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

Optimization of prospective circular economy in sewage sludge to biofuel production pathways via hydrothermal liquefaction using P-graph

Safdar Abbas[a]*, Paraskevi Karka[b], and Stavros Papadokonstantakis[a]

[a] TU Wien, Institute of Chemical, Environmental and Bioscience Engineering, Vienna, Austria
[b] University of Groningen, Engineering and Technology Institute Groningen (ENTEG), Faculty of Science and Engineering, Groningen, Netherlands
* Corresponding Author: safdar.abbas@tuwien.ac.at

ABSTRACT

Hydrothermal liquefaction (HTL) has proven to be an appropriate technology for converting sewage sludge into a valuable resource for renewable energy generation. This study focuses on a prospective analysis of various technological scenarios for sewage sludge-to-fuel pathways via HTL, co-located with a wastewater treatment plant, in support of a circular economy perspective. Four technological foreground scenarios and three prospective background scenarios aligned with the Paris agreement's climate targets REMIND-SSP2-Base (projecting a 3.5°C temperature rise by the end of the century), PKBudg1150 (aiming to limit the rise to below 2°C), and PKBudg500 (targeting a cap below 1.5°C) are analyzed for sewage sludge-to-fuel conversion in 2030, 2040, and 2050. The superstructure problem of the possible combinations of the developed scenarios is solved using the P-graph studio which is based on the branch and bound approach. The goal of this study is to maximize the objective function (OF) by accounting the credits from avoided GHG emissions, the market value of recovered products, while subtracting operational costs and GHG emission penalties incurred during the biocrude production and upgrading processes. The optimal solution shows a potential OF equal to 858 €/ton of sewage sludge for Pkbudg500 under technological foreground scenario 2 by 2040. The P-graph approach demonstrates that HTL treatment of sewage sludge provides an alternative production pathway within the circular economy concept, capable of identifying optimal and near-optimal solutions for addressing trade-offs between future socio-economic policies and practical implementation for 2030, 2040, and 2050, which are often difficult to monetize.

Keywords: Prospective circular economy, integrated assessment models, shared socio-economic pathways, sewage sludge, hydrothermal liquefaction.

INTRODUCTION

Sludge from wastewater treatment plants is a major source of urban waste and the circular economy approach has demonstrated its effectiveness in the waste-to-energy sector as a method to extract value from waste while minimizing fossil fuel consumption [1]. Transforming this sludge into fuels for the transportation sector via HTL can substantially support the renewable energy targets in Europe, presenting an eco-friendly and cost-effective solution over traditional waste management practices [2]. Regarding the market acceptance, the use of sustainable advanced biofuels produced from biocrude is viewed as essential in the shift towards renewable energy, offering a pathway to quick emission reduction while requiring minimal alterations to the existing fossil crude infrastructure [1,3]. As sustainability concerns continue to rise, environmental impacts are gaining increasing attention. Prospective life cycle assessment (pLCA) has emerged as a valuable tool for estimating future environmental performance by accounting for the advancement of current and emerging technologies. It considers both the foreground system e.g., improvements of the investigated technology, and the background systems such as raw material and energy market developments [4]. Regarding the evolution of background systems, the integrated assessment model (IAM), based on shared socioeconomic pathways (SSPs), provides a framework for analyzing climate-related scenario outcomes [6]. One such IAM, the regional model of investment and development (REMIND), describes transformation pathways within the interconnected energy-economy-land-climate system [5]. Addressing climate change requires two key approaches: mitigation, which focuses on reducing greenhouse gas emissions, and adaptation, which involves adjusting economies and societies to meet climate goals [6,7]. Additionally, biogenic carbon removal is increasingly recognized as an essential aspect of mitigation and remains an important area for future exploration. This study employs the SSP2 narrative, known as the "middle-of-the-road" pathway, serving as a useful starting point for exploring solutions that integrate climate mitigation and adaptation while also addressing broader societal objectives throughout the 21st century [7,5,8,9].

The open source LCA tool, activity-browser (AB), modifies the Ecoinvent 3.9.1 database to align with socioeconomic and climate-oriented SSP projections, specifically REMIND-SSP2-Base, Pkbudg1150, and Pkbudg500, for the years 2030, 2040, and 2050 [10].

This study focuses on the conversion of sewage sludge into biofuel using the HTL process, as illustrated in Figure 1. Four distinct technological scenarios for converting sewage sludge to biofuel via HTL are analyzed, as detailed in Table 1. Despite the growing interest in HTL for biofuel production, there remains a gap in the literature regarding a comprehensive, prospective analysis that integrates both economic and environmental factors. The core of this study is the use of prospective assessment to identify the most suitable technological production pathway by considering the economic balance between future demand and the market value of products, alongside externality costs related to GHG emissions and future operating costs (OPEX). To address this, the P-graph framework, combined with prospective assessment, facilitates rigorous superstructure design and efficiently identifies optimal and near-optimal solutions for mid-to long-term scenarios [11,12,13].This approach offers a practical tool for decision-makers to assess trade-offs among technological options, accounting for future socio-economic policies and implementation goals for 2030, 2040, and 2050, which would otherwise be challenging to evaluate both economically and environmentally.

MATERIALS AND METHODS

Technological foreground scenarios

The HTL-based foreground system for sewage sludge valorization, shown in Figure 1, is analyzed across four scenarios as detailed in table 1. In scenarios 1 and 3, natural gas is used to heat the HTL unit, while biomethane is the heating source in scenarios 2 and 4, maintaining a temperature of 347°C [1,3,14]. This process converts sewage sludge into fractions by weight: 42% biocrude, 28% aqueous phase, 24% solids and ash, and small amount of gases [3,14,18]. The solid residues are assumed to be disposed of in a landfill. Other technological options involve recovering valuable nutrients, such as phosphorus, or producing a combined fertilizer product from these solids. While this could enhance sustainability and circular economy concepts, further research is needed to evaluate the technical and economic viability of this option, which is beyond the scope of the current study [3,14,18].

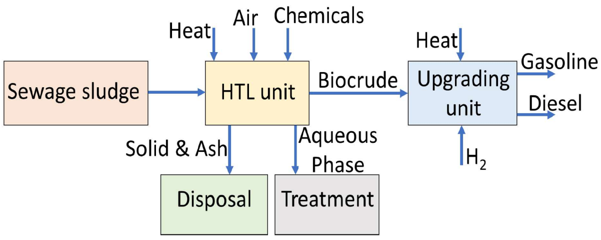

Figure 1. Sewage sludge to biofuel conversion via HTL process.

The aqueous phase treatment varies between scenarios. In scenarios 1 and 3, the aqueous phase, containing effluent water, dissolved organics, ammonia, and metal salts, is treated with lime to raise its pH to 11, releasing ammonia gas. This ammonia is then combusted catalytically in a thermal oxidation unit with a natural gas-air mixture [3,14,18]. In contrast, scenarios 2 and 4 employ dewatering to increase the organic content of the aqueous phase from 7.5% to 45% [3,14,18], followed by anaerobic digestion to produce biogas. After purification, the biomethane generated is used onsite in the HTL and biocrude upgrading units, with any surplus treated as an additional biomethane product. The hydrogen required for upgrading the biocrude differs across scenarios. In scenarios 1 and 2, hydrogen is generated via steam methane or biomethane reforming, while in scenarios 3 and 4, it is produced through electrolysis. The upgraded biocrude is ultimately converted into biogasoline and biodiesel as the primary products, with biomethane included as an additional product in scenarios 2 and 4. The production pathways for sewage sludge-to-biofuel are modeled using P-Graph studio to identify optimal configurations from both economic and environmental perspectives. The analysis evaluates four alternative technological pathways under various future scenarios spanning the years 2030 to 2050. The optimization goal is to maximize the objective function (OF), as defined in Equation (1) [12]. A cradle-to-gate approach is employed in this study to conduct a prospective life cycle assessment (LCA), calculating both the greenhouse gas (GHG) emissions avoided by replacing fossil fuels and the GHG emissions generated during the hydrothermal liquefaction (HTL) process. In this analysis, sewage sludge is assumed to carry no environmental burden, as it originates from wastewater treatment plants (WWTP), where all associated impacts are already allocated. For the alternative approach to biofuel production via HTL, this study specifically examines non-biogenic emission sources, such as chemical inputs and energy consumption. The inputs for converting sewage sludge to biocrude via HTL, upgrading biocrude to biofuels, are detailed in Table 2 and illustrated in Figure 1. Comprehensive life cycle inventories (LCI) for these scenarios are based on data from Karka et al. (2024), Snowden-Swan et al. (2017) and Tews et al. (2014). For cradle-to-gate fossil fuel emissions, the study relies on a prospective LCI database accessed through the open-source software AB.

$$OF = GHG\ avoided\ emissions * C + MV\ product - OPEX - GHG\ emitted\ emissions * C \quad (1)$$

In Equation 1, the term 'OF' does not represent the monetary profit of the entity operating the sludge-to-biofuels facility. Instead, it denotes an objective function that integrates economic aspects (market value minus operational costs) and environmental factors (credits for avoided greenhouse gas emissions minus penalties for emitted greenhouse gases). Both components are monetized to formulate a unified single-objective problem, thereby avoiding the complexity of a bi-objective approach. In OF the term *GHG avoided emissions* refers to the greenhouse gas emissions avoided through the displacement of fossil fuels by biofuels. This is determined by multiplying the annual production of biofuels (e.g., tons of bio-gasoline per year) by the cradle-to-gate emission factor of the fossil fuel being replaced (e.g., tons of CO_2-equivalent per ton of fossil gasoline). These avoided emissions are then multiplied by the carbon tax *C*, measured in €/ton of CO_2-equivalent, to calculate the monetary credits for avoided emissions (€/year). Carbon tax values for 2030, 2040, and 2050 are sourced from the REMIND-SSP2-base, PKBudg1150, and PKBudg500 scenarios [5,15,17].

The term *MV product* is calculated as the revenue generated by biofuel production. This is obtained by multiplying the market price of the biofuel (€/ton), as predicted by the REMIND model for specific years and background scenarios, by the annual production volume (tons/year) for each technological pathway [15,17]. Operating costs *OPEX* include the annual expenses (€/year) associated with biofuel production, considering only the future costs of energy sources such as natural gas and electricity. These costs are derived from REMIND model projections for 2030, 2040, and 2050 under the REMIND-SSP2-base, PKBudg1150, and PKBudg500 scenarios. Material costs for inputs like lime or chemicals, listed in Table 2, are excluded due to insufficient data in the REMIND framework, which primarily focuses on energy-economy modeling [15,17].

The term *GHG emitted emissions* represent the cradle-to-gate greenhouse gas output generated during biofuel production (tons of CO_2-equivalent/year). These emissions are multiplied by the carbon tax (€/ton of CO_2-equivalent) to calculate emission penalties (€/year). Annualized capital costs are not included in this analysis, as their assessment would require a detailed technology learning framework, which is beyond the scope of this study.

Data Collection

The data used in Equation 1, including avoided emission credits, market values of biofuels, operating costs, and emission penalties, is available in the GitHub repository [15]. For convenience, the repository can be accessed directly via this link:[https://github.com/safdar-abbas123/Availability-of-data-for-prospective-circular-economy?tab=readme-ov-file].

Framework of scenarios' modelling using the P-graph software

The P-graph framework is a combinatorial optimization tool based on five core axioms [12,16]. These axioms establish the combinatorially feasible process structures within the P-graph software. Axiom 1 states that every product must be included in the structure. Axiom 2 specifies that a material has no ancestors in the structure only if it represents a raw material. Axiom 3 ensures that every operating unit in the structure is defined in the synthesis problem. Axiom 4 requires that each operating unit in the structure has at least one direct path leading to the final product. Axiom 5 dictates that if a material is part of the structure, it must either be an input to or an output from at least one operating unit in the system [12,16]. These axioms provide mathematically precise guidelines regarding the structural requirements of a problem [12,16]. They are particularly effective in narrowing the structural search space for optimization, allowing the focus to remain on analysing feasible configurations. Figure 2 illustrates the general P-graph structure used to optimize the sewage sludge system. In the first layer, sewage sludge is converted to biocrude via hydrothermal liquefaction (HTL), with heating for the HTL unit provided by either natural gas or onsite-produced biomethane. The second layer involves the upgrading of biocrude, with hydrogen supplied either from natural gas or biomethane through a steam methane reformer (SMR) or electrolysis. In the third layer, product recovery takes place. Four different technological foreground pathways and three prospective background scenarios are considered for the years

Table 1. Scenario description for sewage sludge to biofuel conversion via HTL process included in superstructure.

Scenarios	Heating source in HTL Unit	H_2 source in upgrading Unit	Aqueous phase treatment	Products
Scenario 1	Natural gas	SMR*	Thermal treatment	Gasoline, Diesel
Scenario 2	Biomethane	SBMR**	Anaerobic digestion	Gasoline, Diesel, biomethane
Scenario 3	Natural gas	Electrolysis	Thermal treatment	Gasoline, Diesel
Scenario 4	Biomethane	Electrolysis	Anaerobic digestion	Gasoline, Diesel, biomethane

SMR*: Steam methane reforming
SBMR**: Steam bio-methane reforming
Note: (Sources of these scenarios are mainly from Karka et al. (2024), Snowden-Swan et al. (2017) and Tews et al., 2014).

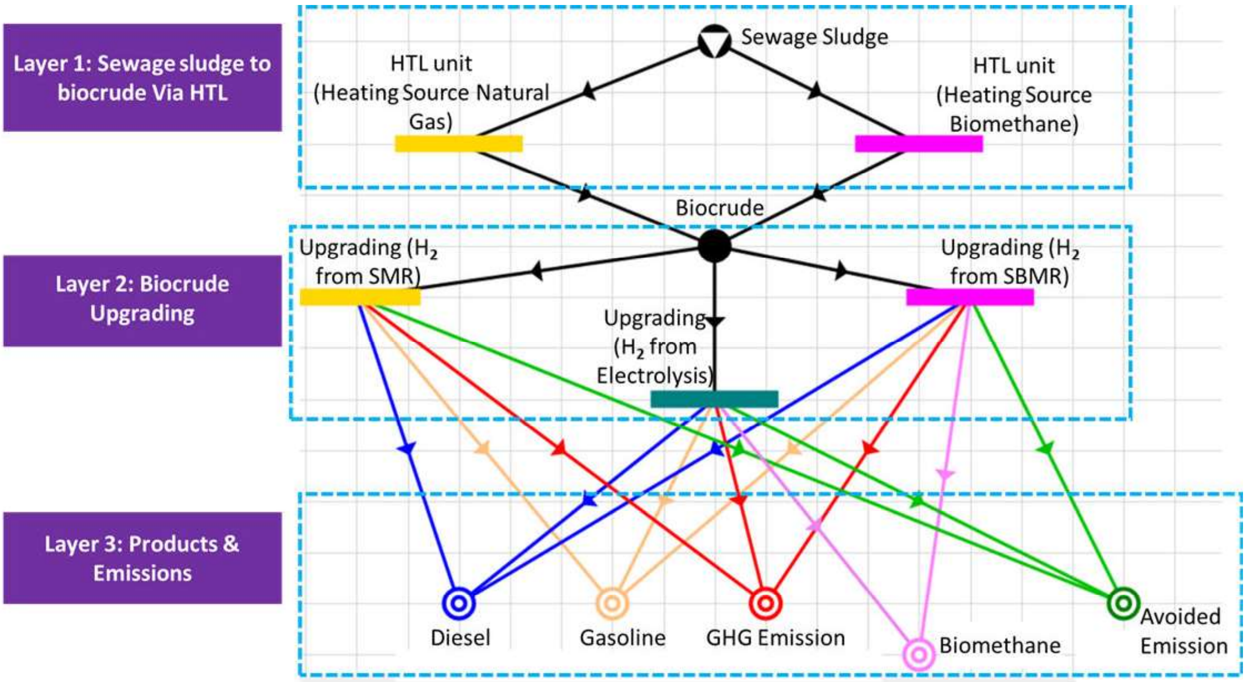

Figure 2. Generic model of sewage sludge to biofuel production using P-graphs: Layer 1 sewage sludge to biocrude via HTL; Layer 2 biocrude upgrading with H_2 sources from SMR, electrolysis, and SBMR; Layer 3 products and emissions.

2030, 2040, and 2050. A total of 36 scenarios are incorporated into a superstructure to find the optimal and near-optimal production pathways.

RESULTS AND DISCUSSIONS

Figure 3 illustrates the optimal and near-optimal solutions for various technological production pathways, modelled using P-graph, across different prospective scenarios for the years 2030, 2040, and 2050. The optimal solution (Scen 2) achieves the highest OF of 858 €/ton of sewage sludge in 2040 under the optimistic REMIND-SSP2-Pkbudg500 scenario, which aims to limit global temperature rise to below 1.5°C. In this technological pathway, biomethane is used in HTL and the biocrude upgrading units. This pathway generates significant revenue from biofuel production (917€/ton of sewage sludge) and credits for avoided GHG emissions through the displacement of fossil fuels (200€/ton of sewage sludge). These benefits outweigh the associated costs, including penalties for cradle-to-gate non-biogenic GHG emissions, primarily resulting from material inputs, as shown in Table 2, during sewage sludge-to-biofuel production via HTL (-253€/ton of sewage sludge) and OPEX (-6€/ton of sewage sludge). The substantial objective function (OF) margin in this pathway is attributed to the optimal alignment of technology and market conditions, maximizing both environmental and economic performance.

Table 2. Material inputs for sewage sludge to biofuel conversion via HTL process.

Material input	Processing unit	Amount
Dewatered sludge	HTL Unit	4158 kg/hr
Air	HTL Unit	4418 kg/hr
Natural gas or biomethane	HTL Unit	221 m3/hr
Chemical organic	HTL Unit	18.7 kg/hr
Electricity, medium voltage	HTL Unit	160.4 kWh
Biocrude	Upgrading unit	1767 kg/hr
Hydrogen	Upgrading unit	96 kg/hr

Note: (Sources of these material inputs are mainly from Karka et al. (2024), Snowden-Swan et al. (2017) and Tews et al., 2014).

The first near-optimal solution yields a slightly lower OF of 804 €/ton of sewage sludge, also in 2040 under the REMIND-SSP2-Pkbudg500 scenario. In this case, scenario 4 is used, where biomethane is utilized in the HTL unit, but electrolysis is employed for the biocrude upgrading unit. While this pathway generates the biofuel revenues (922 €/ton of sewage sludge) and identical avoided GHG credits (200 €/ton of sewage sludge), it incurs the GHG emission penalties (-267 €/ton of sewage sludge) and significantly increased OPEX (-51 €/ton of sewage sludge) due to the additional electricity use. These increased costs reduce overall OF profitability compared to the optimal solution.

Further reductions in OF are observed in the second and third near-optimal solutions, which use technological foreground scenario 2 as also the best solution but under different background scenario years. The second near-optimal solution, under the REMIND-SSP2-Pkbudg500 scenario for 2030, achieves a OF of 735 €/ton of sewage sludge. In this scenario, revenue from biofuel production is (781 €/ton of sewage sludge), and avoided GHG credits drop to (135 €/ton of sewage sludge), reflecting less favorable conditions compared to the optimal solution. Costs include GHG emission penalties (-170 €/ton of sewage sludge) and OPEX (-11 €/ton of sewage sludge). The third near-optimal solution, also using scen 2, occurs in 2050 under the REMIND-SSP2-Pkbudg500 scenario and achieves a OF of 728 €/ton of sewage sludge. Biofuel revenues is (765 €/ton of sewage sludge), while avoided GHG credits fall to (130 €/ton of sewage sludge). Associated costs include GHG emission penalties (-162 €/ton of sewage sludge) and OPEX (-5 €/ton of sewage sludge). The stack bar charts for these solutions demonstrate that the main drivers of OF are revenues from biofuel production and credits for cradle-to-gate avoided GHG emissions. Scenario 2 performs well under the REMIND-SSP2-Pkbudg1150 and REMIND-SSP2-Base scenarios; however, it achieves the highest objective function (OF) in REMIND-SSP2-Pkbudg500, as indicated by the optimal and near-optimal solutions shown in Figure 3.

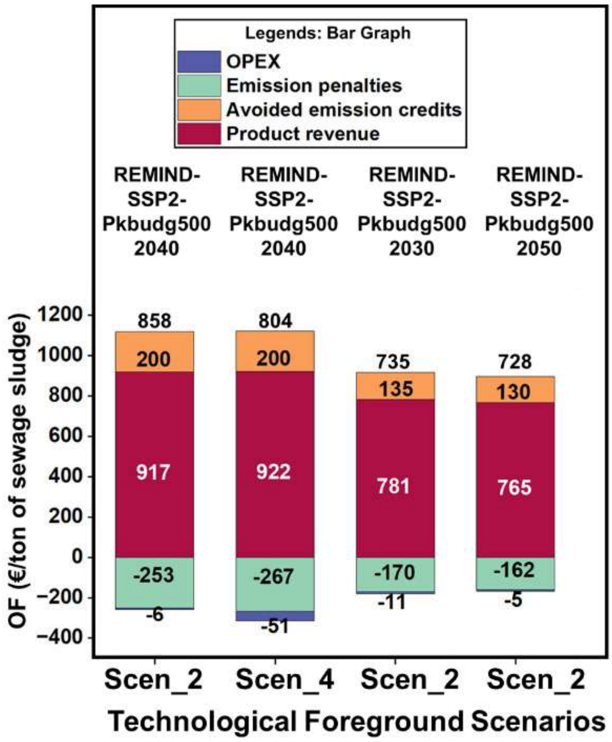

Figure 3. The set of optimal and near optimal solution of different technological foreground scenarios. The bar graph presents the optimal and near optimal solution achieved under the highly optimistic scenario REMIND-SSP2-Pkbudg500 for the year 2030, 2040 and 2050.

Despite costs like GHG emission penalties and OPEX, these revenue streams maintain OF profitability. The key driver for both optimal and first near-optimal solutions in the REMIND-SSP2-Pkbudg500 scenario is the higher biofuel market value in 2040, as outlined in GitHub repository [17]. This increase in biofuel prices significantly boosts revenue, making 2040 the most profitable year. However, biofuel OF are projected to decline in 2050, even under the highly optimistic REMIND-SSP2-

Pkbudg500 scenario, due to reduced demand as the transportation sector increasingly shifts towards electric vehicles and cleaner fuel sources, reducing the reliance on biofuels [5].

CONCLUSIONS

The superstructure-based optimization of sewage sludge conversion to biofuel via HTL, using the P-graph framework combined with prospective assessments, offers valuable insights for circular bioeconomy approaches. The optimal and near-optimal solutions provide valuable guidance for stakeholders offering multiple technological production pathways under various socio-economic scenarios for the years 2030, 2040, and 2050. The optimal solution recommends the conversion of sewage sludge to biocrude through HTL, followed by upgrading biocrude to biofuel, with biomethane being used in both stages. However, a key limitation of P-graphs is its reliance on predefined process structures, which restricts its ability to automatically explore alternative configurations outside the given set. For instance, the present study can be populated with more scenarios regarding the HTL aqueous phase treatment, alternative uses of sewage sludge, and biocrude upgrading product diversification. Despite this, the study illustrates the systematic development and assessment of scenarios, guiding future developments in waste-to-energy conversion and supporting long-term sustainability goals.

ACKNOWLEDGEMENTS

We gratefully acknowledge financial support by TU Wien global budget for PhD research.

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