PhD in ENERGETICS

Research Title: From industrial CO2 streams to added value Fischer-Tropsch energy products and chemicals

Funded by	Dipartimento Energia (DENERG) – ICO2CHEM project (H2020)
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Context of the research activity	The overall aim of the ICO2CHEM project is to develop a new production concept for converting CO2 to white oils and aliphatic high molecular weight waxes. The products are used for wax emulsions and white oils to be used in coatings and sealant materials The properties of the raw materials will be tested against current fossil-based materials. The main raw material for the process is CO2, which is available from processes currently operating at a large industrial site with significant annual CO2 emissions. H2 is obtained as by product from a chlor-alkali plant on the site. Currently H2 is produced in excess and it is used mainly for energy production. Currently at this chemical production site about 2 million tons/a of CO2 is vented to the atmosphere, creating a huge GHG emission reduction potential. The core of this project is a combination of reverse water gas shift (RWGS) coupled with advanced, modular Fischer-Tropsch (FT) technology. The RWGS-step converts CO2 with H2 to carbon monoxide. The following FT-reaction step will be carried out in a novel intensified reactor recently developed and patented by Ineratec. Over 1500 kg of white oils and high-molecular weight wax will be manufactured using a container sized microstructured reactor system. Techno-economic and environmental assessments will be carried out to demonstrate the potential of the new concept in different locations and integration sites. A business plan will be formulated in the project for a follow-up of a commercial industrial demonstration project.
Objectives	Modelling of the whole process concepts for CO2 recovery including the product separation stage is the first task that is required. Mass and energy balances of each process configuration shall be carried out to calculate the expected product yields and energy efficiency of the proposed plant. The modelling work will start with the determination of reaction

	kinetics for RWGS and FT steps with the selected catalysts. Reaction kinetics will be then applied for the construction of the overall flowsheet simulation model including reactors (RWGS and FT) and separation part as well as recycle streams. The simulation model will be used for the optimization of reactor and process performance and for techno-economic analyses of the plant concept. A commercial flowsheet simulation software (e.g., Aspen Plus) will be used for the process simulation task. Energy integration of the system is important for economically and environmentally feasible process. For instance, synthesis reactions produce heat whereas RWGS reactor requires heat. Also, product separation by distillation involves the use of heat sources at different temperature levels. Off-gases from FT-synthesis could be used for energy production (e.g. they could feed an ICE) or as hydrogen source by reforming. Strategies and methodologies for the optimal integration of heat streams and energy contents will be calculated Finally, the techno-economic analysis of the whole plant concept shall be investigated also looking at energy and climate policy implications of a plant able to convert waste CO_2 into energy and chemical products.

Skills and competencies for the development of the activity	The candidate should have a degree that cover the topics of energy technology and energy systems modelling. The candidate should have experience on the process simulation and techno-economic analysis of energy systems. A good attitude toward team working and interaction within in an international framework of English-speaking academics and professionals is also required.