SUSCHEOPE (SUSTAINABLE CHEMICAL OPERATIONS)

Master Thesis Research Topics

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Our current researches, your future technologies

Summary

The SusCheOpe research group is devoted to the development of innovative research topics of potential industrial interest in the field of chemical reactivity, in particular promoted through heterogeneous catalysis, in separations and in process simulation.

- *Chemical reactivity is studied in different kinds of reactors (batch, semibatch and continuous) and is devoted to the production of fuels or materials, searching for raw materials and/or strategies with less environmental impact than traditional processes.*
- *The separation processes concern technologies such as distillation (batch and continuous), absorption and solid-gas separations (adsorption).*
- *The process simulation is based on innovative software through which it is possible to reproduce various kind of processes or parts of them. Process simulation, sometimes coupled with experimental activity, allows analysis and optimization of new technologies and plant schemes.*

Keywords

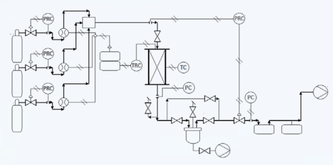
- **Industrial Chemistry**
- **Heterogeneous Catalysis**
- **Chemical Reactors**
- **Separation Processes**
- **Process Simulation**

Description: *Study of new catalytic materials for the conversion of syngas or syngas + CO2 (Biosyngas) to useful products as methanol or hydrocarbons. In this thesis the candidate will conduct the bench scale plant reported in the figure, based on a continuous packed bed reactor able to work until 30 bar and 400°C. The preparation and characterization (TEM, SEM, XPS, TPR, ICP) of the catalysts with traditional and innovative method will be important part of the work. Analytical quantification will be done by micro-GC, GC, TOC, HPLC. Modeling and simulation of the reactor, also in collaboration with POLIMI group, will be performed.*

Keywords: *biosyngas, heterogeneous catalyst, methanol, Fisher-Tropsch, characterization, simulation*

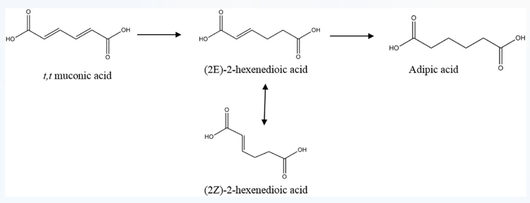
Activities*: plant management and use (40%); catalyst preparation and characterization (30%); analytical activities (10%); literature research, data analysis, modeling and simulation (20%)*

Collaborations in this topic*: Politecnico di Milano, Polytechnique of Montreal, Università di Perugia*



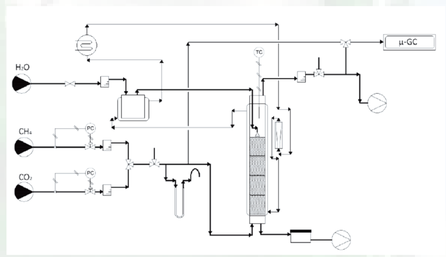
1. Fischer-Tropsch and methanol synthesis by heterogeneous catalysis

Description: Adipic acid is an important building block for the production of Nylon 6. Nowadays, it is produced starting from fossil source with a process characterized by a negative impact from an environmental point of view. New researches are conducted worldwide for its production starting from biomass with green processes. In this context, one possibility is to produce adipic acid in a two phases process. In the first one biomass are transformed in muconic acid by fermentative processes and in the second one muconic acid is reduced to adipic acid in a hydrogenation reactor with heterogeneous catalyst. Our group is working in this second step with different reactors and different catalysts.
Keywords: adipic acid, biomass, heterogeneous catalysis, reactor, simulation, LCA
Activities: literature research, data analysis, modeling and simulation (30%); experimental activities (70%)
Collaborations: Politecnico di Milano,



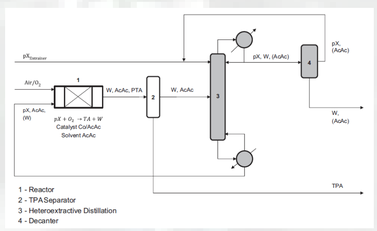
2. Production of adipic acid from biomass

Description: The purification of air from Volatile Organic Compounds (VOC) is a classical industrial problem for several processes. Among other technologies, the removal of these compounds using an absorption column is a highly interesting possibility. Different VOC compound or VOC mixture will be used in two different absorption columns, 1 m height, with classical water absorption or new innovative technology as the use of water/oil mixture to increase the solubilities of long hydrocarbons. Experimental activities and simulation studies will be performed to optimize the technology both from a chemical and economical point of view.
Keywords: absorption columns, VOC, water-oil mixtures, , simulation, LCA
Activities: literature research, data analysis, modeling and simulation (30%); experimental activities (70%)
Collaborations: Politecnico di Milano,



3. Purification of VOC by absorption columns

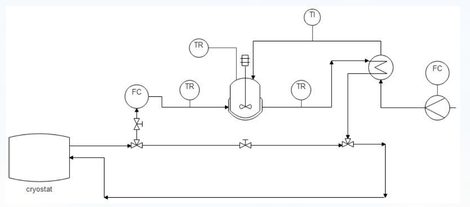
Description: The production of terephthalic acid occurs by the catalytic reaction of p-xylene with oxygen (or air), using acetic acid as a solvent, with the production of water as the main co-product. The acetic acid-water mixture thus produced must then be separated by means of an expensive distillation column. Our group proposed a new distillation configuration based on the use of the same p-xylene as an extractor solvent. This technology has been optimized through experimental activities, process simulation and techno-economic optimization. Now, we should check the entire terephthalic acid plant configuration. New experimental tests and new process simulations are necessary to continue the application study of the new technology.
This topic is to be considered as an example of the working method and of the thesis topics available, to be defined, in this line.
Keywords: terephtalic acid, distillation column, azeotropic distillation, reactor, simulation, economical analysis
Activities: literature research, data analysis, modeling and simulation (50%); experimental activities (50%)
Collaborations: Politecnico di Milano



4. Terephtalic acid optimization process by improvement in distillation column

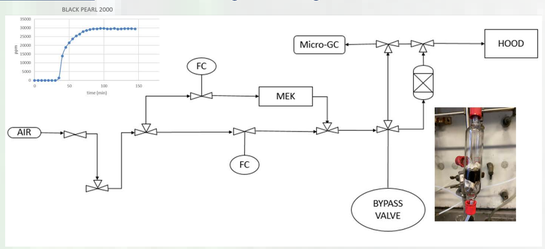
Description: A semi-batch reactor (SBR) is a variant of a batch reactor in which a reagent is added intermittently or continuously to another content as a batch in a vessel. The reactor developed in the research group can be conducted in batch or semibatch mode and is suitable for the collection of kinetic data and the verification of heat balances between the heat produced by the reaction and that disposed of in the external exchange jacket.It is possible to take into consideration in the research work different types of reactions for the data collections that will be the basis of the design of the industrial reactor and its optimization.

Activities: literature research, data analysis, modeling and simulation (30%); experimental activities (70%)
Collaborations: Università dell'Insubria



5. Semibatch reactors for kinetic data and heat balances

Description: Normal filter hoods for air purification are limited by the need for periodic regeneration or replacement of the adsorbent material. In this topic we want to produce a photocatalytic adsorbent material capable of adsorbing polluting molecules with high efficiency during the functioning of the hood and enter into photocatalytic regeneration during the period of non-activity of the hood. The balance between adsorbing properties and the presence of photoactive material represents the main point to be optimized in the work.
Keywords: Adsorption processes, activated carbon, air purification, regeneration, titanium dioxide, photocatalysis.
Activities: literature research, data analysis, modeling and simulation (10%); experimental activities (90%)
Collaborations: Prof. Mariangela Longhi



6.Air purification by photoactive adsorption processes

Collaborations

- Prof. Claudia Bianchi (Chem. Dep.)
- Prof. Ermelinda Falletta (Chem. Dep.)
- Prof. Ilenia Rossetti (Chem. Dep.)
- Prof. Mariangela Longhi (Chem. Dep.)
- Prof. Alberto Villa (Chem. Dep.)
- Prof. Flavio Manenti (Politecnico di Milano)
- Prof. Alessandro di Michele (Università di Perugia)
- Prof. Sabrina Copelli (Università dell'Insubria)
- Prof. Federico Galli, Daria Boffito (Polytecnique du Montreal, Canada)

References

- Purification of air from volatile organic compounds by countercurrent liquid gas mass transfer absorption process, INTERNATIONAL JOURNAL OF THERMOFLUIDS (2020).
- Toward Scaling-Up Photocatalytic Process for Multiphase Environmental Applications, CATALYSTS (2021)
- Experimental Methods in Chemical Engineering: Process Simulation , THE CANADIAN JOURNAL OF CHEMICAL ENGINEERING (2020)
- EYE4EDU: la realtà virtuale immersiva nell'impianto chimico ICP (2020).
- Sonophotocatalytic degradation of sodium diclofenac using low power ultrasound and micro sized TiO2, ULTRASONICS SONOCHEMISTRY (2020)
- Immersive virtual Crude Distillation Unit learning Experience: the Eye4edu project, COMPUTER CHEMICAL ENGINEERING (2020)

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