Master Thesis subjects 2022-2023 proposed by

Department of Chemical Engineering VUB (CHIS)

Topic 1: Computational Fluid Dynamics-aided Design of Microfluidic Chip-Detector Interfaces

Summary:

In this topic you will, after a thorough training on a commercial package for fluid simulations (Ansys Fluent=the international standard in flow simulations), collaborate with our spin-off company to design a new method to couple their high-tech separation chip to the latest mass spectrometry instruments for applications in the proteomics area. A second student can work on a similar topic, but now in collaboration with a Japanese multinational company, who want to design their next generation chromatography instruments for the pharmaceutical industry and need to minimize the axial dispersion in the fluidic connections within their instrument.

Contact: Prof. Gert Desmet (VUB, Room 5G214 gedesmet@vub.be , tel: 02/629.32.51)

Topic 2: 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 (D_{rad}) in chromatographic columns is strangely enough ill-known and poorly studied, the present project aims at making a comprehensive study of the dependency of D_{rad} 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 D_{rad}-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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Prof. Ken Broeckhoven (VUB, Room 5G205, ken.broeckhoven@vub.be, tel: 02/629.37.81)

Topic 3: 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 Nanotechnology 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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Topic 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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Topic 5: Development of continuous chromatography method

Summary:
HPLC is the most powerful analytical separation method in life sciences, but can unfortunately not be used for (industrially relevant) preparative or unit process separations. We recently proposed 2 innovative (so far unpublished) approaches to convert the method in a continuous one and microfabricated silicon devices for this, which will be fluidically characterized in the thesis, eventually aiming for a continuous separation of bio-based building blocks. This topic is supported by a Catalisti SBO project (co-supervisors Jo Christiaens, Dr. Ilyesse Bihi).

Contact: Prof. Wim De Malsche - wim.de.malsche@vub.be

Topic 6: Use of vortices for next generation HPLC

Summary:
Chromatographic performance has recently reached a plateau, due to limitations in (slow) diffusional mass transport. Our group has recently developed electroosmotic and acoustic methods to induce lateral flows in microfluidic channels. This approach has been shown to reduce the dispersion sensitivity to analysis speed by a factor of 5, meaning that much faster analysis can be performed, or that higher resolution can be achieved in a given time. In the thesis we aim to develop and validate the method for large molecules as HBa1c, the most prominent biomarker for follow up and diagnosis of diabetes. Aim is not only to improve performance dramatically , but also to develop low pressure point of care instruments. This topic is supported by 2 European projects involving 5 partners (co-supervision Dr. Pierre Gelin and Dr. Ilyesse Bihi) and will be conducted in close collaboration with diabetes expert Prof. Ilse Weets (UZ Brussel).

Contact: Prof. Wim De Malsche - wim.de.malsche@vub.be

Topic 7: 3D printing of microfluidic chips for liquid chromatography

Summary:

3D-printing is a novel method for the fabrication of layer-by-layer three-dimensional features with high precision. The main scope of this master thesis will be to explore Digital Light Processing (DLP) 3D printing to create of micro-devices. The manufactured devices will be integrated with monolithic stationary phase and/or packed with particles with the objective to perform proof-of-concept spatial multi-dimensional separations of biomolecules.

Contact: Prof. Sebastiaan Eeltink - seeltink@vub.be

Topic 8: Establishing the next-generation LC-MS at ultra-low flow rates

Summary:

Liquid chromatography coupled to mass spectrometry (LC-MS) is one of the most powerful analytical techniques. In this project novel very narrow capillary columns will be developed allowing to operate LC and ultra-low flow rate. This will significantly enhance the ionization process in the ESI interface between LC and MS allowing to increase detection limits with 2 orders of magnitude. We will develop porous polymer structures in capillary column formats and study the effects of flow rate on chromatographic resolution and MS detection sensitivity. Proof-of-concept for low-flow nanoLC-MS using the developed column will be demonstrated for analyzing HeLa cell lysates.

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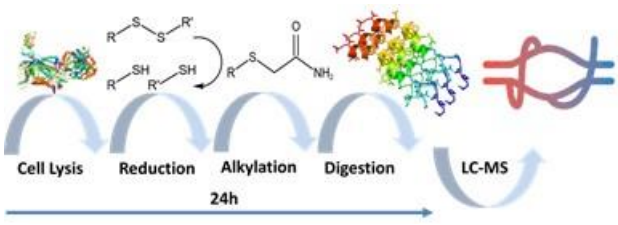
Topic 9: Development of a novel on-line protein preparation interface for proteomics analysis by liquid chromatography-mass spectrometry (LC-MS)

Summary:

Proteomics is arguably the biggest growing area of bioanalysis globally, utilized as the primary tool to determine fundamental behaviors of a huge array of biological systems such as immunity, metabolic systems, drug-protein interactions, and bacterial bio-catalysis. The M.Sc. thesis will involve the development of an integrated sample preparation device which combines protein reduction, alkylation and proteolytic digestion in a single fluidic system in less than 10 minutes. The student will learn to synthesize and optimize polymer monolith bioreactors, perform protein reduction and alkylation protocols as well as work with and gain immensely valuable experience in state- of the art LC-MS instrumentation to analyze complex protein samples.



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***General information on Topics 10-11 (Topics Prof. Broeckhoven*)**

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_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.

Topic 10: **Investigating diffusion and axial dispersion 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_2 (sCO_2), SFC employs mixtures of sCO_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 goal of this study is to investigate in detail the diffusion behavior in SFC mobile phases and in separations columns and develop a model, using experimental measurement and numerical simulations, of the separation performance in SFC.

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Topic 11: Numerical study of separation performance in SFC

Summary:
A challenging aspect when investigating the separation performance in SFC is the strong dependence of the physico-chemical parameters with operating pressure. Whereas for traditional liquids, used in HPLC, it can be assumed that properties such as density and viscosity are independent on pressure, this not the case in the supercritical mobile phase used in SFC. These effect not only result in varying flow rates and non-linear pressure drop in the column, but also phase equilibria (retention), speed of diffusion and mass transfer are effected. As these parameter shave a strong effect of separation performance and quality, it is a challenging task to understand the overall separation performance in SFC as a function of velocity of column length, which both affect the pressure drop over the column and thus the variation in pressure during the separation. If desired, the simulations in this project can be supplemented with experiments work.

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Topic 12: Separation of ethane/ethene and propane/propene mixtures

Summary:
Olefins such as ethene and propene as 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 CO_2-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/propene 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)

Topic 13: Novel nanomaterials for CO_2 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 CO_2 capture and conversion efficiency. Novel solid CO_2 sorbent materials (e.g. Metal Organic Frameworks, MOFs) for operation in low CO_2 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 N_2 and CO_2, several impurities such as SO_X, NO_x 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 an the performance in the CO_2 capture process.

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Topic 14: 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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Topic 15. 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, ZIF-67 onto different metallic and non-metallic substrates. Thus, in this thesis subject will be development of structured MOF composites for separations of different gas mixtures.
Work will include: (I) In-situ growth and/or deposition of different MOFs onto a porous substrate such as melamine formaldehyde sponge (II) Investigating adsorptive gas separation via dynamic breakthrough experiments.

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Topic 16: Development of structured adsorbents for biogas separation

Summary:
Biogas is seen as one of the important future renewable energy carriers. Biogas is obtained via the digestion of organic waste, and contain a significant amount of methane. This stream has to be purified and separated to allow injection of high grade methane in the gas grid. Amongst the various separation technologies, Pressure Swing Adsorption has a number of advantages.
One of the main challenges in biogas upgrading is the removal of N_2. To that purpose, kinetic adsorbents can be used, for which the separation between N_2 and the other compounds is achieved via differences in intra-crystalline diffusion rate, in nanoporous solids such as zeolite ETS-4. Recently, we developed the capacity to synthesize such small pore materials in our own lab. Classically, such materials are used in packed beds.
In this thesis, structured kinetic adsorbents will be developed and tested in the upgrading of biogas, starting from the kinetic adsorbents that we have synthesized. Structured adsorbents (monoliths, 3D-printed structures) have a number of particular advantages such as lower pressure drop and better heat and mass transfer. This research contains lab experimentation and/or process modelling.

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Topic 17: Hydrogen and methane storage in clathrates supported by mesoporous solids

Summary:
Clathrate hydrates are inclusion compounds consisting of a host lattice, formed by hydrogen bonded water molecules, in which gas molecules, such as CH_4, CO_2 and H_2 can reside by attractive van der Waal's forces with the host. Typically, these structures are formed at elevated pressures and temperatures around or below the freezing point of water. In the past, clathrates were merely regarded an obstacle in gas and oil transportation due to spontaneous formation in pipelines leading to flow assurance problems. Recently, however, they have received increased attention as medium to store gases, given their non-explosivity, environmentally benign nature, moderate storage conditions, low production cost, low risk of handling and high volumetric storage capacity, i.e. up to 160 m^3 CH_4 (at 0 °C and 1 bar) is stored in 1 m^3 CH_4 clathrate. It should be stressed that hydrogen is seen as one of the future energy carriers; hydrogen storage is high on the agenda of the European Research Council.

Recently, we have built a novel and unique experimental setup that allows the study of methane and hydrogen clathrate formation. In this thesis, the kinetics of methane and/or hydrogen clathrate formation will be studied. It will generate crucial data, that will allow to evaluate the potential of this approach for energy storage. Very promising results have been obtained very recently in our lab. Research will be performed using advanced mesoporous solids provided by academic partners from other universities of our research consortium (collaboration with UGent, KU Leuven and UAntwerpen).

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Topic 18: CO_2 capture via Temperature Swing Adsorption (TSA) using a Microwave heating 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.
In this thesis, the use of microwaves for the regeneration of solid adsorbents for CO_2 capture will be evaluated. Using lab scale proof of concept setups, cyclic TSA experiments (combing 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, iii) the effect of the structure and geometry of a monolithic adsorbent on microwave absorption on CO_2 recovery.

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Topic 19: Mathematical Modelling and Simulation of Adsorption/Membrane Hybrid process for CO_2 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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Topic 20: 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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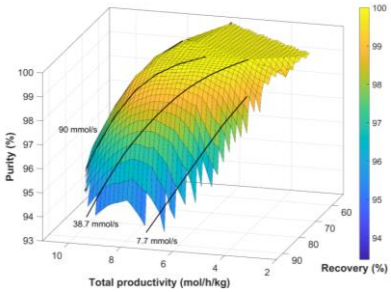
Topic 21: Performance simulation of pressure swing adsorption (PSA) units for biogas separation

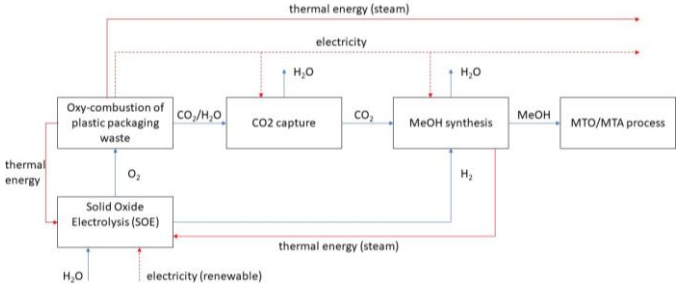
Summary:
Pressure swing adsorption (PSA) is a powerful separation technique, applied on industrial scale since the 1950's. Currently, PSA processes hold a prominent place in the context of carbon capture to combat climate change, as well as biogas separation. For the latter, a solid adsorbent (often zeolite) is used to capture CO_2 from the biogas formed in digesters. Due to the intrinsic dynamic behavior of PSA units, their performance is notoriously complex to understand. To this purpose, we use dynamic process simulations via Aspen Adsorption. Prior experience with the software is not a perquisite (but certainly a plus): former master students have produced 1 published and 1 submitted research article in the last two years. We are seeking a new candidate interested in process simulations. For this campaign we are interested in the trade-off between productivity and efficiency via PSA cycle design. Practical supervisor: ir. Niels De Witte.



Contact: Prof. Tom Van Assche - tom.van.assche@vub.be

Topic 22: Feasability study of new integrated processes (*collaboration with BSOG*)

Summary:
Together with the Brussels School of Governance (BSOG), specialized in providing strategic and policy advice, we are looking for a candidate with an interest in modelling, process simulation and beyond. Using simulation software (Aspen), we aim to study the mass/energy balances of an innovative process design in the field of plastic waste management, possibly coupled with a first techno-economic study and comparison to other processes. Is the process design, shown below, a realistic approach for plastic waste handling? During sorting and mechanical recycling of plastic packaging waste (mainly PE, PP, PS and PET), about 20 % is lost. This loss can be converted to high value chemicals (HVCs), such as olefins and/or aromatics, starting from a combustion process. Oxy-combustion increases the concentration of CO2 in flue gases and reduces the energy consumption of its capture. Via CO2 hydrogenation, methanol is obtained which can be used for MTO (methanol-to-olefins) or MTA (methanol-to-aromatics). The hydrogen and oxygen could be delivered simultaneously via water electrolysis, operating on renewable electricity. Practical supervisor: ir. Stijn Van Der Perre.



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Topic 23: Matlab study on segmented heating in temperature swing adsorption (TSA) processes

Temperature swing adsorption (TSA) is popular technique to remove trace component, widely applied on industrial scale. The adsorption group has a strong research activity on novel heating methods as inductive heating, microwave heating or Joule heating. These methods, in contrast to a hot gas purge, offer a unique opportunity to directly heat the adsorbent pellets, and to apply different temperature programs to various layers or segments of the bed, radically transforming the TSA method. Via proprietary Matlab codes, you will adapt the existing codes, and study the potential of such non-uniform heating on the adsorptive separation. We are looking for a candidate, preferable with some prior Matlab experience , with interested in simulation studies, aiming to expand his/her simulation skills. An interest in coding is a plus.

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