Internship subject - Attention aux titres et contenus détaillés des sujets qui doivent être sans lien direct et immédiat avec une application industrielle. Donner un contenu uniquement basé sur des verrous scientifiques.

Multicriteria Analysis and Relationship / Models between Chemical Structure, Rheology and Standard Characterization on Novel Bituminous Binders

Internship Supervisor
Alain Quignard / Jérémy Barbier

Internship Context
The high sulfur heavy fuel market is continuously decreasing, especially with the implementation of the worldwide mandatory use of very low sulfur marine fuel from January, 1, 2020. The heavy ends conversions and purification is used to transform low value products with a decreasing market towards high value clean transportation fuels and products. The internship will focus on the study of converted heavy products to be used as bituminous binders.

Internship Description
The main objective is to understand the relationship between chemical structure, rheology and standard
characterization of converted heavy-ends to be used as bituminous binders. The internship will consist on three main steps:

- To perform an extensive bibliographic subject in the field
- To settle a multicriteria analysis on an existent in-house data base related to the conversion of heavy-ends in order to understand the relationship between chemical structure (i.e. Size Exclusion Chromatography (SEC) hyphenated to Mass Spectroscopy, High Performance Liquid Chromatography (HPLC), C\textsuperscript{13} NMR,…), rheological behavior and measurements (viscosity, elastic modulus,….) and standard characterization used for bituminous binders, such as softening point, penetration,….
- To propose and to develop models to understand the behavior of these novel binders and to link chemical structure, rheology and standard characterization

Scientific skills
Analysis, correlation, model, process & refining processes

Background
Chemical school / university with an interest toward analysis, data analysis and process

Other Information
- Duration: 4 to 6 months (preferred)
- Date: since February 2020
- Location: IFP Energies Nouvelles – Etablissement de Lyon
- Please submit your application with a resume and a motivation letter to the IFPEN internship supervisors:
  
  Alain.quignard@ifpen.fr
  Jeremie.barbier@ifpen.fr
Characterization of diffusion properties of catalyst supports by PFG-NMR

<table>
<thead>
<tr>
<th>Internship supervisor</th>
<th>name: Leonor DUARTE</th>
</tr>
</thead>
<tbody>
<tr>
<td>function:</td>
<td>Research Engineer</td>
</tr>
<tr>
<td>service:</td>
<td>IFPEN</td>
</tr>
<tr>
<td>e-mail:</td>
<td><a href="mailto:leonor.duarte-mendes-catita@ifpen.fr">leonor.duarte-mendes-catita@ifpen.fr</a></td>
</tr>
</tbody>
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<thead>
<tr>
<th>Location</th>
<th>Solaize – Lyon area (France)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Starting date:</td>
<td>2020-03-01</td>
</tr>
<tr>
<td>Duration:</td>
<td>5-6 months</td>
</tr>
<tr>
<td>Application deadline:</td>
<td>2020-01-31</td>
</tr>
<tr>
<td>Traineeship grant:</td>
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</tr>
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</table>

Abstract/work package/short bibliography/illustration:

Heterogeneous catalysts have applications in very different fields, such as the production of fuels and of chemical intermediates, synthesis of drug molecules or decontamination of liquid or gaseous effluents. These type of catalysts are porous solids, in which molecules diffuse in order to reach the catalytic sites (see Figure 1). The performance of the catalytic process can therefore be strongly impacted by the properties of their complex pore network, such as pore size distribution and multi-level organization. It is hence of great interest to better characterize the pore network and the diffusive properties of the catalysts supports.

The objective of this internship is to characterize the diffusion properties of different molecules in catalysts supports, namely in gamma-alumina type supports. For this purpose, the so-called pulsed field gradient NMR technique (PFG-NMR) at high magnetic field will be used. This work will focus on different aspects: a) effect of the molecule size, b) effect of the mean square displacement of the molecules and c) effect of the molecule-surface interactions. The aim of this work is to relate these data to the porous network properties and to give new insights on the relation between the mass transfer properties of catalyst supports and the geometry of their porous network. The student's work will cover several aspects: bibliographic study, preparation of samples and measurement of diffusion coefficients by PFG $^1$H NMR.

Figure 1 – Representation of a porous solid

References:


<table>
<thead>
<tr>
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<th>Heterogeneous Catalysis, Characterization of Porous Solids, Diffusion, PFG-NMR</th>
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<tr>
<td>Required skills for the internship (max 30 keywords)</td>
<td>Rigour, organization, proactivity, curiosity</td>
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</table>
DETECTION OF GASOLINE ADULTERATION USING HIGH RESOLUTION MASS SPECTROMETRY AND CHEMOMETRICS

<table>
<thead>
<tr>
<th>Internship supervisor</th>
<th>name: LACOUE-NEGRE Marion, BERLIOZ-BARBIER Alexandra</th>
</tr>
</thead>
<tbody>
<tr>
<td>function:</td>
<td>Research Engineers</td>
</tr>
<tr>
<td>service:</td>
<td>IFPEN</td>
</tr>
<tr>
<td>e-mail:</td>
<td><a href="mailto:marion.lacoue-negre@ifpen.fr">marion.lacoue-negre@ifpen.fr</a></td>
</tr>
<tr>
<td>Location</td>
<td>Solaize – Lyon area (France)</td>
</tr>
</tbody>
</table>

Starting date: 2020-04-01 ________________________ Application deadline : 2020-01-31 _______________
Duration: __5-6_________ months Traineeship grant:________ YES

Abstract/work package/short bibliography/illustration:
Gasoline adulteration is a frequent problem world-wide due to its environmental, health and economic effect. Adulterated fuels often result in low engine performance and engine life. It has also been proven that combustible engines with adulterated fuels often produce excessively high quantities of vapors and toxic gases, i.e. CO and NO\(_X\), hence its environmental concerns. Gasoline dilution can be easily achieved with cheap and less taxed solvents of similar composition, such as mineral spirits, kerosene, rubber solvents, petrochemical naphtha, diesel, and thinner or larger amounts of alcohol, mainly ethanol. It is then needed to have valuable analytical methods to detect adulteration of gasolines.
Petroleum products such as gasolines are complex mixture containing tens of thousands of chemically distinct organic compounds. The study of such products requires fast and accurate chemical fingerprinting of hydrocarbons, specifically, distributions of heteroatoms, rings, and double bonds. These information can potentially highlight the adulteration of gasolines. The characterization of such petroleum products requires resolving analytical techniques such as Fourier Transform Ion Cyclotron Resonance Mass Spectrometry (FT-ICR/MS). The main benefit of FT-ICR/MS analysis is also its main drawback: numerous peaks are detected and identified then providing thousands of molecular formulas. However, classical data processing methods are often not sufficient to visualize simultaneously all data generated and explore fully the resulting FT-ICR MS analyses. In this context, chemiometric tools are required.
Thus, this study aimed the development of an analytical method to detect the adulteration of gasoline associated to chemometric methods to i) classify the gasolines according to their source of contamination and ii) evaluate the potentiality of quantification of the adulterant. Various chemometric tools will be used such as Principal Component Analysis (PCA), Hierarchical Cluster Analysis (HCA), Least Discriminant Analysis, Soft Independent Modeling of Class Analogy (SIMCA) and Partial Least Squares regression (PLS). Previous to the analytical part, a Design of Experiment will be developed to create the most relevant mixtures taking into account all the variability of the study. The student will be able to rely on the recent work done on the exploitation of HRMS data by chemometric approach at IFPEN\(^1\).

References:
\(^1\) Guillemant, J. et al., Chemometric Exploration of APPI(+)-FT-ICR MS Data Sets for a Comprehensive Study of Aromatic Sulfur Compounds in Gas Oils, *Analytical Chemistry* (2019), 91, 18, 11785-11793

<table>
<thead>
<tr>
<th>Keywords, areas of expertise</th>
<th>Gasoline adulteration, high resolution mass spectrometry, chemometrics, classification, regression</th>
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</thead>
<tbody>
<tr>
<td>Required skills for the internship</td>
<td>Knowledge in mass spectrometry and/or chemometrics, Rigour, organization, strength of proposal</td>
</tr>
</tbody>
</table>
TRANSMISSION ELECTRON MICROSCOPY STUDY OF THE STRUCTURAL DEFECTS AND POROUS NETWORK OF ZEOLITE CRYSTALS THERMALLY INDUCED BY A WATER VAPOR TREATMENT

Internship supervisor

name: Virgile ROUCHON  
function: Research Scientist  
service: Materials characterization department  
e-mail: virgile.rouchon@ifpen.fr

Location

Solaize – Lyon area (France)

Starting date: 2020-02-01  
Application deadline:  
Duration: 5-6 months  
Traineeship grant: YES

Abstract/work package/short bibliography/illustration:

The valorization of biomass into fuel or molecules for chemistry requires the use of catalytic solids with acidic properties. Among these solids, zeolites are a family of minerals consisting of bridged silicon and aluminum oxide tetrahedra forming structures with exceptional microporous and acidic properties. The primary acidity of the zeolites stems from the charge compensation of the structure by protons bound to bridged oxygen atoms between the aluminum and silicon atoms of the structure. In order to optimize the acidity of the zeolites, chemical and thermal treatments are carried out, inducing defects in the crystalline structure, while generating a porosity additional to the structural porosity, in particular via the expulsion of the structural Al. The relationships between the formation of this porosity, structural defects and the evolution of acid properties are poorly understood today.

In order to bring new elements of understanding, we propose to use high-resolution transmission electron microscopy on samples subjected to thermal treatments under water vapor in order to characterize on the one hand the distribution of the secondary pore network induced by the treatment, and secondly the local structure modification at the immediate periphery of these pores. Both approaches will require the use of electron tomography and electron crystallography based on the acquisition of high resolution TEM images. Particular attention will be paid to the research and optimization of the observation conditions in order to identify an optimum for the observation of zeolites, a material very sensitive to the electron beam irradiation.

This internship will be hosted in the CARMEN joint research laboratory between CNRS, Université de Lyon, Université de Strasbourg, ENS Lyon and IFPEN, bringing together the Villeurbanne CRMN laboratories, PHENIX in Paris, IPCMS in Strasbourg, and IFPEN in Lyon. The internship will take place mainly at IFPEN, and will include several stays at the IPCMS, co-advised by Ovidiu Ersen. This internship may be followed by a PhD thesis on the same topic.

Keywords, areas of expertise (max 30 words)

Zeolite, transmission electron microscopy, tomography, electron crystallography, méso and nanoporosity

Required skills for the internship (max 30 keywords)

Rigour, organization, strength of proposal
Chemical recycling of plastics: Purification of monomers obtained from polyethylene terephthalate (PET) depolymerization

Supervisors
David Chiche, david.chiche@ifpen.fr, (+33) 4 37 70 22 89

Context
The production of plastics or polymers has been growing rapidly for several decades, and accounted for 350 million tons worldwide in 2017. In Europe, the consumption of plastics represents around 100 kg per year and per inhabitant. As a consequence, plastics recycling has become a major issue, in order to reduce the ecological and environmental impacts related to their production and consumption. These include finding solutions to increase the collection rate of plastics, their sorting, and the development of dedicated recycling processes adapted to the different types of polymers.

In the scope of this internship, we will focus on the specific case of PET (polyethylene terephthalate). PET, which constitutes ~7% of the plastics produced, is extensively used for the packaging of food and cosmetic products. Recycling processes exist at industrial scale for the treatment of non-colored transparent PET, such as that commonly used for water packaging. The treatment of colored and/or opaque PET still remains an issue, as this PET contains additives which prevent its recycling in closed loop (mainly organic dyes and/or mineral pigments). These additives alter the final appearance of the recycled PET as well as other properties of the polymer (mechanical properties, ...).

The development of recycling processes dedicated to colored and opaque PET is a major challenge for reducing waste, developing new resources for the production of recycled PET, and therefore reducing the use of fossil resources to produce PET.

Description
The aim of this internship is to study the purification of monomers resulting from a depolymerization based PET recycling process. The impurities might originate from the remaining additives initially in the PET to be treated, such as polymerization catalyst, dyes, pigments, ... and/or the degradation of the monomer or side reactions that might occur during the depolymerization process. The monomers obtained after purification can be reused in a polymerization process for the production of recycled plastic.

Different possible routes allowing monomer purification will be studied (purification by crystallization, adsorption of impurities, ...). A bibliographic study will be performed by the student. An experimental work will be carried out to study the different selected routes.

Monomers before and after purification will be mainly analyzed using gel permeation chromatography and HPLC-MS (quantification of oligomers and other organic molecules), ICP (elemental analysis), UV-visible spectroscopy, and colorimetry. The solids used in the scope of the adsorption study will also be characterized (Hg porosimetry, N₂ adsorption, XRD, SEM, elemental analyzes, etc.).

Desired profile
Master 2 level in chemical science, polymer science, materials science, analytical science, chemical engineering

Required education
See desired profile.

Additional informations
Duration: 5-6 months
Period: February to July 2020
Place: IFPEN, Solaize (69360), France
Transportation: shuttle Lyon-Feyzin (10 min) then bus line GE2 (5 min)
Candidature: Thank you for sending your CV and cover letter to the aforementioned supervisors
Sujet de stage
Synthèses, caractérisations et évaluations de catalyseurs zéolithiques pour la production de biocarburants

Responsable de stage
Christophe BOUCHY (christophe.bouchy@ifp.fr) – Direction Catalyse, Biocatalyse et Séparation
Raquel MARTINEZ FRANCO (raquel.martinez-franco@ifp.fr) – Direction Catalyse, Biocatalyse et Séparation

Contexte du projet
Les enjeux climatiques globaux nécessitent notamment la réduction des émissions des gaz à effet de serre dans le secteur du transport. L'émergence de filières de production de biocarburants s'inscrit dans cette problématique. Des biogazoles de synthèse peuvent ainsi être obtenus par hydrotraitement d'huiles végétales ou de graisses animales ou encore par conversion thermochimique de la biomasse par gazéification et synthèse Fischer-Tropsch. Dans les deux cas les effluents produits sont constitués de paraffines à longues chaînes carbonées et nécessitent d'être isomérisés afin d'améliorer leur propriétés à froid et de pouvoir les incorporer dans le pool carburant.

L'isomérisation des paraffines longues est effectuée grâce à des catalyseurs bifonctionnels qui mettent en jeu une fonction acide de type zéolithe associée à une fonction métallique. On souhaite développer des catalyseurs les plus sélectifs possibles envers l'isomérisation, au détriment du craquage. Les réactions de craquage conduisent en effet à des produits de plus faible valeur et doivent être minimisées. Il est connu que les propriétés de fonction acide sont clés pour contrôler la sélectivité du catalyseur.

Description du projet
L'objectif du stage est de modifier la zéolithe en ajustant son acidité afin d'améliorer la sélectivité du catalyseur. Cette modification pourra être effectuée par différents traitements comme par exemple la désalumination. Cette étude aura également pour but la compréhension des phénomènes pouvant conduire à l'amélioration de la sélectivité en isomérisation du catalyseur. Le travail de l'étudiant sera majoritairement expérimental, au sein des laboratoires de l'IFPEN-Lyon, et concernera donc toutes les étapes nécessaires à l'étude : la modification de zéolithe, la préparation de catalyseurs, leurs caractérisations physico-chimiques, la réalisation de tests catalytiques et l'analyse des résultats.

Profil recherché
Compétences en chimie minérale, synthèse de matériaux, catalyse hétérogène, méthodes de caractérisation physico-chimiques. Rigueur, autonomie, esprit d'initiative.

Ecole(s), formation(s) souhaitée(s)
Élève ingénieur : ECPM (Strasbourg), ESPCI (Paris), ENSCP (Paris), ENSCL (Lille), ENSCM (Montpellier), ENSCR (Rennes), ENSMu (Mulhouse), ENSCPB (bordeaux), CPE (Lyon), IST Lisbonne

Informations complémentaires
Durée souhaitée : 6 mois
Période souhaitée : 2 mars 2020 / 28 août 2020

Lieu : IFPEN, Solaize (69360), France
Transports : voiture conseillée. Train TER Lyon-Feyzin (10 min) puis bus ligne GE2 (5 min)

Lieu : IFPEN, Rueil-Malmaison (92500), France
Transports : ligne RER A station Rueil-Malmaison et prendre le bus 244 arrêt Geneviève Couturier, ou le bus 27, arrêt Bois-Préau. Vous pouvez également emprunter les lignes 144 et 467arrêt Rueil-Ville

Candidature : Merci d’adresser votre candidature (CV et lettre de motivation) aux responsables de stage
Training topic
Synthesis, characterizations and catalytic evaluation of zeolitic catalysts for biofuels production

Supervisors
Christophe BOUCHY (christophe.bouchy@ifp.fr) – Catalysis, Biocatalysis and Separation Division
Raquel MARTINEZ FRANCO (raquel.martinez-franco@ifp.fr) – Catalysis, Biocatalysis and Separation Division

Context
Environmental concerns about climate change require, among other things, the reduction of greenhouse gas emissions in the transport sector. The emergence of biofuel production at the industrial level can help to deal with this problem. Biodeisels can be obtained by hydrotreating vegetable oils or animal fats or by thermochemical conversion of the biomass by gasification and Fischer-Tropsch synthesis. In both cases, the effluents produced consist of paraffins with long carbon chains. They need to be isomerized in order to improve their cold properties before their incorporation into the fuel pool.

The isomerization of long chain paraffins is carried out by means of bifunctional catalysts. Such catalysts involve an acid function like a zeolite associated with a metal function. It is desired to develop a catalyst as selective as possible for the isomerization reaction. Indeed cracking reaction is undesired as it produces shorter paraffins of lower value. It is known that the acid function properties are key for controlling the selectivity of the catalyst.

Description
The aim of the internship project is to modify the zeolite by adjusting its acidity in order to improve the selectivity of the catalyst. This modification can be carried out by different treatments such as dealumination for instance. This study will also aim at understanding the phenomena that can lead to the improvement of the isomerization selectivity of the catalyst. The work of the student will be mainly experimental and performed within the laboratories of IFPEN-Lyon. It will therefore concern all the steps necessary for the study: the zeolite modification, the catalyst preparation, their physicochemical characterizations, the catalytic tests and analyzing the results.

 Desired profile
Skills in mineral chemistry, material synthesis, heterogeneous catalysis, physicochemical characterization methods. Rigor, autonomy, initiative, dynamic and highly motivated by experimental work.

Required education
Engineering school, Bachelor of Science (BSc)

Project leader  N° project/ study  Department’s head  Section
J.P. HERAUD  PKA02.002  E. GUILLON  R065

Additional informations
Duration : 6 months  Period : March 2, 2020 / August 28, 2020

Place : IFPEN, Solaize (69360), France (10 km south of Lyon)
Transportation : shuttle Lyon-Feyzin (10 mins) then bus line GE2 (5 mins)

Place : IFPEN, Rueil-Malmaison (92500), France
Transportation : RER line A station Rueil-Malmaison and take bus 244 get off at Genevieve Couturier, or bus 27 get off at Bois-Préau. You can also use lines 144 and 467, get off at Rueil-Ville

Candidature : Thank you for sending your CV and cover letter to the aforementioned supervisors
TRAINEESHIP OFFER - 2019

IFPEN – Catalysis, Biocatalysis and Separation Division

Training topic
Creating porosity in NaY zeolites

Supervisors
Gerhard Pirngruber (gerhard.pirngruber@ifpen.fr)
Mathias Dodin (mathias.dodin@ifpen.fr)

Context
UltraStable Y zeolites are used as acid catalysts in numerous applications, in refining, petrochemistry, biomass conversion, etc. Zeolite Y is prepared in its Na-form NaY and subsequently transformed into an acid catalyst (called USY) by a series of ion-exchange steps and thermal treatments. These steps change the chemical composition of the zeolite and generate defects, which lead to the creation of mesopores within the (microporous) zeolite structure. Further chemical treatments can be applied to adjust composition (i.e. acidity) and porosity of the zeolite. It is, thus, possible to tune the catalytic properties of USY zeolites over a large range.

Description
The objective of the research project is to explore and combine novel methods of dealumination and creation of mesopores, with the aim of generating USY zeolites with original combinations of porosity and acidity. The project will make the student familiar with zeolite chemistry, chemical and thermal treatments as well as with the numerous analytical methods (XRD, porosity measurements, IR spectroscopy, NMR, etc.) used to characterize the zeolites before and after the modification steps.

Desired profile
Chemist or Chemical Engineer with affinity for Heterogeneous Catalysis, Zeolite Science, Physical/Analytical Chemistry

Required education
Master in Chemistry, Chemical Engineering or Material Science

Project leader
Guichard Bertrand
N° project/ study
PIV02/002
Department’s head
Méthivier Alain
Section
R064

Additional informations
Duration: 5 – 6 months
Period: between february and august 2019

Place: IFPEN, Solaize (69360), France
Transportation: shuttle Lyon-Feyzin (10 mins) then bus line GE2 (5 mins)

Place: IFPEN, Rueil-Malmaison (92500), France
Transportation: RER line A station Rueil-Malmaison and take bus 244 get off at Geneviève Couturier, or bus 27 get off at Bois-Préau. You can also use lines 144 and 467, get off at Rueil-Ville

Application: Please send your CV and cover letter to the aforementioned supervisors
Internship title
Evaluation of the performances of foam catalyst supports through kinetics, heat and mass transfer modeling

Advisor
Florent Allain, Yacine Haroun

Context
The context of this project is the performance evaluation of foam catalyst supports for different catalytic reaction application using multi-physics computational modeling.

Internship description
The goal of the internship is to:
- Realize multi-physics simulations using COMSOL software to evaluate the performances of foam catalyst supports for different applications in terms of kinetics, as well as heat and mass transfer.
- Study the impact of the different physical and shape properties of the foam support on the catalytic performances.

Domaines de compétences recherchés
- Chemical engineering
- Modeling and simulation
- Kinetics, heat and mass transfer
- COMSOL software knowledge would be appreciated

Ecole(s), formation(s) contactée(s)
Engineering schools, Master’s degree in chemical engineering
Informations complémentaires

- How long: 5-6 months
- When: 1st semester, 2020
- Location: IFP Energies Nouvelles – Lyon
- Transportation means: IFP Energies Nouvelles center of Lyon is located at 20 km to the south of Lyon. IFPEN is not easily accessible by public transportation. Therefore, a personal transportation mean is recommended, but not required. An IFPEN shuttle is accessible to all interns.
- Compensation: internship compensated by IFPEN
- Application: please send your application with CV and cover letter to the internship’s supervisor

Please contact: florent.allain@ifpen.fr, yacine.haroun@ifpen.fr
COMPETENCY OF XAS IMAGING AND RAMAN MAPPING ON HYDROTREATING CATALYSTS: IMPACT OF MOLYBDENUM CONTENT

Internship supervisor

- name: Christèle Legens and Elodie Devers
- function: Research Engineers
- service: IFPEN
- e-mail: christele.legens@ifpen.fr; elodie.devers@ifpen.fr; valerie.briois@synchrotron-soleil.fr

Location

IFPEN - Rd point de l’échangeur de Solaize, BP3, 69360 SOLAIZE Solaize – Lyon area (France) and Synchrotron SOLEIL L’Orme des Merisiers, 91190 Saint-Aubin (near Paris, France) – time repartition 2 months IFPEN /3 months SOLEIL

Starting date: 2020-02-01 or 2020-03-01
Application deadline: December 2019
Duration: 5 months
Traineeship grant: YES

In order to reduce the energy consumption of catalytic processes, one of the levers is to optimize catalysts. This optimization is accompanied by an ever-increasing need to characterize these solids. This is particularly the case for hydrotreating catalysts (sulfide molybdenum promoted by cobalt, doped with phosphorus and supported on alumina) that produce fuels and chemical intermediates with low environmental impact. The preparation of these catalysts is composed of a series of unit steps that will design the future properties of the solid: from impregnation on the alumina support of metal species based on molybdenum heteropolyanions (HPA) to activation in a sulfo-reducing medium to obtain the active phase, through maturation and drying. These steps of impregnation and maturation of the oxide catalysts are undergone and lead to a heterogeneous distribution of species on the support that can have a negative impact on the catalytic activity. However, the identification and quantification of these species remain a major challenge. To meet this challenge, we propose to characterize a series of CoMoP supported oxide catalysts with various Mo contents using 2 techniques:

- **2D mapping by Raman spectroscopy** will be used to identify and localize the molybdenum heteropolyanions at the surface of a sliced extrudate (Figure 1).
- On the same samples, spatially resolved **X-ray absorption chemical imaging** technique on the Quick-XAS ROCK beamlime of the SOLEIL synchrotron will be implemented to achieve the relative quantification of the different species identified previously (Figure 2). Thanks to a set of synthesized bulk references, this can be done by linear combination fittings.

![Figure 1](image1.png)
![Figure 2](image2.png)

The student will have to:
- Use the Raman spectroscopy technique and analyze the data on a series of about 7-8 catalysts
- Participate to synchrotron run for X-ray absorption chemical imaging and become familiar with data processing
- Synthesize solid HPAs references according to protocols from the literature

A PhD thesis is being considered as a continuation of this internship.

References:

2. L. Catita et al., Applied Catalysis A, General 547 (2017) 164-475

Keywords, areas of expertise

- Chemical/Process Chemical engineer, Catalysis, knowledge in spectroscopy is appreciated

Required skills for the internship

- Rigour, organization, strength of proposal, experimentation affinities, synthetic spirit
Internship vacancy announcement (IFPEN financed)

IFP Energies Nouvelles
Direction Conception et Modélisation de Procédés
BP3 – Rond-point de l'échangeur de Solaize
69360 SOLAIZE

Internship subject
Experimental study of solid liquid fluidization: particle shape effect. Local hydrodynamic measurements

Supervisor
Rim BRAHEM

Contexte
Particulate flows are widely encountered in industrial processes (catalytic, adsorption, combustion reactors...). Both Experimental and modeling efforts have been focused mainly on the description of hydrodynamic, thermal and / or reactive behaviors of spherical particles. However, in practice, various particle shapes are used, mainly based on extrudates with different shapes such as cylinders, trilobes or quadrilobes. The lack of appropriate laws taking into account a shape factor, presents a hindrance to the development of predictive CFD (computational Fluid Dynamics) models aimed at optimizing industrial process design and technologies.

Within the ANR project MUSCAT (IFPEN, IMFT (Institute de Mécanique des Fluides de Toulouse) and LGCT (Laboratoire de Génie Chimique de Toulouse)), the development of these lacking laws is intended through a multiscale approach associating both experimental and numerical methods.

Description
As the shape strongly influences the reactor hydrodynamics. We propose in this internship to investigate experimentally the particle shape effects on a liquid solid fluidized bed. Both spherical and cylindrical particles will be tested on a small rectangular column (width a~10 cm/ height H~2m/ number of particles~100000 particles). Expansion behavior under several superficial liquid velocities will be studied. The results will be used for the validation of a DEM-CFD model (not included in the internship).

Objectives:
A prior internship will provide overall measurements (overall expansions, pressure drop profiles) and initial results for local measurements. These latter are based on liquid velocity profiles and fast-imaging tracking for the evaluation of particles trajectories, velocities and orientations. This second internship aims at acquiring precise and exhaustive local measurements. Thus the candidate will be working at:

- the set-up of the experimental methods (in collaboration with the first internship candidate)
- providing a comprehensive and well written internship report with an appropriate bibliography on the subject
**Required competences**
Fluid mechanics, process / chemical engineering, experimental rigor, image processing

**Targeted schools**

**Complementary information**

- Internship duration: 6 months

- Desired period: starting from May-June 2020

- Place: IFP Energies Nouvelles – Lyon

- Transport: IFP Energies Nouvelles Lyon is located about 20 km south of Lyon. The institute is poorly served by public transport, a personal means of transportation is recommended but not compulsory. A public shuttle is available 2 hours in the morning and 2 hours in the afternoon.

- Financial compensation: compensation provided by IFPEN

- Application: If you are interested, please address your CV and motivation letter to the supervisor rim.brahem@ifpen.fr
**Sujet de stage**


**Responsable du stage**

O Thinon

**Contexte du stage**

In the development of a new chemical process, the most economically profitable and environmentally responsible process is generally preferred. For that, a techno-economic evaluation is done in order to estimate the costs of the process through the design of equipment and the consumption of utilities. This work is often based on the simulation of the process and needs experimental to establish the material and energy balances. The operating conditions and the nature of catalysts, if used, can significantly impact the result of the economic evaluation. By using screening method, like high-throughput experiment, a lot of conditions can be tested rapidly. However, the simulation and the design of process is a time-consuming work, especially with complex process producing several valuable products. As a consequence, with present methodology and tools, it is not possible to evaluate as many cases as expected.

**Descriptif du stage**

The objective of the training is to contribute to the development of a tool allowing to rapidly estimate and compare the cost of different processes schemes from well-defined parameters. For that, an applied case, based on petrochemical processes like the steam cracking, is proposed. Previous training work has already been done in 2017 and 2018 with the creation of a large data base and process design correlations for several operating units of the steam cracking process. The trainee will have to :

- complete the data base and correlations by simulation and design of further operating units
- integrate an economic evaluation methodology
- implement the correlations in a excel tool with a user-friendly interface

The training will require to make simulation and program writing in VBA excel macro.

**Domaines de compétences recherchés**
Chemical Engineering
Process Engineering
Process simulation : Pro II, ProSim
Programming language: Visual Basic or Visual Basic for Application (VBA Excel Macro)
Knowledge in Petrochemical

Ecole(s), formation(s) contactée(s)

Informations complémentaires

- Durée souhaitée : 6 month max
- Période souhaitée : From January 2020
- Lieu : IFP Energies nouvelles – Lyon
- Transport : le centre IFP Energies nouvelles Lyon est situé à environ 20 km au sud de Lyon. L’ IFPEN étant très mal desservi par les transports en commun, un moyen de transport personnel est recommandé mais non requis, une navette IFPEN étant accessible à tous les stagiaires
- Indemnisation : stage indemnisé par IFPEN

- Candidature : merci d’ adresser votre candidature avec CV et lettre de motivation à :
  olivier.thinon@ifpen.fr
# Internship Proposal

**IFP Energies Nouvelles**  
**Direction Conception et Modélisation de Procédés**  
**BP3 – Rond-point de l’échangeur de Solaize**  
**69360 SOLAIZE**

## Topic of the internship
Modeling of an aerated bioreactor under non-ideal mixing conditions: Application to the growth of the filamentous fungi *Trichoderma Reesei* followed by enzyme production used for biomass hydrolysis

## Supervisor
F.Augier and R.Rousset

## Context
The context of the internship is the scale-up of bioreactors for Ethanol Production from lignocellulosic biomass (also called 2nd generation ethanol).

The enzymes used for cellulose hydrolysis are produced by the filamentous fungi *Trichoderma Reesei*. The scale-up of the bioreactor requires to model precisely both the growth of the fungi and the enzyme secretion.

Furthermore, the modeling will have to handle simple fermentation broths (well homogenized) but also large fermentation broths as in industrial fermenters of hundreds of cubic meters (heterogeneously mixed).

## Internship description
The topic of the internship is to improve an existing bioreactor model in order to adapt it to heterogeneous conditions. This will be done by adding metabolism bio-kinetics mechanisms in the reactor model, and by developing a multi-zone framework able to mimic large bioreactors.

The topic is related to a current PhD dealing with the so called scale-down methodology and performing fungi cultures with dual-zone bioreactor or under unsteady substrate feed rate conditions. The present study will aim to simulate this scale down approach.
**Required skills**

Chemical Engineering and/or Biochemical Engineering  
VBA Programming / other language

**Background**

Chemical Engineering and/or Biochemical Engineering Schools

**Additional information**

- **Duration**: 5 – 6 months
- **Dates**: March-August 2020
- **Location**: IFP Energies Nouvelles – Lyon
- **Transport**: IFP Energies Nouvelles Lyon is located at 20km in the south of Lyon. A shuttle bus serve the TER train station of Feyzin which is connected to city center.
- **Salary**: Depending on the Education (from 750 to 1000€ /months)
- **Please send your CV and cover letter outlining your motivation to**:

  Frederic.Augier@ifpen.fr  
  Romain.Rousset@ifpen.fr
Internship offer

IFP Energies Nouvelles
Direction Conception et Modélisation de Procédés
BP3 – Rond-point de l'échangeur de Solaize
69360 SOLAIZE

Topic
Computational Fluid Dynamics modeling of two-phase flow in catalytic packed bed reactors

Supervisors
Yacine Haroun, Hanane Bouras

Context
The context of this project is to develop validated numerical tool able to simulate two-phase flow through fixed packed catalytic bed with different shape of catalyst. The purpose of the internship is to use Computational Fluid Dynamics modeling to improve the understanding of the impact of particle shape on gas and liquid flow (hydrodynamics, wetting) in fixed bed reactors.

Description
The purpose of the Internship is:

- To perform Computational Fluid Dynamics simulations of gas-liquid flow through fixed bed with different shapes of catalyst
- Compare simulation results to experimental measurement previously done,
- Improve the understanding of the impact of particle shape on gas and liquid flow (hydrodynamics, wetting) in fixed bed reactors.

The numerical model has been developed in ANSYS Fluent 19.2 CFD code, using some User Defined Functions “UDF”

Qualifications
- Chemical engineering
- Fluid mechanics
- Numerical simulation, CFD codes
- ANSYS Fluent knowledge is required

**Ecole(s), formation(s) contactée(s)**
Engineering schools (ENSEEIHT, ENSPG, ENSIACET, ENSIC, UTC, European University…), Master’s degree in fluid mechanics or chemical engineering

**Informations complémentaires**

- **Duration**: 5-6 months
- **Period**: 1st semester, 2020
- **Location**: IFP Energies Nouvelles – Lyon
- **Transportation means**: IFP Energies Nouvelles center of Lyon is located at 20 km to the south of Lyon. IFPEN is not easily accessible by public transportation. Therefore, a personal transportation mean is recommended, but not required. An IFPEN shuttle is accessible to all interns.
- **Compensation**: internship compensated by IFPEN
- **Application**: please send your application with CV and cover letter to the internship’s supervisor
  
yacine.haroun@ifpen.fr, hanane.bouras@ifpen.fr
# INTERNSHIP OFFER

**IFP Energies Nouvelles**  
Direction Conception et Modélisation de Procédés  
BP3 – Rond-point de l’échangeur de Solaize  
69360 SOLAIZE

## Subject

Study and optimization of distillation process schemes for the production of bio-products from enzymatic fermentation

## Supervisor

Ester TOTH

## Context

This internship is proposed within the framework of the development of bio-based products for the petrochemical industry for reducing energetic dependence on fossil fuels. However such development is facing technical and cost issues, requiring intensive R&D works. Research efforts are oriented towards both the development of more productive and more selective enzymes and towards process optimization.

## Internship Description

Many process schemes (using smart fractionation schemes with heat integration; process intensification with use of vapor recompression; dividing wall columns, In Situ Product Recovery…) are proposed in academic literature and in recent patents. However, many of them are at a conceptual stage only and need to be further investigated. The purpose of this internship is to simulate and evaluate those process schemes via the use of the Pro II process simulation software and IFPEN internal tools for AIBE production. A sensitivity analysis versus main process control parameters (e.g. alcohols yields and concentrations) and cost and market environment parameters (e.g. sugar cost, cost of steam and electricity…) will also be performed.

## Competences

Chemical Engineering; Process Design; Process Simulation; Economic evaluation; Innovation

## School / Education

Master students from Chemical Engineering Schools
Complementary Information

- **Duration**: 6 months
- **Période souhaitée**: anytime from January till October
- **Location**: IFP Energies nouvelles – Lyon
- **Transport**: the IFP Energies Nouvelles Lyon is located approximately 20 km south of Lyon. The IFPEN is poorly served by public transportation, so personal transport is recommended but not required, and an IFPEN shuttle is accessible to all apprentices.
- **Indemnisation**: stage indemnisé par IFPEN
- **Candidature**: merci d’adresser votre candidature avec CV et lettre de motivation au responsable du stage

Eszter.Toth@ifpen.fr
# Internship vacancy announcement

**IFP Energies Nouvelles**  
Direction Conception et Modélisation de Procédés  
BP3 – Rond-point de l’échangeur de Solaize  
69360 SOLAIZE

## Internship subject
Study of sulfur elimination reactions for the reduction of polluting emissions of fuels.

## Supervisor
Adrien Gomez, Ph.D., Process Design and Modeling Division  
Clementina Lopez-Garcia, Ph.D., Process Experimentation Division

## Contexte
This internship focuses on the study of thermodynamic equilibrium decomposition of sulfur compounds in fuel treatment processes.

## Description
As part of the development of eco-friendly processes and to limit the impact of fuels on the environment, IFPEN conducts intensive research to reduce pollutant emissions from thermal engines. The objective of this internship is to carry out a study focused on describing the thermodynamic equilibrium involved during elimination reactions of sulfur compounds. This study will contribute to the understanding of the experimental tests (in collaboration with the Process Experimentation Division).

The main objectives of this internship are:
- Carry out a bibliographical study on the thermodynamic modeling of the reactions of elimination of sulfur compounds,
- From experimental data available, a first thermodynamic modeling (tools available) based on some key sulfur species will validate the approach.
- A more complete study will aim to model the sulfur elimination equilibrium based on tests carried out on a real feeds.

## Required competences
Process engineering, chemical engineering.  
Good knowledge of thermodynamics and process simulation.
Complementary information

- Internship duration: 6 months
- Desired period: starting from March-April 2020
- Place: IFP Energies Nouvelles – Lyon
- Transport: IFP Energies Nouvelles Lyon is located about 20 km south of Lyon. The institute is poorly served by public transport; a personal mean of transportation is recommended but not compulsory. A public shuttle is available 2 hours in the morning and 2 hours in the afternoon.
- Financial compensation: compensation provided by IFPEN
- Application: If you are interested, please address your CV and motivation letter to the supervisor adrien.gomez@ifpen.fr
Sujet de stage - Attention aux titres et contenus détaillés des sujets qui doivent être sans lien direct et immédiat avec une application industrielle. Donner un contenu uniquement basé sur des verrous scientifiques.

CFD simulation of solid circulation control by using L-valves

Responsable du stage
Sina Tebianian - Benjamin Amblard

Contexte du stage
Controlled solid circulation rate in Chemical Looping Combustion is one of the most important aspects that determines the reliable operation. Non-mechanical devices such as L-valves represent simple, cheap and reliable means to control the solid circulation rate around the flow loops. However, their design, especially for large units, must take into account the operating conditions such as particle properties, pressure profile and solid circulation rate in order to be able to control the flow in the range of operation.

Descriptif du stage
In this work previously obtained experimental results obtained during operation of different L-valves will be compared with CFD simulations for validation. The CFD tool will be then used to simulate the system at large scale and study the effect of aeration geometry on its performance.
Domaines de compétences recherchés

Chemical engineer with understanding of multiphase flow, solid separation unit operations and CFD

École(s), formation(s) contactée(s)

Informations complémentaires

➢ Durée souhaitée : 5 mois

➢ Période souhaitée : Février – Juillet 2020
➢ Lieu : IFP Energies Nouvelles – Lyon

➢ Transport : le centre IFP Energies Nouvelles Lyon est situé à environ 20 km au sud de Lyon. L’IFPEN étant très mal desservi par les transports en commun, un moyen de transport personnel est recommandé mais non requis, une navette IFPEN étant accessible à tous les stagiaires

➢ Indemnisation : stage indemnisé par IFPEN

➢ Candidature : merci d’adresser votre candidature avec CV et lettre de motivation au responsable du stage

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