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Modelling of the Use of Renewable Energies and Energy-Saving Measures for Polymer Chemical Plant

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This study investigates the utility system of the pyrolysis unit of a polymer plant and assesses the decarbonization options of the utility system. The method is based on an integrated approach that includes a steady-state digital twin (SSDT) of investigated process and an update of the existing steam cascade to apply renewable energy and power-to-x. Pyrolysis gas composition was obtained from online analyzers and simulated in a UniSim environment. The simulation model of the whole process, from pyrolysis of liquid feedstock to final monomer separation, was developed and verified on plant data. The energy-saving potential was assessed based on SSDT, and energy-saving measures were proposed. The updated steam cascade of the investigated process was developed, and decarbonization options accounting for steam generation and waste heat utilization were proposed. The final solution gives the energy targets for e-boilers and low-grad heat for Organic Rankine Cycle (ORC).

1. Introduction

Global environmental challenges speed up a new paradigm of resource circularity. It covers the transition to clean energy and a low-carbon economy (Schneider et al., 2016). In the industry, this forces digital transformation, electrification, and transition to renewable and sustainable energy use. The chemical industry is one of the major pollutants, and transforming existing plants is more environmentally vital while developing new processes. For instance, the European Union’s (EU) chemical industry generated total revenue of 500 × 10^9 € in 2020, consuming 51 × 10^6 toe of primary energy (Statista, 2020). The chemical sector is the third largest industry subsector regarding direct CO_2 emissions (IEA, 2021). Synthetic polymers are a huge part of the chemical sector and the components suppliers for other industries. The energy input in plastic production mainly comes from obtaining the basic monomers. Many approaches for energy saving in polymer production are based on modeling using data-driven methods, mechanism methods, and a combination of them (Han et al., 2020). The machine learning and surrogate modeling of digital twins speed up the time to convergence and can be realized, including the commercial simulator and supplementary coding in Python (Galeazzi et al., 2022). Several recent research demonstrated the progress in the simulation of gasoline pyrolysis, delivering an experimental study (Hu et al., 2022) and unsteady-state modeling (Bunaev et al., 2022) to get a more predictable composition and physical properties of pyrolysis gas. This may be beneficial for further assessment of chemical process sustainability, simulating the process flow diagram (PFD) of the entire processes, as expressed by Varbanov et al. (2020). Despite the numerous simulation research of the pyrolysis process, the modeling of whole monomer plants with gasoline pyrolysis is not described in the literature. This complicates finding the theoretical energy gap and the assessment of energy-saving measures (Khripko et al., 2016) in polymer production. Apart from the application of the energy-saving measures, further decarbonization of industry is possible through renewable energy intervention, as was studied in copper mining (Vergara-Zambrano et al., 2022) or the pulp and paper industry (Sonsale et al., 2021). The electrification options are the priority for further development of the biggest chemical producers, including synthetic polymers (BASF, 2021). This new electrically heated steam cracker furnace may cut CO_2 emissions by 90 %. Existing chemical plants need

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improvement to cut the emission rapidly, while developing new sustainable processes. The present paper is trying to fill a research gap in the assessment of possible renewable energy use at monomer production with gasoline pyrolysis. It is realized by the development of the existing plant model supplemented by energy-saving measures, which are proved by real plant data. An updated steam cascade was built based on digital twin solutions to find renewable energy in the existing process.

2. Research methods

The proposed method is based on an integrated approach for digital twin development and energy-saving solutions. It is used for the update of existing steam cascades and finding the possibilities for renewable energy integration to the process. The general workflow is presented in Figure 1.

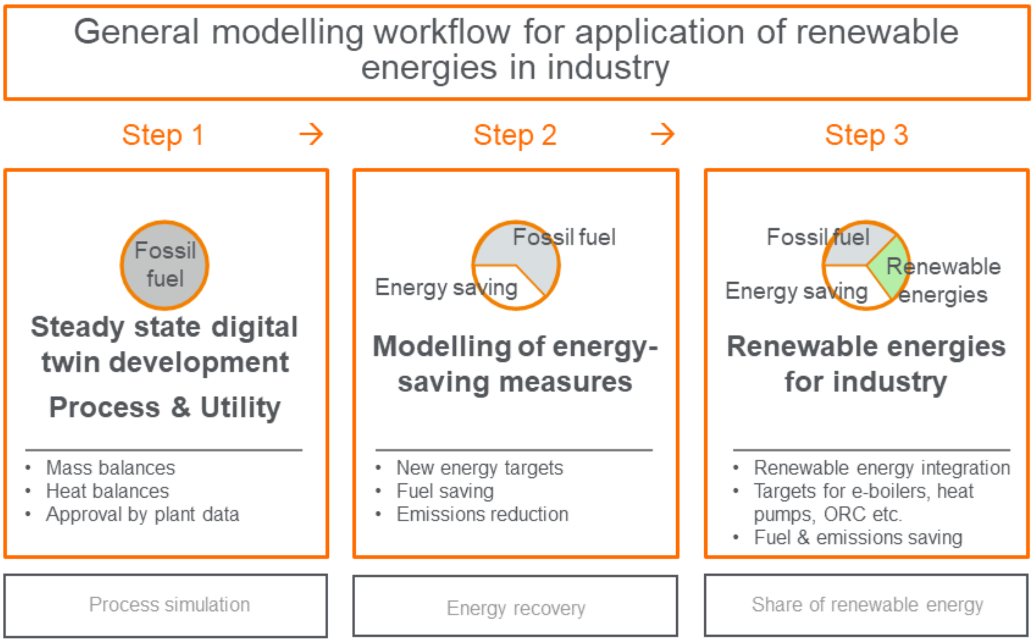

Figure 1: A graphical representation of the general workflow

2.1 Process simulation

The obtained plant data was used for the simulation of the existing process. The simulation strategy is based on the grey box, and white box approaches depending on plant and literature data availability. UniSim Design environment was used as a basic simulation tool, where the Peng-Robinson Stryjek-Vera (PRSV) equation of state was selected as a basic work package, and Zudkevitch Joffee was used as a supplementary work package for high hydrogen-containing systems (UniSim Design R490, 2022). The simulation of the feedstock's physical properties was done based on the measurements of the composition of the pyrolysis gas after chemical reactions in furnaces. The modeling of main process units, e.g., columns, heat exchangers, and compressors, was performed based on the mechanical design and efficiency of the equipment. The chemical reactors for the hydrogenation of alkanes and obtaining of hydrogen-containing gas were simulated based on conversion and components stoichiometry. The cold heat recovery block was simulated with the use of a multi-stream exchanger balance and pressure drop. 22 nested loops were implemented to simulate the recycling of products and by-products. Processes with recycle are vulnerable to process control problems when the overall mass balance of the system containing the recycle is not correctly managed (Bolton and Smith, 2022). The convergence of the model was checked on 3 operation sets of plant data to turn and finalize the steady state digital twin (SSDT). The final heat and mass balances of the existing process were proved.

2.2 Energy saving measures

Based on the developed SSDT, the energy-saving measures were developed and simulated in the modeling environment. All solutions were checked on potential operational problems that may occur when retrofitting and revamping the process flowsheet. Before the development of energy-saving measures, the assessment of the energy gap was performed by process and interplant integration to find thermodynamically available energy for recovery (Boldyryev et al., 2022). The selected measures were shortlisted from the pull of technically viable ones and the final selection was performed based on economic efficiency. The sensitivity of economic parameters was checked for different trends in energy prices, as proposed by Gil et al. (2021). The digital twin was updated to prove the final list of energy-saving measures.

2.3 Electrification of the utility

The existing heat cascade of the monomer plant was revisited and updated according to selected energy-saving measures. The initial steam system expands the steam from very high to low pressure and distributes it to consumers. Since the steam turbines generate the electricity and drive the refrigeration compressors, the shifting of steam extraction was performed, decreasing low-pressure steam saving and increasing very high-pressure steam saving to apply the electrification option for steam boilers. The renewable energy supply is considered to replace fossil fuel for steam generation, and additional electricity generation or power-to-x options are considered for the decarbonization of the facility.

2.4 Assumptions and Constraints

The next assumptions are used when developing the simulation model:

- The quality and quantity of products are not changed;
- Electricity production by steam turbines remains constant;
- Reactor modeling utilizes the grey-box approach with constant productivity;
- The threshold of energy-saving measures is the internal rate of return (IRR) ≥20 %;
- The minimum steam flow through the valves of very high-pressure steam (VHPS) is 2 t/h, it is required by process reliability;
- Electricity supply from renewables is constant.

3. Case study of polymer chemical plant

Considered monomer plant has a nominal capacity of ethylene of 37.5 t/h and propene of 17.4 t/h. The pyrolysis unit consists of 11 reactor furnaces, of which 7 are in operation and the other 4 units are in cleaning mode. The flowsheet of gas compression and separation includes 9 chemical reactors, 18 distillation columns, 86 heat exchangers, and other equipment. The block diagram of monomer production with main process flows is presented in Figure 2. The feedstock is gasoline, with a density of 753.47 kg/m^3. The simulation result of gasoline and pyrolysis gas quality is presented in the true boiling point curve (Figure 3). The mass balance of SSDT of the monomer plant is shown in Table 1.

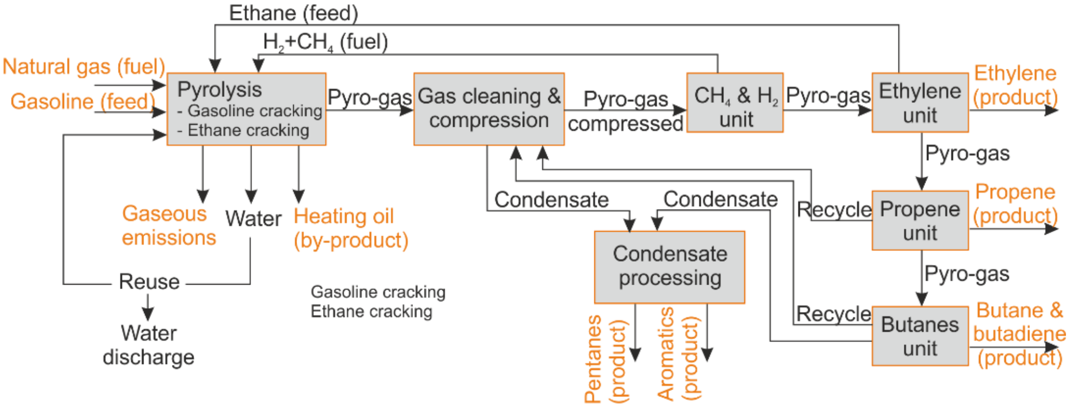

Figure 2: Block diagram of monomer production and main material streams

The utility system of the monomer plant is intended for heating and cooling of process streams and electricity generation. Primary energy sources are natural gas and electricity. Natural gas is used by pyrolysis furnaces and steam boilers. VHPS (110 bar) is generated in heat recovery sections of furnaces (59 %) and steam boilers (41 %). VHPS is released to heat cascade for electricity generation, driving refrigeration compressors, and expansion valves. Exhaust steam is used by different consumers at high pressure (HPS) (25 bar), medium-pressure (MPS) (15, 12 bar), and low-pressure (LPS) (4 bar). The cooling capacity is provided by the cooling water (CW) cycle, air coolers (AC), and propene (P) and ethylene (E) refrigeration cycles with isotherms at +6, -18, -37, -55, -75, and -102 °C.

Table 1: Mass balance of monomer plant

Inlet streams						
Stream name	Pyrolysis gas from furnaces					
Rate, kg/h	196,128					
Outlet streams						
Stream	LP methane	MP methane	HP methane	Ethane	Ethylene	Propene
Rate, kg/h	1,863	924	15,744	10,264	36,288	18,727
Stream	Propane	Butanes	Pentanes	Aromatics	Water	Blowdowns
Rate, kg/h	2,236	8,402	4,359	16,363	79,180	1,778

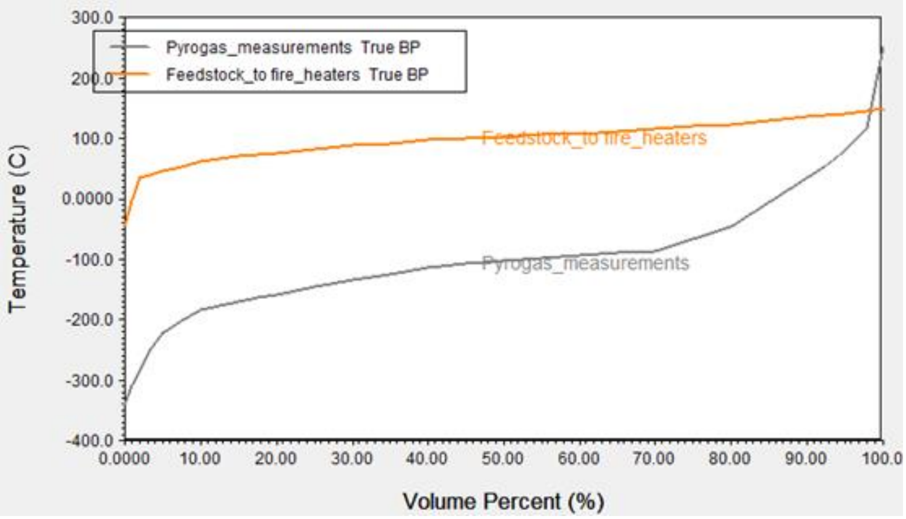

Figure 3: True boiling point curves of the feedstock and pyrolysis gas after furnaces

4. Results and discussion

The summary of energy-saving measures developed based on SSDT, which technically proved and met an economic threshold, is demonstrated in Table 2. The energy-saving is linked to the directly saved heat carriers. Nevertheless, the final saving should be reconciled with the steam cascade, converted to the saving of the primary energy, and assessed for decarbonization options. The final steam cascade indicating the steam savings and supplementary decarbonization options is presented in Figure 4. The initial process, energy-saving measures, and steam cascade were simulated UniSim. The final steam cascade was adjusted with UniSim minimizing VHPS generation to decrease the heat load of e-steam boilers and electricity supply from renewable energies. After the application of energy-saving measures in the main process, the steam cascade was rearranged to keep power production and compressors requirements. The final saving of VHPS is 8.1 t/h compared to the base case, and the VHPS production in gas boilers (142.5 t/h) is substituted by e-boilers that use renewable energies. There is a saving of LPS (7.7 t/h) due to the application of energy-saving measures and rebalancing of the steam cascade. This saving is utilized via ORC unit to produce the electricity or intermediates. There is condensate being released at all steam pressure levels. The condensate is sent to the condensate release network and is used for steam generation.

The energy-saving obtained from energy-saving measures cannot be directly converted to steam or fuel saving due to steam cascade restrictions. After the application of energy-saving measures, the steam cascade was adjusted to maximize VHPS saving. This is the only utility that can be converted to primary energy reduction (gas fuel), other steams are generated by cascading VHPS, and their saving is a waste heat, which cannot be directly used and needs to be utilized. A full load of all steam turbines and minimum steam flow through the VHPS expansion valve are additional process restrictions limiting final energy-saving.

The valves are still present at the VHPS line of the updated steam cascade. They degrade energy quality, but the steam cascade was developed for the real process of a polymer plant, and there are no technical possibilities to exclude steam flow through these valves.

Table 2: Results of the different utility savings after the application of energy-saving measures

Energy saving measure	Heat energy saving, kW						
	Gas fuel	LPS (4 bar)	MPS (12 bar)	VHPS (110 bar)	CW	P (+6 °C)	P (-18 °C)
Waste heat of pyrosis unit	3,734	1,915	1,218	-	6,369	-	-
Acetylene hydrogenation	-	1,326	-	-	1,437	-	-
Hydrogenation of dienes and olefins	-	75	312	-	1,500	-	-
Preheating of columns feed	-	5,405	-	-	5,630	-	-
Ethane column condenser	-	-	-	1,395	-	2,023	2,061
Flue gas profile optimization	7,614	-	-	-	-	-	-

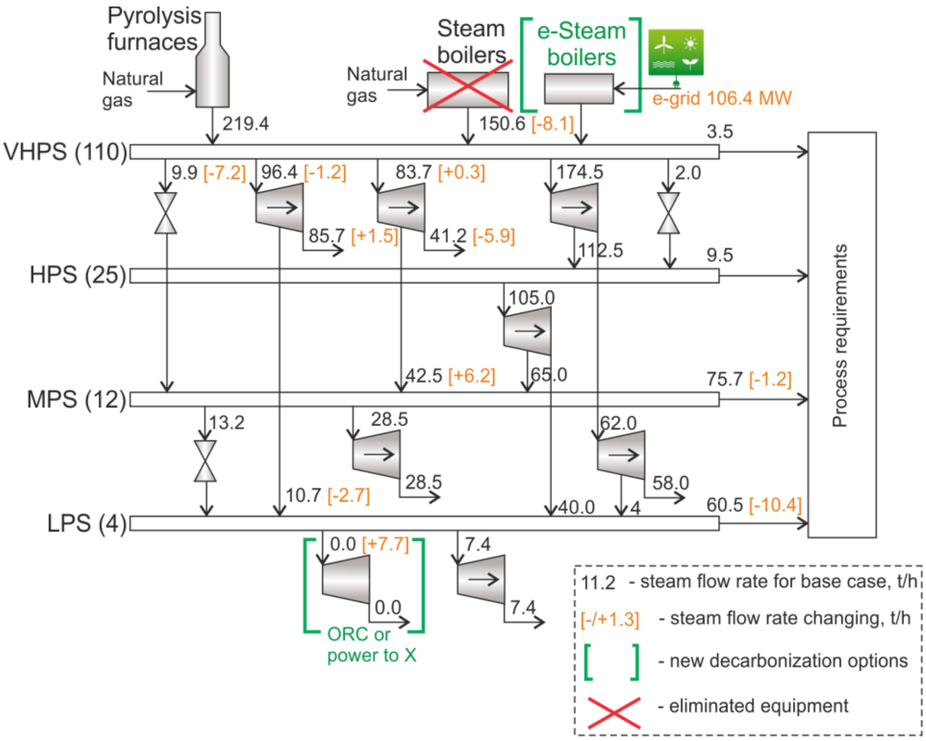

Figure 4: The steam cascade of the monomer plant with steam flow rate changes after the application of energy-saving measures and decarbonization options

Table 3: Economic results and CO_2 savings of developed process retrofit

Scenarios	Economic indicators					
	CAPEX, (EUR)	OPEX saving, (EUR)	CO_2 saving, (kt/y)/(%)	NPV, (EUR)	IRR, (%)	DPP, (y)
Optimistic scenario	1,491,515	20,452,982	18.6 (4 %)	6,006,801	103	3.25
Pessimistic scenario	1,491,515	14,717,617	18.6 (4 %)	3,983,994	70	3.92

5. Conclusions

As a result of energy-saving measures implemented in monomer production, the generation of high-pressure steam was reduced by 8.1 t/h, and the consumption of gas fuel was decreased by 1,712 m^3/h. The amount of low-pressure steam for utilization via ORC is estimated to of 7.7 t/h. The potential share of renewable and sustainable energy was estimated at 40.7 % via using electric boilers for high-pressure steam that corresponds to electricity targets of 106.4 MW. The CO_2 saving from the energy-saving options is 18.6 kt/y or 4 %, and additional potential savings from ORC and electric boilers with renewable energies is 182.4 kt/y or 41 %. The results of this research can be used for the improvement of existing petrochemical plants to achieve sustainable energy goals. However, bottom-up modeling and investigation of specific chemical processes are needed to account for retrofit viability and result accuracy.

Nomenclature

EU – European Union;
toe – t of oil equivalent;
PFD – process flow diagram;
SSDT – steady state digital twin;
IRR – internal rate of return;
VHPS – very high-pressure steam;
HPS – high-pressure steam;
MPS – middle-pressure steam;
LPS – low-pressure steam;
CW – cooling water;
AC – air coolers;
P – propene;
E – ethylene;
NPV – net present value, EUR;
CAPEX – capital expenditure, EUR;
OPEX – operation cost, EUR;
DPP - discounted payback period, y.

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