Systems & Control Transactions

Research Article - Peer Reviewed Conference Proceeding
ESCAPE 35 - European Symposium on Computer Aided Process Engineering
Ghent, Belgium. 6-9 July 2025
Jan F.M. Van Impe, Grégoire Léonard, Satyajeet S. Bhonsale,
Monika E. Polańska, Filip Logist (Eds.)

PSE PRESS

Olefins production through sustainable pathways: techno-economic and environmental assessment

Oktay Boztaş[a*], Meire E. G. R. Domingos[a], Daniel A. Flórez-Orrego[a] and François Maréchal[a]

[a] Industrial Process and Energy Systems Engineering, EPFL, Sion, Valais, Switzerland
* Corresponding Author: oktay.boztas@epfl.ch.

ABSTRACT

This study presents a comparative analysis of various configurations for sustainable olefins production via chemical recycling of plastic/biomass wastes, integrating CO_2 capture, storage and management technologies. The co-gasification, methanol synthesis and methanol-to-olefins process models were developed on the Aspen Plus® software. Optimization of processing conditions is achieved through the OSMOSE Lua platform, for minimizing the total cost of operation while accounting for seasonal variability in the electricity prices. CO_2 valorization processes have been shown to increase carbon efficiency from 55% up to 97% compared to steam naphtha cracking, making chemical recycling of plastics an appealing alternative. In addition, direct CO_2 emissions can be fully eliminated, resulting in up to 70% lower net CO_2 emissions even when fossil-based plastic waste is used as feedstock. Seasonal CO_2 storage can extend the economic benefits by acting as a buffer against high electricity costs and serving as a feedstock for CO_2 valorization processes when excess renewable electricity is available. The benefits of the proposed configurations are expected to become increasingly significant with the decarbonization of the electricity generation, relying more on renewable resources.

Keywords: Plastic Waste, Light Olefins, Gasification, Renewable and Sustainable Energy, Process Integration, Circular Economy

INTRODUCTION

Currently, plastic usage exceeds 400 Mt and with continued economic growth, the production is expected to triple in volume by 2060 [1]. Steam cracking is the dominant method for producing olefins, with naphtha—derived from oil refineries—as the primary feedstock in Europe. This process, however, is highly energy-intensive, as cracking furnaces use fossil fuel combustion to provide the necessary reaction energy. Annually, 400 Mt CO_2 is emitted to produce light olefins, which represents 30% of the emissions of the chemicals sector[2]. Chemical recycling of plastic waste offers an alternative that fosters a circular economy, reduces emissions, and enhances resource efficiency. Waste plastic gasification, followed by methanol synthesis and methanol-to-olefins (MTO), is one of the alternative pathways that can promote waste valorization, minimizing the need for virgin plastics. CO_2 capture and storage, when combined with processes such as methanation, rWGS, and co-electrolysis, can broaden the benefits of sustainable chemical recycling. This study presents a comparative analysis of various configurations for sustainable light olefins production, accounting for the changing electricity prices driven by renewable energy availability.

METHODS

Process Modeling and Simulation

The superstructure for olefins production based on plastics and biomass wastes is presented in Figure 1. The inputs to the overall process are represented by High-Density Polyethylene (HDPE) for the waste plastics and pinewood for the biomass (see Table 1). The downdraft co-gasifier is modeled in Aspen® Plus, featuring 4 main stages, namely internal drying, pyrolysis, tar reforming, and reduction. Modeling of pyrolysis of plastic waste is based on experimental data at 500-550 °C, yielding 11% gas, 47% oil, and 42% wax, which is further broken down

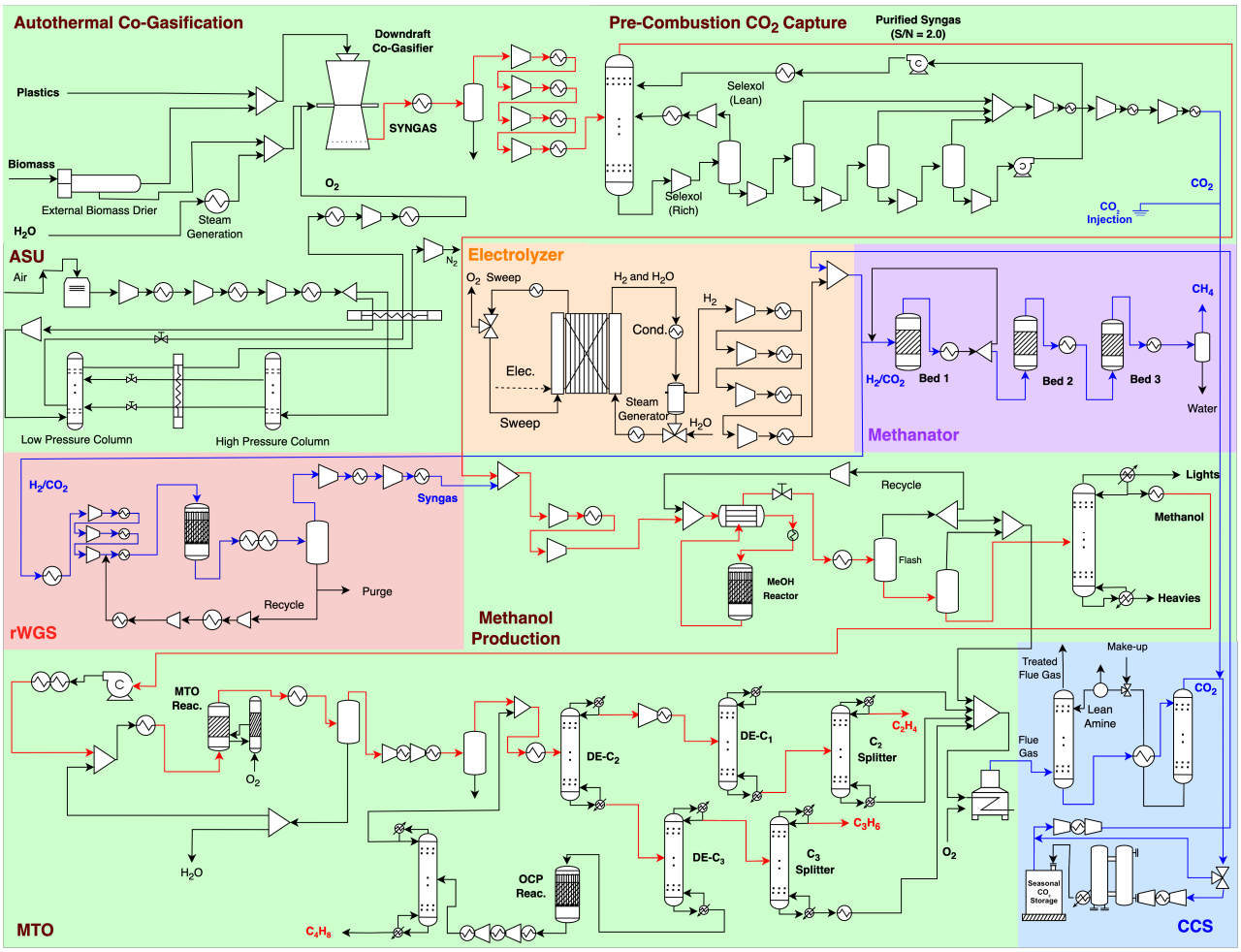

Figure 1: Superstructure for olefins production from plastic and biomass wastes mixture through gasification, methanol synthesis and MTO process.

in the tar reforming stage into solid carbon, CO, CO_2, and H_2 [3]. Biomass pyrolysis yields are determined by temperature-dependent empirical relations using FORTRAN subroutines [4]. The steam reduction stage is modeled using a REquil reactor with water-gas, water-gas-shift(WGS), and steam methane reforming reactions, for which the approach-to-equilibrium (ATE) temperature difference is tuned through sensitivity analysis compared with the experimental data [5]. The model exhibits a relative error of 4.7% and a root-mean square error (RMSE) of 2.2 under operating temperature of 850 °C, pressure of 1 bar, steam-to-feed ratio of 1.0, and plastics-to-feed ratio of 0.5 (dry mass basis). The gasifier is autothermal and the heat is supplied by combustion of char and syngas with O_2 supplied from the air separation unit. The dry molar composition of the syngas is 58.4% H_2, 18.0% CO, 22.7% CO_2, and 0.5% CH_4. The stoichiometric number, defined as:

$$SN = (x_{H_2} - x_{CO_2})/(x_{CO} + x_{CO_2})$$

which favors methanol synthesis when slightly > 2.0. This condition is met by CO_2 removal via physical absorption using Selexol® solvent at 30 bar, resulting in a syngas composition of 69.2% H_2, 21.2% CO, 9.9% CO_2, and 0.1% CH_4.

Table 1: Proximate and ultimate analysis of biomass and plastic feedstocks (dry mass basis)[6]

Composition		Pinewood	HDPE
Proximate Analysis [%]	M	11.5	0.02
	FC	15.4	0.30
	VM	84.2	99.7
	Ash	0.45	0
Ultimate Analysis [%]	C	51.4	84.9
	H	4.90	15.1
	N	0.90	0
	O	42.4	0

Methanol synthesis is modeled based on Lurgi's Mega-Methanol® technology and the kinetic modeling by

Kiss et al., occurring at 210°C and 90 bar [7, 8]. The process could reach 96% methanol yield (depending on CO_2 content in the feed), including a recycle loop with a purge stream that is combusted with pure oxygen, releasing CO_2. After the distillation step providing >99.5% w/w purity methanol, it is sent to MTO process for light olefins synthesis.

This stage consists of a MTO reactor integrated with a catalyst regenerator that uses pure O_2 to combust deposited coke, an olefin cracking reactor for breaking down C_4+ olefins into valuable light olefins, and a series of cryogenic distillation columns to produce polymer-grade final product. The MTO reactor is modeled with a RYield reactor based on experimental data[9]. The yields based on infeed methanol are 19.0% for polymer-grade ethylene and 19.5% for polymer-grade propylene. H_2O formed within the MTO reactor is recycled back into the process as steam. The undesired organic products, such as alkanes and out-of-spec natural gas are combusted with pure oxygen to recover waste heat, whereas CO_2 in the flue gas is captured and valorized after heat recovery.

CO_2 abatement and other energy technologies are integrated to improve process efficiency and offset emissions. The two possible routes for capturing CO_2 are pre-combustion carbon capture, operated at 30 bar using Selexol® solvent, where CO_2-rich solvent is decompressed, flushed and recycled, and post-combustion carbon capture, with 90% efficiency, using chemical absorption in an absorber-desorber column configuration with a di-ethanol amine (DEA) solvent, which enables a high adsorption rate while reducing desorber energy requirements [10]. Pre- and post-combustion captured CO_2 can either be injected for permanent geological storage, upgraded into CH_4, or used as feedstock for syngas production to enhance olefins production. The possible configurations considered in the scope of this work are given bellow:

1. **pre-combustion carbon capture and injection (preCCS & Inj):** Pre-combustion CO_2 captured during the syngas treatment is injected for geological storage, while combustion gases are released into the environment, therefore no CO_2 upgrading is considered. Seasonal CO_2 storage is not implemented in this configuration.

2. **methanation-based:** Both pre-combustion and post-combustion captured CO_2 is seasonally stored in liquid form or upgraded with methanation process depending on the electricity prices.

3. **reverse water gas shift-based (rWGS):** Both pre-combustion and post-combustion captured CO_2 is seasonally stored in liquid form or upgraded with rWGS process for syngas production depending on the electricity prices.

4. **co-electrolysis-based (co-SOEC):** Both pre-combustion and post-combustion captured CO_2 is only seasonally stored in liquid form or upgraded with co-electrolysis process for syngas production depending on the electricity prices.

5. **steam naphtha cracking (SNC):** steam fossil naphtha cracking without CCS unit.

Permanent CO_2 storage is considered only in configuration 1, as CO_2 is already captured as a requirement for methanol synthesis. Unlike other configurations that aim to increase olefins production by eliminating CO_2 emissions, no additional technologies for CO_2 capture from flue gases are included in configuration 1.

The necessary H_2 for configurations 2 and 3 is supplied with a solid oxide electrolyzer (SOEC), which operates at 800°C and 1 bar, with a specific electricity consumption of 35.2 kWh/kgH_2 [11, 12]. In terms of CO_2 and energy management, since most configurations entail high electricity consumption, they are vulnerable to fluctuations in electricity prices. As an alternative to buffer against these costs, CO_2 can be seasonally stored in liquid form at 7 bar and -50 °C during periods of high electricity prices, and processed when prices are lower [13]. A steam network system is also considered to recover waste heat for electricity generation.

Optimization Problem Definition

The process integration of the proposed configurations is handled by Osmose Lua platform [14]. It works out the optimal operating conditions of the technologies of the superstructure, based on an objective function that minimizes the total cost.

$$\min Cost_{tot} = \sum_{u \epsilon Units} \left[\sum_{t \epsilon Time} \left[\left(Cop1_u \cdot Y_{u,t} + Cop2_u \cdot M_{u,t} \right) \Delta t + Cinv1_u \cdot Y_u + Cinv2_u \cdot M_u \right] \right]$$

- $Cop1_u$ [EUR/h]: fixed operating cost of unit u,
- $Cop2_u$ [EUR/kWh or EUR/kg]: variable operating cost of unit u,
- $Y_{u,t}$ [-]: integer variable standing for the activation of the unit u at a time t,
- $M_{u,t}$ [kg/h or kW]: continuous variable standing for the load of the unit u at a time t,
- $Cinv1_u$ [EUR/y]: fixed annualized cost of unit u,
- $Cinv2_u$ [EUR/kWh or EUR/kg]: variable annualized cost of unit u,
- Y_u [-]: integer variable for the activation of the unit u, maximum value of $Y_{u,t}$,
- M_u [kg/y or kWh/y]: maximum load of the unit.

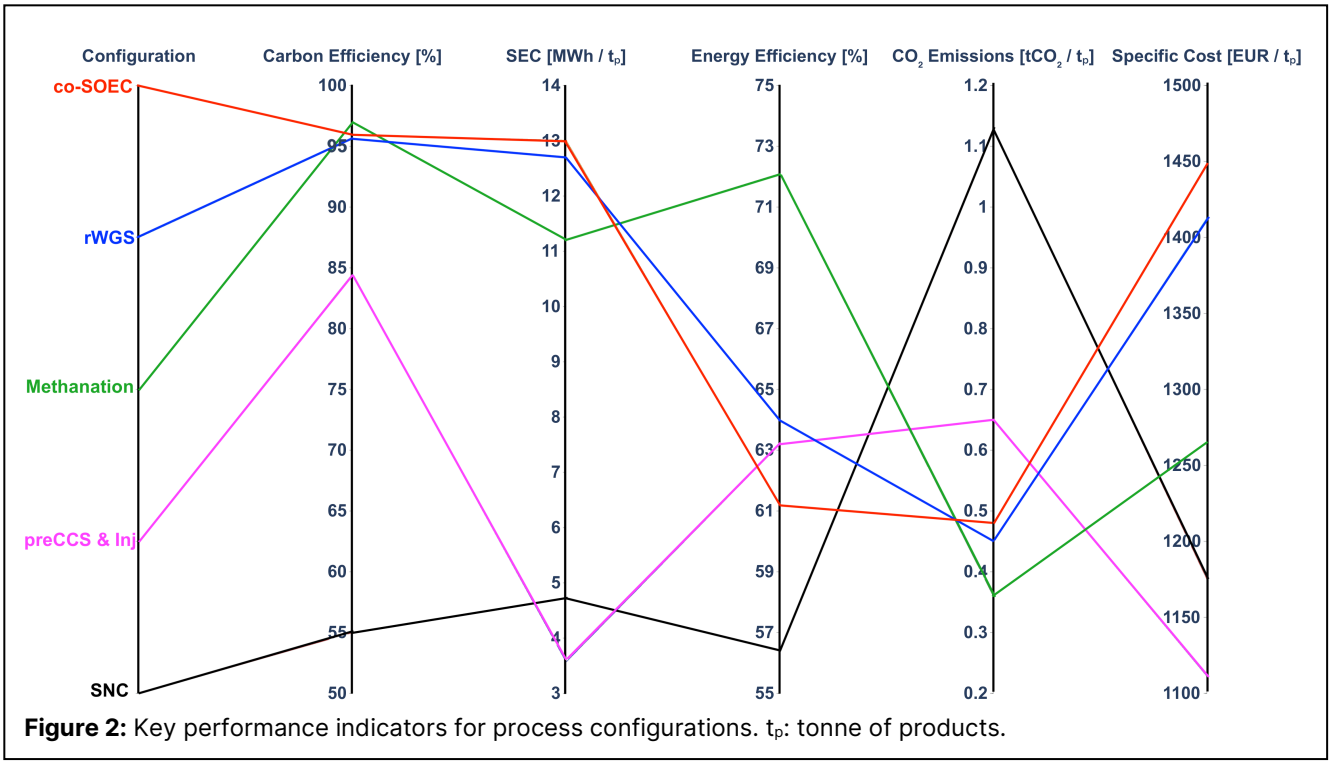

Figure 2: Key performance indicators for process configurations. t_p: tonne of products.

The defined problem is solved over an entire year (8760 h), divided into 12 monthly periods. Based on the availability of renewable electricity throughout the year, the electricity cost is set at 0.05 EUR/kWh from March to October and 0.15 EUR/kWh from November to February. The energy mix is based on the Swiss grid, with an environmental impact of 0.048 $kgCO_2e/kWh$. A carbon tax of 120 EUR/t_{CO2} is assumed. The prices set for the main products and raw materials are as follows: ethylene at 1,200 EUR/t, propylene at 1,100 EUR/t, butene at 1,000 EUR/t, CH_4 at 0.07 EUR/kWh, permanently stored CO_2 with a carbon permit valued at 8.4 EUR/t, plastic waste at 454 EUR/t, and biomass at 73 EUR/t.

Key Performance Indicator Definitions

For comparing the proposed configurations, several key performance indicators (KPIs) are established. These are carbon efficiency (CE), specific energy consumption (SEC), process energy efficiency (η_{Energy}), environmental impact (CO_2e), and specific cost (SC). The definitions of the established KPIs are provided below:

- CE [%] = $\frac{Carbon\ in\ products}{Carbon\ in\ feedstock}$
- SEC $\left[\frac{kWh}{kg}\right]$=$\frac{E_{el}}{m_{products}}$
- $\eta_{Energy}[\%] = \frac{m_{products} \cdot LHV_{products}}{m_{feed} \cdot LHV_{feed} + E_{el}}$
- $CO_2e\ \left[\frac{kgCO_2e}{kg}\right] = \frac{Direct\ CO_2\ . + Indirect\ CO_2\ . - \text{Avoided } CO_2}{m_{products}}$
- SC$\left[\frac{EUR}{t}\right] = \frac{CAPEX + OPEX}{m_{products}}$

Where E_{el} is the electricity consumption of the overall process within a year [MWh]; m is the total mass within a year [kg or t], LHV refers to the total lower heating value within a year [MWh]. For calculation, the considered specific LHVs are: 5.42 kWh/kg for biomass, 9.47 kWh/kg for HDPE, 13.1 kWh/kg for C_2H_4, 12.7 kWh/kg for C_3H_6, 12.6 kWh/kg for C_4H_8 and 13.9 kWh/kg for CH_4. The considered impact factors are: 0.048 $kgCO_2e/kWh$ for electricity, 1.6 $kgCO_2e/kg$ for HDPE and 0.05 $kgCO_2e/kWh$ for pinewood. The total products could consist of olefins, and CH_4 depending on the configuration.

The carbon content within biomass, is biogenic, therefore capture of biogenic carbon within product or with injection, it is counted towards avoided(negative) emissions, however since carbon content within plastic is fossil based, it cannot contribute to negative emissions. It is also assumed that, initially the carbon content within plastics is consumed for product formation and injection. After all the fossil carbon is accounted for, additional carbon is considered to be consumed from biogenic source. Therefore, if the carbon contents within the product is exceeds the carbon content of plastics, all emitted CO_2 should incorporate biogenic carbon, leading to zero direct CO_2 emissions. For indirect CO_2 emissions, the impact of electricity, fossil HDPE production and biomass supply chain are accounted.

RESULTS AND DISCUSSION

The key performance indicators of the optimal configurations are provided in Figure 2. By integrating CO_2

management technologies, the carbon efficiency can reach up to 97%, nearly doubling the produced amount of olefins considering the same amount of feedstock.

CO_2 Emissions, Capture and Utilization

As shown in Table 2, none of the alternative configurations entails direct CO_2 emissions. Moreover, the net CO_2 emissions for the proposed setups are 40-70% lower compared to 5. SNC process. Particularly, in the 2. methanation configuration, lowest CO_2 emissions are reached, due to capturing the highest amount of biogenic carbon within the products.

Since the feedstock consists of waste plastics derived from fossil resources, indirect CO_2 emissions are significant for all configurations. The impact associated with plastics waste accounts for 60-80% of the emissions depending on the studied configurations. The introduction of SOEC introduces an additional impact of 0.5-0.6 tCO_2/t_p due to the high electricity consumption. However, the increased process carbon efficiency offset the impact of raw materials, leading to lower indirect CO_2 emissions in the configurations with SOEC when compared to the 1. preCCS & Inj case.

Table 2: Fossil CO_2 emissions balance for the process configurations[15].

CO_2 emission (t_{CO2}/t_p)	**1**	**2**	**3**	**4**	**5**
Direct	0	0	0	0	0.50
Indirect	2.21	1.46	1.58	1.63	0.63
Avoided (-)	1.57	1.10	1.14	1.14	-
Net	**0.64**	**0.36**	**0.44**	**0.49**	**1.13**

Figure 3 highlights that the optimal strategy during high electricity price periods is to store liquid CO_2, which can later be used to enhance syngas production capacity when electricity prices drop.

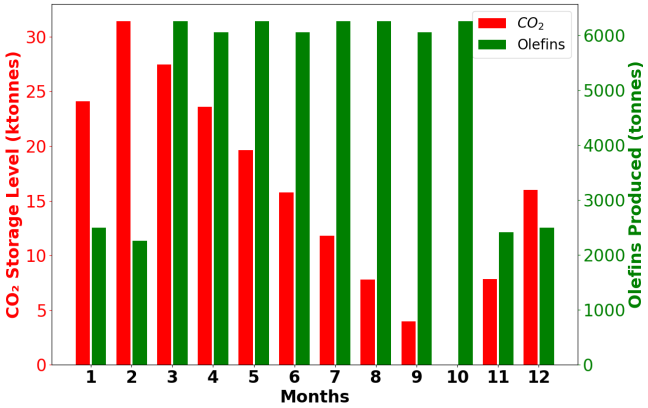

Figure 3: Monthly storage level and olefins production capacity for co-SOEC configuration.

Energy Input and Management

The integration of SOEC causes an increase in energy consumption, making up 60-70% of the overall electricity demand. On the other hand, SOEC boosts the carbon efficiency by 75% compared to 5. SNC and 15% compared to the 1. preCCS & Inj configuration while the energy efficiency is improved by 4 to 16 percentage points with respect to 5. SNC. 1. PreCCS & Inj configuration shows the lowest SEC, due to not leveraging SOEC, and a good integration of the steam network, which provides 78% of the electricity demand of the process. Meanwhile, this power self-generation ratio is limited to 15-20% for the other configurations. None of the processes requires heat from combustion and are autothermal in meeting their heating demands thanks to extensive internal waste heat recovery.

Economic Evaluation

The specific cost of production for SOEC-integrated processes show an increase of 20-50% compared to the 5. SNC. The 1. preCCS & Inj setup has the lowest SC (1111 EUR/t_p), while 4. co-SOEC exhibits the highest cost (1450 EUR/t_p). Operating expenditures (OPEX), account for 65-75% of the total specific cost, mainly due to electricity costs, leading to higher impact for all SOEC-integrated configurations. The capital expenditure (CAPEX) is annualized for 40 years with an interest rate of 6%. The highest CAPEX is linked to the 3. rWGS configuration (504 EUR/t_p), and the lowest cost is that of the 1. preCCS & Inj configuration (318 EUR/t_p).

CONCLUSIONS

This study proposes and analytically compares various routes for the chemical upgrading of plastic wastes to olefins, integrating CO_2 management and energy technologies. This approach offers a globally applicable process that consumes plastic wastes as a widely available feedstock and reduces the dependency on fossil fuels. Furthermore, these configurations not only prevent direct CO_2 emissions but also cut down the emissions linked to the virgin plastic production and the treatment of plastic waste, establishing the foundations of plastics circular economy.

The alternative configurations evaluated using high temperature electrolyzers (SOEC) require a significant amount of seasonal, renewable electricity. However, seasonal CO_2 storage can address this issue by optimizing the process for both process efficiency and operational costs, increasing the production capacity by 40%. In the long term, with increased share of renewable electricity mixes, these routes are expected to economically outperform traditional processes of plastics manufacturing and plastics waste treatment.

REFERENCES

1. OECD (2022) Global Plastics Outlook: Policy Scenarios to 2060. OECD Publishing, Paris
2. Flores-Granobles M, Saeys M (2023) Quantitative analysis of CO2 emissions reduction potential of alternative light olefins production processes. Green Chem 25:6459–6471
3. Jiang G, Wang J, Al-Salem SultanM, Leeke GA (2020) Molten Solar Salt Pyrolysis of Mixed Plastic Waste: Process Simulation and Technoeconomic Evaluation. Energy Fuels 34:7397–7409
4. Trninic M, Stojiljkovic D, Manic N, Skreiberg Ø, Wang L, Jovovic A (2020) A mathematical model of biomass downdraft gasification with an integrated pyrolysis model. Fuel 265:116867
5. Ajorloo M, Ghodrat M, Scott J, Strezov V (2022) Modelling and statistical analysis of plastic biomass mixture co-gasification. Energy 256:124638
6. Pinto F, Franco C, André RN, Miranda M, Gulyurtlu I, Cabrita I (2002) Co-gasification study of biomass mixed with plastic wastes. Fuel 81:291–297
7. Kiss AA, Pragt JJ, Vos HJ, Bargeman G, Groot MT de (2016) Novel efficient process for methanol synthesis by CO2 hydrogenation. Chemical Engineering Journal 284:260–269
8. Domingos MEGR, Flórez-Orrego D, Santos MT dos, Oliveira S de, Maréchal F (2022) Techno-economic and environmental analysis of methanol and dimethyl ether production from syngas in a kraft pulp process. Computers & Chemical Engineering 163:107810
9. Hannula I, Arpiainen V (2015) Light olefins and transport fuels from biomass residues via synthetic methanol: performance and cost analysis. Biomass Conversion and Biorefinery 5:63–74
10. Flórez-Orrego DA, Domingos MEGR, Nakashima RN, Santos MT dos, Junior S de O (2023) Chapter 2 - Syngas purification by common solvents. In: Rahimpour MR, Makarem MA, Meshksar M (eds) Advances in Synthesis Gas : Methods, Technologies and Applications. Elsevier, pp 27–72
11. Domingos MEGR, Flórez-Orrego D, Sfeir S, Maréchal F (2024) Integration of biodigestion, gasification, renewable energy, reversible solid oxide cell and CO2 management strategies for sustainable natural gas production.
12. Flórez-Orrego D, Dardor D, Domingos MEGR, Germanier R, Maréchal F (2024) Integration of renewable energy and reversible solid oxide cells towards decarbonizing the secondary aluminium production and urban systems.
13. Domingos MEGR, Flórez-Orrego D, Santos MT dos, Júnior S de O, Maréchal F (2023) Multi-time integration approach for combined pulp and ammonia production and seasonal CO2 management. Computers & Chemical Engineering 176:108305
14. Dardor D, Flórez-Orrego D, Terrier C, Ribeiro Domingos ME, Platteau C, da Silva JC, Lopez M, Maréchal F (2024) ROSMOSE: A web-based decision support tool for the design and optimization of industrial and urban energy systems. Energy 304:132182
15. Young B, Hawkins TR, Chiquelin C, Sun P, Gracida-Alvarez UR, Elgowainy A (2022) Environmental life cycle assessment of olefins and by-product hydrogen from steam cracking of natural gas liquids, naphtha, and gas oil. Journal of Cleaner Production 359:131884