MSc in Chemistry and Materials engineering
Master Thesis subjects 2021-2022 proposed by Prof. Wim De Malssche - μFlow/Chemical Engineering Department (CHIS).

1. Overcoming diffusion limitations in liquid chromatography chips using electroosmotic acoustic flows

Summary: During the past 10 years, our group has eliminated 2 of 3 dispersion sources by replacing the disorderly packing of classic chromatographic columns with organized radial stretched structures, manufactured by in-house developed etching and lithography processes. To further increase the performance, the mass transport mechanism should be altered. The aim is to achieve faster transport rate than that of for pure diffusion, a current limitation in laminar flow systems. In this master thesis electro-osmotic flows will be used to enhance mass transport. Planned activities include characterization of the chips, simulation and modeling of electric and liquid flows and experimental characterization of dispersion behavior with an in-house-designed set-up.

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Advisor: Eiko Westerbeek (Eiko.Westerbeek@vub.be)

2. Overcoming diffusion limitations in liquid chromatography chips using acoustic flows (topic 2)

Summary: To further increase the performance of chromatographic separation devices, the mass transport mechanism should be altered. This requires a faster transport rate than that occurring at the situation of pure diffusion, a current limitation in laminar flow systems. In this master thesis either acoustic flows will be used to enhance mass transport. Planned activities include characterization of chips, simulation and modeling of acoustic and liquid flows and experimental characterization of dispersion behavior with an in-house-designed set-up.

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Advisor: Pierre Gelin (Pierre.Gelin@vub.be)

3. Single image parasite quantification separation device (room for 2 students)

Summary: According to World Health Organization (WHO), more than 1.5 billion people, or 24% of the world’s population, are infected with soil-transmitted helminths (STH) worldwide. In the present project, a recently developed device based on centrifugal forces and buoyancy for the quantification of parasites (worm eggs) present in stool will be fluidically characterized, modeled and improved. This device has shown to be effective in controlled lab conditions, but also requires integrated and automated sample preparation functionalities. Well established techniques in the group based on acoustic flows and flow focusing will be explored to facilitate this critical purification step. This device will be used for new field tests on close collaboration with 2 local academic partners in Tanzania to detect soil transmitted helminths in humans and animals and the results will be compared to theoretical predictions.

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MSc in Chemistry and Materials engineering
Master Thesis subjects 2021-2022 proposed by Prof. Sebastiaan Eeltink
Department of Chemical Engineering (CHIS) (www.eeltinklab.com)

1. Developing microreactor technology for protein digestion and implementation in an on-line digestion nanoLC-MS/MS workflow

Summary: Mass spectrometry (MS) is an important method for the accurate mass determination and characterization of the amino acid composition of proteins. During the MSc project you will learn how to set-up and conduct nano-liquid chromatography and how to realize good protein i.d.’s with mass-spec technology (spectra interpretation, use of data bases). Different smart digestion procedures will be developed and a novel microreactor for on-line enzymatic digestion will be developed to advance protein identification scores. The latter involves polymerization of a macroporous monolith in-situ in capillaries, tuning the flow-through pore size, functionalization of surfaces with reactive molecules that will cleave proteins. This immobilized enzyme reactor will be incorporated in an LC-MS workflow and efficacy testing involves investigating carryover, recovery, protein i.d. scores.

Contact: Supervisor: Sebastiaan Eeltink (seeltink@vub.be)
Advisor: Daniel Meston (daniel.meston@vub.be)

1. Chip prototyping using 3D printing technology

Summary: Downsizing liquid chromatography allows the incorporation of different miniaturized components (for example, injection loops, stationary phases, valves, detectors, etcetera) into a single modular microfluidic platform. This project aims at developing a microfluidic chip for 1D-LC using 3D printing technology. 3D printing will be applied to create innovative devices integrating injection, a micromixer and the separation channel. Afterwards a polymer monolith will be synthesized nanoLC separation will be conducted and separations will be performed.

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3. Design and engineering of polymer monolithic stationary phases in very narrow capillary columns for ultra-low-flow nano-HPLC-nanoESI-MS

Summary: The goal is to establish a radical novel column technology, i.e., nanostructured polymer monoliths in 15-30 µm i.d. capillary HPLC columns that yields high resolving power but can be operated at ultra-low-flow conditions. Column development involves polymerization of a polymer precursors solution in a capillary and optimizing of the ratio’s monomers, porogen composition, and the amount of initiator. Scanning electron microscopy will be performed to assess the pore structure. When operating at sub nanoliter flow rates the ionization efficiency (in the interface to the mass spectrometer) is greatly enhanced and much higher MS sensitivity will be obtained. This will be tested in a nanoLC-nanoESI-MS set-up. Conditions will be investigated and optimized and finally separations of peptides and proteins will be pursued yielding unparalleled separation efficiency and sensitivity.

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MSc in Chemistry and Materials engineering
Master Thesis subjects 2021-2022 proposed by Prof. Ken Broeckhoven - Chemical Engineering Department (CHIS).

General:
Recent years have seen a renewed interest in supercritical fluids as a medium for analytical and preparative scale separations (e.g. chiral separation, cannabis analysis and extraction). Supercritical fluid chromatography (SFC) offers unique advantages compared to conventional liquid chromatography (LC), such as lower viscosity, less organic solvent consumption and a high volatility of the eluent, which enables easy solvent removal in preparative applications. Supercritical CO\textsubscript{2} is used as solvent in SFC, replacing the use of large amount of organic solvents and minimizing the processing of solvent waste, making this technique a green alternative to current separation systems. Although SFC was already proposed fifty years ago, fundamental understanding of the parameters determining the performance is still lacking. The main difficulty is the high compressibility of the mobile phase and its resulting effects on phase equilibria, mobile phase properties (viscosity, density), decompression cooling etc.

1. Investigating diffusion in supercritical fluid chromatography (SFC)
Summary: Although SFC has been around for several decades, the difficulty of handling the mobile phase (elevated pressures > 100 bar) has limited the investigation into the physicochemical properties of the system. Although a larger amount of data is available for e.g. diffusion coefficients ($D_{mol}$) in pure supercritical CO\textsubscript{2} (sCO\textsubscript{2}), SFC employs mixtures of sCO\textsubscript{2} with a polar co-solvent, often methanol or other small alcohols such as ethanol or isopropanol. It was found that the presence of only small amount of modifier (5%) has a very large effect on $D_{mol}$, reducing it by a factor of 50% or more, strongly affecting the separation conditions and performance. The effect of this modifier also depends strongly on the properties of the analyte (polarity, H-bonding capacity). The goal of this study is to further develop and optimize an experimental set-up to measure molecular and effective bed diffusion in SFC-conditions a and to investigate the effect of different parameters (T, P, co-solvent, additives...).

Contact: Ken Broeckhoven, ken.broeckhoven@vub.be, Advisor: Timothy Januarius

2. Experimental and modelling study of extra-column dispersion SFC and LC devices
Summary: The advances in column technology over the past decades have allowed significant improvements in the separation performance and speed that is achievable for analytical scale separation systems. Further improvements are currently however limited by the dispersion processes occurring outside the separation column, i.e. in the instrumental fluidic path from injector to detector. Although approximate models are available for these effects, the fine details of these processes are still unknown, limiting technological innovations to improve current and future chromatographic systems. In addition, in the emerging field of multidimensional separations (e.g. 2D-LC), these aspects have not yet been investigated and significant improvements can still be achieved. The thesis project therefore aims at gaining a better understanding of these contributions, using an experimental approach, supplemented with numerical simulations to model the behavior.

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MSc in Chemistry and Materials engineering

Master Thesis subjects 2021-2022 proposed by Prof. Gert Desmet - Chemical Engineering Department (CHIS).

1. Simulation and measurement of flow and mass transfer processes in novel packed bed column systems

Summary: Liquid chromatography is a separation technique that can separate mixtures of a quasi unlimited complexity in all its individual components. The Chemical Engineering department of the VUB is one of the world's leading groups in the modelling and development of novel chromatographic separation systems. In the planned thesis project proposal, the student will first experimentally characterize one or more new chromatographic column systems that are currently under development in the industry. Secondly, he or she should build a mathematical model describing the performance of the columns under evaluation. The model should subsequently be solved using computational fluid dynamics (CFD). In this Master thesis, the student will learn to cooperate with industry at a high international R&D level, and will be trained in the basic skills of computational fluid dynamics.

Contact: Prof. Gert Desmet (VUB, Room 5G214 gedesmet@vub.be, tel: 02/629.32.51) & Prof. Ken Broeckhoven (VUB, Room 5G205, ken.broeckhoven@vub.be, tel: 02/629.37.81)

2. Chip-based Chromatography: use of micromachining technology to produce perfectly ordered chromatographic columns in silicon (1 to 2 students)

Summary: Amongst all unit operations, liquid chromatography is undoubtedly the most sensitive to the microscopic structure of the device, in which the operation is performed. More specifically, the separation efficiency that can be achieved in liquid chromatography could be drastically improved if it would be possible to produce columns that are perfectly ordered. Together with its spin-off company, Pharmafluidics, the Chemical Engineering department of the VUB is developing such a column using advanced micromachining techniques (i.e., the same techniques as those used in the clean rooms of the micro-electronics industry). If desired, this Master thesis can be combined with an Erasmus exchange to the MESA+ Institute for Nano-technology of the University of Twente (The Netherlands). The planned work may involve computer-aided design, fabrication and testing of the columns. This separation technique can separate mixtures of a quasi unlimited complexity in all its individual components. The Chemical Engineering department of the VUB is one of the world’s leading groups in the modelling and development of novel chromatographic separation systems.

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3. Chip-based Experimental study and modelling of the radial dispersion in packed bed columns for liquid chromatography

Summary: Liquid chromatography is most probably the chemical process whose performance is most sensitive to the micro- and macroscopic shape of the column packing. This sensitivity manifests itself as the axial dispersion or band broadening, which directly determines the separation efficiency of the column. This axial dispersion originates from the many sources of radial differences in axial velocity that inevitably exist in a column. Fortunately, these differences in axial velocity are countered by the radial dispersion process, as this helps to average out the differences in axial velocity. Since the value of the radial dispersion coefficient (Drad) in chromatographic columns is strangely enough ill-known and poorly studied, the present project aims at making a comprehensive study of the dependency of Drad on the species retention equilibrium, the liquid velocity, and the diffusion coefficient in- and outside the particles. Data will be collected on real columns using a simple yet effective measurement principle, as well as via computational fluid dynamics, which offer the advantage to investigate the phenomenon under exactly known geometrical and physicochemical conditions, as well as to impose some "exaggerated" conditions that cannot be realized in practice but provide a stringent test for the improved mathematical Drad-models that will be established. A fully parallel study will be undertaken to also establish improved models for the radial heat transfer coefficient.

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4. Nano-Precision Construction Engineering at the 1-Micron Scale: New Hierarchical Materials and New Applications

Summary: Being able to position micron-sized functional particles with nano-precision in well-defined 3D networks is a feat that has not been realized before and is nearly unexplored territory in terms of dedicated fabrication and engineering. Finding a method that can achieve this would open the road to produce materials with new, unexplored possibilities in chemistry (e.g., chromatography, catalysis) or physics (e.g., photonics). In this PhD project, it is planned to investigate the possibilities and challenges of a number of potential strategies that would enable large-scale construction engineering with micro-scale building blocks (uniform micron-sized spheres). The project will start with a design phase wherein a number of strategies targeting simple aims (positioning and fixing one microsphere, a single layer of 10x10 microspheres,…) will be devised. The proposed structures will subsequently be fabricated using state-of-the-art micromachining technology (photolithographic etching) and will then be used in a dedicated nano-precision displacement set-up. In later stage, the set-up will be equipped with a picodroplet dispenser or a two-photon laser to provide to dispatch nanopatches of photosensitive glue to fix and position the micro-particles. Visual inspection of the constructions will be carried out using SEM.

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MSc in Chemistry and Materials engineering
Master Thesis subjects 2021-2022 proposed by Prof. Joeri Denayer & Prof. Tom Van Assche

1. Separation of light olefins and paraffins

Summary: Olefins such as ethene and propene are massively produced and used for the production of plastics. Before their use in the polymerisation reactor, olefins have to be separated from the paraffins which are also obtained in the production process. This separation between light olefins and paraffins of the same carbon number is industrially done via cryogenic distillation, which is extremely energy intensive given the small difference in boiling points. Olefin purification accounts for 0.3% of the global energy use. Any improvement in efficiency will have a large impact on energy consumption and global CO₂-emissions. In this thesis, we will focus on the use of mixed matrix membranes for the separation of light olefins and paraffins. Mixed matrix membranes consist of a porous polymer containing a (micro-)porous solid that enhances the separation. The role of the porous solid in the separation will be investigated. Transport and adsorption of ethane/ethene and propane/propane mixtures will be studied experimentally, by performing breakthrough and pressure decay experiments. A possible extension of the project includes the modelling of the separation process.

Contact: Joeri Denayer (joeri.denayer@vub.be)

2. Novel nanomaterials for CO₂ capture and utilization: multicomponent adsorption equilibria

Summary: This thesis topic fits in the Nano-CCU research project, aiming at the development of high-throughput electrolyzers for CO₂ capture and electrocatalytic conversion directly from the gas phase for deployment at point sources and eventually directly from air. The project aims at the development of novel gas-diffusion-electrode architectures to enhance CO₂ capture and conversion efficiency. Novel solid CO₂ sorbent materials (e.g. Metal Organic Frameworks, MOFs) for operation in low CO₂ concentration gas atmospheres will be developed by one of the research partners. In this thesis, the adsorption and transport/diffusion properties of these materials will be studied. Real flue gases contain, beside N₂ and CO₂, several impurities such as SO₂, NOₓ and water. The competition between these compounds is largely determining their global performance. Therefore, this thesis aims at the development of an efficient method to study competitive adsorption and diffusion of the compounds present in flue gas. The method will then be applied to a number of promising Metal Organic Frameworks which are optimized for optimal selectivity, to obtain a better understanding of the relationship between the properties of the MOFs and the performance in the CO₂ capture process.

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3. Synthesis of structured adsorbents for CO₂ capture

Summary: Major global changes will be required to reach the goal of carbon neutrality by 2050. CO₂ is by far the most contributing gas to the greenhouse effect. Therefore, carbon capture and storage (and utilization) processes are seen as a potential for climate change mitigation. All of these include a CO₂ capture step. Adsorption technologies using porous solids in cyclic processes are known to be more energy-efficient than conventional absorption technologies. The adsorbent used in this process is essential and plays a role on multiple levels: capacity, selectivity, mass transfer characteristics, ease of desorption,... Next to the properties of the adsorbent itself, also the shape and size is essential. Conventional packed beds, filled with beads or granules, are associated with some important drawbacks. An alternative approach focuses on creating structured adsorbents with specific geometries, wherein the thin wall dimensions promise rapid mass and heat transport while keeping the pressure drop low. Synthesis of these structures is a challenge, but crucial to be able to tune materials for specific purposes. In this thesis different materials will be synthesized and characterised in the scope of CO₂ capture.

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4. Hierarchically porous metal organic frameworks (MOFs)-sponge for adsorptive gas separation

Summary:
Separation processes are considered as the backbone of the world’s manufacturing industry. These processes are used for essential chores such as removal of contaminants from raw materials and recovery and purification of primary products. However, when adsorbent materials are used in the form of beads, pellets or granules, efficient gas separation processes operating at high throughput are compromised. System performance reduces rapidly due to high pressure drop associated with gas flow through a packed bed and mass transfer limitations related to gas diffusion into or out of the beads. Therefore, with the global community’s pursuit for a more energy- and carbon-efficient economy, development of efficient structured adsorbent is necessary.

Metal Organic Framework (MOFs) are a new class of promising adsorbents which present high surface area, tailored topologies, tuneable functional groups and good mechanical and thermal properties. Typically, MOFs are prepared as powders but in the view for more efficient and faster adsorptive gas separations, a MOF based hierarchically porous structured adsorbent is pursued. In our group, so far we have successfully achieved coatings of different MOFs such as ZIF-8, ZIP-67 onto different metallic and non-metallic substrates. Thus, in this thesis subject will be development of MOF-sponge composite for separations of different gas mixtures.

Work will include:
- In-situ growth and/or deposition of different MOFs (MOF-74, CuBTC) onto a porous substrate such as melamine formaldehyde sponge
- Investigating adsorptive gas separation via dynamic breakthrough experiments.

Contact: Joeri Denayer (joeri.denayer@vub.be), Ravi Sharma (ravi.sharma@vub.be)

5. Theoretical study of carbon capture via an electrified adsorptive carbon capture process

Summary: Since by 2050 Europe want to be carbon neutral, there must be an electrified carbon capture method to capture the CO$_2$ from the sectors in which the CO$_2$ is a product of a chemical reaction or where the electrification has not been done (possible). Post-combustion carbon capture process is one of the promising methods to efficiently capture CO$_2$. Prof. Denayer’s group focusses on developing and studying electrified adsorptive processes for carbon capture based on the use of electrified heating methods such as resistive heating, induction heating, and microwave heating for the sorbent regeneration. The well-equipped research lab contains all possible tools for the in-depth study of adsorption, separation processes, and recently decent set of experimental data were measured. In the next step, these processes can be more investigated via a simulator software to study the effect of different cycle steps and operating conditions on the performance of such a process. The developed models can be used for (i) identification of the most efficient cycle steps, (ii) investigation on operating conditions (iii) and a theoretical study of the influence of adsorbent type and size on separation efficiency. Models can be validated using experimental data previously generated at CHIS, however the performance of some extra experiments can also be envisaged.

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6. CO$_2$ capture via Temperature Swing Adsorption (TSA) using an innovative regeneration step

Summary: The increasing concentration of CO$_2$ (a predominant greenhouse gas) in the earth’s atmosphere via anthropogenic activities is causing dramatic climate changes. As a consequence, a significant reduction in its emission is a critical task that must be addressed. In order to limit the effects of impending climate crisis, there is a dire need for efficient CO$_2$ capture technologies. Prof. Denayer’s group focusses on developing and studying sophisticated adsorptive processes based on the use of alternative (resistive, inductive, and microwave) heating and regeneration methods for CO$_2$ capture. The well-equipped research lab contains all possible tools for the in-depth study of adsorption, separation processes. During this thesis, a selection of promising porous adsorbent materials (various shapes and sizes) will be made available (commercial and/or in-house synthesized/modified) that can be efficiently heated using alternative methods (microwaves and/or induction). Using lab scale proof of concept setups, cyclic TSA experiments (combining the adsorption and desorption/regeneration) steps will be conducted with focus on several aspects of the process such as, i) effect of heating on process efficiency (heating rate, cyclic capacity, cycle time, CO$_2$ recovery etc.), ii) CO$_2$ desorption kinetics, energy consumption, and CO$_2$ adsorption capacity as function of process parameters.

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7. Mathematical Modelling and Simulation of Adsorption/Membrane Hybrid process for CO₂ Removal from Biogas

Summary:
Adsorption processes have demonstrated attractive results in terms of process performance and are regarded as viable candidates for biogas upgrading. Proper design of an efficient adsorption process is best achievable through development of robust theoretical models that can describe well the governing transport phenomena and dynamics of the process. While development of such mathematical models in not trivial, such models encompassing equilibrium and kinetic parameters would provide fantastic opportunities for predictive analysis and simulation of the process performance without need for expensive experimentations and time consumption. Thus, mathematical models can be a exploited as useful tools for exploring the effect of various operational parameters and for process optimizations. Like many processes, mathematical modeling and simulation of adsorption processes has attracted many attentions. This is especially true in the case of biogas upgrading. Due to the attractive features and ever-growing importance of biogas upgrading, modeling and simulation studies have been extended and applied to the various aspects of the processes dealing with biogas upgrading. These efforts have made great contributions to the progress of the process performance in addition to providing valuable understanding about the various aspects of this process.

This project relies primarily on mathematical modeling and simulation of the adsorption process based on a set of partial differential equations (PDEs) representing materials, momentum and energy balances to be solved using corresponding boundary conditions. Several simplifications and assumptions will be applied to facilitate the simulation studies. In addition, the effect of various parameters defined in the models will be obtained. In contrast to the prior works in the literature, a novel aspect of this project would be to extend the mathematical models to the interface of adsorption-membrane hybrid process. The findings in this project would provide insights to the researchers about the best configurations of this hybrid process for biogas upgrading and applications alike.

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8. Design and Development of Structured Adsorbents from polymeric precursors for gas separation

Summary: Separation and purification of gases constitutes one of the major industrial processes with wide and attractive applications particularly in the fields of Energy and Environment. Majority of the separation technologies rely on the concurrent advancements in both process design as well as materials engineering. This is especially true in the case of adsorption separation which its efficiency is largely governed by the type and characteristics of the adsorbents employed. Despite the progress made over the years led to the emergence of diverse ranges of adsorbents, yet an attractive root is to achieve high performance adsorbents is through engineering of polymeric based precursors and turning them to adsorbents. One of the main features of this approach is that it enables selective design and controlled modification of the process to achieve adsorbents with desirable characteristics for targeted species.

The steps in this project include exploring the properties and identification of appropriate polymeric materials that can be turned into carbon molecular sieves. Next, precursors in the form of thin films will be fabricated from the ideal candidates through casting. The important step in conversion of the precursors into adsorbents is the pyrolysis process and the goal is to optimize the parameters that could yield best adsorbent morphology and pore structures. Finally, instrumental techniques and tests will be used for characterization of the produced adsorbents in terms of physico-chemical properties, sorption isotherms and separation efficiency for targeted gas pairs.

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9. Process optimization and integration options for new industrial processes

**Summary:**
Individual process facilities typically consist of several unit operations having individual specifications/requirements on feed or product streams and utilities. Furthermore, such facilities are often clustered in industrial zones for mutual benefits. With upcoming new technologies, the possibility for optimization and integration needs to be revisited from a macroscopic point of view for decision making, well beyond the view of the process engineer. In this master thesis, you will be at the unique interface of chemical engineering and strategic governance.

In a new collaboration between the department of chemical engineering (VUB) and the Brussels School of Governance (VUB), you are to establish first macroscopic models for a preselected list of facilities/clusters to estimate their mass and energy (utility) balances and identify integration opportunities. These macroscopic models may be built using the Matlab/Excel package. Critical data absences and/or interesting cases are studied and refined using the Aspen Plus process simulator. We are looking for a unique candidate with interest in chemical engineering, modelling and policy making. Prior experience with Aspen Plus is not a prerequisite but certainly a plus.

**Contact:** Tom Van Assche (tom.van.assche@vub.be), Tomas Wyns (tomas.wyns@vub.be)

10. Technology evaluation matrix for carbon capture and utilization (CCU)

**Summary:** Carbon capture and utilization aims at converting contaminated and low concentrated CO₂ streams to concentrated streams meeting the EU and local legislative standards and commercial/technical specifications. Separation technologies have their own advantages and disadvantages, depending on the stream types. In this master thesis, you will be at the unique interface of chemical engineering and strategic governance.

In a new collaboration between the department of chemical engineering (VUB) and the Brussels School of Governance (VUB), you are to establish an evaluation matrix for the CCU technologies for various streams to identify suitable processes (low or high TRL). To this purpose, a techno-economical analysis and process modelling can also be used. We are looking for a unique candidate with interest in chemical engineering and policy making.

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11. Investigation of small-pore zeolites with tuneable Al-distribution

**Summary:** Zeolites are microporous, aluminosilicate materials with widespread use in petrochemical, pharmaceutical and agro-food industry. The confined spaces of zeolite allow for adsorption of molecules, and can be exploited to separate mixtures or convert molecules (catalysis). Examples are CO₂/CH₄ separations, (bio)alcohol upgrading and cracking of hydrocarbons. Small-pore zeolites are of great interest as the molecular confinement increases as the zeolites pore size goes down, sometimes leading to unusual phenomena in adsorption. The location of the aluminum in the structure of zeolites can play a role in its acidity and accessibility, and thus ultimately its activity. Recent advances in zeolite synthesis offer the potential of creating small-pore zeolites with tunable aluminum(Al)-distribution. The aim of this thesis is to determine the impact of Al-distribution in small-pore zeolites on their adsorption and separation behavior. The behavior will be studied using low- and high-coverage experimental techniques.

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