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Total Site Analysis as a Synthesis Model to Select, Optimize and Integrate Processes in Multiple-Product Biorefineries

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The paper presents a new approach to apply Total Site Analysis (TSA). The incentives of this work originate in biorefineries, where numerous alternative processing routes are possible to get integrated in new plants. The fact that energy targets in Total Sites are exclusively estimated using the graphical tool of Site Sources and Sinks Profiles (SSSPs) as well as that TSA assumes fixed processes in integration procedure causes significant limitations in new applications. The problem requires the re-development of conventional TSA approach into a synthesis tool to systematically evaluate the energy targets of numerous alternative process combinations rather than solely estimate steam savings of given process portfolios. Given a set of candidate processes – possible to get integrated with an existing plant or across a new one – the conventional approach would require the exhaustive use of SSSPs to estimate steam savings of each potential process combination. Instead, the proposed approach introduces a new representation to combine thermodynamics of Total Site integration with mathematical programming and systematically screen the infinite process combinations. As a result, the processes portfolio that improves steam savings and minimizes energy cost can be detected. The proposed model was used for the development of a real-life biorefinery yielding in structures with 9 % and 14 % lower hot and cold utility demands, respectively, compared with the solution obtained by using SSSPs.

1. Introduction

Biorefineries constitute the most promising route for the commercially viable valorisation of bio-sources and the replacement of fossil-oil in any application of chemicals and fuels production. The incentives for the utilization of food crops and production of 1G biofuels continuously abate, while the valorisation of 2G (lignocellulosic and organic wastes) and 3G (aquatic) non-food biomass has been significantly increased. Several biorefineries in Europe, USA, China and Brazil have already taken off proving the economic and environmental benefits of the upcoming industry. Biorefineries are capable to utilize up to 80 % less non-renewable sources growing the expectations for a tremendous reduction of GHG emissions from 60 % to 100 %. Only for the EU (2020), the benefits from 2G Ethanol production are estimated to 1000 biorefineries, 1 million new jobs and € 32 billion of revenue (EuropaBio, 2011). 2G biorefineries are capable to valorise a wide range of bio-sources like forestry and agricultural residues, civil and industrial wastes, as well as aquatic biomass (algae). Moreover, several bio-chemical and thermo-chemical routes can be integrated in biorefineries generating a wide spectrum of conventional and novel bio-products that include bulk chemicals, cosmetics, polymers, plastics, coatings, surfactants, pharmaceuticals, probiotics, enzymes, fuels etc.

The integration of multiple processes and products can benefit the overall biorefinery by exchanging raw/auxiliary materials and energy among them. In this scope, Process Integration will play a crucial role for the improvement of sustainability and robustness of the upcoming industry in new markets by providing insights for savings in capital and operating expenses. The development of synergies among processes may result in reduction of up to 90 % in CAPEX (EuropaBio, 2011) and 84 % in energy consumption (Kokossis et al., 2015). However, provided that numerous bio-sources, conversion technologies and bio-products can get integrated across the same plant, critical questions rise about which biorefinery portfolio offers the highest efficiencies. Due to the high impact of energy cost of biorefining on sustainability, this paper focuses on integration techniques that build energy efficiencies in upcoming industrial applications.

The application of energy integration among multiple processes naturally relates to Total Site Analysis (Dhole and Linnhoff, 1993). Besides direct integration of hot-cold streams of each process, TSA investigates for additional benefits by exchanging heat among processes via steam production and reuse. The graphical tool

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of SSSPs is used to estimate steam targets in Total Sites. SSSPs were used in the biorefinery study of Hackl and Harvey (2011) to assess energy benefits (up to 37 % less steam consumption and 15 % improved shaft-work) at the replacement of oil-based feedstocks with renewables in a cluster of six processes in Sweden. Total Site integration was also used to examine and build efficiencies in biorefinery scenarios that valorise lignocellulosic feedstocks (Michael et al., 2014). The multi-stage methodology of Kokossis et al. (2015) uses synthesis models to detect bio-products of high economic potential, while Total Site integration models are next used to fathom in process combinations and detect biorefinery portfolios with high steam savings.

However, the use of SSSPs assumes processes as fixed (given) options of the integration problem. This makes the conventional approach impractical and/or ineffective for the integration of upcoming applications, since processes are not given and constitute significant degrees of freedom. Each process features different energy demands (quantitatively and qualitatively) leading in different steam savings according to the number and energy profiles of processes that are integrated together. Under these conditions, heat exchange options does not refer to a fixed cluster of processes but further extend among all candidates that are possible to get included in the plant. In fact, the biorefinery problem constitutes a synthesis problem and typically requires the exhausting use of SSSPs to evaluate the energy targets of all combinations. However, this approach is time consuming and impractical and inefficient to detect better solutions that can be detected by mathematically formulating thermodynamics of Total Site integration.

The biorefinery problem is represented in the form of value chain paths that incorporate all candidate routes from raw materials (biomass) to intermediate and final products. The value chain paths of Figure 1.a present the conversion routes of biomass into three competitive chemicals (2, 3 or 4) by following alternative processing routes. This example requires three alternative SSSPs to estimate targets for each potential biorefinery. Apparently, the use of SSSPs becomes impractical for large and complex problems, where the candidate combinations explode. Moreover, this paper proves through an illustrative example the existence of infinite combinations that need to be assessed. In this scope, SSSPs are not only time consuming but actually incapable to address the combinatorial synthesis and integration problem.

The development of biorefineries brings new challenges in integration procedure and requires the re-development of TSA concept into a synthesis tool to systematically address the additional degrees of freedom. The paper presents two comprehensive representations (i) to systematize the synthesis of alternative biorefinery routes and (ii) to describe the thermodynamic constraints in Total Site integration serving a holistic energy analysis of the problem. The target of proposed approach is not (exclusively) to optimize energy consumption of involved processes but to synthesize the Total Site (processes portfolio) that minimizes energy cost of the under-construction plant.

2. Problem description: selection of processes to save energy

Energy targeting in upcoming plants is essentially translated into searching for complementary processes that minimize energy consumption, if collocated and integrated together. This means that screening of process combinations and energy integration of involved hot/cold streams should occur simultaneously to identify promising energy synergies among candidates. Synergies may also allow processes enter the plant without additional energy cost by using excess heat from others involved. Though SSSPs could technically evaluate all possible combinations, the combination of thermodynamics with mathematical programming is capable to reveal additional energy savings than cannot be detected by the conventional TSA approach. The potentials for higher efficiencies are presented through the following illustrative example.

Let the candidate biorefinery paths of Figure 1b. Chemical 1 (ex. biomass) is converted through process 1 (p1) into chemical 2 (ex. xylose), which can be next converted to chemicals 3 (ex. ethanol) and 4 (ex. xylitol) through processes 2 (p2) and 3 (p3), respectively. For the purposes of the illustrative example each candidate process includes one hot and one cold stream. The thermal data of processes are as follows: Process p1: T_{supply_1} = 155.01 °C, T_{target_1} = 80.00 °C, Q_1 = 20 MW; T_{supply_2} = 40.00 °C, T_{target_2} = 160.00 °C, Q_2 = 17 MW; Process p2: T_{supply_3} = 147.88 °C, T_{target_3} = 40.00 °C, Q_3 = 3.2 MW; T_{supply_4} = 30.00 °C, T_{target_4} = 137.88 °C, Q_4 = 12 MW; Process p3: T_{supply_5} = 160.00 °C, T_{target_5} = 105.00 °C, Q_5 = 3 MW; T_{supply_6} = 95.00 °C, T_{target_6} = 170.00 °C, Q_6 = 9 MW. The case assumes three steam levels at 100, 130 and 180 °C for heating and cold water for cooling. The Grand Composite Curve of each process is shown in Figure 2. According to conventional TSA approach, two SSSPs are developed: (i) for p1 and p2 (Figure 3(a)) and (ii) for p1 and p3 (Figure 3(b)). In both scenarios, steam generated by p1 is consumed for the heating needs of p2 and p3, while the remaining needs are covered by external utilities. Steam savings range to 47 % and 20 % for cluster p1-p2 and p1-p3, respectively. The utility needs of individually and Total Site integrated processes are summarized in Table 1.

Though individually integrated process p3 appears more promising than p2 from an energy cost point of view (see Table 1), the integration of p2 with p1 yields in higher steam savings and lower energy cost compared to

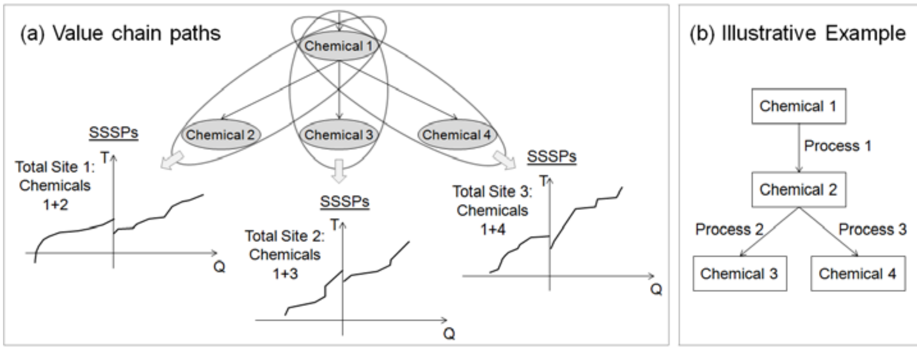

Figure 1: (a) Value chain paths and understudied SSSPs, (b) Value chain paths of illustrative example

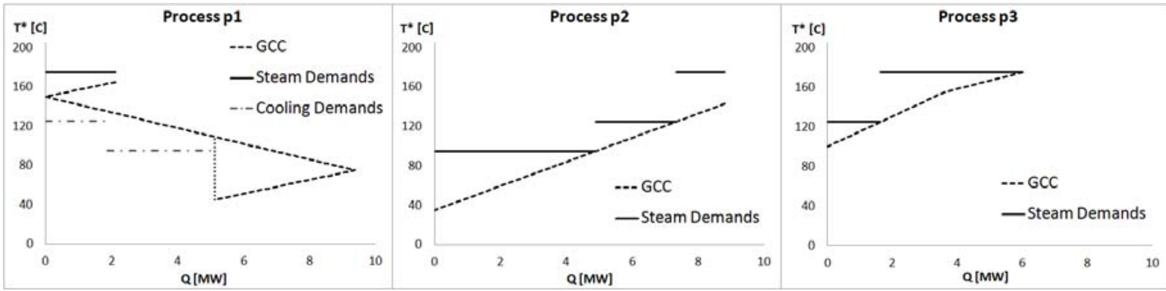

Figure 2: Grand Composite Curves of processes included in illustrative example

integration of p3 with p1 (see Table 1). The use of SSSPs proves that Total Site p1-p2 is the best solution. At first, this proves the importance of addressing TSA as a synthesis tool to investigate promising process portfolios that are not obvious by solely observing the utility needs of individually integrated processes. Secondly, there are additional incentives to search for higher steam savings by sharing upstream chemical 2 among competitive processes p2 and p3. For this reason, the coexistence of p2 and p3 (p1 is always included) is investigated by splitting chemical 2 among processes and, hence, changing their capacities and energy contents in different ways. A step of 10 % is selected for the splitting strategy and a linear dependence of energy demands with process capacity is assumed. The energy targets of all p1-p2-p3 combinations were estimated using SSSPs and the utilities consumption and cost are plotted in the diagram of Figure 4. Though the conventional approach showed above that Total Site p1-p2 is the most promising, a better solution is obtained when p2 and p3 share chemical 2 in the ratio of 70 % - 30 % (Table 1). This grows the expectations that an optimal solution exists in the neighbourhood of this ratio. Apparently, this solution cannot be detected by using the graphical tool, since the construction of Grand Composite Curves and SSSPs require fixed/known capacities (and energy content) of integrated processes. Total Site integration should be mathematically formulated to investigate all synthesis options addressing process capacities as continuous variables rather than as binary options. The proposed concept could be interpreted as if SSSPs were formulated by variable curves.

The proposed methodology introduces two representations to simultaneously describe both the synthesis and integration problem. The first, a Biomass Bipartite graph Representation (BBR), involves disjoint sets for products and processes, and translates arcs, which connect products with processes, into chemicals flows to describe mass balances along value chains. The second representation constitutes a properly modified cascade, Total Site Representation (TSR), which describes all heat exchange options among hot-cold streams of candidate processes and enables the development of energy balances involved in Total Site integration. The mass and energy balances are constructed as an optimization model that is solved using mixed integer linear programming (MILP) and yields the optimal processes portfolio that minimizes the energy cost of the overall plant.

For the case of illustrative example (Figure 1(b)), the proposed model yields the optimal portfolio than includes p1 as well as p2-p3 in the ratio of 66.4 % - 33.6 %; the relevant SSSPs are presented in Figure 3(c). The optimal solution yields in 16 % lower hot utilities consumption and 7 % lower energy cost compared with portfolio p1-p2 that was proved as good solution by using SSSPs for the two alternative combinations p1-p2 and p1-p3.

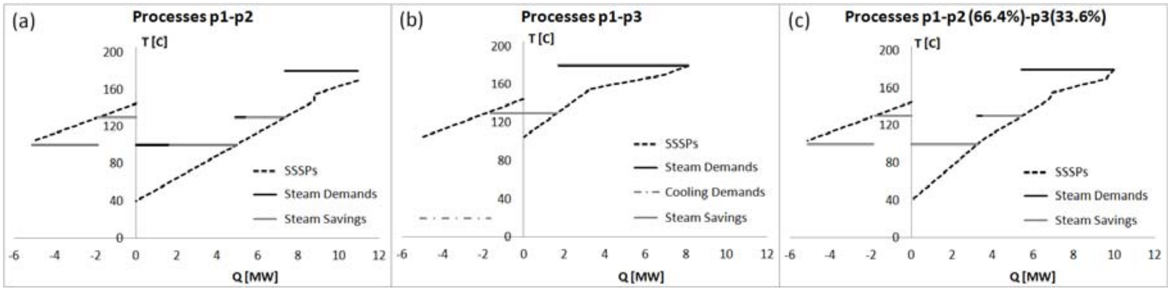

Figure 3: Site Sources and Sinks Profiles of process portfolios in illustrative example

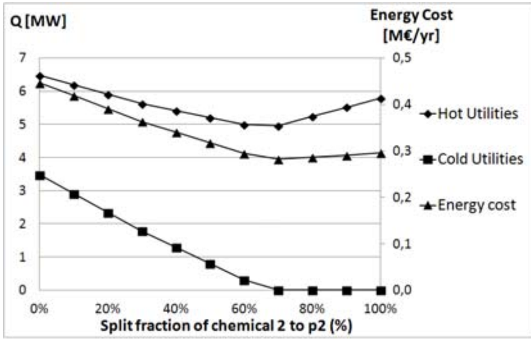

Figure 4: Utilities and energy cost of several p1-p2-p3 process combinations in illustrative example

Table 1: Energy results of individually and Total Site integrated processes in illustrative example

	Individually integrated			Total Site integration			
				SSSPs (Binary combinations)		SSSPs (10% splitting step)	Proposed model
Processes	p1	p2	p3	p1-p2	p1-p3	p1-p2 (70 %)-p3 (30 %)	p1-p2 (66.4 %)-p3 (33.6 %)
Hot utilities [MW]	2.12	8.80	6.00	5.80	6.49	4.96	4.86
Cold utilities [MW]	5.13	0.00	0.00	0.00	3.49	0.00	0.00
Energy cost [M€/y]	0.213	0.362	0.306	0.278	0.418	0.263	0.259

Utilities	Steam 180 °C	Steam 130 °C	Steam 100 °C	Cold Water
Cost [M€/MW/y]	0.0541	0.0430	0.0364	0.0191

3. Methodology

The Biomass Bipartite graph Representation (Kokossis et al., 2015) was properly adjusted for the needs of this work. The graph uses three building blocks: product nodes (chemicals), process units (paths) and interconnections (arcs), to translate the unclear value chain paths into comprehensive representations. Accordingly, the following sets are defined: PR={pr| product nodes of value chain}; P = {p| process units of value chain}; and T = {t| interconnections that transfer chemicals between product nodes and process untis}. For the case of illustrative example (Figure 1(b)), the transformation of the understudied value chain into BBR (Figure 5(a)) requires 4 product nodes (pr1-pr4), three process units (p1-p3) and nine interconnections (t1-t9). At next, let $\mathrm{f_t}$ and $\overline{\mathrm{f_t}}$ be the actual and maximum flowrates of interconnection t. Given the annual capacity of the raw material of value chain and the conversion rates (given by experimental groups) of feed-chemicals of each process to downstream chemicals, the maximum flowrates of interconnections can be estimated in advance. Eventually, the mass balances at each product node and process unit can be recorded. For the BBR of Figure 5(a), the mass balances at each node are: $f_{t1} = f_{t2}$ *(for pr1)*, $f_{t3} = f_{t4} + f_{t5}$ *(for pr2)*, $f_{t6} = f_{t8}$ *(for pr3) and* $f_{t7} = f_{t9}$ *(for pr4)*; and for each unit are: $\frac{f_{t2}}{\overline{f_{t2}}} = \frac{f_{t3}}{\overline{f_{t3}}}$ *(for p1)*, $\frac{f_{t4}}{\overline{f_{t4}}} = \frac{f_{t6}}{\overline{f_{t6}}}$ *(for p2) and* $\frac{f_{t5}}{\overline{f_{t5}}} = \frac{f_{t7}}{\overline{f_{t7}}}$ *(for p3)*. Given the maximum capacities of each process, the maximum energy content of involved hot/cold streams ($\overline{Q_p^{hot/cold}}$) can be also estimated in advance. Assuming that the mass and energy flows within a process linearly depend on its capacitiy, the actual energy content of streams can be expressed through the actual flowrates of interconnections that feed each process as: $Q_p^{hot/cold} = \frac{f_{feed\_t\_of\_p}}{f_{feed\_t\_of\_p}} \cdot \overline{Q_p^{hot/cold}} \quad \forall p \in P$. This generic expression defines the communication between mass balances of BBR and energy balances of Total Site representation and actually activates/deactivates the heat contribution of streams of selected processes (when $f_{feed\_of\_p} \neq 0$) in the integration procedure.

Integration in Total Site Analysis occurs in two levels: (i) direct integration between hot-cold streams that belong to each process and (ii) indirect integration between hot-cold streams that belong to different processes via steam production/reuse. Though several models concerning direct integration are available in literature, Total Site Analysis misses of a mathematical formulation. For this purpose, the paper introduces a new super-interval representation, called Total Site Cascade (TSC), which is composed by the intervals of all individual cascades of candidate processes (Figure 5(b), left). The proposed cascade enables the mathematical formulation of Total Site integration as an optimization model using a properly modified transshipment model.

Each interval of TSC incorporates heat flows related with direct heat exchange among contributed hot-cold streams excluding heat exchange options among streams belonging to different processes. As a result, TSC estimates the total utility needs of individually integrated processes that contribute. At the same time, a parallel set of blocks, called utility operators (Figure 5(b), right), is applied together with TSC to supervise utility needs of TSC and proceed with indirect integration among contributed processes. In particular, the blocks (i) translate excess heat from TSC into steam production, (ii) estimate the maximum overlap between generated and demanded steam and (iii) call for external (Total Site) utilities to cover the remaining demands. The combined system of TSC and utility operators constitute the TSR.

Since processes are addressed as additional degrees of freedom (through variables f_t), the utility operators indentify steam-source/sink-processes that improve steam savings and avoid processes that charge the Total Site with non-steam (namely, non-recoverable) utilities.

The objective function estimates the energy cost, E^{TS}, and involves the Total Site utilities weighted by their unit costs. While BBR develops all feasible Total Sites (TS'), TSR searches for the prime Total Site, TS'^*, that minimizes energy cost; namely: $\exists\, TS'^* \in TS'$: $E^{TS'^*} = min[E^{TS'}]$. The problem can be alternatively formulated by further including in the objective function – preserving the linearity of model – basic economic characteristics of candidate processes (CAPEX, OPEX and profits from product sales) to select the portfolio that maximizes profitability of the plant.

4. Case Study

The proposed methodology was used to select processes for a real-life lignocellulosic biorefinery that involves 7 candidate paths and 9 chemicals (Figure 6). Each process was simulated using Aspen plus V8.6 according to its maximum capacity; thus, the maximum heat contents of all hot/cold streams are estimated beforehand. On one and, the portfolio with the lowest energy cost that obtained by using the SSSPs tool for each process combination (assuming processes as binary options) involves p1, p2, p4 and p6 at their maximum capacities (shaded processes in Figure 6.a). The hot and cold utilities of this portfolio range to 47.3 MW and 60.8 MW, respectively; steam production ranges to 12.8 MW; the energy cost is 3.73 M€/y. On the other hand, the proposed model selected p1, p2, p4, p5, p6 and p7 at 100 %, 100 %, 28 %, 72 %, 100 % and 72 %, respectively, of their maximum capacities (shaded processes in Figure 6(b)). The hot and cold utilities range to 42.9 MW and 52.4 MW, respectively, while steam generation increases to 13.8 MW; the energy cost is estimated at 3.67 M€/y.

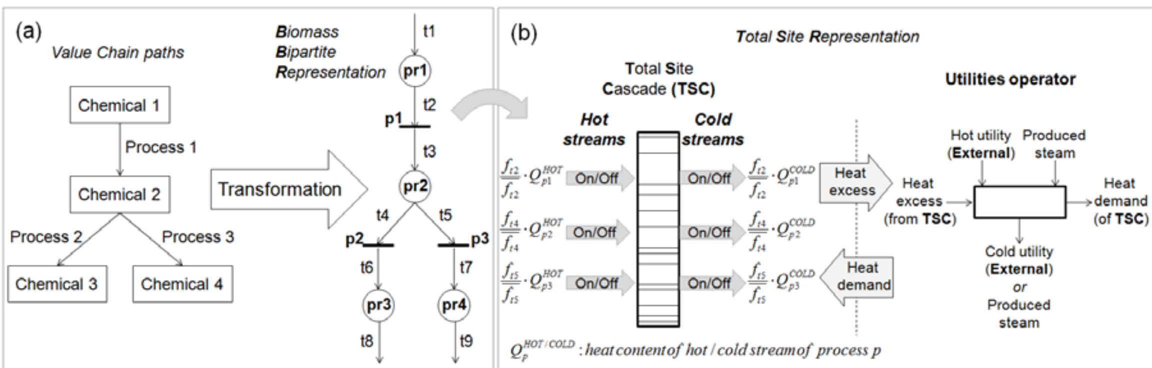

Figure 5: (a) Transformation of value chain paths into BBR, (b) Total Site Representation

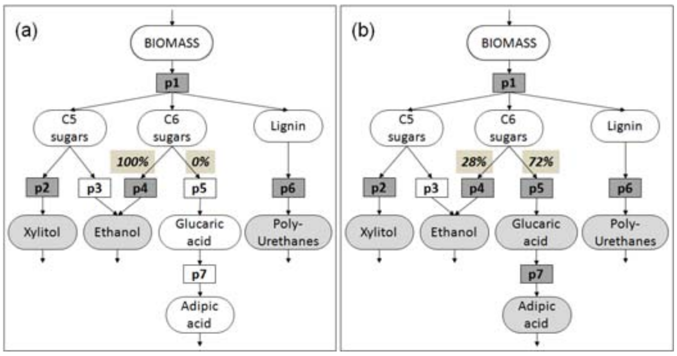

Figure 6: BBR of lignocellulosic biorefinery: (a) solution obtained by using SSSPs, (b) solution obtained by proposed model

The optimal solution obtained by proposed model yields in higher energy efficiencies compared to solution obtained by using SSSPs in any level: 9 % (hot) and 14 % (cold) lower utilities consumption, 8 % higher steam production and 2 % lower energy cost. Moreover, the optimal solution involves a bigger products portfolio by further incorporating adipic acid. The improvements in generation of steam that detected by using the proposed model are due to the selection of p7 (1 MW of steam is additionally generated). The conventional approach was incapable to predict this benefit, since the steam-source-process p7 becomes beneficial only if the upstream process, p5, is selected together with p4 in the ratio of 28 % - 72 %. This particular mix of processes properly adjusts excess heat from p7, which in combination with steam generated by p1 and the steam demands of p4 and p5, yields the highest overlap between generated and demanded steam. Moreover, high cold utility demands coming from p4 are significantly reduced by reducing its capacity from 100 % to 28 %.

5. Conclusions

This paper presents a new methodology to apply TSA as a synthesis tool to address the combinatorial synthesis and integration problem, when candidate processes need to be assessed. TSA is formulated as a mathematical model to estimate energy targets in clusters of processes instead of using the graphical tool of SSSPs. The methodology introduces novel representations to aid with the mathematical formulation of heat exchange options in Total Sites considering involved processes as additional degrees of freedom. Given a range of candidate products and processes, the proposed optimization model (MILP) selects the capacities of the best portfolio of heat-source/sink-processes that minimizes the utilities consumption of the overall under-construction plant. Treating heat contents of involved streams as additional (continuous) variables of the integration problem results in better solutions with higher energy efficiencies compared to solutions obtained by the conventional graphical approach. The model not only detects processes with high steam generation potentials, but also adjusts process capacities to optimally valorise generated steam across the site subsequently minimizing the cost of external utilities.

Acknowledgments

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