MSc in Chemistry and Materials engineering
Master Thesis subjects 2019-2020

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2. Prototyping of microfluidic chips using 3d printing technology
3. Pareto optimality optimization of 2d-lc and 3d-lc separations using matlab
4. Operation strategies for industrial PSA separation units
5. Synthesis and testing of nanoporous coatings for adsorber packings
6. Desorption of bio-chemicals with (super-/subcritical) liquid CO_2 and 2-step purification
7. Development of a new technology for the abatement of CO_2
8. Modelling and optimisation of processes combining adsorption columns with a different selectivity
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10. Pressure Swing Adsorption for the upgrading of biogas
11. Simulation and measurement of flow and mass transfer processes in novel packed bed column systems
12. Chip-based Chromatography: use of micromachining technology to produce perfectly ordered chromatographic columns in silicon (1 to 2 students)
13. Development of a computer-controlled "automatic problem solver machine" to solve chromatographic separation problems
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35. Modelling of nucleate boiling: single vapour bubble growth on a superheated substrate
36. Experimental and/or theoretical analysis of “tears of wine” in alcoholic beverages
37. Microencapsulation of pharmaceutical active compounds by spray drying. A numerical and experimental optimization of the process.
38. Intermittent drying of Baker’s yeast pellets. A new way to improve the quality of the dried product?

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40. Development and characterisation of novel adaptive bio-based composites
41. Advanced thermal characterization of materials for organic photovoltaics and/or NIR photodetectors
42. Study of dehydration of Portland cement paste and the fines obtained from recycled concrete.
43. Recovery and study the properties of the sand obtained from the fines of recycled concrete.
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45. Additive manufacturing of reversible polymer network composites for sensing applications
46. Rheokinetics and reactive modelling of additive manufacturing techniques

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48. “Greener” and affordable materials for thermochemical heat storage
49. Towards the electrochemical valorization of valuable elements from secondary sources: electrochemical properties of critical elements in non-conventional solvents
50. Additive manufacturing technology for aeronautical applications: Influence of heat treatments on microstructure and mechanical properties of Al- and Ti-alloys
51. Development of nanostructured and multiphase glasses
52. Thermomechanical treatment of a high-entropy alloy: link between process parameters, microstructures and mechanical properties
53. Quenching and Partitioning steels: Investigation of microstructural development and mechanical properties.
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59. Drop-by-drop manufacturing and testing of double-layer ultra-capacitors
60. Smart management of de-icing systems for aeronautical and marine applications
61. Microparticles uptake by complex fluids under periodic excitation
62. Supercritical carbon dioxide as a green solvent
63. Why molecules move along a temperature gradient?
64. Dynamic weting properties in pulsating heat pipes
65. Oscilllating mass transport in a temperature gradient
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67. Green deep eutectic solvent for the regeneration of waste wool fiber
68. Implantable natural polymer-based electrode for stimulation and repair of neurons
69. Glycerol fermentation from lignocellulose biomass
70. Microbial degradation of recycled PET plastic: applied biochemistry/fermentation
71. Mathematical modeling for optimizing intracellular trehalose accumulation in yeast fed-batch cultures
72. Metabolic model-based optimization of hybridoma cell fed-batch cultures
73. Analysis and development of methods for estimating the fluxes in food webs describing coastal ecosystems

Details

Department of Chemical Engineering (CHIS) – VUB

1) development of native lc methods for the separation of macrobiomolecules

Summary: Chromatographic techniques such as size-exclusion chromatography (SEC), ion-exchange chromatography (IEX), and hydrophobic interaction chromatography (HIC) are the gold standard for the characterization of aggregates and higher order structures, charge variants and structural variants arising from post-translational modifications (PTM's). During the analysis the protein 3D structure is maintained. Hence the technology can be used to assess the biological activity of target biomolecules in complex life-science matrices, and to analyse protein-protein interactions. In this research project the possibilities and limitations of novel (MS compatible) salt systems will be investigated for profiling of biomacromolecules.

Contact: Prof. dr. Sebastiaan Eeltink (sebastiaan.eeltink@vub.be)

2) Prototyping of microfluidic chips using 3d printing technology

Summary: Traditional chip manufacturing procedures often involve a multi-step, labor-intensive and costly process, which currently hinders the rapid and widespread development of new applications using microchip devices. 3D printing is a novel prototyping tool, allowing to rapidly fabricate and easily modify the microfeature design of prototype microfluidic chip devices. The benefits of the technique include rapid feedback, allowing channel layout changes to be quickly tested, and cost-effectiveness to create devices with interwoven microchannels. By pushing the limits of printing resolution and substrate material science, novel devices for liquid chromatographic separations can be created offering an unparalleled multichannel arrangement with on-chip integrated multi-purpose microfluidic design features.

Contact: Prof. dr. Sebastiaan Eeltink (sebastiaan.eeltink@vub.be)

3) Pareto optimality optimization of 2d-lc and 3d-lc separations using matlab

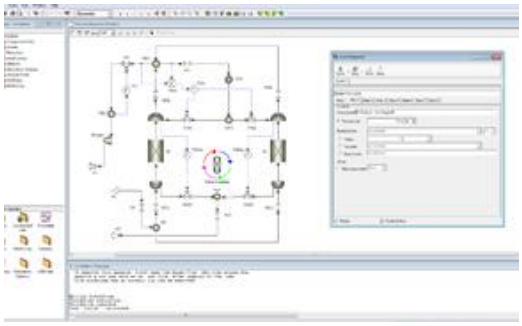
Summary: In spatial three-dimensional chromatography, components are separated in the space domain with each peak being characterized by its coordinates in a three-dimensional separation body. Spatial three-dimensional (3D-)LC has the potential to offer uniquely-high resolving power when orthogonal retention mechanisms are applied, since the total peak capacity is the product of the three individual peak capacities. Due to parallel developments during the second- and third-dimension separations, the analysis time is greatly reduced compared to a coupled-column multi-dimensional LC approach. In this study, matlab scripts will be developed to get information on design parameters (channel length, gradient time, particle diameter HPLC columns, etc, etc) of spatial 3D-LC chips that yield the best possible performance in the shortest possible analysis time.

Contact: Prof. dr. Sebastiaan Eeltink (sebastiaan.eeltink@vub.be)

4) Operation strategies for industrial PSA separation units

Summary: We are looking for a candidate with a keen interest in modeling and process simulation. Using the AspenTech process simulator, industrial sized pressure swing adsorption (PSA) units are to be operated more efficiently by implementing control and operation strategies. This project starts with analyzing the potential of predefined control strategies on existing models of the industrial units. The performance of the unit, with and without the new operation methods, is to be mapped for varying settings (customer industries) and the gains in operational costs determined. The candidate assists in developing test comparison (*from pilot unit*

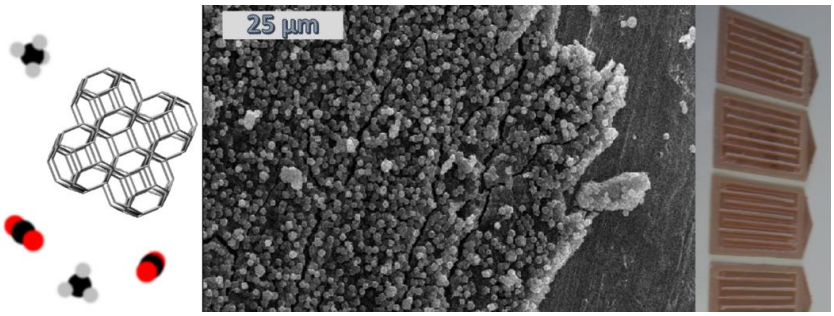
and/or production unit) and data analysis strategies. Prior experience with Aspen is not a prerequisite but certainly a plus.



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

5) Synthesis and testing of nanoporous coatings for adsorber packings

Summary: To reduce the footprint and increase effectiveness of separation units, columns with advanced structured packings are widely used within industry. In this master thesis project we seek to develop a proof of concept (POC) device with a novel structured packing for adsorption units. Thin sheets (laminates), spaced less than 1 mm apart, offer high mass transfer characteristics and low pressure drop. Due to these characteristics, the POC device aims at rapid thermal cycles (RTSA) to adsorb CO_2. The candidate is to test current and new synthesis methods to obtain hybrid nanoporous coatings. Examples of methods are room temperature mixing, solvothermal synthesis and electrochemical synthesis. The core concept aims at 30-100 µm layers on various supports: metal foils, glass fiber sheets *etc*. Besides synthesis, the candidate assists in developing analysis methods (with respect to the adsorption capacity and kinetics of the foils), and in the assessment of the POC potential in CO_2 adsorption applications. This work is mainly experimental, involves pragmatic skills, data analysis and may be extended towards modeling.



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

6) Desorption of bio-chemicals with (super-/subcritical) liquid CO_2 and 2-step purification

Summary: Bio-chemicals have been identified as promising, sustainable substitutes for fossil feedstocks. Their production still faces a series of challenges, such as in the downstream processing. The adsorption phenomenon (i.e. the concentration of molecules on the surface of solid (porous) materials) has been pinpointed as the most energy-efficient process. A key step in adsorption technology is the recovery of the product from the pores of the adsorbents, the so-called desorption. In this master thesis, we will investigate the desorption of bio-chemicals using alternative technologies (e.g. liquid CO_2 and/or combined adsorption columns). Besides mainly experimental work, the student may also develop mathematical models to fit experimental data and perform simulations of an adsorption-desorption process.

Contact: Benjamin Claessens, Benjamin.Claessens@vub.be ; Joeri Denayer, joeri.denayer@vub.be

7) Development of a new technology for the abatement of CO_2

Summary: Carbon dioxide is one of the most important greenhouse gases, produced in nearly every human activity. Its emissions should be drastically reduced. In collaboration with a major chemical company, Prof. Denayer is developing a new and highly advanced technology for the separation of CO_2 from flue gases. Innovative aspects of the process are based on an ultrafast desorption step, allowing to tremendously reduce cycle time in combination with a smaller volume for the industrial plant and the use of new nanoporous structured adsorbents. Many aspects (heat and mass transfer, regeneration, adsorption and diffusion in the nanopores of the adsorbent, effect of poisons, effect of humidity, cycle optimisation,….) of the process are currently investigated. In this particular project, we will study the use of microwaves for the regeneration step in the adsorption process, to obtain a faster and more efficient CO2 capture process.

Contact: Joeri Denayer, joeri.denayer@vub.be

8) Modelling and optimisation of processes combining adsorption columns with a different selectivity

Summary: Both renewable and traditional chemical processes often yield complex mixtures of different reaction products. A one-step separation process is therefore often insufficient to allow full purification of the end products. In the case of the production of the platform chemical 1-butanol from renewable resources, a two-step adsorption/desorption process was very recently developed at CHIS. In this process, two fixed bed adsorption columns containing zeolites with a complementary selectivity were combined to fully purify 1-butanol from a model mixture. For this project, the development of mathematical models describing the behaviour of such multicolumn adsorption systems in the context of 1-butanol purification is envisaged. The developed models will allow for (i) identification of the most efficient column combinations, (ii) optimisation of process conditions (iii) and a theoretical study of the influence of adsorption kinetics and equilibrium 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.

Contact: Benjamin Claessens, Benjamin.Claessens@vub.be ; Joeri Denayer, joeri.denayer@vub.be

9) Purification of hydrogen with ion-exchanged zeolites

Summary: Hydrogen is a very useful molecule and might gain an enormous share in the future energy market. It is, for example, used in space shuttle jet-fuel, fuel cell electricity generation and in the semiconductor industry. Currently, hydrogen is mainly produced as a by-product from steam-reforming of hydrocarbons. Prior being used, hydrogen needs to be purified from impurities present in the product stream. In this work, the student will explore how zeolites can be used for the removal of a hydrogen chloride impurity from a hydrogen stream. The performance will be carried out with packed columns and breakthrough experimentation. Making use of ion-exchange, the students will explore how cations presents in the zeolite structure may influence the purification performance of these materials.

Contact: Julien Cousin-Saint-Remi, jcousin@vub.be; Joeri Denayer, joeri.denayer@vub.be

10) Pressure Swing Adsorption for the upgrading of biogas

Summary: Even though the amount of CO_2 present in the atmosphere is greater than CH_4, the global warming potential of CH_4 is 21 times higher than that of CO_2 and therefore, the emission of CH_4 to atmosphere must be reduced. The major source of CH_4 to atmosphere is biogas, which is composed of around 55 - 70% CH4, 30 - 40 % CO2 and smaller amounts of NH_3, H_2S, N_2 depending on the source of production. To increase the energy content and also to avoid the pipeline and equipment corrosion, the CO_2 content for pipeline grade biomethane should be less than 2 – 3%. Adsorption, especially pressure swing

adsorption (PSA) or vacuum swing adsorption (VSA), is a commercially established process for the separation of gas mixtures in chemical industry. In this project, PSA separation of CH_4 from its gaseous mixture with CO_2 will be studied using different adsorbents like zeolites, MOFs etc. New types of structured adsorbents (e.g. monoliths) will be tested. This research fits in a collaboration with a large company.

Contact: Joeri Denayer, joeri.denayer@vub.be

11) 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 (http://vubchemicalengineering.be/). 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.ac.be , tel: 02/629.32.51)

12) 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 (http://vubchemicalengineering.be/) 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.

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

13) Development of a computer-controlled "automatic problem solver machine" to solve chromatographic separation problems

Summary: Liquid chromatography is the most widespread analytical technique used in science and technology. The liquid chromatograph is the third most sold laboratory item (after the weighing balance and the pH meter). The Chemical Engineering department of the VUB is one of the world's leading groups in the area of liquid chromatography (http://vubchemicalengineering.be/). The standard practice of a chemical analyst consists in seeking the right combination of packing material and carrier solvent (chemical nature) to separate a mixture. Given the many operational variables, and given the fact that the different components of a mixture respond in a highly unpredictable way to any change in packing material and carrier solvent, this

is a very time and labour consuming activity which up to now mainly occurs via trial-and-error. The aim of the presently proposed thesis project is to contribute to either the software or the hardware part of the "automatic problem solver machine" the department is currently developing.

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

14) 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.

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

15) 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.

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

16) Overcoming diffusion limitations: towards a 1000 times higher separation efficiencies?

Summary: During the past 10 years, our group has eliminated 2 out of 3 dispersion sources in chromatography by replacing the disorderly packing of classic columns with organized radially stretched structures, manufactured by in-house developed etching and lithography processes. To further increase the performance, the mass transport mechanism now needs a more drastic change change. This requires a faster transport rate than that of for pure diffusion, a current limitation in laminar flow systems. In this master thesis electro-osmotic flow will be used to enhance mass transport, which is a patented concept. Planned activities include electrical characterization of chips, simulation and modeling of electric and liquid flows and experimental characterization of dispersion behavior with an in-house-designed set-up. The student will function in an interdisciplinary team (expertise in electronics, electrochemistry, optics, microfluidics and chromatography) in close interaction with the Mesa+ Institute in Enschede (NL), (visits and stays can be organized).

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

17) Development of particles for sustained drug release

Summary: Poly-lactic-glycolic particles have been used in the context of cell therapy. These FDA approved particles are slowly decomposed whereby incorporated chemicals are slowly released, influencing the further development of cells. A disadvantage of current PLGA methods is the very limited control on the size of the particles, which limits the efficiency of cell therapy. In this thesis a number of developed (and patented) microreactor designs will be validated experimentally and further refined. The influence of flow characteristics on the development and growth of PLGA clusters will be studied by using the newest generation high-speed camera and particle image velocimetry. The flow will be created by piezoceramic actuators and segmented pressurized systems and in electro-osmotic mixers, systems that each generate a unique flow profile. This thesis will be performed in close collaboration with Prof. Karine Hellemans of the Diabetes Research Centre (VUB Jette) who incorporates particles in beta-cells.

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

18) Experimental and modelling study of the performance of SFC and LC devices

Summary: In SFC, Supercritical CO_2 (sCO_2), which has liquid like properties, is used as a solvent. Although SFC was already proposed 50 years ago, fundamental understanding of the parameters determining the performance and separation mechanisms is still lacking. The high compressibility of the sCO_2 strongly affects phase equilibria, solvent properties (viscosity, density), causes decompression cooling etc., making it challenging task to understand the fine details of this technique. The project aims at better understanding these effects using an experimental approach, supplemented with numerical simulations and modelling.
Contact: Ken Broeckhoven, ken.broeckhoven@vub.be

19) Novel sample injection techniques in LC and SFC

Summary: With the introduction of new, highly performant chromatographic column, separation performance in LC and SFC has improved to such an extent that instrumental contributions to dispersion become the dominant factor. One the most challenging contribution factors that often has a large effect on the obtained performance is the sample introduction. Increasing the amount of sample introduced in the system increases the number of molecules reaching the detector and thus improves detection sensitivity. Too large sample injection volume, that additionally very often has a different solvent composition as the separation medium, however gives rise to a loss in separation resolution. This project investigates the novel

"feed stream" injection technique, recently introduced by Agilent Technologies, which directly injects the same in the mobile phase stream, for both LC and SFC using experimental and simulation approaches.

Contact: Ken Broeckhoven, ken.broeckhoven@vub.be

20) Development of novel techniques to characterize column performance and packing quality

Summary: After the leap in separation performance that was achieved in liquid chromatography with the introduction of the so-called ultra-high pressure or ultra-high performance liquid chromatography (UHPLC), a stalemate was reached in the development of novel separation columns. Further decrease in column diameter or particle size does not provide expected increase in separation performance and in fact often yield worse performance. To better understand the limitations of column development and the underlying reasons for poor column performance, a non-invasive method is needed to characterize the packing quality of these small volume columns packed with sub-2µm sized particles. Although the so-called total pore blocking method shows promising results, this technique is limited to small flow rates outside the range of interest. In this project, a novel technique using an in-column polymerisation method to develop a monolithic structure inside the particles or by templating the whole column structure will be investigated.

Contact: Ken Broeckhoven, ken.broeckhoven@vub.be; Gert Desmet, gedesmet@vub.be

21) Extreme Pressure LC (up to 3000bar): breaking the pressure limits of HPLC

Summary: The most straightforward way to improve separation performance in liquid chromatography is to increase the maximum operating pressure of the chromatographic system. Besides fundamental challenges (viscous heating, pressure induces changes in retention), the mechanical requirements for the development of pumps, injectors and durable chromatography is enormous and will be investigated in this project

Contact: Ken Broeckhoven, ken.broeckhoven@vub.be ; Gert Desmet, gedesmet@vub.be

Electrochemical and Surface Engineering (SURF) – VUB:

22) Aging Study of Lithium Ion Battery Materials:

Summary: Lithium ion batteries are currently used to power most portable electronic devices and are also very promising candidates for electric vehicles. Due to unwanted reactions during discharging or charging, aging of the materials occurs, limiting the lifespan of the batteries. To further optimize the utilization of the batteries, a better understanding of the interior aging processes is necessary. Aged batteries will be analysed by multiple techniques to have a deeper insight into the origin of the aging phenomena. Electrochemical impedance spectroscopy (EIS) is one of the main tools for characterization of the ongoing processes. In this work, EIS will be performed using the in-house developed Odd Random Phase EIS (ORP-EIS). This technique allows, next to post-mortem analysis, also *operando* measurements, meaning that measurements can be performed during discharging or charging. In support, multiple surface analysis techniques like SEM, XPS, AFM, Raman…can be applied for the batteries detailed chemical characterization down to the nanoscale.

Contact: Xinhua Zhu (xinhua.zhu@vub.be), Annick Hubin (annick.hubin@vub.be)

23) Multifunctional and environmentally friendly corrosion inhibitor systems:

Summary: This project aims to design new, environmentally friendly coating systems for steel in marine environments by incorporating novel, non-toxic pigments that can be combined to protect against both corrosion and microbial attack. Structural requirements for these compounds will be determined through the use of advanced characterisation techniques to identify the largely unknown mechanisms of attachment and protection on steel surfaces. The components may themselves be dual active, or be combined to capitalise on individual protection mechanisms that provide a synergy whereby the combination leads to better protection outcomes. Such coatings have the potential to significantly improve the lifetime of marine infrastructure. The subject is together with Professor M. Forsyth Daikin University Australia. Inhibitors will be synthesized at Daikin University. The student will focus on the electrochemical and surface characterisation to determine the inhibitor mechanism.

Contact: Herman Terryn (herman.terryn@vub.be), Annick Hubin (annick.hubin@vub.be), Maria Forsyth (Daikin University)

24) Conversion layer treatments on novel grade stainless steels for automotive industry:

Summary: Automotive industry is continuously looking for novel materials for their car bodies, in order to lower greenhouse gas emissions during the life-time as well as to improve their mechanical strength. Press hardened stainless steels offer a valuable alternative to steel and aluminium cars, having a high strength to low thickness ratio. Such stainless steels, composed of a low chromium content, have to be protected against corrosion. In a car manufacturing line, the whole body is treated in the same production line. Therefore, it is important to know whether and how traditional cleaning, pretreatment, e-coat and final coating procedures are of equal quality compared to traditional metals. This study focusses on the understanding of the mechanism of fluoride-induced zinc phosphate conversion coatings (as used on the Volvo car line) on a special, novel grade stainless steel from Aperam. State-of-the-art surface sensitive techniques as well as in situ (electrochemical) analysis will be performed to understand the behaviour of the new materials in commercial car manufacturing production lines.

Contact: Mohadesse Nabizadeh (mohaddese.nabizadeh@vub.be) , Tom Hauffman (tom.hauffman@vub.be)

25) Mechanical and corrosion study of 3D printed steel using WAAM (Wire Arc Additive Manufacturing) technology:

Summary: Metal 3D printing using WAAM technology is mainly applied for large structures as WAAM allows a very rapid printing and a flexible design, does not require special atmosphere and can also be used as repair technique for structures on which damaged parts can be re-printed. WAAM is based on metal wires being molten and rapidly solidified together into a 3D structure. In the present master project the research will be done **in collaboration with OCAS/ArcelorMittal**. The aim of the research is to fully characterise the WAAM steel microstructure and link it to the mechanical behaviour and surface properties such as corrosion and possible corrosion protective measures.
In this project characterisation of the microstructure and composition will be done using various surface analysis methods (SEM, AES, XPS, EBSD…), mechanical testing using tensile and hardness analyses, and corrosion investigation using electrochemical approaches such as potentiodynamic polarisation, cyclic voltammetry, and/or local methods such as SVET, SECM, SKPFM.

This topic can be fine-tuned for one or two students.

Contact: Iris De Graeve (Iris.De.Graeve@vub.be), Stephane Godet (sgodet@ulb.ac.be)

26) 3D printing of stainless steel using LMD (Laser Metal deposition) hybrid additive-subtractive manufacturing:

Summary: The fully new hybrid additive-subtractive manufacturing setup based on LMD is operational at VUB. LMD is a powder-based 3D printing technology that allows printing of various metals, with flexible design and properties. As for all 3D printing methods, the microstructures of the additive manufactured (AM) metals are very different from conventional wrought or cast products. As such, also the performance properties are very unique, reflecting significant influence of the unique printing microstructures. Stainless steel produced by powder-based AM has a very fine microstructure and interesting mechanical and surface properties. Stainless steel, being 'stainless' because of its added chromium forming a passive chromium oxide surface layer, shows different corrosion properties compared to rolled SS. The aim of this master project is produce LMD printed 316L samples and to investigate the surface composition & microstructure and link it to the surface properties, using various surface analysis methods (SEM, EDX/WDX, AES, XPS…) and electrochemical analyses (polarization, impedance, and local methods SECM, SKPFM…).

This project is part of a large consortium project on AM of metallic structures where different research groups of VUB are participating. This topic can be fine-tuned for one of two students, with potential collaboration with the dept of Mechanical Engineering.

Contact: Iris De Graeve (Iris.De.Graeve@vub.be), Reynier Revilla (Reynier.Inocente.Revilla.Castillo@vub.be)

27) Hydrogen embrittlement of oxidized (stainless) steel:

Summary: The risk of hydrogen embrittlement (HE) occurs when the metal is exposed to a hydrogen containing environment. This is for example critical in applications where the steel structure is under cathodic corrosion protection, but also for hydrogen storage containers – required for the production of 'green' hydrogen based energy - it is a concern.
Hydrogen being a very small mobile element can enter metal microstructures, and depending on the type of crystalline lattice, defects, grain boundaries, precipitates etc. the hydrogen can diffuse inside the material and/or become trapped. Typically, when accumulation can occur the metal can suddenly become brittle during deformation or loading processes and fracture. The surface properties of the metal are also playing an essential role in this HE investigation, but are less studied than the bulk metal influences. Especially for stainless steel, the surface is a complex mixture of oxides that will potentially influence the uptake and release properties of the hydrogen. The aim of this project is to study the influence of the surface state of the SS alloy by deliberately changing the surface oxides in a controlled and characterized manner

(characterization using ellipsometry, Raman, XPS, AES etc) and quantifying the impact on the HE using various electrochemical methods (polarization, SKPFM etc).

Contact: Iris De Graeve (Iris.De.Graeve@vub.be), Tim Rubben (Tim.Rubben@vub.be)

28) Hydrogen embrittlement of aluminium:

Summary: The risk of hydrogen embrittlement (HE) occurs when a metal is exposed to a hydrogen containing environment. This is for example critical in applications where the metal structure is under cathodic corrosion protection, but also for hydrogen storage containers – required for the production of 'green' hydrogen based energy - it is a concern.
Hydrogen being a very small mobile element can enter metal microstructures, and depending on the type of crystalline lattice, defects, grain boundaries, precipitates etc. the hydrogen can diffuse inside the material and/or become trapped. For aluminium, research on HE is much more limited than for steel because initially it was believed that HE is not a concern for aluminium with its FCC crystalline lattice structure. In FCC the hydrogen is very soluble and has a very low diffusion rate, hence once inside the FCC lattice the hydrogen remains and cannot cause any problems. However, this believe has proven to be incorrect and even in natural corrosion conditions where hydrogen gas develops as the cathodic reaction, HE has been observed in certain alloys. The aim of this project is to study the interaction of hydrogen and aluminium using various electrochemical methods (polarization, CV, SKPFM etc).

Contact: Iris De Graeve (Iris.De.Graeve@vub.be), Tim Rubben (Tim.Rubben@vub.be)

Engineering of Molecular NanoSystems Laboratory (EMNS) – ULB

29) Elaboration of micellar nanodevices for biomass conversion in water:

Summary: There is currently great interest in development of environmental-friendly synthetic processes and, in this context, the replacement of commonly-used volatile organic solvents by water is of prime interest. Water is a solvent with little environmental impact but its use has been limited because organic substrates are often poorly soluble in water. Micellar systems represent one of the simplest methods to achieve organic transformation in an aqueous environment. In collaboration with the University of Padova, we are investigating the potential of vanadium-based catalysts in aqueous micellar media for the hydrolysis of lignin. The work will consist in monitoring the conversion using model substrates in order to identify the key parameters to control for optimum conversion. This will entail work in the wet-lab and the set-up of HPLC and NMR protocols to characterize the systems and reactions.

Contact: Kristin Bartik, kbartik@ulb.ac.be

30) Transmembrane transporters for phosphates:

Summary: The cell membrane is an apolar barrier for the free diffusion of ions. In-vivo, specialized proteins embedded within the cellular membranes take care of the transport of ions. In our laboratory, we seek to mimic the action of these proteins with synthetic organic molecules that can transport ions across membranes. The aim of this project is to develop and test potential anion transporters. We are particularly interested in molecules that can carry chloride and phosphate anions across lipid bilayers. After the organic synthesis of a transporter, you will evaluate if the compound is able to bind anions and if it can function as a transporter. For this, you will prepare liposomes, spherical assemblies of lipids, as models for cell membranes. The transmembrane transport of the anions will be studied with fluorescence spectroscopy by monitoring the emission of dyes which are encapsulated in the liposome. The mechanism of transport will be investigated by varying salt solutions and lipid composition.

Contacts: Hennie Valkenier; hennie.valkenier@ulb.ac.be
Luis Martinez Crespo; lumartin@ulb.ac.be

31) Preparation of Giant Unilamellar Vesicles using microfluidics:

Summary: In the EMNS laboratory, vesicles prepared from natural lipids (liposomes) are used as models for cell membranes to study processes like transmembrane transport and cell targeting. With standard procedures, vesicles with diameters of up to 200 nm are easily made, but the preparation of giant unilamellar vesicles (GUVs, ~10 µm) is still a challenge. The TIPS laboratory is specialized in microfluidics, which can be used to prepare droplets and vesicles. The aim of this collaborative project is to develop a method to prepare GUVs as membrane model system by microfluidics. You will use a home-made 3D-printed micro-emulsion generator to produce double emulsions and screen the conditions (fluid viscosities, lipid solutions and concentration, flow rates, geometry) to identify the optimal regime for generating stable GUVs, with minimal organic solvent present. You will characterise these GUVs (DSC, ^{1}H NMR spectroscopy) and compare transmembrane transport into these GUVs with those prepared by classical methods.

Contacts: Benoit Scheid (TIPS); benoit.scheid@ulb.ac.be
Hennie Valkenier (EMNS); hennie.valkenier@ulb.ac.be

32) Nucleic acids driven assembly of nanoparticles at the surface of biological membranes:

Summary: Gold nanoparticles (GNPs) are of particular interest for biomedical diagnostic and therapeutic applications because of their remarkable optical properties, ease of surface functionalization and presumed biocompatibility. In particular, the photothermal properties of GNPs and ease of detection using photoacoustic imaging make them an ideal theranostic tool. For in vivo applications however, the plasmon

band (LSPR) of GNPs, which falls in the visible range, is not ideal and the near-IR would be more suitable. This shift can be obtained by the controlled assembly of the GNPs. This project will aim at controlling the assembly of GNPs at the surface of a target membrane using a bioinspired strategy based on the use of nucleic acids. Nanoparticles will be synthesized and functionalized with different DNA oligonucleotides encoding for the targeting of membranes functionalized with a complementary strand but also for their assembly at the surface.

Contact: Gilles Bruylants, gbruylan@ulb.ac.be

33) Design of nucleic acids coated nanoparticles for miRNA delivery in ovarian cells:

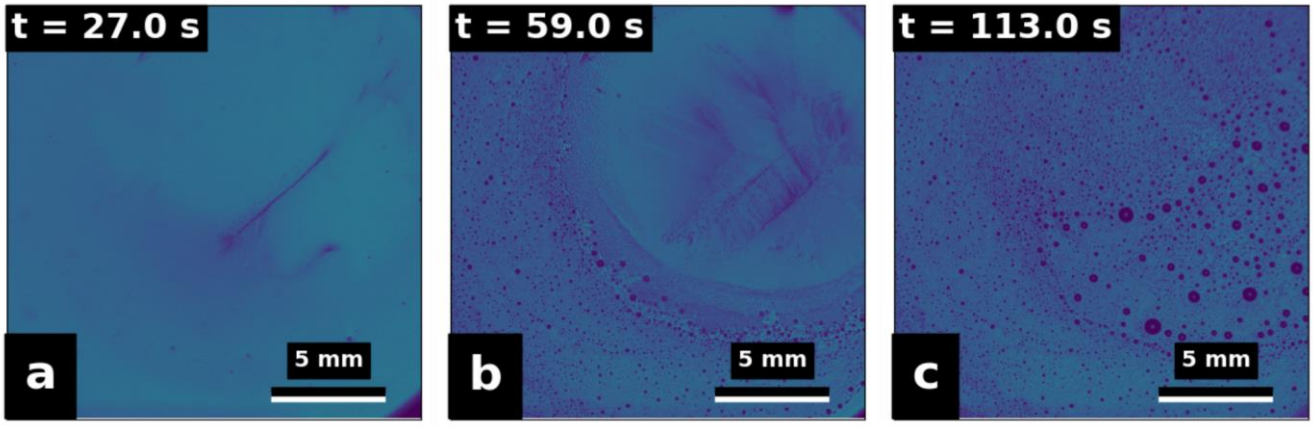
Summary: Chemotherapy drugs such as cyclophosphamide are highly gonadotoxic and can lead to ovarian reserve depletion, causing infertility and thus strongly affecting the quality of life in young patients. The EMNS laboratory works in collaboration with the Laboratory of Human Reproduction from the Erasme hospital that has recently identified microRNAs as therapeutic options to preserve fertility during chemotherapy exposure. MiRNAs are small non-coding molecules, which offer new promising approaches in cancer therapy but also in fertility preservation, as they play a key role in ovarian function. However, these miRNA have to be delivered to the ovarian cells, which requires the development of new delivery systems. Gold nanoparticles (GNPs) are promising vectors, which have already been successfully used for nucleic acid delivery. In this study, we propose a new approach of GNPs surface functionalization based on calix[4]arenes which can be used to control the anchoring of synthetic miRNA nucleotides and/or of other ligands (peptides) for organ specific targeting. The goal of this project is to create novel ovarian protective drugs by combining the favorable characteristics of miRNAs and the cutting-edge technology of GNPs.

Contact: Gilles Bruylants, gbruylan@ulb.ac.be

Transfers, Interfaces and Processes (TIPS) – ULB

34) Liquid-liquid phase separation in partially miscible mixtures

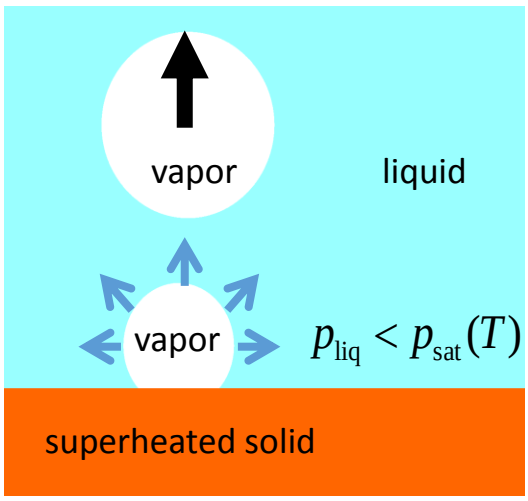
Summary: Controlling the deposition of liquids is an attractive topic due to its applications in industry. Managing nano-particle deposition, generating thin layers of semiconductors, and delivering therapeutic agents in human body are just some examples benefiting from it. A new approach in deposition control is demixing (phase separation) phenomenon. For a partially miscible solution, phase separation can occur through demixing, which is controlled by composition and temperature of the mixture. Setting the right conditions for certain mixtures leads to controlling the deposition of a low volatile solute (residue). Below figures show the demixing process in a thin liquid layer. As the volatile solvent evaporates, the solute forms a scattered pattern on the surface. In this project, we are experimentally (possibly theoretically) looking for answers to these questions: i) what are the physical mechanisms behind the phenomenon, ii) how the size and distribution of the isolated sub-milliliter drops are controlled, iii) what is the effect of evaporation rate on the pattern. At TIPs, you will be trained to use different experimental techniques such as Schlieren and infrared thermography. This project will be performed in collaboration with University of Liège, with funding from F.R.S. – FNRS.



Contact: H. Sadafi (m.sadafi@ulb.ac.be), P. Colinet (pcolinet@ulb.ac.be)

35) Modelling of nucleate boiling: single vapour bubble growth on a superheated substrate

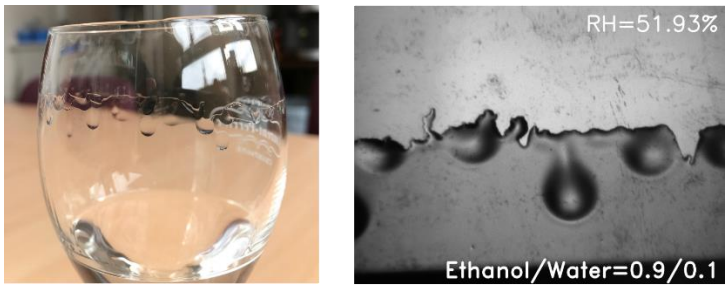
Summary: For a superheated liquid, when the saturated vapour pressure is greater than the ambient pressure, there erupts a violent process known as boiling: vapour bubbles are formed at nucleation sites on the heated bottom of the container, grow in size by liquid evaporation and finally, when sufficiently large, detach under the action of gravity. Getting rid of gravity would permit observation of larger bubbles without detachment and a better understanding of the intricacies of the boiling process. This is one of the objectives of the RUBI experiment to be flown by the European Space Agency on board the International Space Station in 2019. The activities of the ULB-TIPs department as a partner in the project are in particular concerned with modelling of bubble growth, which is hereby proposed as a MT subject. The study is to be carried out in the framework of the multiscale approach currently being developed at TIPs and using the COMSOL Mutiphysics® software. The approach is based on a separation of micro- (contact line vicinity) and macro- (bubble) scales.



Contact: Pierre Colinet (pcolinet@ulb.ac.be), Alexey Rednikov (aredniko@ulb.ac.be)

36) Experimental and/or theoretical analysis of "tears of wine" in alcoholic beverages

Summary: Spinning a glass of wine to smell the aroma would leave a thin film of wine deposited along the glass walls. Over time, the alcohol in this film being more volatile evaporates leaving the water behind. This results in a difference in the surface tension between the edge of the film (concentrated with water so high surface tension) and the bulk of the wine (low surface tension) resulting in formation of tears as shown in Fig.1 (a). The detailed analysis of these patterns would reveal certain aspects such as alcohol content (quality) and viscosity (taste). However, we have found that these tear patterns are also affected by the ambient conditions such as temperature and relative humidity. This master thesis would be based on the analysis of these patterns for different initial alcoholic content and ambient relative humidity. Experiments will be conducted with commercial alcoholic beverages of different alcoholic content (typical wine: 10% alcohol to Vodka about 50% alcohol). A simple experimental setup consisting of a controlled cell will be used to initiate and visualize these wine tears on a reflective substrate. The image similar to Fig. 1 (b) will be used for analysis. A suitable numerical model will be developed in order to estimate the film thickness and its variation with the relative humidity.



(a) (b)

Figure 1 (a) Tears of wine as created by Gin tonic (about 37.5% alcohol) **(b)** Wine tears generated on reflective substrate in laboratory for analysis.

Contact: Senthil Kumar (sparimal@ulb.ac.be) and Pierre Colinet (pcolinet@ulb.ac.be)

37) Microencapsulation of pharmaceutical active compounds by spray drying. A numerical and experimental optimization of the process.

Summary: Microencapsulation is a formulation operation commonly encountered in the pharmaceutical industry. It typically consists of adding an "encapsulating" agent to a liquid solution containing a dissolved pharmaceutical active ingredient. Then, the solution is dispersed as fine drops in a hot air stream (in a device called a spray dryer). The subsequent evaporation of the solvent generates an increase of the encapsulating agent concentration within the drops (especially at the liquid-gas interface), until the onset of a sol-gel transition. The finished product is therefore a powder, with each particle composed of a "shell" of the encapsulating agent, containing the active ingredient, thus protected from the environment. Although used for a long time in industry, the physical and chemical mechanisms taking place during microencapsulation are still poorly understood today. Therefore, the goal of this Master thesis is to improve this understanding, through experimental studies (at different scales) and mathematical modelling. The aim is also to use, in a combined way, the experimental and modelling results in order to optimize the microencapsulation operation in a specific case: the encapsulation of gallic acid, a polyphenol with anti-oxidant and anti-oxidative properties.

Contact: Benoit Haut (bhaut@ulb.ac.be)

38) Intermittent drying of Baker's yeast pellets. A new way to improve the quality of the dried product?

Summary: Yeasts are microorganisms widely used in the food industry (e.g. in the making of bread and beer). Yeasts are produced by fermentation. At the end of the fermentation, the culture medium is filtered and the filtration cake obtained is converted into small cylindrical or spherical pellets of one or two millimetres in diameter. Each of these pellets is an agglomeration of yeast cells, with water between them. In order to extend the shelf life of this product, the yeast pellets can be dried. However, this drying should be done with caution, as exposure to too high temperatures or too much removal of water can have a significant negative impact on the quality of the product (e.g. the ability of the yeasts to release CO_2, as part of bread making). In collaboration with the Puratos company, the aim of this Master thesis is to analyse the impact of an intermittent realization of the drying of yeast pellets on the kinetics of this drying and on the quality of the end product. By "intermittent", it is understood that the drying is carried out by successive phases of drying at high rate and drying at low (or zero) rate. It has already been shown for several products that such an intermittent drying can have beneficial effects on the quality of the end product. This analysis will be performed by the combination of drying experiments, at different scales (scale of a part of the porous medium, pellet scale and dryer scale), and mathematical modelling. The comparison of the experimental and modelling results should make it possible to highlight the key phenomena involved during an intermittent drying of yeast pellets and to understand their impact on the kinetics of the drying and on the quality of the end product.

Contact: Benoit Haut (bhaut@ulb.ac.be)

Physical Chemistry and Polymer Science (FYSC) – VUB

39) Explorative study of self-healing powder coatings:

Summary: Traditionally, powder coatings are applied by heating up thermoplastic or thermosetting particles to induce flow, and eventually to cure (i.e. crosslink) the material in the case of thermosets. In the latter case, this results in processing temperatures above 150 °C, unsuitable for heat sensitive substrates (e.g. wood). In this master thesis, the feasibility of self-healing powder coatings based on reversible Diels-Alder (DA) bonds will be investigated. The working hypothesis is that by using such materials, flow at high temperatures (= breaking of the reversible bonds) can be decoupled from cure at lower temperatures (= formation of the reversible bonds) enabling a coating process at lower temperatures than traditional thermoset powder coatings, which is crucial for heat sensitive substrates. The following will be explored: rheometric study of flow, dynamic mechanical analysis (DMA) of cure during cooling, study of thermo-mechanical stability and upper temperature limitations, role of side reactions, …

Contact: Jessica Mangialetto (Jessica.Mangialetto@vub.be), Niko Van den Brande (npvdbran@vub.be)

40) 2. Development and characterisation of novel adaptive bio-based composites:

Summary: This master thesis project will focus on the development and characterization of adaptive wood-based composites made of renewable binders and fibres. Both renewable binders and fibres will originate from wood-based sources and therefore contribute to a more carbon-neutral material production. By the integration of adaptive properties, such as self-healing and reshaping based on either reversible Diels-Alder (DA) or supramolecular chemistry, the service lifetime of the final wood-based composites will be increased and such composites may be reprocessable. The following will be explored: preparation of adaptive wood-based composites (from e.g. solvent or extrusion), determination of fibre dispersion quality in the composite, characterization of thermomechanical behaviour by rheometry and dynamic mechanical analysis (DMA), …
This project is defined in the frame of a collaboration with the Flemish Institute for Technological Research (VITO). Based on the student's mobility, some work may take place in VITO, but this is not a requirement.

Contact: Marlies Thys (Marlies.Thys@vito.be), Niko Van den Brande (npvdbran@vub.be)

41) Advanced thermal characterization of materials for organic photovoltaics and/or NIR photodetectors:

Summary: Solution-processable organic photovoltaics (OPV) and photodetectors (OPD) have gained ever-increasing attention due to advantages over their inorganic counterparts, such as printability, flexibility, light weight, and low cost. The final morphology will greatly influence the performance and stability of a device. A thorough characterization of such materials (polymers or small molecules) is therefore required to gain insight into the phase behaviour, and link this to device performance. FYSC has extensive experience in the characterization of OPV materials by advanced thermal analysis (e.g. rapid heat/cool DSC and chip calorimetry) and complementary techniques (e.g. SEM, AFM, etc.). While the research will take place in FYSC, it is part of a collaboration with research groups at Hasselt University, who are specialized in synthesis of novel materials and device manufacture. This subject will make students familiar with the exciting and quite recent field of organic electronics, and their study by advanced thermal analysis techniques.

Contact: Zhen Liu (Zhen.Liu@vub.be), Niko Van den Brande (npvdbran@vub.be)

42) Study of dehydration of Portland cement paste and the fines obtained from recycled concrete.

Summary: Due to enormous growth of cement demand, its production represents 5% of annual anthropogenic global CO_2. Recycling of cementitious material in construction waste can be an efficient pathway to lower CO_2 emission, protect natural resources and reduce environment pollution. After thermal treatment, hardened cement can regain its hydration capacity. So, this work will emphasizes on studying the cementitious characteristics and the relative rehydration capability of dehydrated cement paste and also a dehydrated fine fraction obtained from recycled concrete rich in cement at different temperatures ranging. For the characterisation of the hydrated and dehydrated cement physicochemical and mechanical tests will be carried out.

Contact: Eduarda Baptista – eduarda.baptista@vub.be
Hubert Rahier – hrahier@vub.be ; M.P. Delplancke - mpdelpla@ulb.ac.be

43) Recovery and study the properties of the sand obtained from the fines of recycled concrete:

Summary: Concrete is a hardened building material created by combining a chemically inert mineral aggregate (usually sand, gravel or crushed stone), a binder (natural or synthetic cement), chemical additives, and water. Once concrete is the most widely used man-made material its production has a huge environmental impact. Thus, from the global environmental point of view of preservation and effective utilisation of natural resources, it is beneficial and necessary to recycle it. However, concrete recycling can be very challenging especially the fine fraction obtained after crushing. This fraction is a mixing of hydrated cement, sand and aggregates. So, this work will emphasizes on studying the sand recover and its characterisation. For the characterisation of the recovered sand physicochemical and mechanical tests will be carried out.

Contact: Eduarda Baptista – eduarda.baptista@vub.be
Hubert Rahier – hrahier@vub.be ; M.P. Delplancke - mpdelpla@ulb.ac.be

44) Low-CO_2 hybrid cements, from waste products:

Summary: Our world is built upon concrete. Concrete is the most-used man-made material in the world. The main component is ordinary Portland cement (OPC) which is responsible for 8-10% of global anthropogenic CO_2 emissions. One way to reduce the CO_2 emissions is to lower the cement content by using SCM (supplementary cementitious materials), i.e. by-products from other industrial processes such as fly ash or slag. However, due to their limited reactivity the amount of OPC that can be replaced is limited (approx. 30%). To achieve higher replacements, alkali-activation could be a path forward. In this subject you will focus on the production and properties of a new type of cement, starting from a solid waste (non-ferrous metallurgical slag) and a liquid activator. The mechanical properties of the cement must be optimized (ratio solid waste to activator). This implies some physicochemical characterization, as well as mechanical characterization. The aim is to minimize the eco-footprint of the final product, while retaining decent mechanical properties.

Contact: Jorn Van De Sande (Jorn.Van.De.Sande@vub.be)
Hubert Rahier (Hubert.Rahier@vub.be)

45) Additive manufacturing of reversible polymer network composites for sensing applications:

Summary: The addition of electrically conductive nanomaterials (carbon black, graphene, CNT) to reversible polymer networks (RPN) results in conductive polymer nanocomposites (cPNC) with dynamically reversible properties that could be used for advanced processing and manufacturing. Feasibility studies have proven the possibility to extrude the RPN into filaments that can be used for filament printing. cPNC's based on the same polymer matrices show prove to be promising candidates for additive manufacturing
Sensor designs will be printed using conductive and non-conductive RPN to assess the feasibility of sensing damage inside the printed materials and structures. The focus of this project will be on the materials

production and characterization, the optimization of the printing process and the assessment of the quality of the printed structures. This project is performed in parallel to a master thesis project at the R&MM group for validation towards applications for strain and damage sensors and self-healing assessment of the printed structures.

Contact: Joost Brancart (joost.brancart@vub.be)
Guy Van Assche (guy.van.assche@vub.be)

46) Rheokinetics and reactive modelling of additive manufacturing techniques:

Summary: Recent explorative studies have demonstrated the possibility to extrude filaments from in-house developed self-healing materials for fused deposition modelling (FDM) of soft robotic devices. The reaction kinetics of the reversible polymer networks (RPN) are well-understood, however, a detailed understanding of the rheological processes during processing (reactive filament extrusion) and manufacturing (3D printing) are required to improve the quality of the produced filaments and the properties of the manufactured products. In this study a thorough rheokinetic evaluation will be performed of the reversible polymer networks (RPN), modelling the development of the material properties (viscosity, (de)gelation, elastic modulus) with respect to the progress of the reversible network-forming reactions. Modelling of the production and manufacturing processes.
This project is partially in collaboration with KU Leuven.

Contact: Joost Brancart (joost.brancart@vub.be)
Guy Van Assche (guy.van.assche@vub.be)

Materials Engineering, Characterization, Synthesis and Recycling (4MAT) – ULB

47) Ultimate fine-grained residues left after treating street-sweeping solids could be valorized after all: exploration of a thermal mode of treatment dealing with their actual contaminant physico-chemical composition, including the effect on specific surface:

Summary: The Suez Remediation company located in Grimbergen treats contaminated soils and street sweeping residues coming from the Brussels-Capital Region. After treatment, there are a number of sub-product residuals which are currently not valorised at all. The fine-grained output material has to go to landfill. Reusing this matter, or at least a portion of it, would constitute an eco-friendly proposition, contributing to the circular economy. However, to achieve this aim, the contaminants which are present in these treatment
residuals have to be destroyed or to be extracted. Thermal treatment could constitute an interesting track to do this and will be explored in the Master thesis. A detailed physico-chemical characterization of these solid residuals will help identifying what would eventually be the valid reuse and valorization options.

Acronym : Desorb

Contact: M. VERBANCK (mikeverb@ulb.ac.be), P. D'ANS (pdans@ulb.ac.be), G. DIELIE (gdielie@ulb.ac.be)

48) "Greener" and affordable materials for thermochemical heat storage:

Summary: The reduction of greenhouse gases emissions imposes stringent conditions on the thermal performances of dwellings. In addition to a deep thermal insulation, non-fossil sources of heat are required. Solar heat is a good candidate but generates heat mostly during summertime, while the demand is during wintertime. To solve this, thermal batteries can be designed based on hygroscopic chlorides, bromides or sulphates, encapsulated in a porous matrix like silicagel, metal-organic frameworks,... At the scale of a dwelling, several tons of materials are needed. Their production must be extremely efficient to improve the "value for money" of the stored heat. In this work, the candidate will select one such material and identify the most promising route for its large scale production. The proposed strategies include the use of secondary materials, the improvement of well known processes or the identification of new cheap matrices. For this work, the interested student will access 4MAT facilities, including reactants, recycled materials and characterization tools (SEM-EDX, XRD, XRF, ICP and porosimeter). A life-cycle analysis and a cost analysis are strongly advised to validate the propositions.

Contact: P. D'ANS (pdans@ulb.ac.be), F. BASTIN (frbastin@ulb.ac.be)

49) Towards the electrochemical valorization of valuable elements from secondary sources: electrochemical properties of critical elements in non-conventional solvents:

Summary: The scarcity of resources leads to the need of new solutions for the recycling of "rare" metallic elements, notably rare earths and elements like tantalum. This issue is crucial for electronic waste, but also for other waste flows like wind turbine magnets, batteries,… Processes are difficult to develop because these elements are generally dispersed and their value is still too low to justify short term developments. This situation may change rapidly in case of shortage. There is thus a need of understanding of the extraction processes of these elements. Recent developments in the field of electrolytes (deep eutectic solvents) may open new ways in their recovery. In this work, we propose to select a relevant secondary resource of a given element and to consider its electrochemical behavior in a non-conventional electrolyte. This can be done either based on components from secondary sources or model samples. Techniques are available for the electrochemical testing at CHANI department (Fac. Science) where similar studies were carried out for precious metals using cyclic voltammetry. In addition, and depending on the preliminary results, the interested student will access 4MAT department equipment: SEM-EDX, XRD and ICP for sample characterization.

Contact: P. D'Ans (pdans@ulb.ac.be), T. Doneux (Thomas.Doneux@ulb.ac.be)

50) Additive manufacturing technology for aeronautical applications: Influence of heat treatments on microstructure and mechanical properties of Al- and Ti-alloys:

Summary: Additive manufacturing (AM) is very promising in aeronautics in order to build light 3D metallic parts with complex geometries. Electron Beam Melting (EBM) and Selective Laser Melting (SLM) are additive manufacturing techniques that print the parts layer-by-layer based on a 3D computer model. Titanium alloys (e.g. Ti6Al4V) and aluminum alloys (e.g. AlSi10Mg) are widely studied depending on the mechanical requirements of the part.
However, AM processes generate particular microstructure inducing anisotropic mechanical properties. AM parts also present defects such as lack of fusion or gas porosities that are inherent to the process and that are detrimental for mechanical properties, especially in fatigue. In those (2) master theses, the students will work on the optimization of heat treatments in order to tune the microstructure and improve the mechanical properties of the parts. The underlying mechanisms of material deformation in traction and the microstructure evolution will be investigated.

Contact: Promotor: Stéphane Godet (sgodet@ulb.ac.be tel: 02 650 36 48)
Supervisor: Gaëlle Couturiaux (gaelle.couturiaux@ulb.ac.be tel: 02 650 39 82)

Industrial partners: Safran Aero Boosters, SABCA

51) Development of nanostructured and multiphase glasses:

Summary: Window glasses traditionally consist of a fully amorphous structure. It makes them transparent but also intrinsically brittle. In the present project, a new approach will be followed and aims at producing glasses with enhanced mechanical properties and interesting optical properties. The strategy consists in introducing interfaces in the glass by phase separation and/or crystallization. Those processes should take place over very short distances (a few nanometers) in order to preserve the transparency of the glass. The phase separation and crystallization will be studied and characterized using high resolution scanning and transmission electron microscopy together with calorimetry and X-Ray diffraction. The optical and mechanical properties will also be studied. A particular interest will be devoted to the checial and thermal tempering of those multiphase structures.
This final year project has to be coupled with an internship at AGC

Contact: Promotor: Stéphane Godet (sgodet@ulb.ac.be tel: 02 650 36 48)
Supervisor: Gaëlle Couturiaux (Gaelle.Couturiaux@ulb.ac.be , tel: 02 650 39 82)

Industrial partner: AGC FlatGlass

52) Thermomechanical treatment of a high-entropy alloy: link between process parameters, microstructures and mechanical properties:

Summary: High-entropy, also called multi-principal element alloys, are a combination of 5 or more chemical elements in near equiatomic ratios. Those new alloys show interesting properties that can challenge and sometimes even exceed properties presented by conventional alloys in different domains as cryogenic or high-temperature mechanical properties, resistance to irradiation… The mechanisms responsible for such good properties are not completely understood. While in some aspects high-entropy alloys resemble closely conventional alloys, it is probable that new mechanisms are to be discovered.
The alloy we are interested in is the equiatomic CoCrFeMnNi which shows exceptional strength, ductility and tenacity at cryogenic temperatures. However, its strength at ambient temperature is much smaller than in

conventional alloys. In order to strengthen the structure, alloying elements (Al, Si…) are added in CoCrFeMnNi in order to form new hard phases.
In this project, thermomechanical treatments (rolling, annealing steps) will be used in order to finely tune the distribution and size of those new phases. Those microstructural features will be characterized using Optical Microscopy, SEM, EBSD and XRD and the mechanical properties measured in tension and by hardness indentation. Linking process parameters, microstructural and mechanical properties is the key to fully understand the mechanisms involved in this new type of alloys.

Contact: Promotor: Stéphane Godet (sgodet@ulb.ac.be tel: 02 650 36 48)
Supervisor: Dorian Hachet (dhachet@ulb.ac.be , tel: 02 650 65 50)
Industrial partner: Aperam

53) Quenching and Partitioning steels: Investigation of microstructural development and mechanical properties:

Summary: The constant query for cheap, strong and ductile materials in the automotive industry led to the last generation of Advanced High Strength Steels (AHSS): the quenching and partitioning steels. The heat treatment consist of a partial quench from full or partial austenitization, to form a control fraction of martensite. The material is then kept at an intermediate partitioning temperature to allow for austenite stabilization, achieved via carbon enrichment from the supersaturated fraction of martensite. The final microstructure should ideally consist of carbon depleted martensite and retained austenite at room temperature. The process is however not ideal; competing reactions occurs such as bainite transformation and carbide precipitation.
Up to now, it is well known that all these microstructural processes are occurring simultaneously and there is a strong interest for a deeper understanding of each of the separated processes as well as their simultaneous occurrence. A deep understanding of the complete process is needed in order to optimize the carbon enrichment of the austenite, and therefore to optimize the combination of strength and good ductility of the material.
The proposed master thesis consists in the first hand of a complete microstructural characterization of Q&P steel in relation with its process parameters. The characterization techniques used are dilatometry, X-Ray diffraction, Electron Backscatter Diffraction (EBSD), Scanning Electron Microscope (SEM), Optical Microscope, and others. In the second hand, a modeling approach will be used to push further the understanding of the thermodynamics and kinetics of the microstructural processes (martensite transformation, carbon diffusion, austenite stabilization, and bainite transformation). Finally, the tensile properties in relation with the microstructural development and process parameters will also be investigated.
Contact: Promotor: Stéphane Godet (sgodet@ulb.ac.be tel: 02 650 36 48)
Supervisor: Eve-Line Cadotte (Eve-Line.Cadotte@ulb.ac.be)
Industrial partner: CRM Group, Arcelor-Mittal

54) Nitrogen fixation by inductively coupled RF plasmas:

Summary: Nitrogen is a crucial element in the growth of plants and living organisms. Unfortunately, atmospheric nitrogen (N_2) is hardly accessible to most living beings because of its extremely stable triple bond which requires very high activation energies to break. To become available nitrogen should be bonded to oxygen or hydrogen through a process called nitrogen fixation. Most of the non-biological ammonia is produced by the Haber Bosch process at high pressure, medium temperature and in presence of an iron based catalyst. This process consumes almost 2% of the world total energy production and emits 300 million metric tons of CO_2 per year. New approaches are necessary. Among several alternatives, non-thermal plasma processes are considered to be very attractive for N_2 fixation. The theoretical limit of energy consumption of N fixation via non-thermal plasmas is more than 2,5 times lower than the energy consumption of the Haber Bosch process. In this project, we will explore the possibility to fix nitrogen through oxidation in an inductively coupled plasma. The gas phase composition will be investigated by chromatography and mass spectroscopy. The plasma itself will be characterized by optical emission spectroscopy and Langmuir probe. The effect of various parameters (pressure, proportion N_2/O_2, injected power…) will be studied.

Contact: Promotor: Delplancke Marie-Paule (mpdelpla@ulb.ac.be, tel 02 6502902)

55) Study of efflorescence in modified cementitious materials:

Summary: Efflorescence is a phenomenon observed on cement-based material, which leads, upon exposure to water, to the whitening of freshly prepared cement-based materials (mortar, concrete). In most cases, absorption of water into the cement matrix, is followed by dissolution of the calcium hydroxide (always present in a cement matrix), transfer to the surface and crystallization at the surface upon water evaporation. This crystallization of calcium hydroxide, which converts into calcium carbonate upon reaction with CO_2, leads to strong whitening of the surface.
Silicone-based additives are used as post treatment and integral water repellent to reduce water penetration of cement-based material. Reduced water penetration is expected to lead to reduced efflorescence. However, there are situations where, despite the use of silicone integral water repellent and despite a strong reduction of water penetration, a strong efflorescence is observed upon water penetration.
The objective of the work is to understand how efflorescence can happen, despite low water penetration and based on the understanding study, to propose and test new solutions to reduce efflorescence. Analytical testing of surfaces showing efflorescence or not, impact of degree of cement hydration, impact of integral water repellent, can be considered in this study.

Contact: Promotor: Delplancke Marie-Paule (mpdelpla@ulb.ac.be, tel 02 6502902)
Industrial partner: Dow

56) Dimensional stability of glasses for large interactive displays:

Summary: Modern communication technology uses larger and larger interactive screens (up to 2300*1500 mm^2) including a large number of functionalities. Those screens are based on sheets of glass that could be subjected to chemical tempering, which induces a compressive stress at the surface by ion exchange. This treatment drastically improves the mechanical properties such as scratch resistance of the glass. Thermal treatments are also applied to the glass. Unfortunately, the dimensional changes induced by these high temperature treatments are not fully reversible and cannot be predicted up-to-now. Nevertheless these changes must be taken into account in the production line to provide products that fulfill requirements of the display industry.
In this master thesis, we will investigate the influence of process parameters, such as treatment time, glass thickness, treatment temperature, quenching…, on the dimensional stability of one industrial glass composition used for large display devices. The work will involve the fine characterization of the process itself and of the resulting materials. The depth of treatment will be measured by EDX coupled to the scanning electron microscopy and optical method. Correlations between the treatment conditions and the dimension variation will be proposed.
This master thesis will be developed in close collaboration with the European Technovation Center of AGC, which is located in Gosselies (Belgium).

Contact: Promotors: Delplancke Marie-Paule (mpdelpla@ulb.ac.be, tel 02 6502902)
Stéphane Godet (sgodet@ulb.ac.be tel: 02 650 36 48

Industrial partner: AGC

57) Synthesis of Hydroxymethylfurfural by reaction of cellulose with hydrogen sulfate:

Summary: Hydroxymethylfurfural, also named 5-(hydroxymethyl) furfural, is a potential carbon-neutral feedstock for the production of fuels and other chemicals. It has attracted lately a lot of attention as it is also regarded as having potential therapeutic properties. This compound results from sugar degradation and can be found in sugar-containing food after a thermal treatment.
Synthetizing this molecule from recycled materials would be of interest. In this master thesis, we propose to explore the degradation of cellulose in concentrated sulfuric acid to evaluate the yield in hydroxymethyl furfural and to identify by-products of the reaction.
Different characterization methods will be applied to identify the products and the starting materials.

Contact: Promotors: Delplancke Marie-Paule (mpdelpla@ulb.ac.be, tel 02 6502902)
Schmitz Guy

Physical chemistry / Microgravity Research Center (MRC) – ULB

58) Vizualisation through in blood vessels by digital holographic microscopy:

Summary: Digital holographic microscopy allows to refocus objects recorded out of focus and to measure, with a nanometric accuracy, the optical thickness of transparent particles. For those reasons, it is a valuable technology to measure fluxes in 3D. In particular, it is used to analyze dynamical fluxes of platelets and red blood cells. However, actual vessels are covered by an epithelium that may disturb the imaging quality. For this master thesis proposed in collaboration with the Laboratoire de Médecine Expérimentale (ULB – CHU Charleroi), we propose to study the methods to improve the image quality in presence of such disturbing layers. The master thesis will target both experimental and software works.

Contacts: Prof. Frank Dubois, frank.dubois@ulb.ac.be,
Prof. Karim Zouaoui Boudjeltia, Karim.Zouaoui.Boudjeltia@ulb.ac.be

59) Drop-by-drop manufacturing and testing of double-layer ultra-capacitors:

Summary: Additive manufacturing – a technique for manufacturing complex 3D object "layer-by-layer" – was first introduced in the '70, but it is only at the beginning of the XXI century that this technique became widely used in many industrial applications, thanks to the introduction of more advanced tools and processes such as stereo-lithography and laser sintering. In recent years, 3D-printing triggered a real technological revolution still on-going.
An intriguing possibility to achieve layered structures opportunely functionalized could consist in depositing and evaporating successive layers/drops of fluid dispersed with micro/nano particles. Playing on the dispersed phase materials (conductive/dielectric) it will be possible to manufacture a composite ultra-capacitor for hand-held devices and photovoltaic systems.
The proposed work will then focus on characterizing those assemblies and their properties respect to current load, self-discharge, and lifetime.

Contacts:
Dr. Carlo Saverio Iorio, ciorio@ulb.ac.be
Dr. Christophe Minetti cminetti@ulb.ac.be

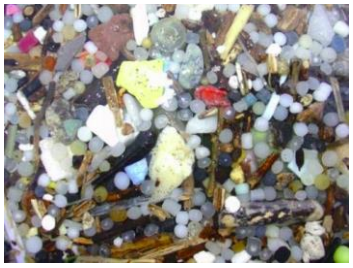
60) Smart management of de-icing systems for aeronautical and marine applications:

Summary: The formation of ice on airfoils is detrimental for the overall aerodynamics performances because it dramatically decreases the ability of the airfoil to create lift while sharply increasing drag. For an airplane to be approved to flight into icing conditions, it should be equipped with special ice-control systems that are extremely costly and inefficient in terms of power consumption. In general, the anti-icing system is turned on before the flight when ice is visually detected by direct inspection, a procedure that has been often criticized, especially after the air crash due to icing condition of Air Ontario Flight 1363 and American Eagle Flight 4184.
The purpose of this work is to develop a smart management de-icing system, which is capable of detecting the formation of ice in real time as well as counteracting to eliminate the icy spots in an energy-efficient way. The device, based on an integrated thermoelectric matrix, is able to detect ice by sending power pulses across the matrix and analyze the response signals. Those latter should determine the position in the matrix of the icy spots and trigger the heaters closer to the detected point of ice formation.

Contacts:
Dr. Carlo Saverio Iorio, ciorio@ulb.ac.be
Dr. Christophe Minetti cminetti@ulb.ac.be

61) Microparticles uptake by complex fluids under periodic excitation:

Summary: The proposed project is devoted to the investigation of the uptake of microparticles by vidcoelastic fluids under periodic excitations. The technological, medical and environmental applications of this work are far-reaching. One of the examples is the uptake of microplastics by the aquatic environments, which leads to disruption of ecological systems and accumulation of microplastics in tissues of marine organisms and even humans. The spectrum of sizes and shapes of microparticles is extremely broad. For example, there is a plethora of microplastics that can be shaped as beads, disks, bullets, rods, cubes, dumbbells and fibres, while the majoring of secondary microplastics in oceans have irregular shapes, see figure below. Their sizes vary from a few of micrometres up to a few millimetres. The proposed work will focus on a topology of particles in viscoelastic liquid under external shaking. The experimentally observed structures will call for the theoretical explanation.



Contact: Dr. Valentina Shevtsova (vshev@ulb.ac.be)

62) Supercritical carbon dioxide as a green solvent:

Summary: The current practical interest in CO_2 application is driven by peculiarly high solvent strength of CO_2 in near- and supercritical conditions. The solvent strength of CO_2 is highly tuneable, which allows easy separation of solute and solvent. This makes CO_2 a highly desirable new 'green' solvent. We aim to make the breakthrough in comprehension of dynamics of mixtures in the states far from their thermodynamic equilibrium. We will finalize development of novel high-pressure set-up designed for measurement of the diffusion in CO_2-rich liquid mixtures. These measurements are vital in view of CO_2 sequestration in saline aquifers and depleted oil reservoirs. The proposed work will focus on study diffusion of hydrocarbons in supercritical CO2.

Contact: Dr. Valentina Shevtsova (vshev@ulb.ac.be)

63) Why molecules move along a temperature gradient?

Summary: Molecules drift along temperature gradients, an effect called thermophoresis, the Soret effect, or thermodiffusion. The molecules of the mixture redistribute, forming concentration gradient that normally follows thermal one. The effect is slow and can play a visible role in large, geological, scales. It affects redistribution of species in underground oil reservoirs staying millions of years in geothermal gradient; it can affect redistribution of salinity in ocean producing impact on climate change. Finally, thermodiffusion allows the microscale manipulation of small particles. In liquids, its theoretical foundation is the subject of a long-standing debate initiated by Belgian Nobel prize winner I. Prigogine. The proposed work can be focused either on experimental or numerical side. An optical diagnostics of superior sensitivity and precision, namely interferometry, will be used for measurements of thermodiffusion coefficients in hydrocarbon mixture. On numerical side the redistribution of mixture components will be analysed using open software.

Contact: Dr. Valentina Shevtsova (vshev@ulb.ac.be)

64) Dynamic weting properties in pulsating heat pipes:

Summary: Heat pipes are sued to transfer heat and are present in many installations, as in each personal computer, trains, chemical plants etc…. Two phase flows are ensured the process, and the properties in pulsating heat pipes depend a lot on the wetting properties. Finding the good fluid is essential in particular in pulsating heat pipes. Also, dynamic behaviour, to be viewed and understood with our fast camera is essential for any improvement and adaptation.

Contacts: Prof Stefan Van Vaerenbergh svanvaer@ulb.ac.be
Dr. Quentin Galand qgaland@ulb.ac.be

65) Oscilllating mass transport in a temperature gradient:

Summary: Mass transfer in solution is occurring in binary solution as a result of the temperature gradient, a process named thermodiffusion. By interferometry and relevant model analysis, we want to investigate what occurs when the temperature gradient is socillating nd deduce interesting properties for later usage.

Contacts: Dr. Quentin Galand qgaland@ulb.ac.be
Prof Stefan Van Vaerenbergh svanvaer@ulb.ac.be

66) Study of demixtion by shadowgraphy.

Summary: Demixtion in binary mixtures occur when changing temperature or compositin. In preparation of an experiment that will be carried on the Chinese Space Station, the work will be carried experimentally and with the available image processing tools

Contact: prof Stefan Van Vaerenbergh svanvaer@ulb.ac.be

Subjects proposed by 3BIO-BioControl /Modelling and Control of Bioprocesses – ULB: Pages

67) Green deep eutectic solvent for the regeneration of waste wool fiber:

Summary: Wool is a renewable, protein-rich material with great potential to be used for producing environment-friendly materials. A large quantity of wool wastes are produced annually, leading to the discard of protein resources and environmental contamination. The recycling of wool is of great significance for the application of keratin. This project focuses on the development of a benign deep eutectic solvent (DES). The candidate will acquire various skills related to physiochemical characterization techniques such as thermogravimetry/differential scanning calorimetry, protein electrophoresis, scanning electron microscope, and amino acid analysis. We hypothesize that the results of the study can lead to a green approach for the regeneration of wool keratin without damaging the long chain of peptides leading to possible reuse of waste wool for production of natural fiber.

Contact: Amin Shavandi amin.shavandi@ulb.ac.be

68) Implantable natural polymer-based electrode for stimulation and repair of neurons:

Summary: Peripheral nerve injuries can be repaired by autograft, allograft, or nerve conduits. This project aims to develop implantable hydrogels for nerve tissue engineering applications using natural polymers such as chitin, keratin, and carbon nanotubes (CNTs). Knowing that electrical stimulation can enhance nerve regeneration and stimulate neural stem cells, in this study electrically conductive biomaterials will be fabricated for neural stimulation and neural tissue engineering applications. In order to manufacture a soft and biocompatible chitin-keratin based electrically conductive scaffold, deep eutectic solvents will be used for dissolution of the polymers and dispersion of CNTs. The physiochemical properties of the developed biomaterials such as morphology, mechanical stability and chemical composition will be evaluated. The proposed biomaterial should be nontoxic and able to attract neurons in order to regenerate nerve tissue, therefore in vitro cell cytocompatibility assays will be performed. We hypothesized that chitin-keratin biomaterial provides a matrix that is well tolerated by the cells, and that it would be suitable for cellular infiltration.

Contact: Amin Shavandi amin.shavandi@ulb.ac.be

69) Glycerol fermentation from lignocellulose biomass

Summary: Glycerol is considered a green chemical commodity and therefore inserted into the list of the top 30 chemical compounds of most interest from the world green chemistry society. In this thesis the student will attempt at producing glycerol using a complete bio-based process starting from lignocellulosic biomass via yeast fermentation. The glycerol so obtained will be subject of further catalysis for its conversion into other interesting chemicals in a joint collaborative research project with University of Namur and UCLouvain. The student will have the opportunity to dialogue daily with professional scientists and professors, will mostly learn how to operate CSTR bioreactors at various scale from 100ml to pre-pilot 20L, and learn analytical techniques based on state of art HPLCs, GC and IC. The thesis should be preferably written in English

Contact: David Cannella, david.cannella@ulb.ac.be

70) Microbial degradation of recycled PET plastic: applied biochemistry/fermentation

Summary: In our lab we pioneer biochemical methods for increasing the reactions rate and final yields of several polymer degrading enzymes by applying new chemical and physical stimuli and ultimately design the reactor better tailored for polymer conversion into smaller molecules or their direct fermentation. The

biochemical mechanisms behind the enzymatic hydrolysis of PET chains remember closely the enzymatic degradation of biological biopolymers, therefore in this thesis the candidate will deal with applying the technology developed for the biochemical degradation of lignocellulose to the PET plastic degradation using newly isolated plastic degrading bacteria. Besides the microbiological skills the student will also learn the basis of dielectric spectroscopy in collaboration with the physics department at the faculty of Sciences-ULB. Moreover the student will have the opportunity to collaborate scientifically with foreign institutes located in Denmark (Aalborg and Aarhus Universities). For this and thesis writing purposes a high fluency in English is preferable.

Contact: David Cannella, david.cannella@ulb.ac.be

71) Mathematical modeling for optimizing intracellular trehalose accumulation in yeast fed-batch cultures

Summary: The general context of this study concerns yeast cell cultures in fed-batch bioreactors, i.e. within reactors which are fed over time with liquid culture medium containing the required species for an efficient yeast growth. There exist a lot of applications, from baker's yeast production to the one of therapeutic molecules, or biofuels. The general goal is to mathematically analyze the key factors influencing the accumulation of trehalose (TRE) within Saccharomyces cerevisiae cells cultured in bioreactor, and to deduce feeding profiles which allow maximizing this accumulation. Several studies have proved the key role of TRE whose accumulation allows increasing yeast cell resistance to diverse stresses caused by the surrounding environment. The main goal is to build a mathematical model which allows predicting the time profiles of S. cerevisiae yeast concentration, of the main extracellular species involved in the bioreactor culture medium (glucose, ammonium, ethanol) and of intracellular TRE. This model will have the following features: description of overflow metabolism phenomena, description of glucose and ammonium coordinated uptakes, description of intracellular TRE accumulation, use of continuous differentiable kinetic models. It will take inspiration on former results obtained at 3BIO-BioControl (A. Richelle et al., Computers and Chemical Engineering, 61, 220-233, 2014). The model will be used to determine the optimal bioreactor feeding conditions which maximize TRE accumulation. Experimental validation of the obtained results will be performed based on data available at 3BIO-BioControl (and possibly data collected from new experimental campaigns). This work is part of a collaboration with Puratos company.

Contact: Philippe BOGAERTS (philippe.bogaerts@ulb.ac.be), 3BIO-BioControl, UD5.111a, 02/650.4076

72) Metabolic model-based optimization of hybridoma cell fed-batch cultures

Summary: Hybridoma cell fed-batch cultures are used in biopharmaceutical industries for producing monoclonal antibodies. Dynamical macroscopic models of such processes are of outmost importance for their monitoring, optimization and control. Macroscopic models have been identified and validated at 3BIO-BioControl for hybridoma cell fed-batch cultures (Z. Amribt et al., Biochemical Engineering Journal, 70, 196-209, 2013; Richelle and Bogaerts, Biochemical Engineering Journal, 100, 41-49, 2015) based on available experimental data. The first one has been used for determining optimal feeding profiles which maximize the biomass productivity obtained at the end of the process (Z. Amribt et al., Bioprocess and Biosystems Engineering, 37, 1637-1652, 2014). Another dynamical model has been recently developed based on a simplified metabolic network and metabolic flux analysis tools (Bogaerts et al., Journal of Process Control, 60, 34-47, 2017). The aim of this work is to revisit the process optimization based on this newly available model and to compare optimal solutions derived from macroscopic models and metabolic models.

Contact: Philippe BOGAERTS (philippe.bogaerts@ulb.ac.be), 3BIO-BioControl, UD5.111a, 02/650.4076

73) Analysis and development of methods for estimating the fluxes in food webs describing coastal ecosystems

Summary: The analysis of marine ecosystems involves food webs which describe the mass flows between different trophic compartments. For low trophic levels, these compartments are phytoplankton, zooplankton, bacteria, detritus, etc., while for higher trophic levels they concern different fish species which are directly linked to the former levels through the zooplankton they predate. Quantifying these web flows allows understanding the behavior of many types of marine and coastal ecosystems and the impact of natural and anthropogenic changes (climate, fishery intensity, nutrient enrichment, etc.). Similarly to metabolic networks, food webs are generally underdetermined as the number of unmeasured web fluxes is higher than the available linear equality constraints (mass balances and available measurements). Even by considering the inequality constraints representing physiological constraints like lower and upper bounds on bacterial growth efficiency or detritus degradation rate, it is not possible to determine unique values for the web fluxes. Linear Inverse Models (LIMs) consist of the set of equality and inequality equations which link the web fluxes (van Oevelen et al., Ecosystems, 13, 32-45, 2010). Different algorithms have been proposed to tackle the underdeterminacy problem. The goal of this work is to test and/or develop different algorithms for determining the food web flows in some practical case studies for which the food web and data / constraints are available in the literature (e.g., Soetaert and van Oevelen, Oceanography, 22(1), 128-143, 2009).

Contact: Philippe BOGAERTS (philippe.bogaerts@ulb.ac.be), 3BIO-BioControl, UD5.111a, 02/650.4076