EMBEDDING ADVANCED WASTEWATER TREATMENT TECHNOLOGY MODELS INTO P-GRAPH FRAMEWORK

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Abstract

Process Network Synthesis for Wastewater Treatment Networks encompasses the sequence of technologies (operations) to remove contaminants via the differences in their physical or chemical properties. These differences in properties contribute to the driving forces that aid in the separation of contaminants and water recovery. Traditional methods of process synthesis have limitations due to simplified technology model equations and deficiency in the incorporation of entire structural properties. To this end, we have developed rigorous technology models via discretization and combinatorial methods for operating units such as sedimentation, filtration, adsorption, and activated sludge. The functionality and accuracy of these rigorous models are demonstrated via a coffee wastewater treatment case study. Furthermore, the P-graph axioms lead to the identification of all plausible wastewater treatment networks as well as provide information regarding their structural feasibility for the concerned case study. The problem is solved via the SSG (Solution structure generation) algorithm in combination with NLP (nonlinear programming) solvers, which leads to the determination of ranked optimal and feasible structures based on well-established process economics including capital and operating costs and the SPI (Sustainable Process Index) sustainability metric.

Keywords: Process Synthesis, Nonlinear Programming, P-Graph

Introduction

According to the World Economic Forum (2020) report, water availability, scarcity, and management are among the top ten global issues that humankind is facing, and if not addressed soon, these challenges will aggravate further. Wastewater treatment (WWT) for water recovery and reuse is one of the ways to help mitigate these concerns (Crini and Lichtfouse, 2018). Treating wastewater for reuse should be recognized as part of the sustainable solution to the quantitative and qualitative problem of water availability (Aboagye et al., 2021; Balkema et al., 2002; Bartholomew and Mauter, 2016; Yan et al., 2017; Yenkie, 2019). Traditionally, wastewater treatment networks are designed based on heuristics and considering previous designs for problems with different specifications. This strategy results in inefficient designs since the selected technologies, and their sequence, highly depend on the properties of the raw

wastewater and the discharge requirements. Due to this, it is highly relevant to employ systematic and advanced methods for synthesizing wastewater treatment networks. In solving problems relating to wastewater treatment, Furthermore, handling nonlinearities and binary variables within the synthesis problem often presents a challenge as global optimality is not guaranteed. In addition, most problems pertaining to wastewater treatment often implement linear models which sometimes are insufficient to describe the treatment process for reliable results. Finally, having ranked options based on both cost and a sustainability metric can help decision-makers implement informed decisions at the onset of projects and help in trade-offs between the economics and environmental burden of the process. Finally, solving a wastewater treatment synthesis problem with multiple products is often challenging as ideally the treated water is to be discharged. However, reusing part of the treated water for subsequent processes which do not require higher purity specifications can help improve the sustainability of industrial processes. Thus, to help address these challenges, we implement the P-graph framework.

In this work, the P-graph framework is employed as a synthesis tool for wastewater treatment networks, as it can exploit the combinatorial properties of the problem's structure to accelerate the optimization and to find a ranked list of the n-best solutions (Friedler et al., 1993, 1992). Furthermore, the use of the combinatorial properties of the problem reduces the search space and decreases the risk of convergence to local optima. Hence, a structural examination of the synthesis problem effectively generates a holistic overview of the problem and provides essential information to the designer (Yenkie et al., 2021).

Methodology

The P-graph framework has two major principles: its graphical representation and the sets of combinatorial axioms and algorithms. A brief introduction to the framework is presented here; for further details, the reader can refer to the work of Friedler et al. (2022). The P-graph representation is deployed to depict the structures of the synthesis problem unambiguously, thus enabling its combinatorial manipulation via the algorithms of the methodology. This graphical representation comprises two types of nodes, i.e., the M-type and the O-type. The first group represents the materials (or streams) in the process, which are represented as circles in the graph; the second group represents the operating units (i.e., units or technologies) involved in the distinct structures. These nodes are shown as horizontal bars in the illustration of the process. The two types of nodes are connected by arcs (i.e., arrows) that indicate the flow direction of the material. Figure 1 shows the graphical representation of P-graph.
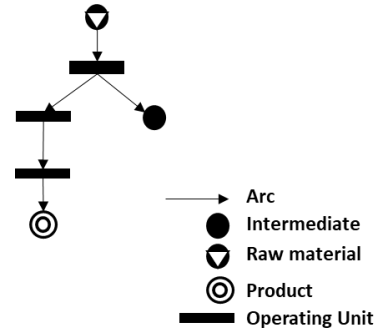

Figure 1. Graphical representation of P-graph showing the materials (intermediate, raw material, product), arc, and operating units

The second major principle of the framework is the set of axioms of combinatorially feasible solutions, which constitute a set of conditions that the structure of every process must fulfill. The framework algorithms are formulated based on these combinatorial axioms; exploiting them to exclude structural infeasibilities beforehand. In this work, two of the t hree P-graph algorithms are employed. Firstly, the MSG algorithm which constructs the maximal structure of the problem by excluding the infeasible nodes. Such a structure contains every feasible structure derived from the units and connections specified. The SSG algorithm is then used to enumerate all combinatorially structurally feasible processes encompassed in the maximal structure. In this work, the enumeration capacity is employed to identify the combinatorially feasible solution structures, which are then individually solved using NLP solvers. Since generated structures are combinatorially feasible, the framework guarantees the inclusion of the optimal structure. Hence, local optima values encountered when MINLP is employed can be avoided (Pimentel et al., 2022).

Example of Technology Model

Naturally, the solution yielded by the structural examination heavily depends on the mathematical models selected to describe the performance of the units. Here, this performance is evaluated using nonlinear functions that relate the parameters of the units with their total annualized cost. An example of the advanced model implemented in this work is demonstrated for the sedimentation unit.

Sedimentation: This model is formulated assuming discrete particle size and laminar flow. The terminal settling speed u_{ts_i} of a particle of diameter D_{p_i} and density ρ_s can be estimated using the Stokes equation (McCabe et al., 2005).

$$u_{ts_i} = \frac{g D_{p_i}^2 (\rho_s - \rho_W)}{18\,\mu} \tag{1}$$

where μ is the viscosity of the fluid. The flow of solids is partitioned in component flows according to particle size distribution, diameters, and their settling speed, regarded as

parameters. The settling time of solids in a tank of depth H is

$$t_{ts} = \frac{H}{u_c} \qquad (2)$$

where u_c is the critical settling velocity of the particle. The residence time in the tank must be equal to or greater than the settling time of the solids. The area of the tank A_{sed}, is given by:

$$A_{sed} = \frac{Q}{u_c} \qquad (3)$$

All particles whose terminal settling speed is higher than u_c, settle completely, whereas the rest of the particles are removed partially with a proportion $\frac{u_{ts_i}}{u_c}$ (Metcalf & Eddy Inc., 2003). Consequently, the constraint for the mass balance of the members of the set of solids, S is given as:

$$a^i \, max \left[0, \left(1 - \frac{u_{ts_i}}{u_c} \right) \right] - b^i = 0 \; \forall i \in S \qquad (4)$$

whereas for those components that do not belong to S it is

$$a^i - b^i = 0, \quad \forall i \notin S \qquad (5)$$

Where a^i and b^i are input and output flowrates, respectively. The annualized capital cost of the settling tank is then estimated as a function of the area according to the expression

$$C_{Sed}^C = 14041.05 + 362.54 \, A_{sed}{}^{0.83} \qquad (6)$$

The operating cost includes pumping and flocculants for settling, which are proportional to volumetric flowrate, Q, and sedimentation area:

$$C_{Sed}^{Op} = 281.1 + 2.01 \, A_{sed}{}^{0.73} + 103.68 \, Q \qquad (7)$$

The total annualized cost of the settling tank is then calculated as the sum of capital and operating costs

$$C_{Sed} = C_{Sed}^C + C_{Sed}^{Op} \qquad (8)$$

In addition to estimating the cost for each feasible structure, we incorporated the Sustainable Process Index (SPI), an ecological footprint that maps the entire process to land area (Krotscheck and Narodoslawsky, 1996; Narodoslawsky and Krotscheck, 2004). This ecological footprint typically comprises seven areas, namely: areas needed for raw materials and energy consumption, areas required for equipment installation and staff accommodation, and areas needed to embed air, water, and soil emissions (Narodoslawsky, 2015). However, in this work, we only considered areas needed for raw material, energy, staff, and equipment installations. Thus, SPI was estimated for each feasible structure investigated to help analyze the environmental burden of each process.

Case Study

We illustrated the methodology described using a synthesis of a coffee wastewater treatment network. The coffee production process requires approximately 15,000 L of water per ton of coffee fruit (Rattan et al., 2015). Hence the coffee production process results in huge wastewater generation. In this work, the case study is adapted from Wisniewski et al. (2020) where they investigated the possibility of using a vibratory nanofiltration unit to recover water for reuse from a soluble coffee manufacturing wastewater stream. The total flowrate for this case study is 1,323 m³/day. Table 1 shows the composition of the inlet wastewater stream. There are two outlet requirements: the first product should meet the required purity needed for recycling, while the second is to meet the purity requirements set by the US EPA before releasing into the environment.

We implemented a stage-wise treatment approach where the first stage comprises technologies capable of removing solid contaminants. Thus we considered sedimentation (Sed) and membrane processes (Mbr) for the primary stage. The secondary stage, which is predominantly used for the removal of both chemical and biological contaminants, comprises a rotating biological contactor (Rbc), activated sludge (Asl), and membrane bioreactor (Mbrt) units. The final stage, mainly used to improve the efficiency of removal and aesthetics of the purified water, involves advanced oxidation and ion exchange units. Furthermore, we provided bypasses at each stage of the treatment process to prevent a mandatory technology selection. In addition, we implemented auxiliary units to help with the connectivity between technologies and flows. The "MM_" symbol depicts these auxiliary units (see Figure 2).

We first use the Maximal Structure Generation (MSG) algorithm to generate the maximal superstructure, as shown in Figure 1. Then, the Solution Structure Generation (SSG) algorithm is used to enumerate all the combinatorially feasible structures. Next, these feasible structures are used to automatically generate GAMS® models in MATLAB using MATLAB-GAMS API. These generated GAMS models are then solved using the ipopt solver. According to the results, the combinatorially feasible solutions are partitioned into three groups: i) feasible solutions: structures that rendered an optimal answer by the solver; ii) redundant solutions: structures in whose solution one or more units were excluded as a result of the optimization; consequently, they are equivalent to another combinatorially feasible solution; iii) Infeasible solutions: structures for which the NLP solver selected converged to an infeasible point.

Table 1. Inlet and Outlet Composition

Contaminant	Inlet Component	Outlet 1	Outlet 2
COD (mg/L)	1140	≤228	≤230
TSS (NTU)	22	≤4.4	≤10
Conductivity (µS/cm)	940	≤188	≤188

Figure 2 shows the generated maximal structure for the coffee wastewater treatment case study. From this maximal structure, 151,848 combinatorially feasible structures were identified and analyzed for this case study.
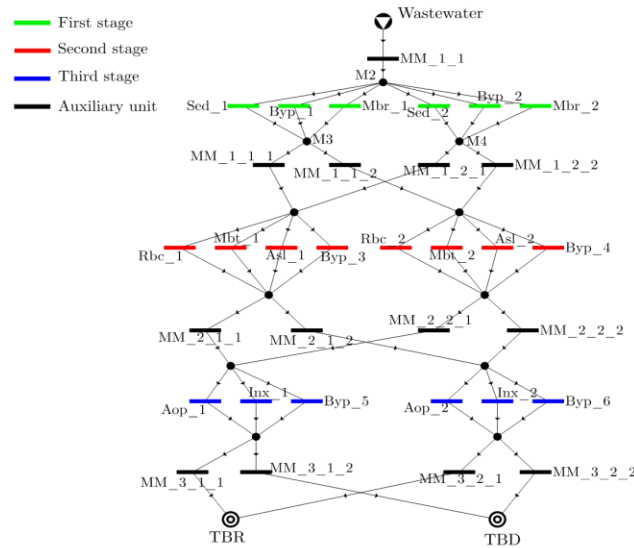

Figure 2. Maximal structure synthesized for coffee wastewater treatment. TBR – To Be Recycled; TBD – To Be Discharged

Result and Discussions

The total cost of the treatment process entails both capital and operating costs per annum. In addition, the total SPI entails the area needed for staff accommodation and equipment installation and areas needed for raw material and energy consumption. We used cost as the objective function because the process has to be viable before it can be implemented. In this work, the cost functions for each technology are functions of the capacity and other peripheral units such as pumping and consumables. To further present different perspectives on how environmentally friendly a selected process will be, we have incorporated the SPI metric to help with trade-offs.
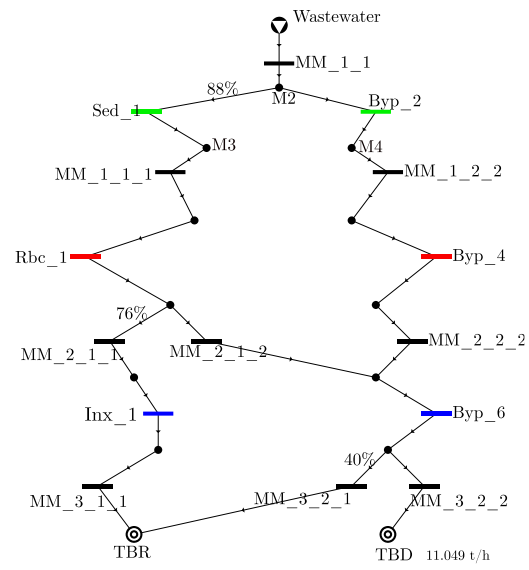

Figure 3. Feasible structure with the least cost of treatment

The most cost-effective solution has an annual cost of $ 54,892/y as shown in Figure 3. The total SPI value corresponding to this feasible structure is 38.84 km^2/y. The technologies selected for this process are sedimentation, rotating biological contactors, and ion exchange. We do observe some interesting features with this structure as more water is to be processed for recycling compared to being treated for discharge. Furthermore, we observe some non-intuitive mixing of diverted streams from the Rbc with the outlet stream from bypass 4.
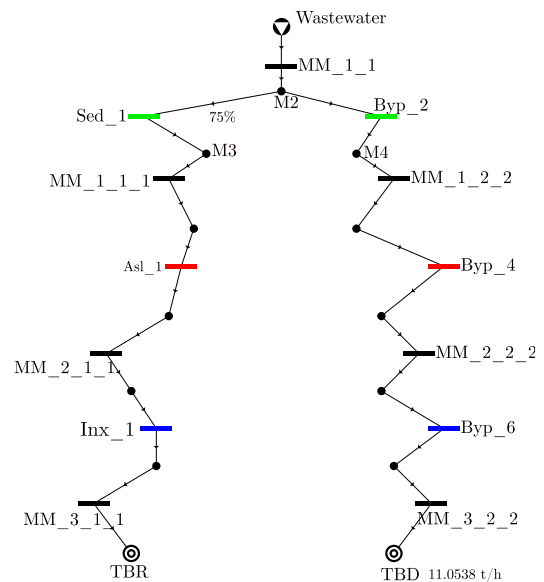

Figure 4. Feasible structure with the least SPI value

Figure 4 shows the feasible structure with the lowest SPI value of 31.50 km^2/y. Thus in terms of reducing the ecological footprint of this wastewater treatment network, a

sedimentation unit followed by activated sludge and ion exchange presents the best solution; however, this comes at an extra cost of $ 6,095/y.

Conclusion

This work integrates detailed nonlinear technology models for separation of contaminants from water as well as exhaustive structural enumeration for the synthesis of cost-effective, and sustainable wastewater treatment networks. The novelty of the work lies in the ability to predict all feasible networks and rank them in order based on the desired metric of cost or sustainability. Furthermore, capturing the driving forces of the separation technologies in terms of nonlinear model equations provides a more realistic cost and efficacy estimate as compared to simplified linear models. All this is possible with reasonable computational complexity and time needed to evaluate the solutions, which is a noteworthy accomplishment in process synthesis. Furthermore, we have used a combination of coding and interactive platforms such as GAMS, Excel and MATLAB. All the features of the work are demonstrated via a soluble coffee wastewater treatment case study. Additionally, we observe trade-offs as certain structures are economically favorable but are less sustainable based on the SPI value estimated.

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