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Towards a Sustainable and Defossilized/Decarbonized Chemical and Process Industry

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ABSTRACT

This work presents an overview of the path towards the use of renewable and nonconventional resources for a sustainable chemical and process industry. The aim is not only to lead the way to meet the sustainable development goals but also to maintain the style and quality of life achieved by the technologies and products developed within this sector. Alternative raw materials are to be used and processed differently while a new paradigm for utilities is to be established. The development of technologies and their deployment faces several barriers that we as process engineers can help overcome by providing insight into the alternatives, the thresholds to achieve to become competitive, and strategic analyses.

Keywords: Process Design, Renewable and Sustainable Energy, Modelling, Process Synthesis, Energy Storage

INTRODUCTION

The current chemical and process industry stands at a crossroads. Over the last decades its products have provided a lifestyle and wellbeing to society non precedented. Even though there are thousands of chemicals, most of them can be directly related to eight building blocks (ammonia, methanol, ethylene, propylene, benzene, toluene, and mixed xylenes) that are typically produced from fossil resources. Energy intensive chemical production processes consumed 14% of global oil and 9% of global gas and released 13% of global industrial direct CO_2 emissions in 2020,[1,2] it represents the largest energy consumer and the third largest direct CO_2 emiter.[3] Adding to production the use of the product, the chemical industry accounts for 45% of global greenhouse gas (GHG) emissions. Therefore, reducing the use of resources this sector, it is possible to cut the global emissions by 39% (22.8 Bt).[4] These processes can be divided into different business such as chemicals (including consumer products and pharma), food and beverage, petroleum refining, iron and steel, cement, among others that required utilities of different grades.[5] Thus, the transition towards a new process industry starts from the raw materials but it also must include the utilities required to process them into the final products, such as thermal and electrical energy or water, see Figure 1.[6]

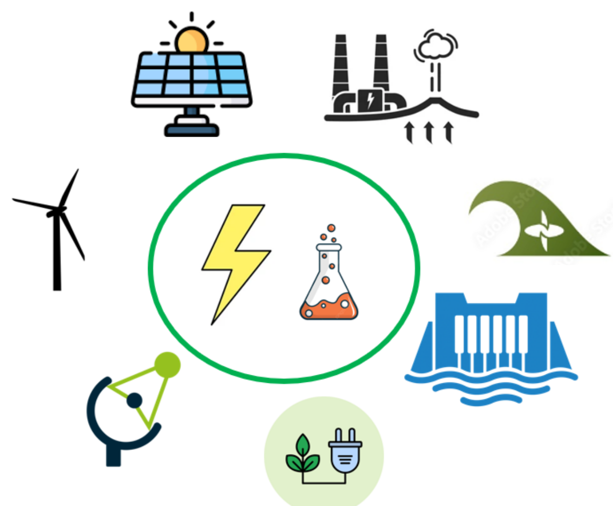

Figure 1. More sustainable production system

In the path to meet the sustainable development goals both aspects are to be addressed simultaneously. However, the problem has been addressed by pieces by different research groups. The efforts have been placed either on evaluating alternative sources for the chemicals or the production of utilities. A wider and more systematic view[7] is required for the integration of resources and technologies, and the selection of the best use of the natural resources towards sustainability.

In this perspective, we present the different efforts and challenges at process scale and at strategic level as well as the barriers[8] new technologies face that include the social perspective.[9] Once the information is on the table, the opportunities that process system engineering has to offer to help overcome those barriers and contribute to the sustainable transformation of the chemical industry are presented. Chemical engineering has contributed to the past industrial transitions, there is no reason to think why it is not possible to do that again.

STATE OF THE ART ON THE TRANSFORMATION TECHNOLOGIES

In the path towards a sustainable chemical and process industry there have been several efforts in parallel, raw materials, utilities and the process design itself, but that are intrinsically related. Over the last years there has been a trend to evaluate the possibility of substituting the production of basic chemicals from biomass and waste, specifically the major building blocks, see Figure 2.

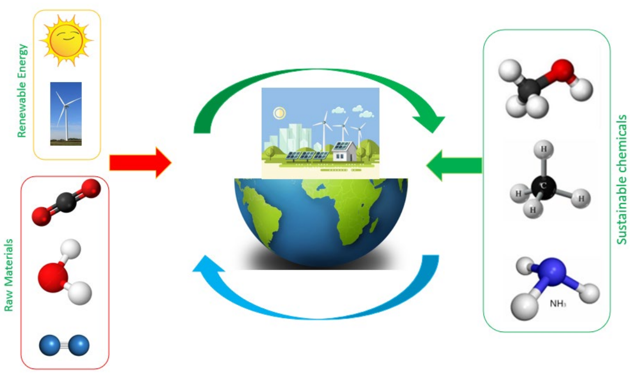

Figure 2. Use of CO_2 as raw material

Renewable Raw Materials

It is expected that by 2050 the chemical system will reduce the use of fossil feedstock down to 10-42%.[1] While the early works focused on the use of biomass and wastes to produce biofuels such as ethanol or biodiesel[1], the extension of the application to substitute fossil fuels has been limited so far. Beyond ethanol and glycerol, as biodiesel major byproduct,[10] that can be used as a source of other chemicals including monomers, (i.e. ethylene, butadiene), the production of platform chemicals from biomass (i.e. Dimethyl furfural, xylitol)[11], as well as specialty chemicals, (i.e. limonene, phenols)[12,13] has been the follow-up effort. So far two main barriers have been identified, their economics, the higher production cost[1] and the tight margins of the bulk chemicals [14] together with the fact that the petrochemical industry and the related business are well established. The additional processing steps required in waste processing add cost to the final product, even if the raw material is cheap or even free,[15,16] so that the use of residues is first and foremost a waste management strategy before a true starting point for a circular economy. Only in the case of high added value products it is interesting to use biomass as a resource and biorefineries that produced them as principal product, together with others including biofuels and/or utilities are the most interesting processes.[12,13] The similarities between the crude oil refineries and thermochemical biorefineries have provided the opportunity to retrofit conventional facilities into biobased ones.[17]

The discussion extends and holds true for CO_2 as raw material.[18,19] The increase in the CO_2 concentration in the atmosphere is one of the major concerns because of its effect on global warming. While it is possible to capture it from point sources such as industries (cement, steel) and power plants, direct air capture (DAC) has become an interesting technology to reduce the CO_2 already in the atmosphere. However, recent works show that the energy consumption to capture and further use of the CO_2 can represent a high share leading to a high level of related emissions due to the capture step unless less carbon intense technologies and resources are used to produce PV panels and wind turbines.[20] Utilization of CO_2 rather than just sequestration[21] can provide a way to create a circular economy around it, once the levels in the atmosphere are back into acceptable ones. The use of renewable energy to process CO_2 is one of the first cases of integrating alternative energy sources as utilities within major chemical processes. As a result, CO_2 has been the base for e-fuels including methane, methanol, Dimethyl ether (DME), Fischer Tropsch-fuels among others. The reduction of CO_2 via hydrogenation[14] or electroreduction[22,23] are possible technologies that have been evaluated towards the production of methanol or ethylene and all the way to polymers. However, some are still at low TRL. In addition, most of them can be produced also from biomass, several studies compare both alternatives.[14]
Comparing CO_2 and biomass as raw material for the same product, biomass-based processes require more processing stages to prepare the syngas, but in general they are more mature technologies while the need for renewable based electricity results in higher investment costs in Solar panels and wind turbines. In addition, the need to overdesign of the units to operate over a year or the storage of hydrogen represents an additional burden. Biomass based products show lower production costs[14,24] but biomass availability is limited, and it has a wider spectrum of final products represents a decision on the best use is yet to be taken. But it has to be made not at process level, but a more strategic one which calls for a multiscale approach.

Sustainable Process Design

Process design towards efficiency in the use of energy and raw materials is and has been the first step towards sustainability. Selection of processing paths and technologies is an important synthesis problem to be solved. The catch is that novel technologies present a lack of information on their operation and/or the uncertainly in their performance. Modelling and simulation are key for process synthesis and represent a challenge when dealing with novel technologies, but first principles can help and provide the first approach while artificial intelligence (AI) is becoming a powerful tool also. Apart from the economic feasibility, the distributed availability of the resources also jeopardizes the facilities using alternative resources. No longer scale-up and economies of scale play an important role but scale down and the effect that it has on the selection of technologies to build a process.[25] Distributed production and modularization are part of the new design approaches for the exploitation of biomass, solar and wind energy.[26] This is also true for the case of small nuclear reactors[27], see Figure 3, which also adds the social acceptance as a variable to the deployment of non CO_2 based technologies. To help in the path, circular process design, such as the effort in plastic recycling,[30,31] creating a circular economy around CO_2, process integration to avoid the use of external chemicals[2] and intensification[32] are additional tools to be developed an implemented.

Renewable Utilities

It is also important to highlight another line of work that typically progresses in parallel with the production of chemicals. The transformation processes require energy and cooling. Even if the raw material is a residue or a renewable resource, the utilities required must also be provided avoiding fossil-based CO_2 emissions. This has been a common weakness in the analysis of the process. Either the utilities are decarbonized and/or new technologies are to be implemented. However, even new processes using unconventional raw materials have been built based on the same principles, so that the same utilities are used.[28,29]

Utilities refer to electricity and heat representing 20 % and 80% respectively of the total energy consumption in the production of chemicals.[29] Therefore, utilities decarbonization means heat decarbonization,[28,35,36] all the way from steam decarbonization,[37] either using biofuels[20] or hydrogen for high temperature requirements[38], to the electrification of the units, refrigeration cycles[39] including heat pumps cycle lay out and fluid selection,[40] or the use of Solar based ones such as gasification or reforming or to provide energy for endothermic reactions in general.[41] In addition, recovering heat from waste streams to produce power[33], and water network[34] design require additional analysis but is proven to reduce the need for external resources.

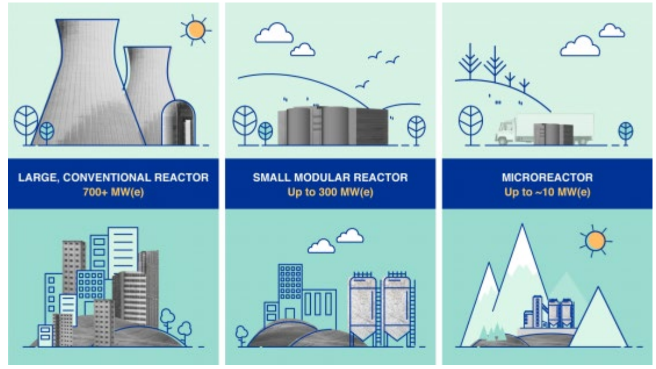

Figure 3. Scale down of technologies. effect on the facility and on the surroundings[27]

As in the case presented for the transformation stages, the use of nonconventional utilities requires unit and process design. In addition, novel process approaches such as intensification, plasma technology, ultrasound microwaves and others have reduced the costs and the generation of wastes.[29] Some of them are related to the use of utilities differently. The design of such novel units is still in their infancy and involves the concept of process and product design and requires considering additional principles beyond traditional chemical engineering since solar and electrical heating are involved. Transport phenomena, unit operations and reactor engineering need to team up with electrical engineering and electro chemistry and can play an important role for the new technology to become competitive. The role of minerals and their availability to build these units can represent another limitation on the extent of the expansion of the penetration of renewable energy.[42] So far only pilot plant scale studies are available. The MeOH is among the fist examples of defossilization considering both the raw materials and the utilities involved.[24]

CO_2 utilization as well as utilities decarbonization is linked to the use of renewable energy and electricity and green hydrogen. Carbon capture and utilization (CCUS) involves the production of chemicals out if it, including methane, DME, methanol or urea creating a circular economy for CO_2. But it is also possible to fully avoid the use of carbon-based chemicals developing non-carbon-based based power plants[44,45] via the temporal storage of hydrogen ammonia, MgH_2[44] or Liquid organic hydrogen Carriers (LOCHs). In all these cases, the integration of solar and wind within the chemcial transformation is key and affects process design.

Challenges of Process Operation Integrating Variable Resources

Management of highly volatile resources such as wind and the Sun calls for process and resource integration[46] as well as smart storage, where chemicals can play an important role[47] to reduce the need to build batteries beyond the minerals availability.[48] The operation of processes that rely on variable resources, variable because of their composition, i.e. biomass, or availability, solar and wind, results in demand site management problems that have been addressed at small scale[45] due to their complexity. In addition, most of the work in heat integration of power to heat for process industries integration has used the pinch technology, but the use of mathematical optimization has proven a powerful tool that has been used traditionally in the petrochemical industry and for the penetration of renewables but the full electrification results in problems that are mathematically really complex due to the variability of the resources and novel tools are being developed[49,50]

Assessment of Process Sustainability

One question arises here, when a new process is more sustainable than the one is trying to substitute. Recent studies have posed that question and presented interesting results for several examples.[51,52] Further analysis is required to cover the entire spectrum. One on the current limitations is the tools to quantify the environmental impacts. LCA analysis present limitations when novel technologies are evaluated due to the lack data to characterize them. Similarly, the technoeconomic analysis of processes involving novel biomass pretreatments, energy collection technologies as well as new units that substitute the current state of the art to provide utilities[53] to the process represent an additional challenge.

DEPLOYMENT OF TECHNOLOGIES

Process level provides the feasibility analysis of the technology and the economic and environmental evaluation that can establish the need for improvements until it can become competitive. But for the production of really high added value products, i.e. polymers or active ingredients for food or the pharma industry,[12,13] additional incentives are needed to substitute/modify production processes that require several years amortization. By enforcing emission levels and providing incentives[54] is how Europe,[55] or the US have been moving towards net zero emissions. However, the transition, the deployment of a decarbonized chemical industry, is to be carried out at a larger scale, at strategic scale. It is at this scale that the incentives need to be designed.

Multiscale approaches have been typically presented within the process community to be able to present strategic decisions to the decision makers, either stakeholders or the governments, see Figure 4.[17] These models require real data, that sometimes are not easy to find, the proper scale-up of the process so that the comparison among alternatives is consistent,[56] an issue that is sometimes overlooked, and the problem, if formulated, is highly complex to solve. Several cases of study are available for biofuels, power at country and continental level[57,58,59] showing certain limitations as how far we can get. European size examples for electricity and fuels alone are the work of many groups and special solution techniques, variable aggregation, reduced area and time discretization are to be implemented.[57]

However, these studies use the resources towards a particular target. The actual issue is when the raw materials are to be shared to meet the current demand of all products, how far is it possible to get using waste biomass, residues, and renewable resources in general[1]. The ultimate question is what is the best use of the limited resource? what to produce out of it? Therefore, the decision boils down to the availability of natural resources required[60], including water[61], area, or mineral among others and the social, environmental, and economic advantages of producing it via that path. Area, water, and nutrients are needed to grow biomass, area is required to install PV panels and wind turbines as well as heliostat fields. To build these units as well as others such as electrolysers, or bateries[62] we need minerals. Preliminary studies show that it is not possible to cover the first generation of electrified systems, the one that will allow start recycling.[60] On the one hand the actual availability of area, harvesting sites and soil properties have lately been analyzed via GIS, originally for food production[63] but also as a potential for energy crops[64]. To reduce the use of area several strategies arise such as the use of the residues from food production, beyond the needed for animal feed, as well as novel developments in PV panels that are transparent and allow for biomass growing in the same field[65]. On the other hand, planetary boundaries have been presented as a way to evaluate how far it is possible to go with the natural resources,[60,66] but show several issues on how we allocate the possible growth. Such a problem is basically the combination of some of the ones presented for the different cases but has not been addressed so far.

Strategic studies also allow evaluating the social issues that the deployment of the new system can bring to regions that host the new facilities[44]. How to measure circularity and the social impact of the transformation of industry require further analysis and metrics beyond the ones available such as job based[5] indexes and marginalization.[67] The challenge may not be to decarbonize industry but to get to zero net emissions and to create an economy that makes the best use to the resources substituting those that are harmful for the system creating circular economies for those wastes to avoid accumulation in the system.

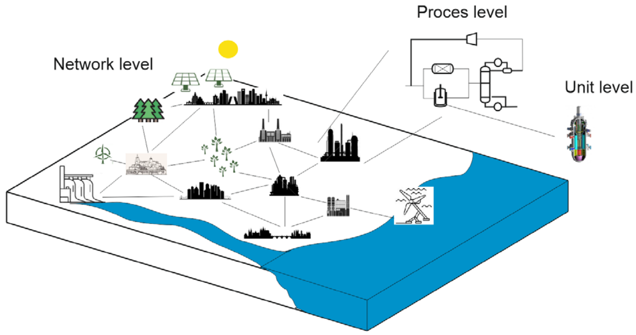

Figure 4. Deployment of technologies

OVERCOMING THE BARRIERS: INCENTIVIES AND SOCIAL IMPACT

The transition to a new system presents opportunities in terms of generation of wealth and jobs due to the installation of transformation facilities. But at the same time, the transition is closing down business, i.e. coal mining and thermal power plants.[44] As such, the decision on where to install them poses a number of social impacts. The first barrier to address is *the social or behavioral one*. Acceptance of a technology has been related to the psychology in product selection, that has been a field of study over the last decades. There is a high activation energy to change. This is similar to customer loyalty to a brand. To address these issues, international agencies campaign to present the need and benefits, such as the United Nations with the SDGs[68] and the effort to convince the population that another production and consumption system is possible. These organizations require systematic studies to provide with reliable data to be able to come to those advertisements. Acceptance of a technology may have an additional positive outcome. On the one hand, society can push their governments to change if the people are convinced. On the other hand, it can be a barrier. One example is nuclear power. Recent efforts focus on small reactors to avoid the society concerns on large facilities close to the cities, see Figure 3.[27] Psychological factors also affect the investors since they need to envision benefits.[54] Apart from this barrier, technical barriers are in place.[69] The *technical barriers* are the ones presented along the first sections of the paper. It is something we as engineers are directly involved in. The third barrier is the so-called *Organizational barrier.* It depends on the companies that are running the business. It is somehow related to the first one in the sense that there is a psychological aspect behind. They need to see the advantage of the new technology. It can also be linked to the incentives that they are going to get.[54,70] Being the first operating a technology provides expertise, at a cost. Technology lock-in only appears when it is widely used[71]. Governments, agencies and other associations, (i.e. EU, UN) play a role in that. The creation of incentives, to reduce taxes or impose ones to certain technologies, help in the development of the technologies and reduce bureaucracy, [54,72] and present targets such as the ones in emissions or temperature increase, has been the usual one. From the systematic studies of the entire system, it is possible to design and define such incentives since they identify the bottlenecks of the technologies themselves as well as their deployment. The competitors also represent a barrier. New technologies come to take a piece of the cake and represent a threat to a running business. However, some of the companies are already diversifying their portfolios to embrace alternative resources.[54] Finally, *political barriers* are somehow linked to the ideology that not all the times is linked to scientific facts and have an effect on the organizational and the social but also on the development of the technologies due to the incentives Governments can assign and the campaign in favor or against it.

We as process system engineers can play a role in most of them by providing tools, and results that can support the selection of new technologies, the breakeven points (the threshold effect) for one technology to be deployed as well as scenario based analysis for the decision makers to be aware of economical, environmental and social issues as well as defining the incentives[73] required for a particular transition to occur or for a technology to enter the market

CONCLUSIONS

In this perspective we aimed at presenting the current trends to pave the way towards a more sustainable production system, but in particular, to transform the chemical and process industry into a more sustainable operation. The barriers new technologies are to face come from society itself as well as the stakeholders. Process system engineering, with its systematic analysis of technologies and multi scale studies, are in a pivotal role to provide insights for the decision makers to select the best use of resources considering not only economics and environmental metrics, but also the social impact that the deployment of the new technologies can have.

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REFERENCES

1. Meng, F et al. (2023) Planet-compatible pathways for transitioning the chemical industry PNAS 120 (8) e2218294120
2. Gabrielli, P., Rosa, L., Gazzani, M., Meys, R., Bardow,

A., Mazzotti, M., Sansavini, G. (2023) Net-zero emissions chemical industry in a world of limited resources, One Earth, https://doi.org/10.1016/j.oneear.2023.05.006
3. Chung, C., Kim, J., Socacoo, B.K., Griffiths, S., Bazilian, M., Yang, M. (2023) Decarbonizing the chemical industry: A systematic review of sociotechnical systems, technological innovations, and policy options. Energy Res. Soc. Sci. 96, 102955
4. https://www.weforum.org/agenda/2023/03/chemicals-industry-low-carbon-economy/
5. Rightor, E., Whitlock, A., Elliott, R.N. (2020) Benefical electrification in industry. ACEEE.
6. USDOE(2022) Industria decarbonization Roadmap. USDOE DOE/EE 2635
7. Martin, M., Grossmann I.E. (2018) Optimal integration of renewable based processes for fuels and power production: Spain case study. Applied Energy 213, 595-610
8. Abdul Qadir, S., Al-Motairi, H., Tahir, F., Al-Fagih, L. (2021) Incentives and strategies for financing the renewable energy transition: A review, Energy Reports, 7, 3590-3606
9. Chung, C., Kim, J., Socacoo, B.K., Griffiths, S., Bazilian, M., Yang, M. (2023) Decarbonizing the chemical industry: A systematic review of sociotechnical systems, technological innovations, and policy options. Energy Res. Soc. Sci. 96, 102955
10. Almena, A., Bueno, L., Díez, M., Martín M (2018) Integrated biodiesel facilities: Review of transformation processes of glycerol based production of fuels and chemicals. Clean Technol. Environ. Pol. 20:1639–1661
11. Galán, G.; Martín, M., Grossmann, I.E. (2021) "Integrated Renewable Production of Sorbitol and Xylitol from Switchgrass. Ind. Eng. Chem Res. 60,15, 5558-5573
12. Criado, A., Martín, M., (2020) Integrated multiproduct facility for the production of chemicals, food and utilities from oranges. Ind. Eng. Chem. Res. 59, 16, 7722-7731
13. Guerras, L.; Sengupta, D.; Martín, M., El-Halwagi, M. (2021) Multi-layer approach for product portfolio optimization: Waste to added value products. Acs. Sust. Chem. Eng. 9, 18, 6410–6426
14. Martín, M (2017) Artificial vs natural reuse of CO_2 for DME production. Are we getting any close? Engineering. 3(2) 166-170
15. Hernández, B., Martin, M .(2017) Optimal Integrated Plant for Production of Biodiesel from Waste ACS Sust. Chem. Eng., *5* (8), 6756–6767.
16. Sánchez A, Martín M.* (2018) Optimal renewable production of ammonia from water and air, J. Clean. Prod., 178, 325-342
17. Floudas, C.A., Niziolek, A.M., Onel, O., Matthews, L.R., 2016, Multi-Scale Systems Engineering for Energy and the Environment: Challenges and Opportunities. AIChE J. 62(3), 602-623
18. Artz, J., Müller, T.E., Thenert, K., Kleinekorte, J., Meys,R., Sternberg, A., Bardow, A., Leitner, W., (2018) Sustainable Conversion of Carbon Dioxide: An Integrated Review of Catalysis and Life Cycle Assessment. Chemical Reviews 118 (2) 434-504
19. Ioannou, I., Javaloyes-Antón, J., Caballero, J.A., Guillén-Gosálbez, G. (2023) Economic and Environmental Performance of an Integrated CO2 Refinery. ACS Sust. Chem. eng. 11 (5) 1949-1961
20. Galán, G., Martín, M., Grossmann, I.E. (2023) Systematic comparison of natural and engineering methods of capturing CO2 from the air and its utilization . Sust Prod. Consumpt. 37, 78-95
21. Gabrielli, P., Rosa, L., Gazzani, M., Meys, R., Bardow, A., Mazzotti, M., Sansavini, G. (2023) Net-zero emissions chemical industry in a world of limited resources, One Earth, https://doi.org/10.1016/j.oneear.2023.05.006
22. Kim, J., Henao, C.A., Johnson, T.A., Dedrick, D.E., Miller, J.E., Stechel, E.B., Maravelias, C.T., (2011) Methanol production from CO_2 using solar-thermal energy: process development and techno-economic analysis. Energy Environ. Sci., 4, 3122-3132
23. Sharp, S, González-Hernández, S., Chen, C., Sheehan, S.W., (2021) Alcohol production from Carbon dioxide: Methanol as a fuel and Chemical Feedstock. Joule, 5 (1), 59-76
24. Chen, C., Lu, Y., Banares-Alcantara, R. (2019) Direct and indirect electrification of chemical industry using methanol produftion as a case study. Appl. Energy. 243, 71-90
25. Sánchez, A., Martín, M. (2018) Scale up and Scale down issues of renewable Ammonia plants: Towards modular design. Sust. Prod. Consump., 16, 176-192
26. Baldea, M., Edgar,T.F., Stanley, B.L., Kiss, A.A. (2017) Modular manufacturing processes: Status, challenges, and opportunities AIChE j. 63 (10), 4262-4272
27. https://www.iaea.org/newscenter/news/what-are-small-modular-reactors-smrs
28. Martín , M. (2023) Heat decarbonization: Towards a sustainable utility system. Joule. 7,1, 15-17 ,
29. Mallapragada D.S. et al (2023) Decarbonziation of the chemical industry though electrification: barriers and opportunities. Joule 7, 23–41
30. Li, H., et al. Expanding plastics recycling technologies: chemical aspects, technology status and challenges (2022) GREEN CHEMISTRY 24 (23), 9329-9329
31. Hernández, B., Kots,P., Selvam, E., Vlachos, D.G.,

Ierapetritou, M.G., (2023) Techno-Economic and Life Cycle Analyses of Thermochemical Upcycling Technologies of Low-Density Polyethylene Waste ACS Sust. Chem Eng. 11 (18), 7170-7181
32. Li, Q., Finn, A.J., Doyle, S.J., Smith, R., Kiss, A.A. (2023) Synthesis and optimization of energy integrated advanced distillation sequences Separation and Purification Technology 315, 123717
33. Anteportalatina-García, V.M., Martín, M (2022) Process synthesis for the valorisation of low-grade heat: Geothermal brines and Industrial waste streams. Renew. Energ. 198, 733-748
34. Ahmetović, E., Grossmann, I.E., Kravanja, Z., Maréchal, F., Klemeš, J.J., Savulescu, L., Dong, H. (2023) Combined water and heat integration in the process industries Frontiers in Chemical Engineering 4, 1012754
35. Madeddu, S., Ueckerdt, F., Pehl, M., Peterseim, J., Lord, M., Kumar, K.A., Krúger, C., Luderer, G. (2020) The CO2 reduction potential for the European industry via direct electrification of heat supply (power- to heat). *Environ. Res. Lett.* **15** 124004
36. Kim, J.K. (2022) Studies on the conceptual design of energy recovery and utility systems for electrified chemical processes. Renew. Sust. Energy. Revs. 167. 112718
37. Pérez Uresti, S.I., Lima, R., Martín, M., Jiménez-Gutiérrez, A. (2023) On the design of renewable-based utility plants using time series clustering. Comp. Chem Eng. 170, 108124
38. Gilbert, T., Menon, A., Dames, C., and Prasher, R. (2022) Heat Source and Application Dependent Levelized Cost of Decarbonized Heat. Joule 7(1) 128-149
39. Chen, B., González-Ayala, J., Calvo Hernández, A., Luo, R., Yang, H., Guo, J. (2023) A novel electrochemical system with adiabatic pre-charging and pre-discharging processes for efficient refrigeration. Energ. Convers. Manage. 293, 117518
40. Vermani, S (2022) thermodynamic modelling of high temperature heat pump systems. Msc Thesis TU Delft
41. Martín, M., (2022) Challenges and Opportunities of Solar thermal energy towards a sustainable chemical industry Comp. Chem. Eng. 165, 107926
42. Chang, I., Taghizadeh-Hesary, F., Mohsin, M. 820239 Role of mineral resources trade in renewable energy development. Renew. Sust. Ener. Revs. 181, 113321
43. Davis, S.J. et al (2018) Net- zero emissions energy systems. Science, 360, eaas9793, 1419
44. Heras, J., Martín, M., (2020) Social issues in the energy transition: Effect on the design of the new power system. Applied Energy. Applied Energy 278 (2020) 115654
45. Sánchez, A., Castellano, E., Martín, M. (2023) Methanol and Ammonia as Emerging Green Fuels: Evaluation of a New Power Generation Paradigm. Renew. Sust. Revs. 175, 113195
46. Rightor, E., Whitlock, A., Elliott, R.N. (2020) Benefical electrification in industry. ACEEE.
47. Sánchez, A., Martín, M., Zhang, Q. (2021) Optimal Design of Sustainable Power-to-Fuels Supply Chains for Seasonal Energy Storage Energy. 234, 121300
48. Michaux, S., (2021) Assessment of the Extra Capacity Required of Alternative Energy Electrical Power Systems to Completely Replace Fossil Fuels GTK Open File Work Report 42/2021
49. Hart, W.E., Laird, C.D., Watson, J.P, Woodruff, D.L., Hackebeil, G.A., Nicholson, B.L., Siirola, J.D., Pyomo optimization modelling in python. Springer
50. Chen, Q., Johnson, E.S., Bernal, D.E., et al. (2022) Pyomo. GDP: an ecosystem for logic-based modeling and optimization development Optimization and Engineering 23 (1), 607-642
51. Tulus, V., Pérez-Ramírez, J., Guillén-Gosálbez, G. (2021) Planetary metrics for the absolute environmental sustainability assessment of chemicals Green Chemistry 23 (24), 9881-9893
52. Cao, G., Handler, R.M., Luyben, W.L., Xiao, Y., Chen, C-h., Baltrusaitis, J. (2022) CO2 conversion to syngas via electrification of endothermal reactors: Process design and environmental impact analysis. Energ. Convers. Manag. 265, 115763
53. Pérez Uresti, S., Martín, M., Jiménez Gutierrez, A (2019) Estimation of renewable-based steam costs. Applied Energy 250 (2019) 1120–1131
54. Abdul Qadir, S., Al-Motairi, H., Tahir, F., Al-Fagih, L. (2021) Incentives and strategies for financing the renewable energy transition: A review, Energy Reports, 7, 3590-3606
55. A.SPIRE Board of Directors (2020) Processes4Planet Transforming the European Process Industry for a sustainable society
56. Martín, M., Taifouris, M., Galán, G. (2023) Lignocellulosic biorefineries: A multiscale approach for resource exploitation. Bioresourc. Tecnol. 385, 129397
57. Potrč, S., Čuček, L., Martin, M., Kravanja, Z. (2021) Sustainable Renewable Energy Supply Networks Optimization – The Gradual Transition to a Renewable Energy System within the European Union by 2050. Renewable and Sustainable Energy Reviews 146,111186
58. Elia, J.A., Baliban, R.C., Floudas, C.A., Gurau, B., Weingarten, M.B., Klotz, S.D., 2013. Hardwood Biomass to Gasoline, Diesel, and Jet Fuel: 2. Supply Chain Optimization Framework for a Network of Thermochemical Refineries. Energy Fuels. 27(8),

4325–4352
59. Marvin, W.A., Schmidt, L.D., Benjaafar, S., Tiffany, D.G., Daoutidis, P. (2021) Economic optimization of a lignocellulosic biomass-to-ethanol supply chain. Chemical Engineering Science 67 (1), 68-79
60. Michaux, S., (2021) Assessment of the Extra Capacity Required of Alternative Energy Electrical Power Systems to Completely Replace Fossil Fuels GTK Open File Work Report 42/2021
61. Di Martino, M., Linked, P., pistikopoulos, E.N. (2023) a comprehensive classification of food-energy-water nexus optimization studies: state of the art. J clean prod. 420. 138293
62. Zhang, C., Zhao, X., Sacchi, R., You, F. (2023) Trade-off between critical metal requirement and transportation decarbonization in automotive electrification. Nature Comm. 14:1616
63. https://geomarvel.com/analyze-food-security-with-gis/
64. Fiorese, G., Guariso, G. (2010) A GIS-based approach to evalaute biomass potential from energy crops at regional scale. Environ. Modell. Soft. 25 (6) 702-711
65. Lee, K., Um, H.-D., Choi, D., park., J., Kim, N., Kim, H., Seo, K. (2020) The development of transparent photovoltaics. Cell reports Phys. Sci. 1 (8) 100143
66. Galan-Martin, A., Tulus, V., Diaz, I., Pozo, C., Perez-Ramirez, J., Guillen-Gosalbez, G. (2021) Sustainability footprints of a renewable carbon transition for the petrochemical sector within planetary boundaries One Earth 4 (4) 565-583
67. Matheson, F.I., Dunn, J.R., Smith, K.L., Moineddin, R., Glazier, RH. (2012) Development of the Canadian Marginalization Index: a new tool for the study of inequality. Canadian Journal of Public Health/Revue Canadienne De Sante'e Publique, S12–6
68. https://sdgs.un.org/goals
69. Chung, C., Kim, J., Socacoo, B.K., Griffiths, S., Bazilian, M., Yang, M. (2023) Decarbonizing the chemical industry: A systematic review of sociotechnical systems, technological innovations, and policy options. Energy Res. Soc. Sci. 96, 102955
70. Erickson, E.D. ,Tominac, P.A., Zavala, V.M. (2023) Biogas production in United States dairy farms incentivized by electricity policy changes Nature Sustainability, 1-9
71. Struben, J., Sterman, J. D. (2008) Transition challenges for alternative fuel vehicle and transportation systems Environment and Planning B: Planning and Design, 35, 1070 – 1097
72. Nicole, T., Jaehyung, A., Igor, V., Oleg, L., Lyubov, K., Sergey, B., Olga, K. (2022) Renewable energy incentives on the road to sustainable development during climate change: A review Frontiers in Environmental Science, 10, 10.3389/fenvs.2022.1016803
73. Martín-Hernández, E., Hu, Y., Zavala, V.M., Martín, M, Ruiz-Mercado, G (2022) Analysis of incentive policies for phosphorus recovery at livestock facilities in the Great Lakes area Resources, Conservation and Recycling 177, 105973