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Synthesis of More Sustainable Total Site

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Heat recovery between different streams of Total Site (TS) can significantly decrease external utility consumption. Decreased utility consumption leads to decreased impact on the environment resulting from lower GHG emissions produced by fuel. The optimal rate of heat recovery can be determined by establishing an appropriate trade-off between utility consumption and investment in heat transfer equipment. Therefore, it can be concluded that both economic and environmental pillars of sustainability encourage the goal of constructing TSs. However, the social pillar of sustainability should also be considered in order to ensure the overall sustainability of a TS. The social pillar is usually not included in the synthesis because different aspects of social performance are quite difficult to quantitatively determine. Safety is an important social aspect when considering TS, especially when TS complexes are located across areas with high population density where any failure is a potential source of events with catastrophic consequences. In order to construct a safe TS, one option is to perform risk assessment before the synthesis and forbid highly risky matches at the synthesis step or to perform the synthesis and the risk assessment simultaneously. In this study, risk assessment was performed simultaneously during the synthesis in order to design TSs with as low risks as are socially acceptable. The synthesis was performed in two steps. In Step 1 a globally optimal solution was obtained based on a simplified trade-off between investment and operating cost while simultaneously considering risk assessment using a mixed-integer linear programming (MILP) TransGen model, while in Step 2 a detailed synthesis considering risk assessment was performed on a reduced superstructure obtained in Step 1 with a mixed-integer nonlinear programming (MINLP) model called Total Site Synthesis model, which explicitly considers risk limits during optimization. The risk depends on the frequency of failures and the severity of the consequences. The former can be reduced by the selection of more suitable equipment and the latter by selecting indirect rather than direct heat transfer, selecting smaller sizes and safer operating conditions. The minimization of total annual costs (TAC) is a primary objective of this synthesis. There are significant differences in the results obtained when safety is not considered and when lower risk limits are set in order to obtain safer designs. It can be concluded that by performing TS synthesis using the proposed synthesis model, the inherent safety of the TS is significantly increased; however, this incurs economic expense.

1. Introduction

Projections of energy consumption indicates that world energy consumption is increasing worldwide; even more alarming is the fact that consumption of fossil based fuels such as petroleum and other liquids, coal and natural gas is still increasing (EIA, 2016). Therefore, with current consumption trends, it is unrealistic to expect decrease in fossil fuel consumption, despite different international energy treaties such as the Kyoto Protocol (UNFCCC, 1998), or the latest attempt, the Paris Agreement, that has not yet been ratified by all Parties (UNFCCC, 2016). These are good initial attempts; however, achieving sustainable development is still in the initial stage. When considering global carbon emissions from fossil fuel burning, it can be seen that it is still increasing (C2ES, 2015). The IEA presented a Blue Map scenarios, where possible technologies for reducing CO_2 emission were listed. In this prediction, the greatest reduction in CO_2 emissions can be obtained by the end-use fuel and electricity efficiency (38 %), in the scenario, when CO_2 emissions would be reduced to 14 Gt by the year 2050 (IEA, 2010). Heat Integration can significantly contribute to the CO_2 emission reduction as a result of utility demand decrease. The savings can be even higher when TS synthesis is considered. However,

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for successful implementation of TS, its heat exchanger network in the proposed design should be feasible and acceptable.

One of the most important aspects of acceptability is the safety of the design obtained. Until now, a great deal of work has focused on enhancing the safety of already existing plans, estimating potential deviation events, and their consequences. However, the application of safety metrics as part of the design of many unit operation and chemical processes is still in an early stage of development (Roy et al., 2016). Moreover, existing metrics are mainly qualitative (Marhavilas et al., 2011). Jung et al. (2010) presented a methodology for optimizing the placement of hazardous processes and other facilities using mixed-integer nonlinear programming considering the risk map of a plant area. Kim et al. (2011) tested a qualitative index-based approach in the case of hydrogen infrastructures, evaluating different scenarios. Shariff et al. (2012) dealt with the identification of critical streams with high explosion potential in order to indicate critical points in networks via Process Stream Index (PSI). A similar study for toxic releases was later conducted by Shariff and Zaini (2013). Strictly focusing on safety in a Heat Exchanger Network, there has been some work conducted by Chan et al (2014) who presented a combined methodology of Stream Temperature vs. Enthaphy Plot (STEP) with risk assessment. Liu et al. (2015) assessed the risk in TS using a step-by-step procedure considering direct or indirect heat transfer. Vázquez-Román et al (2015) used a cause-effect analysis in mathematical programming approach to determine optimal layout of facilities considering toxic releases. Inchaurregui-Méndez et al. (2015) considered inherent safety when synthesizing Heat Exchanger Networks based on layout with allocation of hot/cold streams.

Previously, we developed a sequential step-by-step approach for considering safety in a TS (Nemet et al, 2015). The methodology presented in that work cut off some heat transfer options with the highest heat integration potential as matches were assessed prior to synthesis based on maximal heat transfer.

In this study, risk assessment is performed during the synthesis of TS via modelling the interactions between risk and selected Heat Exchanger Networks, leading to better optima. A two-step procedure was developed for obtaining TS design. In Step 1, a global solution is obtained based on simplified area, pipeline, operating cost and risk assessment using MILP model TransGen, while in Step 2 more detailed synthesis is performed using a MINLP Total Site synthesis model, based on the solution obtained in Step 1 that serves as the initialization and prescreening of the alternatives.

2. Methodology

Obtaining a TS design is a complex problem, especially when synthesizing the HEN at both levels of integration simultaneously, within and between processes. Accounting for pressure/temperature drops, heat losses, and pipe design optimisation leads to a highly non-linear model, capable only of solving very small problems and obtaining poor locally optimal solutions. The two-step approach mentioned above was developed in order to obtain solutions closer to global optima and to solve larger problems. In Step 1 the TransGen model for TS area/energy targeting is thus used to identify promising alternatives to be developed further in the second step. Note that risk assessment is performed simultaneously with the targeting process. As the TransGen model is formulated as a MILP model, the solutions obtained are globally optimal; however, because of model simplifications, the trade-off obtained between operating cost and investment of heat exchangers and pipes is rough and should be improved in the second step based on a detailed MINLP synthesis model. As Step 2 is performed on a reduced superstructure identified from the global solution obtained in Step 1, larger problems can now be solved in a rigorous way and the final solutions can thus be guided close to global optima. Note that risk assessment is performed simultaneously in the second step, too.

In Step 1, the TransGen (Nemet et al, 2016) targeting model for the synthesis based on an extended transhipment model using temperature intervals is used. Although area calculation is simplified, it is still realistic enough in order to achieve a reasonable trade-off between investment and operating cost; moreover, the risk assessment is also based on the determined area. For this purpose, the heat transfers between process streams are explicitly determined as, $q_{i,j,k,kk}$ representing the heat transferred from hot stream *i* released at interval *k* to cold stream *j* consuming the heat at the same or lower temperature interval *kk*. The area is determined for each heat transfer from each interval *k* to the same or lower temperature interval *kk*. Note that besides indirect heat transfer between processes via intermediate utilities, direct heat transfers between processes are also allowed, assuming a transport of cold stream from one process to the hot streams of the other process and after returning to its original process. Heat losses are accounted for in both cases. It should be noted that risk assessment is determined for each heat exchanger. This is defined as a multiplication of the failure frequency and the severity of the consequences (Eq. 1). The failure frequency f^{fail} can be determined based on historical data, while the severity of the consequences is determined based on the amount of the substance present in the heat exchangers and its properties and operating conditions. The amount of the substance is determined by multiplication of the area of the heat transfer A_{hx} and the density of the substance divided by area density β_{hx} of the heat exchanger (ratio between area and volume of the medium in the heat exchanger). The operating conditions and placement of heat exchangers are considered via factors f^1-f^3 and the limiting value G_{risk} for the considered risk type (toxicity, flammability, explosiveness) depending on the properties of the substance.

$$R_{s,hx,risk} = f_{hx}^{fail} \cdot \frac{A_{hx} \cdot \rho_s \cdot f_{hx}^1 \cdot f_{hx}^2 \cdot f_s^3}{\beta_{hx} \cdot G_{risk}} \qquad \forall s \in S,\ hx \in HX,\ risk \in RISK \qquad (1)$$

It should be noted that the area in the first step is somewhat overestimated. Larger heat exchangers lead to higher risk; therefore, they reach the upper limit of individual risk limit earlier compared to the optimised area. Therefore, parallel heat exchangers between the same hot and cold streams are included as an option not to cut off matches with high heat integration potential and still acceptable risk. For this purpose, the number of parallel heat exchangers is selected via binary variable y_p that is related to coefficient k^{phe} presenting the number of parallel heat exchangers.

$$A_{i,j}^{new} = \sum_{phe} k^{phe} \cdot A_{i,j,phe}^{phe} \qquad \forall i \in I,\ j \in J \qquad (2)$$

$$A_{i,j,phe}^{phe} \leq 1/k^{phe} \cdot y_p \cdot A^{\max} \qquad \forall i \in I,\ j \in J,\ phe \in PHE \qquad (3)$$

Another binary $y_{i,j,phe}$, presenting exactly the heat transfer between hot stream i, cold stream j and number of parallel heat exchangers *phe* is introduced in order to enable the risk assessment of pipe when direct heat exchange between process streams belonging to different processes is selected for a heat match.

$$y_{i,j,phe} \leq y_{i,j} \qquad \forall i \in I,\ j \in J,\ phe \in PHE \qquad (4)$$

$$y_{i,j,phe} \leq y_p \qquad \forall i \in I,\ j \in J,\ phe \in PHE \qquad (5)$$

$$y_{i,j,phe} \geq y_{i,j} + y_p - 1 \qquad \forall i \in I,\ j \in J,\ phe \in PHE \qquad (6)$$

The risk for heat transfer between a pair of hot and cold process streams within a process is determined as the risk of substance of the hot process streams in a heat exchanger as well as the risk of medium in the cold process stream. For direct heat transfer between different processes, the risk assessment for a pipe should be added:

$$R_{s,hx,risk} = 2 \cdot f^{fail} \cdot L_{hp,cp} \cdot qm_{\mathrm{cp}} \cdot 600 \cdot \frac{f_{hx}^1 \cdot f_{hx}^2 \cdot f_{cp}^3}{G_{cp,risk}} \cdot \mathrm{y}_{hp,cp,phe}^{phe} \qquad \forall s \in S,\ hx \in HX,\ risk \in RISK \qquad (7)$$

Note that for the risk of a pipe, when utilising indirect heat transfer via steam, a zero value is used as steam is neither toxic, flammable nor explosive.

The objective function is defined as total annual cost, where the additional investment for Heat Integration is considered:

$$TAC = \sum_{hp}\left(Q_{hp}^{\mathrm{CU}} \cdot t^{\mathrm{op}} \cdot c^{\mathrm{CU}}\right) + \sum_{cp}\left(Q_{cp}^{\mathrm{HU}} \cdot t^{\mathrm{op}} \cdot c^{\mathrm{HU}}\right) + \sum_{icup}\left(Q_{icup}^{\mathrm{HU}} \cdot t^{\mathrm{op}} \cdot c^{\mathrm{HU}}\right) + \sum_{Ccond}\left(Q_{Ccond}^{\mathrm{HU}} \cdot t^{\mathrm{op}} \cdot c^{\mathrm{HU}}\right) + f^{annual} \cdot I \qquad (8)$$

3. Case study

3.1 Input data

Different types of heat exchangers are considered during optimisation of the heat exchanger network of a TS (Table 1). The case study consisted of two processes, P1 and P2. Process P1 includes six hot streams and two cold streams, process P2 consists of two hot and four cold process streams. The input data for these processes is presented in Table 2. It should be noted that additional data were required in order to perform risk assessment.

Four different intermediate utilities were available for indirect heat transfer between processes (Table 3). The temperatures of intermediate utilities are fixed during the optimisation in Step 1 ($T^{fix,Step\ 1}$), while in Step 2 they are considered as optimisation variables within given upper and lower temperature bounds as presented in Table 3.

Table 1: Input data for different heat exchanger types

Type of HE	A^{max}/m^2	T^{LO} /°C	T^{UP} /°C	*cf*/ k€	*cv* / k€/m^2	*β* / (m^2/m^3)	f^{fail}/y^{-1}
Double pipe	200	-100	600	46	2.742	80	0.009929
Plate and frame	1,200	-25	250	129.8	0.347	80	0.010908
Fixed plate shell and tube	1,000	-200	850	121.4	0.193	720	0.009029
Shell and tube with U-tubes	1,000	-200	850	100.9	0.304	1,300	0.009929
Evaporator	1,000	-10	600	174.4	0.919	720	0.009929
Condenser	1,000	-10	600	105.6	0.272	720	0.009929

Table 2: Input data for process streams

Process	Stream	T^{in} /°C	T^{out}/°C	*FC*/ (kW/(m^2.K)	*h*/ (kW/(m^2.K))	LC_{50} (rat, inh, 1h)/ (mg/m^3)	*Qexpl* (kJ/kg)	flammable
P1	H1P1	445	303	9	0.33	500	500	Yes
	H2P1	398	25	10	0.36	900	0	Yes
	H3P1	436	297	19	0.35	300	100	Yes
	H4P1	389	32	8	0.42	100	5	Yes
	H5P1	451	300	24	0.38	800	10	Yes
	H6P1	401	44	11	0.44	5000	5	Yes
	C1P1	40	80	45	0.40	500	0	Yes
	C2P1	50	60	15	0.36	600	500	Yes
P2	H1P2	148	90	16	0.33	100	5	Yes
	H2P2	127	75	12	0.4	50	10	Yes
	C1P2	100	248	45	0.43	700	5	Yes
	C2P2	76	325	10	0.38	500	0	Yes
	C3P2	100	236	25	0.45	600	500	Yes
	C4P2	80	318	15	0.38	100	100	Yes

Table 1: Intermediate utility properties

Intermediate utility	T^{LO} /°C	T^{UP} /°C	$T^{fix,Step\ 1}$ / °C	*h* /(kW/(m^2 °C))
Low pressure steam	120	148	136	10,000
Medium pressure steam	148	208	180	10,000
High pressure steam	208	252	230	11,000
Ultra-high pressure steam	252	275	280	11,000

3.2 Solutions

3.2.1 Without risk assessment

First, a solution without risk assessment was obtained that served as a reference from the safety point of view. The optimal scheme of TS is shown in Figure 1. The HEN for the TS consisted of 20 HEs, of which 12 are fixed plate shell and tube, 6 double pipe and 2 are shell and tube with U-tubes type. Note that only direct heat transfer without intermediate utilities was selected. The TAC was 2,659 k€/y with 315 kW consumption of hot utility and 564 kW of cold utility. It should be noted that this scheme enables a 98.26 % reduction of GHG emissions as a result of Heat Integration within and between the processes. The risk recalculated after optimization was 0.048 y^{-1} for toxicity, 0.002 y^{-1} for flammability and 4.44 x 10^{-7} y^{-1} for explosiveness.

3.2.2 Simultaneous risk assessment

In the second case, the risk assessment was performed simultaneously by setting an upper bound on the overall risk at one-half of initial risk in order to obtain twice safer design than in the first case. The safer TS is shown in Figure 2. The safer HEN of TS now consists of an increased number of HEs – 33, of which 11 are fixed plate shell and tube, 6 are plate and frame, 7 are double pipe, 5 are shell and tube with U-tubes, two evaporators and two condensers. Note that besides direct, indirect heat transfer via medium pressure steam (MPS) was also selected with a 70 % recycle of condensate and preheating of fresh water and condensate streams. The TAC was increased to 3,268 k€ as a result of more than double the hot utility consumption, now 851 kW, and cold utility consumption of 754 kW. The reduction of GHG emissions caused by Heat Integration is now slightly worse than the first case, a somewhat smaller 95.29 %.

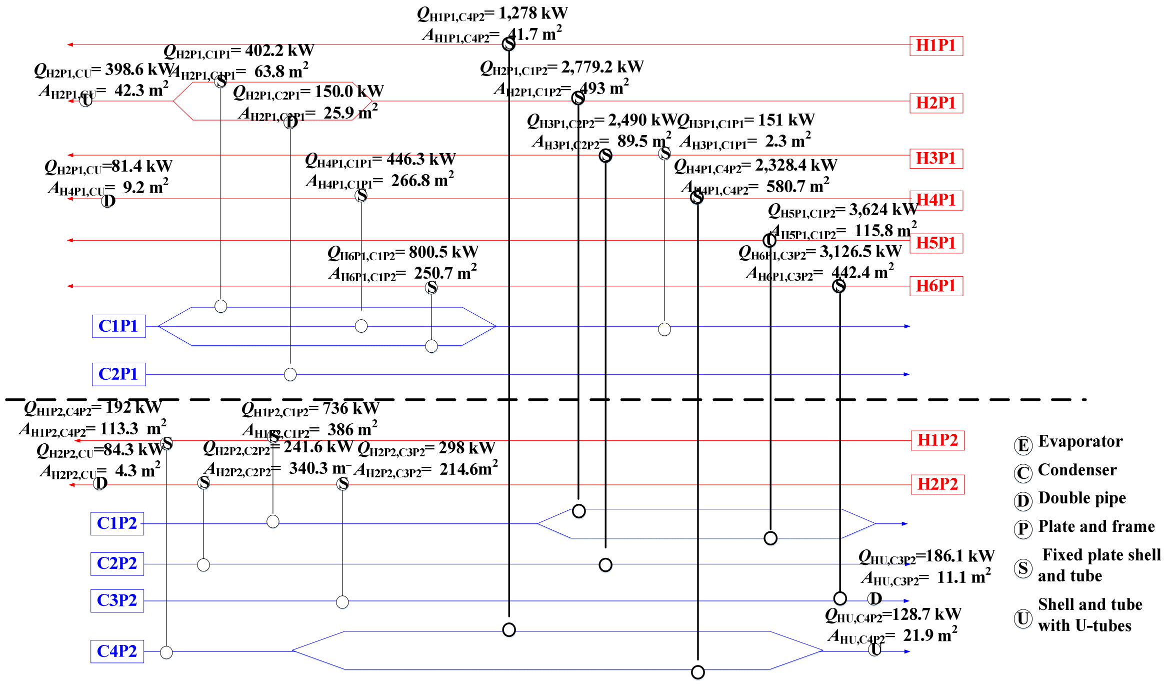

Figure 1: Optimal Total Site when no risk assessment is performed

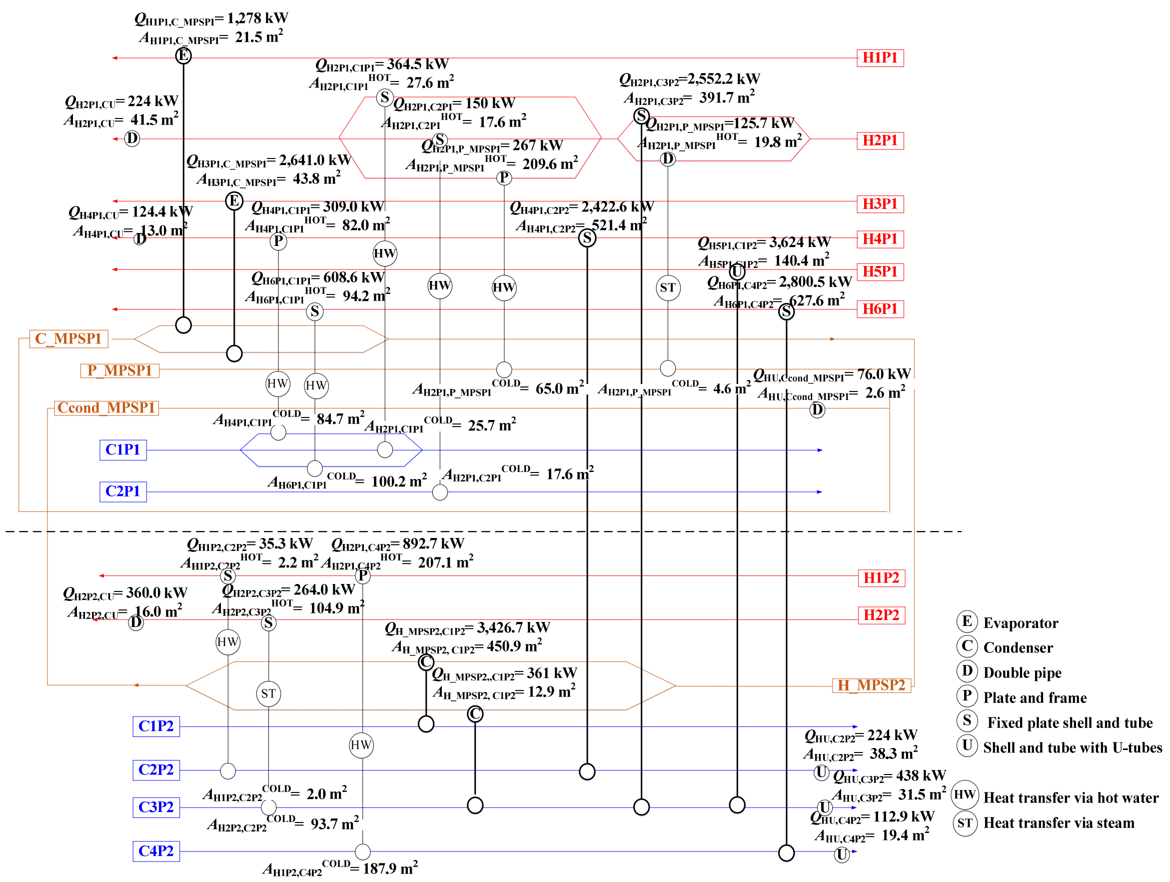

Figure 2: Twice safer Total Site obtained with upper bound on the overall risk set at one-half of initial risk.

4. Conclusion

A two-step procedure for TS synthesis with embeded safety analysis has been developed. The solutions obtained indicate that safety improvements can be obtained at the cost of economic expense. A further observation is that safer designs may exhibit somewhat larger GHG emissions as the level of Heat Integration can be lower.

In future studies, the synthesis of TS, besides setting limits on the overall risk, will be performed also by setting limits on individual units (heat exchangers and pipes), because it may also significantly affect the final design. Also, a composed objective, including both economic and safety aspects directly into the objective function, is planned. This will enable an optimal TS design by performing the synthesis in a single optimization, rather than sequentially by executing Pareto solutions at different risk limits. More appropriate trade-offs between utility consumption, investment and safety can be obtained in this way. The methodology presented here will be extended to other process subsystems as well as to overall process systems.

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