Industrial Processes Design

Process Development and Simulation

KEYWORDS: Energy efficiency / Process integration / Techno-economic analysis/ NETmix

LSRE-LCM has established industrial processes based on mixing technologies developed from CFD simulations. Exploiting these technologies requires assessing their application, so further developments lay on their integration into industrial processes. Process simulation tools were used to make this integration and benchmark new technologies. ASPEN has been used as the workhorse for this line and was mainly applied to integrating NETmix in CO2 capture and transport processes and extraction processes for biobased products. With the acquired expertise, this line has extended to other industries, namely a project with several industries in the packing sector.

Introduction

When the continuous production of hydrates was demonstrated in a lab pilot, in parallel with the process enhancement and optimisation, there was the need to integrate this process in industrial units. Several applications were devised for the hydrates, most related to the capture, transport and sequestration of CO_2. The exploitation of these applications was made by the CoLab NET4CO2, a collaborative laboratory founded by Prof. José Carlos Lopes that has several partners, including FEUP and the leading Portuguese oil company, Petrogal. Within the goals of NET4CO2, it was crucial to benchmark the hydrates production technology in several processes. In this report period, one of the main activities was the integrated process simulation of hydrates for CO2 capture, CO2 transport in hydrate slurries, and water desalination. These activities were developed within the framework of Isabel Fernandes's PhD thesis and Rita Martinho's MSc thesis, which used process simulation data to make LCA of thermal power plants with hydrates continuous production for CO2 capture. The hydrogen production from methane steam reforming was assessed with LCA in collaboration with NET4CO2 under Gustavo Rangel's MSc thesis. The MSc thesis on LCA was carried out in cooperation with Dr Aleksandra Ziemińska-Stolarska from Lodz University of Technology and Prof. Belmira Neto of LEPABE.

For the start-up of this line at LSRE-LCM, several researchers in the group underwent advanced training with ASPENtech in a course organised by LSRE-LCM and hosted at FEUP in 2019. This course covered several advanced features of ASPEN, including programable modules, energy integration and advanced cost modelling. Ten researchers from LSRE-LCM attended this course. With the expertise acquired on process simulation, other projects were carried out. One project consisted on the determination of properties of mixtures with carbon dioxide, which have applications in extraction processes studied in Product Engineering group.

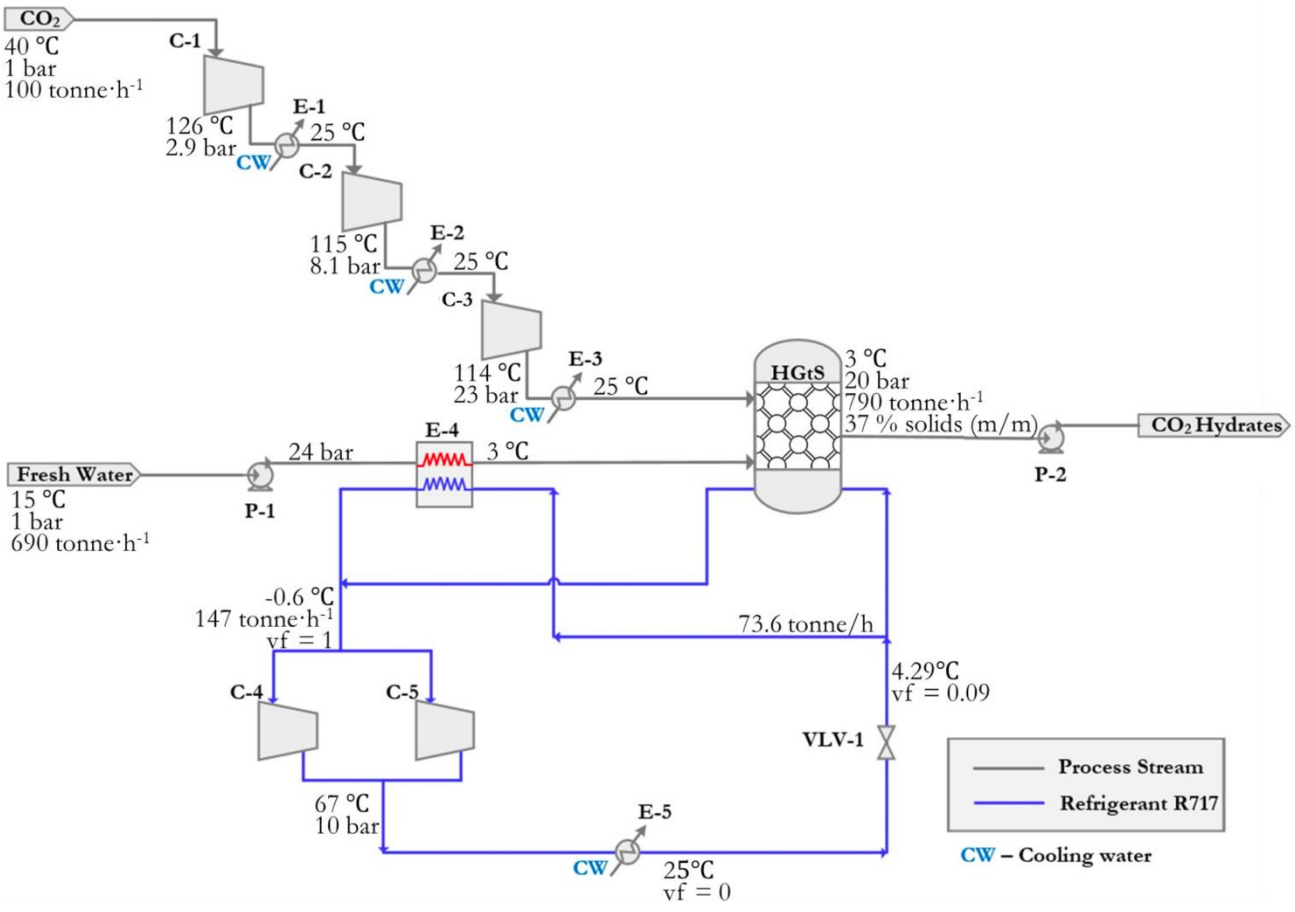

Fig 1. Process flow diagram for the continuous industrial production of CO2 hydrates with NETmix.

Current Development

NET4CO2

A key aspect of the hydrates technology is the heat transfer since the process takes place within a narrow window of temperature values, 0 to 5 ºC, and the pressure for the process is above 20 bar. This brings operational costs associated with chillers, compressors, and respective investment costs. The competitiveness of this technology depends on the best operational conditions, the best choice of equipment and the use of promoters that enable it to operate at more favorable conditions. Fig. 1 shows a layout of a process optimised for continuous hydrate production. The process simulation for the carbon dioxide enclathration is based on the model CSMGem (Colorado School of Mines – Gibbs energy minimisation).

Hidrates processes can also be used to separate CO_2 from other gases. Process simulations with ASPEN showed the ability to perform these operations at a cost of 67€/tonne of CO2. Furthermore, based on process simulation data, LCA showed that the hydrates technology enabled the mitigation of global warming potential by 79% for natural gas plants and 89% for coal power plants.

NETmix technology enables large heat and mass transfer rates with precise control of local conditions. This makes it a technology with considerable potential for application in methane reforming for hydrogen production. The technology assessment for methane reforming was based on the known mass and heat transfer rates of the NETmix technology. Process simulation of the industrial dry methane reforming (DRM) and steam methane reforming (SMR) was performed and coupled to LCA. This study showed a potential global warming reduction of 0.601 kg CO2 eq/MJ PCI for DMR and 1.60 kg CO2 eq/MJ PCI for SMR. These results motivated further advances in the particular design of a NETmix for SMR using CFD, which is being carried out by José Paula, a student of the PhD programme ENGIQ (Refining, Petrochemical & Chemical Engineering) in a project hosted at NET4CO2.

Extraction processes

An appropriate thermodynamic model is vital for simulating the multiple industrial processes involving carbon dioxide. This work used equations of state available in Aspen Plus to determine carbon dioxide's thermodynamic and transport properties (density, viscosity, and specific heat capacity) and its equilibrium in binary mixtures with water and ethanol. Results were compared with literature data for temperatures from 273 to 353 K and pressures up to 30 MPa. The best results for carbon dioxide's pure properties were given by the REFPROP and GERG-2008 models, with less than 0.5% overall relative error. Other models also produced accurate predictions within the global average absolute value of the relative error of less than 5%. Regarding the equilibrium of binary mixtures (carbon dioxide/water and carbon dioxide/ethanol), no model accurately covered the entire pressure and temperature range here considered.

This analysis is a step closer to simulating processes involving carbon dioxide in the Aspen Plus software, allowing the identification of appropriate thermodynamic models for different pressure and temperature ranges. Fig. 2 shows data from binary mixtures properties estimation using the models in ASPEN Plus.

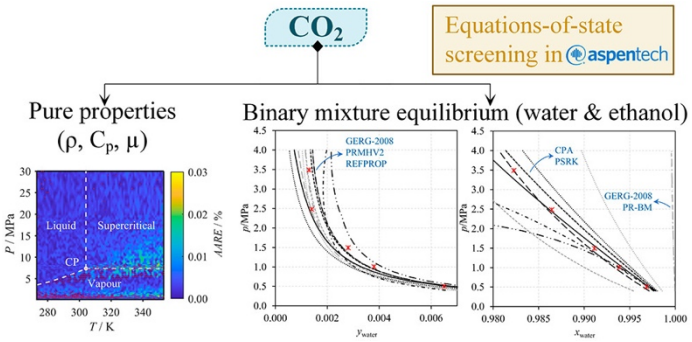

Fig 2. Properties of binary mixtures determined from several models in ASPEN Plus.

Future Perspectives

The LSRE-LCM team integrated a project within the Portuguese Resilience and Recovery plan aiming to make the packing industry more sustainable. An important part of this project is the simulation of industrial processes to improve energy efficiency of enable the usage of raw materials from alternative sources, such as recycling or biomass. Within this project, and because some processes are envisaged to be biobased, the group added another instrument to the process simulation toolbox the software SuperPro Designer.

Recently, the project applications made by this group on biobased products and biovalorization consistently incorporate a component of industrial process simulation, which aims at increasing the impact of the group research in society. The last project proposal, approved in 2023, CyChest, which aims at developing products from resources in chestnuts production, has a strong component of product development associated with process simulation. In this projects SuperPro Designer is an important addition to the tools at our service.

Related Sustainable Development Goals

Outputs

PhD Theses

[1] Isabel Fernandes, Multiphase Flow in NETmix: mixing studies and applications, PDEQB, FEUP, 2023

Master Dissertations

[1] Ana Rita Martinho, Life Cycle Assessment of a novel Co2 Capture Technology (Hgts) on Retrofitting Coal and Natural Gas Power Plants: Portugal Case Study, MIEA, FEUP, 2020

[2] Gustavo Rangel, LCA of a novel F-T Syncrude Pathway using Advanced NETmix Microreactor Technology – Conversion of associated gas destined for flaring into liquid fuels in offshore FPSO operations, MIEA, FEUP, 2020

Selected Publications

[1] C.F. Almeida et al., Journal of Chemical & Engineering Data, in press (2024), Special Issue in Honor of Maria Eugénia Macedo.

Team

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NET4CO2 Service Contract, FEUP/NET4CO2/2020-76537, 2020-2021
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