 pm and 150 pm respectively, making their separation on microporous materials very challenging. To achieve the conditions of draconian purity required in future experiments, new adsorbents with high adsorption capacity and extremely high selectivity for ^{222}Rn are needed.

Porous carbon materials with tailored porosity and heteroatom content must be developed to selectively separate radon. To this end, in the frame of the project IRENE, we study the effect of the heteroatom content, especially oxygen and nitrogen, as well as the effect of their textural properties. Pristine and doped carbons are doped with metallic ions such as silver and mechanosynthesis in order to reduce the quantities of chemicals and the synthesis time needed.

Funding: This work was supported by the project ANR-23-CE31-0022 "Innovative Materials for Extreme Radon Adsorption – IRENE"

Investigation of Physics-informed Neural Networks for Surrogate Modeling of Chromatographic Systems

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This study investigates the potential of physics-informed neural networks (PINNs) as a surrogate modeling method for chromatographic systems. Our aim is to enhance computationally intensive applications, including process optimization, uncertainty quantification, and model predictive process control. PINNs provide a gray-box modeling approach that leverages automatic differentiation during the learning process to calculate solutions to partial differential equations (PDEs) without relying on classical numerical methods. Established by Raissi et al. [1], this method allows physical principles to be incorporated into the network as an additional part of the loss function.

While traditional mechanistic models dominate chromatography simulations, hybrid models like PINNs are gaining increasing attention in the academic community due to their potential speed advantages over mechanistic approaches and greater data efficiency compared to other data-driven methods. However, it is anticipated that they may require longer training times and are difficult to set up due to the complex error function. To investigate these claims, we conducted an in silico study by developing a PINN using simulated chromatography data derived from a fully parameterized mechanistic model; this model's PDEs were discretized and integrated using the open-source tool CADET [2]. For this study, we chose to examine the adsorption of dicarboxylic acids on hydrophobic adsorbents as a physical example. Here, we present initial results and discuss the limitations and potential of this modeling approach.

Binary CO/N_2 separation on Ba-ETS-4 and comparing with 5A and 13X zeolites

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Carbon monoxide (CO) is an essential C1 building block, but in steelmaking off gases, it is commonly mixed with nitrogen (N_2), making recovery challenging due to similar kinetic diameters [1]. Microporous Engelhard Titanosilicate-4 (ETS-4) is a small pore member of the titanosilicate family. ETS-4 has the pore size of 0.3–0.5 nm, which is in the range of the kinetic diameters of CO (3.764 Å) and N_2 (3.64 Å) [2,3]. We investigates Ba-exchanged ETS-4 (Ba-ETS-4) as a CO selective adsorbent against commercial zeolites (5A and 13X).

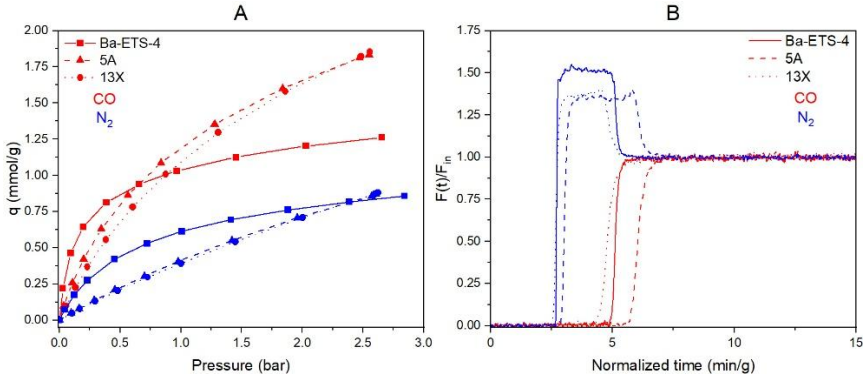

Figure 1: A) Single component isotherms at 25 °C, B) Binary breakthrough curves for 35-65 % composition CO and N2 at 25 °C and 1 bar with feed flowrate of 4.8 nml/min.

Figure 1A shows that at 25 °C all adsorbents preferentially adsorb CO over N_2 under static conditions. Under binary feed (Figure 1B), Ba-ETS-4 exhibited sharp fronts and a short CO mass-transfer zone (0.45 min g^{-1}), shorter than 5A (0.92) and 13X (1.04), which reduced the length of unused bed. Dynamic capacity calculation indicated that, while 5A provided the highest CO capacity at these conditions, Ba-ETS-4 achieves the highest CO/N_2 selectivity (4.2), outperforming both 5A and 13X in separation factor. Ba-ETS-4 also regenerated under very mild conditions. N_2 eluted near ambient temperature, and CO was completely released by 75 °C without high temperature tails. Sequential adsorption and desorption cycles showed stable CO capacity.

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Graphene-Based Metal Oxide Composites for the Adsorptive Elimination of Crystal Violet

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Abstract

Water is an essential element of life, and its pollution due to industrial effluents has posed significant threat to environment. Among various pollutants, synthetic dyes from textile, food, and printing industries are particularly harmful due to their stability, toxicity, and non-biodegradable nature. Herein, graphene-based adsorbents were synthesized for the removal of Crystal Violet (CV) from wastewater. The project commenced with the synthesis of graphene oxide (GO) via modified Hummer's method, followed by in-situ doping of NiO and CuO nanoparticles during the fabrication process. Various analytical techniques, including PXRD, FTIR, and UV-Visible spectroscopy were utilized for structure elucidation, whereas FESEM coupled with EDS mapping was used to confirm the morphology elemental composition of as-synthesized products. After the required characterizations, batch adsorption experiments were performed to optimize the reaction conditions for real-world applications. Different parameters affecting the adsorption, such as effect of pH, contact time, temperature, concentration, and adsorbent dose were studied. Among various kinetic and adsorption models, pseudo-second order kinetic model and Langmuir adsorption models were well-fitted, demonstrating the chemisorption adsorption and adsorbate species were adsorbed on the surface of adsorbents by forming a monolayer surface with no lateral interactions between the adsorbate molecules. Moreover, thermodynamic studies confirmed that adsorption process was endothermic, spontaneous, and entropy driven. All post-adsorption samples were analyzed using UV-Visible spectroscopy exhibiting exceptional adsorption capacities for both adsorbents in the natural conditions (pH = 6 and T = 303 K). Finally, the adsorbents after the successful adsorption of CV were analyzed through FTIR, which has confirmed the surface complexation mechanism of adsorption.

Sustainable Adsorptive Dye Removal Using Walnut Septum-Derived Activated Carbon

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Abstract

Water pollution caused by the discharge of industrial effluents has emerged as a major environmental challenge, affecting ecosystem and human health. Among the variety of contaminants, synthetic dyes are particularly detrimental due to their stable nature. Herein, the activated carbon was derived from the walnut septum and is chemically activated using KOH for the subsequent removal of methyl orange (MO) from wastewater. The synthesized adsorbents were characterized by PXRD, FTIR, and FESEM coupled with EDS mapping to determine its structural, functional, and morphological characteristics. Batch adsorption experiments were performed to analyze the removal of MO under varying pH, contact time, temperature, adsorbent dose, and dye concentration. Kinetic and adsorption modelling, including pseudo-second order, Langmuir, Freundlich, and Temkin models have confirmed the chemisorption adsorption, monolayer surface coverage along with formation of multi layers on some sites of the adsorbent. Afterwards, Vont Hoff plot was applied to analyze the thermodynamics, and it demonstrates that the process was endothermic, spontaneous, and entropy driven. Finally, the post-adsorption samples analyzed through FTIR have confirmed the surface complexation mechanism of adsorption.

Stability of Adsorbents for Direct Air Capture (DAC): Experimental and Modeling Approach

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In recent years, adsorption-based DAC systems have emerged as one of the major focuses of scientific and industrial research, driven by the advantages they offer for scalable CO_2 capture. Nevertheless, a key factor limiting the large-scale deployment of these systems is the long-term stability of solid sorbents. While most research has focused on developing adsorbents with high CO_2 selectivity and capacity, stability aspect has received less attention in the literature, yet it remains a critical challenge. The DAC process is highly sensitive to ambient conditions, namely the properties of the air from which CO_2 is removed. These include variables such as temperature and humidity, which can vary considerably across locations. During adsorption, exposure to air with a much higher O_2 concentration than CO_2 can lead to oxidative degradation. Additionally, adsorbents are subjected to elevated temperatures during the desorption step, the intensity of which depends on the specific regeneration method employed. Moreover, steam exposure during regeneration may further undermine their durability. Insufficient material stability not only raises the cost of captured CO_2 but also diminishes capture efficiency and reduces the net negative emissions achieved. Building on our previously developed DAC process model, we used model-derived data to estimate the impact of adsorbent lifetime on capture cost, thereby highlighting the importance of adsorbent longevity.

Our current research aims to address the critical gap between laboratory studies and real-world implementation of adsorption-based DAC systems. To this end, the literature is first reviewed to identify the main classes of adsorbents used in DAC and to determine the key factors influencing their stability. Subsequently, a dedicated test bench has been developed to systematically evaluate adsorbent stability under different conditions and as an initial case study, the stability of Lewatit® VP OC 1065, a benchmark DAC adsorbent, is investigated.

Furthermore, existing process models of adsorption-based systems often overlook the long-term stability of adsorbent materials, and no practical framework has been proposed in the literature to account for their degradation or deactivation. In this work, we also explore approaches to incorporate adsorbent aging into process modeling, enabling the determination of optimal replacement intervals and preventing unintended positive CO_2 emissions. This methodology further allows for optimization of cycle organization and can be extended to other adsorption-based separation systems beyond DAC.

An analytical design model for biogas upgrading VPSA plants

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A new analytical design model for the quasi-stationary state of a vacuum pressure swing adsorption (VPSA) process for upgrading biogas (CO_2 and CH_4) to biomethane (CH_4) is presented.

A reduced VPSA cycle comprising the steps adsorption, depressurization and evacuation was considered, using a model biogas system of 50% CO_2 in 50% N_2. The mass balance for the gas phase was formulated using an advection-reaction (AR) and for the solid phase using the Linear Driving Force (LDF) model.

The steady-state model provides adsorber dimensioning for maximized bed utilization at a demanded product purity. It is a practical tool for early-stage design and optimization in the basic engineering project phase.

Methanol from Air – The DryHy Project – Water-positive Methanol Generation by Utilizing Amine-based Direct Air Capture

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To reduce CO_2 emissions and mitigate climate change, fossil fuels must be replaced with renewable energy sources like solar and wind. Subtropical regions have significantly higher solar power potential than Europe, making them ideal for large-scale renewable power production. However, utilization and transportation of the generated electricity over large distances is a challenge. To address this, alternative energy carriers like methanol are needed. Methanol is particularly promising due to its high energy density, ease of storage and transport, and existing market demand. Producing green methanol (or other carbon-based energy carriers) requires a carbon source, a proton source like water, and low-cost solar energy. However, water scarcity in sun-rich regions makes it essential to develop a water-conscious approach that avoids competing with drinking water supplies.

A CO_2-negative carbon feedstock can be provided by direct air capture (DAC) of CO_2. In contrast to other technologies, amine-based DAC separates not only CO_2 but also water as a byproduct. Usually, the separation of water is regarded as disadvantageous due to increased energy demand during desorption. However, to produce green energy carriers in sun-rich, arid regions, it is advantageous, as it supplies a proton source without depleting local water reservoirs.

This synergy is one of the innovative approaches that are utilized in the DryHy project. An amine-based DAC plant separates CO_2 and water from air, which are subsequently converted to syngas using solid oxide electrolysis cells (SOEC) in co-electrolysis mode (Figure 1). In a chemical reactor the syngas is converted into methanol. The whole process is only reliant on low-cost renewably generated energy such as solar power. In this contribution, the DryHy process chain is presented and the challenges and synergies of amine-based DAC in the context of this power-to-X process are highlighted.

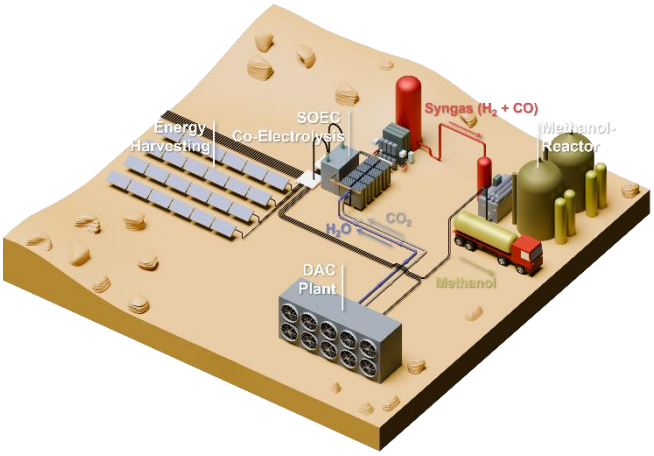

Figure 1: Visualization of the DryHy-process chain. A DAC is separating H_2O and CO_2 from air, while a SOEC converts both into syngas. A chemical reactor converts syngas into methanol.

DISTINCTION: Coal tar distillers in transition: developing new products for a sustainable, carbon-neutral economy

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DISTINCTION aims at supporting coal tar distillers in their transition to economic activities of high added value in a carbon-neutral economy, specifically in the field of energy storage, Na-ion batteries. The action therefore targets supporting the just transition of the coal sector and regions. DISTINCTION, the project has a two-fold purpose, namely, (1) to contribute to the creation of European-based value chains for the Na-ion battery as an incipient new-generation energy storage technology, and (2) to integrate coal tar distillers as a key link into such value chains.

In the frame of DISTINCTION, we develop hard carbon materials from wood and coal tar-derived precursors for use as the battery anode. A large pool of precursor substances is being prepared and processed and used to identify efficient routes to hard carbons with suitable physicochemical features and high electrochemical performance towards sodium storage. Selected materials will be presented, and their gas adsorption results will be discussed in detail.

Adsorption of acetone on silica-alumina gels

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The recovery of CO_2 by carbon capture technologies is gaining increasing importance, particularly in sectors where defossilization is difficult. The captured CO_2 can either be stored or further processed in downstream industrial applications. To protect distribution networks from corrosion, drying of the gas stream is required, which can be achieved by temperature swing adsorption (TSA) using oxidic adsorbents. During this process, accompanying trace components such as ketones and aldehydes are co-adsorbed. Due to their reactive nature, these compounds can polymerize on the surface of the adsorbent, forming permanently chemisorbed structures. The resulting material aging leads to a gradual loss of adsorption capacity during repeated adsorption-desorption cycles, eventually necessitating costly replacement of the adsorbent. For industrial applications, it is therefore of high relevance to understand this reactive system and to develop strategies to mitigate aging effects by adjusting process parameters.

In this study, adsorption and desorption experiments were carried out in a fixed-bed adsorption setup to evaluate the reactivity of various oxygenated hydrocarbons on silica and silica-alumina gels under different process conditions. Since the kinetics of chemical reactions strongly depend on temperature, the temperature swing inherent to TSA processes plays a crucial role in determining reactivity. Consequently, a systematic temperature study was conducted using acetone on a silica-alumina gel, with adsorption temperatures varied between 50 and 175 °C. To analyze the chemical composition of the loading, a sequence of desorption steps was performed: concentration swing desorption (CSD) at the respective adsorption temperature, temperature programmed desorption (TPD) up to 175 °C and thermogravimetric analysis (TGA) up to 800 °C.

At low adsorption temperatures, the breakthrough curves exhibit a predominantly physisorptive character, reaching a plateau at inlet concentration. In contrast, at higher adsorption temperatures, the adsorption kinetics become increasingly governed by chemical reactions, resulting in a very slow approach of the outlet concentration toward the inlet concentration. This behavior indicates a continuous chemical binding of additional adsorptive molecules. Calculated loadings after adsorption and desorption, together with TGA measurements after desorption, underlined the formation of a substantial residual loading at high adsorption temperatures. A large fraction of the reaction products was found to be thermally stable up to 800 °C. At such high temperatures, extensive cross linking of long-chain polymers and cyclic structures can be expected. This suggests that elevated temperatures during desorption are a key factor contributing to material aging effects in industrial applications.

Experimental investigation of the degradation of amine-functionalised adsorbents during direct air capture processes

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A promising technology to compensate for hard-to-abate CO_2 emissions is adsorption-based direct air capture (DAC) in combination with permanent storage [1]. Amine-functionalised adsorbents are particularly suitable for DAC due to their high CO_2 affinity at low concentrations and tolerance towards water vapour [2]. During the DAC process degradation of amine-functionalised adsorbents occurs during process phases with high temperatures and oxygen concentrations [3,4]. This causes higher operation costs due more frequent replacement of the adsorbent.

We investigated the adsorption performance of an industrially relevant temperature vacuum swing adsorption cycle for CO_2 capture from ambient air on Lewatit VPOC 1065 using a kilogram-scale test stand under varying relative humidities (RH) and air temperatures. During repeated measurements, a decrease in adsorption capacity is observed. This decrease in adsorption capacity is due to oxidative degradation of the adsorbent, which is caused by water induced temperature spikes in the presence of atmospheric oxygen concentrations at the start of adsorption.

To further investigate the influences of temperature, RH and oxygen concentrations on the oxidative degradation of amine-functionalised adsorbents, a gram-scale test-stand is being constructed. This test-stand iteratively first induces oxidative degradation and then measures breakthrough curves to determine the adsorption capacity and kinetics. Oxidative degradation is induced by exposing the adsorbent to a stream of premixed air consisting of oxygen, nitrogen and water vapour at a constant RH and adsorbent temperature. The oxygen concentrations, RH and adsorbent temperature can be varied, respectively. The breakthrough experiments are conducted with a gas mixture consisting of CO_2, nitrogen and water vapour at a constant CO_2 concentration, RH and adsorbent temperature. During the breakthrough experiment dedicated sensors for the CO_2 concentration and RH are used to measure the co-adsorption of CO_2 and water.

The aim of the degradation experiments is to determine the rate at which the adsorption capacity and kinetics of amine-functionalised adsorbents decrease depending on adsorbent temperature, RH and oxygen concentrations. These findings can be used to optimise DAC processes in order to increase the lifetime of amine-functionalised adsorbents and lower the cost of DAC.

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Beyond forever sorbents: Capturing the impact of sorbent degradation in adsorption based direct air carbon capture and storage systems

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Current scenarios from the Intergovernmental Panel on Climate Change (IPCC) indicate that achieving the 2 °C target will almost certainly depend on deploying negative emission technologies. A promising negative emission technology is Direct Air Carbon Capture and Storage (DACCS), which captures CO_2 directly from the atmosphere for permanent storage, offering a potential solution to mitigate climate change.

The performance of sorption-based DACCS processes is greatly influenced by the considered sorbent. Amine-functionalized solid sorbents can be more energy-efficient than traditional liquid-based sorbents. Despite their advantages, solid sorbents still require significant energy input and suffer from degradation over time, leading to reduced performance and efficiency. Degradation can occur through multiple pathways, including O_2- and CO_2-induced amine deactivation. In both cases, moisture can prevent or accelerate degradation, depending on the sorbent configuration. Thermal exposure can further result in amine volatilization and promote side reactions such as bond cleavage, cross-linking, and disproportionation. Current assessments often oversimplify the degradation of sorbents by assuming fixed replacement intervals, overlooking the gradual decline in performance during operation. However, sorbent degradation and the cyclic stability of sorbents have been identified as a key factor for DACCS process costs[1].

Within this work, we address this gap by integrating oxidative degradation into an existing dynamic DACCS model developed at our institute and by explicitly accounting for the environmental and economic impacts of sorbent replacement. The model is parameterized for Lewatit VP OC 1065, a commercially available polymeric resin functionalized with primary amines and representative of sorbents used in recent DACCS plants. The extended model enables a quantitative assessment of the oxidative degradation of Lewatit VP OC 1065 in the DACCS process over a plant lifetime of 20 years, revealing a significant underestimation of the cost of carbon removal. The extended model also enables the identification of optimal sorbent replacement intervals, which can mitigate the increased costs of carbon removal.

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Estimation of heat and mass transfer during desorption for direct air capture using the infrared-large-temperature-jump method

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Dynamic process models are widely used for the optimization and design of adsorption-based processes. The capability of such models strongly depends on an accurate description of heat and mass transfer during ad- and desorption. In the field of thermal engineering adsorption applications, the infrared large temperature jump (IR-LTJ) method has been established as a reliable means for determining heat and mass transfer [1-3]. This method allows the identification of independent heat and mass transfer coefficients by using a dynamic model of the experiment to estimate effective coefficients from the IR-LTJ experiments.

So far, the application of the IR-LTJ method has been limited to thermally driven adsorption processes such as adsorption chillers. However, beyond thermal utilization processes, heat and mass transfer during adsorption–desorption cycles are also central to thermally driven separation technologies such as adsorption-based direct air carbon capture (DAC). In DAC processes, the desorption step is of particular importance, as it governs productivity and energy demand. Nevertheless, desorption kinetics are often described using simplified assumptions or inferred indirectly from adsorption data, as experimental methods enabling their direct determination under process-relevant conditions are lacking. Consequently, model parameters are frequently extrapolated or assumed, which limits the predictive accuracy of dynamic process models.

To address this limitation, the IR-LTJ method [3] is applied in this work to estimate desorption kinetics for DAC applications. Since desorption in temperature–vacuum swing adsorption-based DAC processes is driven by rapid temperature changes, the IR-LTJ method inherently reproduces the relevant transient thermal conditions. As a result, desorption kinetics can be estimated under process-relevant operating conditions. The proposed approach is used to determine desorption kinetics of different sorbents suitable for DAC processes under varying operating conditions. Experiments are conducted in both water vapor and carbon dioxide atmospheres, providing a consistent experimental framework for the characterization of sorbent regeneration behavior in DAC processes.

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PSA-PINN: An Integrated Platform for the Collaborative Design, Optimization and Control of Pressure Swing Adsorption Processes and Adsorbents

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Global warming is a pressing challenge. As the primary greenhouse gas, CO_2 has an atmospheric concentration of 420 ppm, making the development and deployment of carbon capture, utilization and storage (CCUS) technologies imperative. Industrial flue gases contain only 10%–20% CO_2, making post-combustion carbon capture the costliest link in the CCUS chain. Pressure swing adsorption (PSA) is the core carbon capture technology for this scenario, and its material selection, process design, optimization and control directly govern the comprehensive performance and energy efficiency of carbon capture.

However, conventional PSA simulation software (e.g., Aspen Adsorption, gPROMS) has two critical limitations. First, it disconnects the full lifecycle of PSA research and deployment. It cannot achieve integrated, streamlined collaboration among material screening, process modelling, optimization and control. Second, it only relies on physics-driven models based on partial differential equations (PDEs). This method has low computational efficiency and cannot support large-scale parameter exploration or real-time control.

To address these two issues, this study proposes the PSA-PINN platform. It is a physics-data dual-driven tool designed for full-lifecycle research and deployment of CO_2/N_2 separation PSA processes. This platform breaks the functional barriers of traditional software. It covers the full workflow, including material screening, process design, simulation, optimization, parameter sensitivity analysis, and control. At its core, a 1D non-isothermal PDE physics model guarantees accurate physical calculations. The platform embeds a physics-informed neural network (PINN) surrogate model for second-level fast prediction, forming a balanced framework that achieves both precision and efficiency. The platform also integrates a parameter inversion function to efficiently solve PSA inverse problems. It supports adsorbent screening using different PSA cycles, enabling rapid identification of optimal adsorbents for specific process performance requirement scenarios.

PSA-PINN effectively overcomes the bottlenecks of traditional physics-driven software (low efficiency, slow computation, single function) and pure data-driven models (poor physical interpretability), providing a high-efficiency platform for the deployment of PSA processes in post-combustion carbon capture.

Keywords

PSA, PINN, CO_2 capture, full-lifecycle, parameter inversion

A decoupled DR-PSA process for upgrading low-quality natural gas using optimized ETS-4

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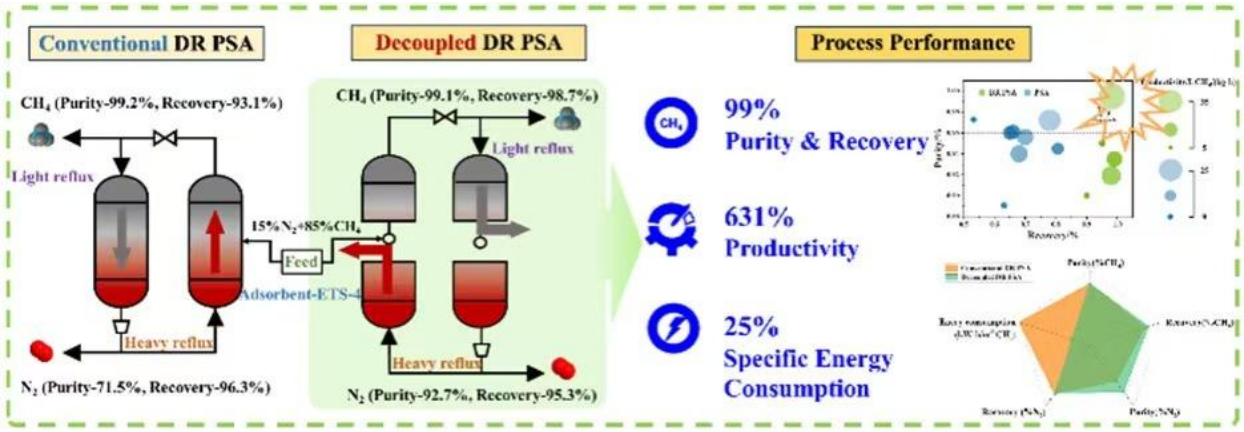
The separation of methane and nitrogen is essential for the upgrading of low-quality natural gas, and its efficiency depends heavily on the selection and preparation of suitable adsorbent materials along with advanced process configurations. We proposed a decoupled DR-PSA process, employing N_2-selective ETS-4 as the adsorbent. The ETS-4 material is synthesized via a seeding method to enhance crystallinity and phase purity. The pore aperture size of ETS-4 can be precisely controlled, enabling selective access for smaller nitrogen molecules while restricting methane diffusion. The process features a mid-feed configuration that divides the column into two functionally distinct zones: an upper stripping section and a lower rectifying section. The two zones operate with decoupled mass transfer behaviors and minimal mutual interference.

By incorporating N_2-selective ETS-4 into the integrated DR-PSA configuration, the redesigned system demonstrated superior separation characteristics when contrasted with traditional process. The N_2 purity was significantly improved from 71.46 to 91.30%, coupled with a CH_4 recovery rate of 98%. Furthermore, the adsorbent productivity of the original process was also markedly enhanced, reaching 30.70 NL CH_4/(kg·h), more than seven times the value achieved under the conventional process (4.48 NL CH_4/(kg·h)).



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Beyond Vycor Glass – New Reference Materials for Adsorption Experiments

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Porous Vycor glasses have been used for decades in applications like catalysis, adsorption or chromatography, due to their chemical inertness and thermal stability as well as their defined pore structure.[1] With the discontinuation of their industrial production, there is an increasing demand for alternative materials. Therefore, we investigated the suitability of porous potassium borosilicate (KBS) glasses as Vycor replacement in the context of adsorption behavior. These alternative Materials require an isodiametric, interconnected pore system with high tortuosity, which enables uniform flow and efficient mass transport processes, as seen in Vycor type glasses. By melting and leaching a borate rich KBS glass (50/43/7 mol-% $SiO_2/B_2O_3/K_2O$) we were able to mimic the pore diameter, average connectivity and tortuosity of a Vycor system (72.5/20.5/7 mol-% $SiO_2/B_2O_3/Na_2O$).[2] A key advantage of the KBS-materials is the ability to tailor the pore volume (V_p) through variation of the SiO_2/B_2O_3-ratio and in the processing parameters of phase separation and leaching. By that we tuned V_p from 0.64 to 0.43 $cm^3\ g^{-1}$, while maintaining pore diameter, connectivity and tortuosity. By further adjusting the processing parameters we intend to fully replicate the adsorption behavior of Vycor glass.

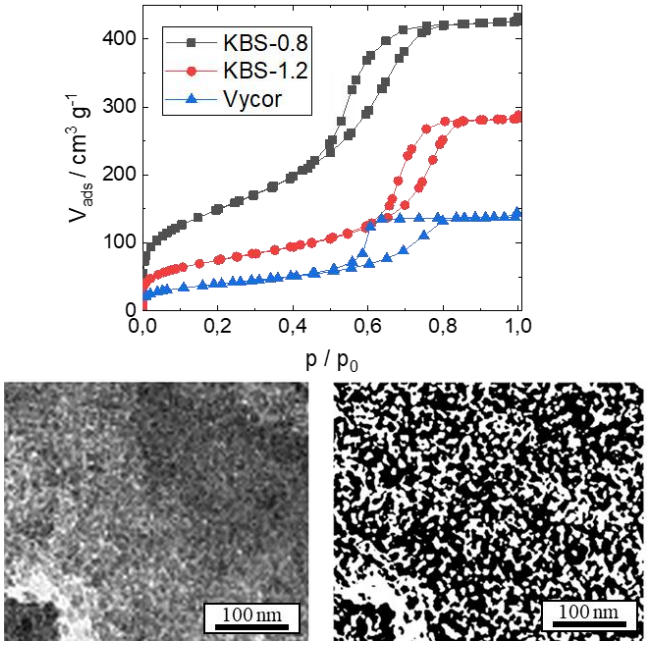

Fig. 1: Top: N_2-sorption isotherms of porous Vycor glass and KBS glasses, with SiO_2/B_2O_3-ratio of 0.8 and 1.2 respectively.
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Adsorption Kinetics Model of Hydrogen on Graphite

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A new kinetic equation for the adsorption and desorption of H_2 on graphite is derived based on the adsorption and desorption equilibrium rates obtained from the molecular dynamics [1]. These rates are proportional to the activity in the gas and the adsorbed phase and thus do not obey Langmuir kinetics although the isotherm is well model with a Langmuir type [2]. The new equation offers a new route for understanding experimental results. It is used to simulate the kinetics under different thermodynamic conditions, both isothermal and non-isothermal. The relation between the kinetics and the mass flow equation is discussed within the framework of the non-equilibrium thermodynamics of heterogeneous systems [3, 4]. Finally, expressions for the transport coefficients are proposed for both the transfer of mass and the coupling between the mass and heat fluxes.

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Kinetics of CO_2 Adsorption and Deformation in Microporous Carbon

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In this work[1], we studied the adsorption and deformation kinetics of microporous carbon materials using a model that combines the classical density functional theory with a diffusion mass transfer approach. We measured a series of adsorption uptakes and, in addition, used literature data[2] on strain uptake to verify our model. We showed that theoretical calculations accurately predict the uptake of CO_2 in the carbon molecular sieve (Shirasagi MSC CT-350). Our analysis accounts for the contributions of various mass-transfer resistances and thermal effects. We concluded that the surface-barrier mass-transfer resistance is the limiting factor in our measurements at higher pressures. Additionally, using a separate dataset, we demonstrated that our model can predict adsorption uptakes measured at the same temperature but at different pressure steps.

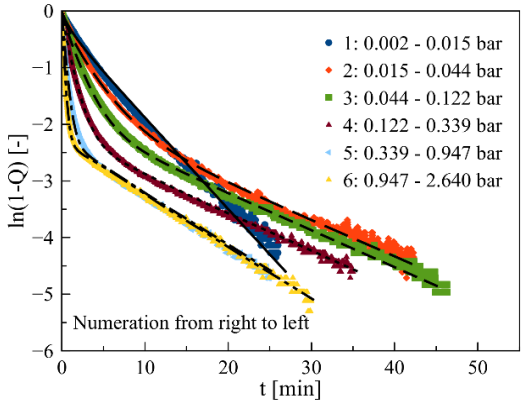

Figure 1: Kinetic uptakes for six measurements taken at 293 K. The symbols are the experimental data, and the lines are the results of our approach.

Finally, we examined the dependence of strain uptake on pore-size distributions, mass-transfer mechanisms, and temperature effects. The proposed theoretical approach can be used to interpret experimental data on adsorption and deformation. It may provide a basis for characterizing the kinetics of carbon materials using joint information on adsorption and deformation.

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Study of adsorption/desorption of carbon dioxide using microwave heating (MSA) on modified Metal Organic Frameworks (MOF's)/ Graphene Oxide (GO) composites

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Combating climate change requires drastic reductions in greenhouse gas emissions, with industrial and energy sectors contributing around 60% of anthropogenic CO_2 emissions (≈40 Gt CO_2-eq yr^{-1}). Among mitigation strategies, **adsorption-based carbon capture** has emerged as a promising option due to its low energy demand and operational flexibility. The main challenge lies in **regenerating the adsorbent**, traditionally achieved by pressure/vacuum (V/PSA) or temperature (TSA) swings. While TSA ensures more complete regeneration, it is slower and less productive because of generally inefficient heat transfer, either through gas heating (low heat capacity) or external heating (poor thermal conduction). To overcome these limitations, **microwave-assisted heating (Microwave Swing Adsorption, MSA)** is being explored. Unlike conventional heating, microwaves penetrate directly into materials, providing rapid, volumetric, and energy-efficient heating. This can drastically reduce desorption times and improve process efficiency. However, MSA introduces new challenges such as temperature control, heating uniformity, and compatibility of adsorbents with microwave energy. This study investigates the enhancement of microwave responsiveness by incorporating 5%wt of **graphene oxide (GO)** into MOFs.

CO_2 and N_2 adsorption isotherms were measured from 0–1 and 0–50 bar and 20–50 °C using a gravimetric setup. In parallel, a **custom MSA apparatus** was developed, featuring a 200 W microwave generator (2.4–2.5 GHz) and a borosilicate column equipped with a pyrometer and mass spectrometer. The study examined adsorption/desorption behavior for CALF-20, and MIL-120(Al), comparing samples with and without GO. While adding GO slightly reduced CO_2 uptake, it enabled significant heating under microwave radiation and much faster desorption. The desorption temperature influenced greatly the desorption peak while the flowrate influenced the tail. A preliminary energetic study showed promising results compared to other carbon capture processes with a capture energy below 550kWh/T CO_2. Finally, water adsorption was also found to **enhance microwave absorption** and, in some cases, CO_2 capacity (e.g., CALF-20 at <25 % RH), suggesting potential for efficient regeneration under humid conditions.

In conclusion, **GO-modified MOFs** enable microwave-based regeneration, reducing desorption time compared to classical TSA, with optimal purge flow and concentration minimizing energy use. This demonstrates the strong potential of MOF/GO composites for fast, energy-efficient CO_2 capture processes.

Textile Dye Desorption to Enable Activated Carbon Reuse

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In the chemical recycling of textile waste, the removal of dyes is crucial to ensure the quality of the recovered monomers and oligomers. Activated carbon (AC) is widely used for decolorization due to its large specific surface area, chemical stability and high adsorption capacity. In terms of a sustainable circular system, its regenerability is becoming increasingly important, as multiple use saves both resources and energy.

Current research shows that dye-loaded activated carbon can be regenerated using various physical and chemical processes. Thermal methods are effective, but often result in structural loss and high energy consumption (da Silva Santos et al., 2022). Alternatively, microwave and electrochemical processes are being investigated, which offer shorter cycle times and lower environmental impact (Durán-Jiménez et al., 2019; Zhou et al., 2019). Particular focus is being placed on chemical regeneration or desorption, in which dyes are dissolved from the pores of the activated carbon using suitable washing liquids, such as alcohol-water or pH-modified solutions (Lu, 2011). This form of desorption is considered a promising approach for reusing activated carbon multiple times and making the decolourisation processes in chemical textile recycling more ecologically and economically efficient.

Most studies on desorption originate from the field of water treatment. To date, there has been no direct transfer of the adsorption and desorption behaviour observed in water treatment to chemical recycling. This study examined the desorption of loaded activated carbon in the context of chemical recycling. Different activated carbons were used in the purification of a solution from the chemical recycling of polyester and specifically loaded with dyes. This was followed by systematic desorption tests. Nine washing solutions, differing in polarity, pH and water solubility, were systematically tested for desorption performance. In addition, cyclic adsorption and desorption tests were carried out with the activated carbon that had previously performed best in order to check its reusability and stability over several cycles of use.

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Confined Geometry Effects on the Supercritical Adsorption Behavior of Hydrogen

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In recent decades, growing concerns about global climate change and the increasing frequency of extreme natural disasters have led society to prioritize the search for low-polluting and renewable energy sources. As a result, hydrogen is emerging as a promising clean energy alternative.

However, the efficiency and safety of H_2 storage are challenging. Several methods for storing hydrogen fuel are currently being researched or are already in practice: compressed hydrogen, liquefied hydrogen, cryo-compressed hydrogen, metal hydrides, complex metal hydrides, liquid organic hydrogen carriers (LOHC), and physisorption-based storage in porous materials [1].

For physisorption-based hydrogen storage supercritical high-pressure adsorption is important, but there is still a lack of understanding of how key textural properties such as surface area and confinement (e.g., pore size/pore geometry) affect details of the shape of supercritical high-pressure adsorption isotherms. A key feature is that experimentally determined surface excess adsorption isotherms may exhibit a characteristic maximum at a certain pressure. For a given temperature and adsorptive/adsorbent system, the surface excess maximum (and the corresponding adsorbed amount) is related to the storage capacity of the adsorbent. In order to investigate the effect of confinement on the supercritical adsorption behaviors, in previous work [2] a systematic experimental study assessing the effect of pore size on the supercritical adsorption isotherms of pure fluids such as C_2H_4, CO_2, SF_6 had been conducted over a wider range of temperatures and pressures utilizing a series of mainly mesoporous model materials exhibiting well-defined pore size. A fundamental result of this work is a unique, fluid-independent correlation between the pressure of the surface excess maximum (at a given temperature) and the effect of confinement.

In this study, we expand our investigations from the mesopore range to the micropore range with the focus on supercritical hydrogen adsorption, i.e., exploring the effects of pore size, geometry, and pore-network characteristics on hydrogen adsorption behavior at 77 K. To achieve this, we employ selected metal-organic-framework materials, which have been characterized through a combination of argon adsorption at 87 K and dedicated non-local-density-functional theory (NLDFT) methods. Additionally, we perform complimentary grand canonical Monte Carlo (GCMC) simulations to to investigate the effect of confinement of supercritical hydrogen

adsorption on a molecular level. Our systematic study reveals significant structure-property relationships, enabling us to determine optimal operating conditions for hydrogen storage applications under specific thermodynamic conditions.

References

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From Powder to Pellet: Impact of Binders on the Structure, Functionality and Robustness of Carbon Nanofiber Molecular Sieves

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Carbon nanofibers (CNFs) have shown great promise as a molecular sieve due to their high surface area and tunable properties. However, handling CNFs in the form of powders or mats, as it is commonly done in small-scale research, poses significant challenges in packed columns, including dust formation, electrostatic charging, and low packing density, resulting in reduced adsorption efficiency and unfavorable process conditions. To address these issues, we propose pelletizing CNFs as a viable solution.

In this study, synthesis routes to create pelletized CNFs using different binder systems are explored. Two distinct approaches are investigated: (1) using polyacrylonitrile as a binder with dimethylformamide as the solvent, utilizing the same base chemicals used to produce the nanofibers by electrospinning, and (2) utilizing carboxymethylcellulose with water as the solvent as a more economic and sustainable approach. For both approaches, CNFs pellets with varying binder contents are produced.

The resulting pellets are characterized thoroughly. Structural information is obtained by argon and CO_2 adsorption measurements to evaluate the pore size distribution and BET surface area. Furthermore, mercury intrusion porosimetry for additional insights into the pore structure is performed. The applicability as a molecular sieve is tested by measuring the gravimetric and volumetric gas adsorption capacity, i.e. CO_2 capacity. Due to friction and strain in the packed bed of adsorbent pellets, the mechanical stability is evaluated as well, including compressive and abrasive strength.

By exploring various synthesis routes, as well as binder systems and contents, followed by a thorough characterization of the resulting pellets, this research offers comprehensive insights into how different binder systems affect the functionality as a molecular sieve, the mechanical properties and therefore the scalability of pelletized CNFs.

Comparative Physisorption Performance of MOR-Type Zeolites and KAUST-7 for Direct Air Capture under Humid Conditions

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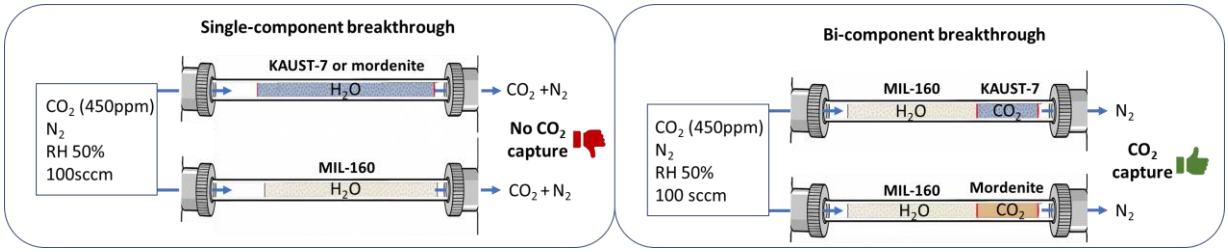
Achieving the European Union's 2050 climate neutrality goal requires transformative technologies capable of mitigating atmospheric CO_2 concentrations. Direct air capture (DAC) offers a promising pathway toward net-zero emissions and negative emission solutions, but its implementation faces the intrinsic challenge of capturing CO_2 at ultra-dilute concentrations (~420 ppm). While traditional chemisorbents such as amine-based systems exhibit strong CO_2 affinity, their high regeneration energy demands and limited stability constrain large-scale deployment. In contrast, recent progress in physical adsorbents, particularly zeolites and metal-organic frameworks (MOFs) has opened new avenues for energy-efficient DAC.

This study investigates the physisorption performance of MOR-type zeolites and the fluorinated MOF KAUST-7 (NbOFFIVE-1-Ni) under DAC-relevant conditions. MOR-type zeolites demonstrate high CO_2 uptake (1.15 mmol g^{-1} at 400 ppm, 30 °C), fast kinetics, and excellent selectivity driven by Na^+ cation sites within 8-membered ring side pockets, maintaining robust performance even at low temperatures. KAUST-7 achieves benchmark CO_2 uptakes (1.3 mmol g^{-1}, 51.4 cm^3 (STP) cm^{-3}) through engineered fluorinated channels that enhance CO_2 framework interactions, coupled with hydrolytic stability and mild regeneration requirements. However, both materials exhibit significant sensitivity to humidity. To address this, the study explores coupling these CO_2-selective adsorbents with a water-harvesting MOF (MIL-160) capable of pre-capturing atmospheric water.

This approach may simultaneously enhance DAC efficiency and enable water collection in arid environments. The comparative evaluation of these advanced physisorbents highlights their adsorption mechanisms, trade-offs, and scalability potential. The findings provide critical insights into the rational design of next-generation materials for sustainable, large-scale DAC technologies.



Physically Consistent Analysis of Water Adsorption Kinetics in MOF-303 under Adsorption Cooling Conditions

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Accurate characterization of adsorption kinetics is essential for the reliable design and modeling of different application like adsorption cooling systems, yet kinetic parameters reported for metal–organic frameworks are often model-dependent and difficult to compare. In this study, the water vapor adsorption kinetics of MOF-303 were systematically investigated under vacuum conditions representative of adsorption cooling operation using dynamic vapor sorption (DVS). Uptake kinetics were measured over a wide range of relative humidities (2–90%) at 25 °C and analyzed using three kinetic models: Fickian diffusion (FD), the classical linear driving force (LDF) model, and a time-adapted LDF (TA-LDF) formulation. To enable physically meaningful comparison, all kinetic parameters were mapped to an equivalent diffusion timescale expressed as D/R^2, using established spherical-particle equivalence relations. The results reveal that MOF-303 exhibits diffusion timescales typically, on average, seven times faster than silica gel across the different humidity ranges, confirming its suitability for fast-cycling adsorption cooling applications. However, a pronounced minimum in diffusion rate is observed near 10–15% relative humidity, coinciding with the step in the MOF-303 adsorption isotherm, highlighting the dominant role of thermodynamic effects and darken effect on transport kinetics. Among the evaluated models, TA-LDF provides the highest fitting accuracy ($R^2 > 0.93$ across all humidities) by capturing both early-time and near-equilibrium uptake behavior. Nevertheless, when interpreted in terms of equivalent diffusion timescales, classical LDF shows closer agreement with FD than TA-LDF, indicating that improved curve-fitting accuracy does not necessarily imply physical consistency. These findings demonstrate that FD remains the most physically representative model, while LDF offers a robust and computationally efficient approximation for system-level and CFD-based simulations. The study provides a unified framework for interpreting adsorption kinetics in MOFs and supports the use of MOF-303 as a high-performance adsorbent for adsorption cooling systems.