CHEMICAL ENGINEERING TRANSACTIONS

VOL. 45, 2015

A publication of AIDIC
The Italian Association of Chemical Engineering
www.aidic.it/cet

Guest Editors: Petar Sabev Varbanov, Jiří Jaromír Klemeš, Sharifah Rafidah Wan Alwi, Jun Yow Yong, Xia Liu

ISBN 978-88-95608-36-5; **ISSN** 2283-9216 DOI: 10.3303/CET1545021

Safety Analysis Embedded in Total Site Synthesis

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Decreasing utility consumptions by Total Site (TS) process-to-process Heat Integration can be performed via several possible configurations, namely: i) Indirect, via intermediate utility and ii) Direct, by transporting either hot or cold process streams from one process to a heat exchanger placed within another process, undertaking heat exchange and afterwards returning them to the original process. The indirect heat transfer requires more complex network compared to direct, whilst the direct configuration can have safety issues. This contribution presents a five-step approach for TS heat exchanger network (HEN) synthesis. During the first steps the risk assessment is determined for each possible heat transfer match between processes. The matches can be classified by applying a risk-ranking matrix to matches with high, medium and low-level risks. In the fifth step synthesis of the Total Site Heat Integration Network is performed by a mixed-integer nonlinear programming (MINLP) model by considering the classifications of the matches obtained during the first step. The matches can be assigned as forbidden (high risk), allowed with penalty (medium risk) and allowed (low-level risk). The objective of the MINLP model is to maximise the Expected Net Present Value of the Total Site. This methodology was tested on an illustrative case study for analysing the impact of risk assessment. The obtained TS heat exchanger networks (HENs) by applying the described methodology were inherently safer and yet economically viable.

1. Introduction

Total Sites Heat Integration can significantly contribute to all three pillars of sustainability - the environmental burden can be decreased, the economic efficiency increased, and the social aspect improved (Čuček et al., 2015). There are two main approaches for Total Site evaluation (Dhole and Linnhoff, 1993).The first is the thermodynamic approach that sets thermodynamically achievable targets at a certain minimal temperature difference (e.g. Klemeš, 2013) and a mathematical programming approach, where different parts or the whole Total Site Heat Exchanger Network can be optimised, usually by applying an economic objective function (e.g. Klemeš and Kravanja, 2013). Whichever approach is applied any of them can lead to solutions that can hardly be implemented due to the high risk rate. The public's interest in risk assessment has been continuously increasing over the last three decades as a result of the need for obtaining safer and more reliable processes (Marhavilas et al., 2011). Despite great interest in risk analysis the majority of scientific publications on risk assessment cover quantitative methods (66 %) whilst the qualitative methods are only present as a smaller proportion (28 %) – see Marhavilas et al, 2011. The majority of work has focused on the risk assessment and analysis method, assuming a retrofit of an already existing or designed plant. It is used for identifying places with high risks regarding operability requirements. However, the possibility of affecting the inherent safety of a process decreases as the decision or investment on design has already been made (Heikkilä, 1999). Risk assessment at an early stage of design can have substantial impact on the later operations of processes. Chan et al. (2014) combined the inherent safety index with Stream Temperature vs. Enthalpy Plot (STEP) analysis developed for HEN design. It is a graphical approach based on a heuristic that can provide a deep understanding of the planned HEN. However, it can become too complex for solving larger problems and obtaining solutions

Please cite this article as: Nemet A., Lee K., Klemeš J.J., Varbanov P.S., Moon I., Kravanja Z., 2015, Safety analysis embedded in total site synthesis, Chemical Engineering Transactions, 45, 121-126 DOI:10.3303/CET1545021

can be left to the engineer's expertise. The framework presented in this work provides a systematic procedure for synthesis of a Total Site regarding a wider scope of Heat Integration, including risk assessment at an early stage during planning. The acceptable solutions are often trade-offs between low-risk designs and economic viabilities. Obtaining designs by considering only risk analysis might not be implemented due to poor economic performance. In order to evaluate this trade-off during Total Site synthesis, the synthesis is performed by adding penalties to heat transfers with high risks by establishing a trade-off between risk level and economic performance.

2. Methodology

The aim of the developed methodology is to consider safety during the process of obtaining a design for a Total Site. For this purpose a five-step approach has been developed in order to obtain a Total Site Heat Exchanger Network. An extension of the Grid Diagram (Linnhoff and Flower, 1978) has been used for the illustration. The Hu represents the heaters whilst Cu stands for the coolers within the graphical presentation (Figure 1).

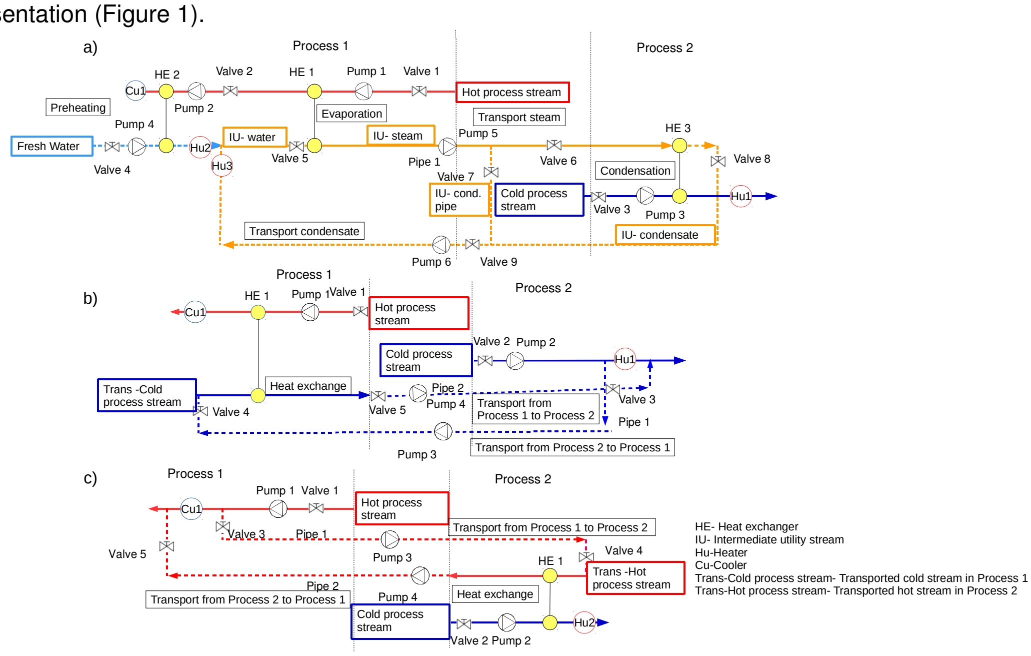

Figure 1: TS HEN, when heat transfer configuration is a) Indirect, via intermediate utility, b) Direct, transport of cold stream and c) Direct, transport of hot stream heat transfer between different processes

Step 0: Total Site description. The Total Site identification and breakdown has to be performed before risk assessment can be performed. On a Total Site three different configurations of heat transfer are possible: i) Indirect, via an intermediate utility (Figure 1a) and direct, by transporting either ii) cold (Figure 1b) or iii) hot (Figure 1c) process streams of one process to exchange heat within another process. In the case of Indirect heat transfer the whole heat transfer process can be composed of five basic operations: preheating, evaporation, transport of steam, condensation and transport of condensate (Figure 1a). In the case of direct heat transfers only three operations occur: transport of cold (hot) stream to another process, heat exchange, and transport of cold (hot) process back to its original process, as presented in Figure 1b (Figure 1c). Moreover, only matches with feasible heat transfer enabled by temperature difference should be included in the further steps of evaluation.

Step 1: Deviations (hazards) identification. The HAZOP (Hazard and Operability study) method is a systematic examination of design documents for identifying and documenting hazards through imaginative thinking. It is the more systemised qualitative technique enabling thorough identifications of deviations (Marhavilas et al, 2011). The specific Guide Words used for Total Site when performing HAZOP analysis are presented in Table 1. They could be extended by more deviation parameters; however, this would also contribute to the complexities of analysis. In this work the temperature and pressure have not been included as parameters. They have rather been treated as a consequence of decreased or no velocity. The planned or emergency shutdown of a process can be treated as the consequence of any failure in this process; therefore, this case has not been included separately as a parameter.

Table 1: Guide words for HAZOP analysis used for Total Site

Parameter	Guide word	Deviation caused by
Flow or velocity	More	Reduced backpressure, surging, controller failure, valve stuck open
	Less	Leakage, partial blockade, fouling, sediment, cavitation, low suction head
	No	Clogging, blockage, pump failure, closed stuck valve, leak
	Reverse	Valve failure or wrongly inserted, poor isolation, wrong routing, control failure
Composition	Other than	Presence of impurities (e.g. air, water, acids, corrosion)
	Part of	Different phases, foaming, change in viscosity or density
	Contamination	Leakage of one media to other

Step 2: Determining frequency and severity of deviation from planned operating conditions. Based on Table 1 and Figure 1 the deviation events can be created for each of the heat exchange matches. The failure frequency is determined based on historical statistical data (e.g. Flemish government, 2009). It should be noted that the pipe failure frequency is determined by considering its length (Flemish government, 2009), which is an important aspect in Total Site. The severity of the leakage is determined following the guideline set in the so-called "Purple book" (Uijt and Ale, 2005). It suggests the calculation of a dimensionless indication number of an installation A_i for a substance *i* as presented in Eq(1) of an installation for substance *i:*

$$A_i = (Q_i \cdot Q_1 \cdot Q_2 \cdot Q_3) / G_i \tag{1}$$

where Q_i is the quantity of the substance *i* present the installation in kg, Q_1 the factor for installation type, whether process or storage, Q_2 the factor for positioning of the installation, Q_3 the factor for process conditions including the amount of substance during the vapour phase after release based on process temperature, atmospheric boiling point, the substance phase and the ambient temperature, and G_i is the limit value representing a measure of dangerous properties on both physical properties and the toxic/explosive/flammable properties of the substance. Determining the risks at each installation can indicate the place/reason for high risks. In the Total Site approach the consequences are not limited only to the loss of some of the media but also the missing of the same media in other places can be critical, due to uncovered heat demand or excess of heat. For this purpose an indication number A^q_i of heat loss or heat cumulating within a system due to cold stream loss is determined by applying the same equation Eq(1), where the loss presents the amount of heat due media loss within 10 min in pipes and the amount of heat present within the mass of media in the heat exchanger. The limiting value is the overall hot or cold utility consumption.
Step 3: Determining the risks of each heat transfer match between processes. The overall risk of one match is obtained by the summation of risk over each installation required for the heat transfer. The total failure frequency for one heat transfer match can be determined as by the summations of failure frequencies of any of the installations involved in the heat transfer. This is done based on the assumptions that a failure of one installation would lead to a failure of the overall network. The total risk should be obtained in order to gain information regarding the total severity of the consequences of deviations for a certain heat transfer between processes. The total severity can then be determined by division of the total risk by the total frequency of failure. The distribution between frequency and severity can still be estimated by revealing the basic problems within a network leading to risk (Figure 2a).

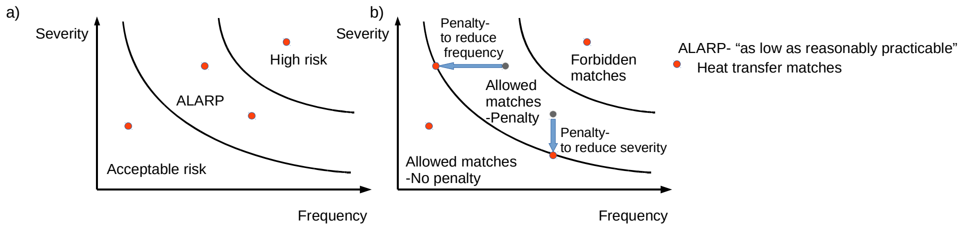

Figure 2: Presentation of possible heat exchanger match as Severity vs. Frequency a) after risk assessment and b) as an input data for TS synthesis

Step 4: Connection between Risk Assessment and Total Site synthesis. The results obtained by risk assessment can be presented as graphical representations Severity versus Frequency (Figure 2a). This plot is divided in three regions: i) high risk, ii) ALARP ("as low as reasonably practicable") and iii) acceptable risk. The same regions are taken as a basis for selecting matches during optimisation to be: i) forbidden matches, with unacceptable high risks, ii) allowed matches with penalties for medium risks, and

iii) allowed matches with acceptable risks. The penalties for medium risk matches are determined as investments required to obtain matches with acceptable risks (Figure 2b). The observed matches can then be transferred to the acceptable risk region. Three types of investments are possible in order to obtain this: i) to decrease frequency, ii) to decrease severity and iii) both simultaneously. The investment to decrease frequency can be a selection of different materials for equipment or increased thickness (diameter) of pipe etc. Decreasing the severity consequences can be more complex as it mostly depends on the media of the process, which would lead to process changes; however, it can be assumed as an investment for additional safety equipment for detection, fire safety equipment etc. Only one type of investment is assumed, representing the minimal investment for obtaining a network with acceptable risk.
Step 5: Synthesis of Total Site considering input data obtained in Step 4. For Total Site synthesis a stochastic mixed integer nonlinear programming model has been used (Nemet, 2015a; Nemet et al, 2015b) considering the risk assessment results.

3. Illustrative case study

This illustrative case study consisted of Process 1 representing a sulphuric acid production plant and Process 2 representing part of a refinery complex. The input data of process streams is presented in Table 2. The utility and cost data has been taken from Nemet et al. (2015a). The distance between processes is assumed to be 2 km.

Table 2: Input data for process streams of the case study

Process	Stream	Type	T_{in}/°C	T_{out}/°C	CP/ kW°C^{-1}	h/kW m^{-2}°C^{-1}	Medium
Process 1	H1P1	Hot	980	430	20	0.065	Sulphuric acid
Process 2	C1P2	Cold	210	368	35	0.62	Oil
	C2P2	Cold	75	95	250	0.5	water

Step 0: All three mechanisms of transfer were considered for the heat transfer between H1P1 and C1P2 as well as for H1P1 and C2P2 (Figure 1). Accounting for the required temperature difference ΔT_{min} = 5 °C the maximal possible heat transfers were determined for all possible heat transfer matches (Table 3).
Step 1: The deviations were determined based on Table 1 for each operation involved in heat transfer, namely: heat exchangers, pipes, and pumps. In regard to heat exchangers the shell and tube types and for pipes the centrifugal pumps with gaskets were assumed. Process streams, trans-streams at direct heat transfer, Fresh W and IU water at indirect heat transfer were all assumed as above ground pipelines, whilst Pipe 1 and Pipe 2 at direct heat transfer and IU steam and IU condensate at indirect heat transfer were assumed as underground pipelines. The valve failure was unconsidered in this case study.

Table 3: Maximal possible heat transfer between all possible process-to-process heat transfers

Match type	Streams involved	Intermediate utility level range	ΔH_{max}/ kW
Direct	H1P1-C1P2	-	5,530
	H1P1-C2P2	-	5,000
Indirect	H1P1-C1P2	LPS: 120-148	0
	H1P1-C2P2	LPS: 120-148	5,000
Indirect	H1P1-C1P2	MPS: 148-208	0
	H1P1-C2P2	MPS: 148-208	5,000
Indirect	H1P1-C1P2	HPS: 208-252	1,295
	H1P1-C2P2	HPS: 208-252	5,000

*At T^{HPS} = 252°C and ΔT_{min} = 5°C
Step 2: The failure frequencies were determined for the above listed equipment. The quantity of substance present in the installation had to be determined in order to determine the severity of consequences of deviations. As the methodology is developed for an early stage design the following simplified correlation for quantities were considered in the heat exchanger. The area of heat exchanger A^{HE} could be determined from the amount of exchanged heat; overall heat transfer coefficient U and the logarithm mean temperature ΔT_{ln}. The correlation between the volume in the tubes and the area could be determined as presented in Eq(4) The more common tube diameter sizes are between 19 mm and 25.24 mm (Edwards, 2008). For a preliminary calculation a 22 mm tube diameter was selected (11 mm radius) for a preliminary calculation.

$$A^{HE} = \Delta H^{\max} / \left(U \cdot \Delta T_{\ln} \right) \tag{3}$$

$$\frac{V^{HE,tube}}{A^{HE}} = \frac{\pi \cdot r^2 \cdot l}{2 \cdot \pi \cdot r \cdot l} = \frac{r}{2} => V^{HE,tube} = A^{HE} \cdot \frac{r}{2} \tag{4}$$

The mass of content can be determined from the volume by multiplication of the $V^{HE,tube}$ by the density of the content. The mass on the shell side can be determined from the mass determined by the ratio between mass flow-rate on the tube side and the shell side of the heat exchanger Eq(5). The mass flow-rate is determined from the heat transferred within the heat exchanger. Sensible heat is determined from Eq(6). If the heat is stored in the form of latent heat (evaporation and condensation of intermediate utility), the mass flow-rate is determined as a maximal enthalpy flow divided by the difference between the specific enthalpy of steam, and water Eq(7).

$$\frac{m^{shell}}{m^{tube}} = \frac{\dot{m}^{shell} \cdot t}{\dot{m}^{tube} \cdot t} = \frac{\dot{m}^{shell}}{\dot{m}^{tube}} => m^{shell} = m^{tube} \cdot \frac{\dot{m}^{shell}}{\dot{m}^{tube}} \tag{5}$$

$$\dot{m} = \Delta H^{\max} / \left(cp \cdot \Delta T\right) \tag{6}$$

$$\dot{m}(T^{steam}) = \Delta H^{\max}\left(T^{steam}\right) / \left(h^{steam}\left(T^{steam}\right) - h^{water}\left(T^{steam}\right)\right) \tag{7}$$

The substance has to be selected carefully for flowing into the tube as it can lead to substantially different results. In regard to pipes the quantity present is determined as the amount within the pipeline, with the length equal to the velocity multiplied by 600 s (Flemish Government, 2009). The mass flow-rate within the pipelines is determined from the heat content in the process pipes. Regarding direct heat transfer the mass flow-rate can be determined similarly as in Eq(6). For the indirect heat transfer the steam mass-flow rate is determined by applying steam tables and maximal possible heat transfer, as presented in Eq(7).
Step 3 The risk is determined for each deviation separately for all the instruments involved during heat transfer covering four major consequences of failure namely toxicity, flammability, explosiveness and additionally for heat loss. The overall risk for a certain heat transfer is determined by summation of all the risks regarding the equipment involved during heat transfer. The frequency of failure is similarly summed up for equipment enabling heat transfer. The average severity is afterwards determined by dividing the overall risk by the overall failure frequency. The obtained results are presented in Figure 3. It should be noted that indirect heat transfer configuration for same match have similar risks, therefore, they can overlap. As can be seen the frequency of the failure is higher in the cases when indirect heat transfer configurations are planned. This is expected as more instruments are involved in heat transfer. However, the severity of the failure is multiple times higher when direct heat transfer occurs. It is a consequence of transporting either sulphur acid or crude between processes. This leads to generally higher risk during direct heat transfer.

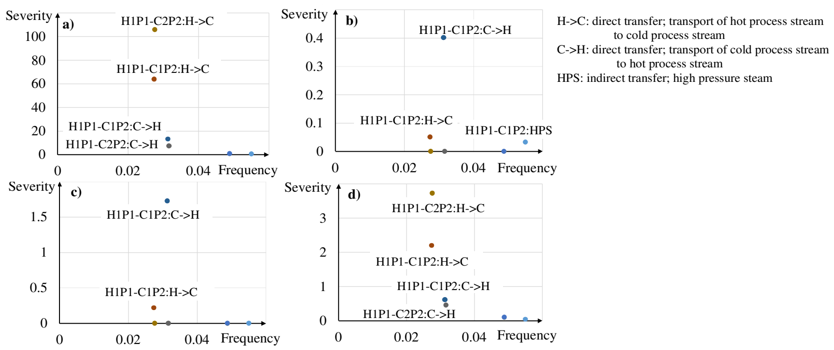

Figure 3: Overall frequency and severity of a certain heat transfer by considering a) toxicity, b) flammability, c) explosiveness and d) heat loss risk assessment.

Step 4: As can be seen in Figure 3 matches H1P1-C2P2 and H1P1-C1P2 have significant risks for toxicity, for direct heat transfer configuration involving heat transport by hot stream. It is a consequence of sulphuric acid being the media in hot stream H1P1. The mentioned matches should be forbidden during synthesis due to the high severity consequences of failure. The flammability risk and explosiveness risk assessment support the decision of forbidding the match between H1P1-C1P2, when cold stream is transported to hot stream, as the media is crude oil that is flammable and might become explosive. The heat loss risk assessment highlights that match where the hot stream is transported having high risk of heat loss.
Step 5: The results of the synthesis indicated that considering risk can provide different solutions compared to those considering only economic criteria. In this particular case, the Expected Net Present

Value of network savings was decreased when considering the risk aspect, namely from 13,853 k€ to 10,831 k€, and the hot utility consumption was increased by 2,369 kW, from 748.5 kW to 3,117.3 kW.

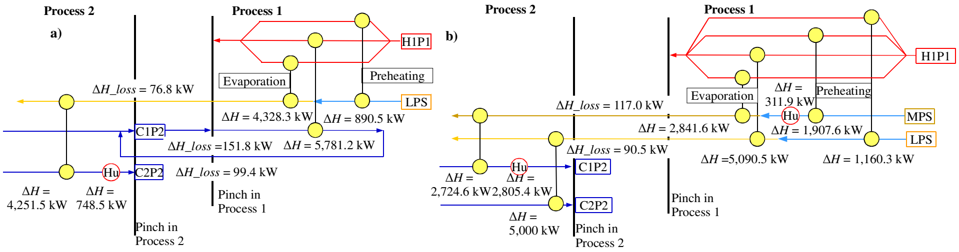

Figure 4: Comparison between solutions obtained considering a) only economic value and b) economic value and risk assessment

4. Conclusions

A framework has been presented for considering safety analysis during Total Site synthesis. The case study indicates that solutions obtained when considering risk aspects can be significantly different compared to those obtained without including the safety aspect-significantly safer solutions can thus be obtained; however, with considerably higher consumption of external utilities.

Acknowledgement

The authors are grateful for the financial support from EC FP7 project FP7-PEOPLE-2011-IRSES “Energy Systems Engineering – ESE”, project No. 294987, EC FP7 project ENER/FP7/296003/EFENIS ‘Efficient Energy Integrated Solutions for Manufacturing Industries – EFENIS’ and from the Slovenian Research Agency (Program No. P2-0032).

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