

Synthesis of Safer Heat Exchanger Networks

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This paper describes the synthesis of safer Heat Exchanger Networks (HENs) accomplished by performing a risk assessment simultaneously during the synthesis. Considering risks during the synthesis of HENs is important because safety, especially inherent safety, can be successfully enhanced at early stages of design. Because risks depend on the types of heat transfer and equipment selected, a superstructure has been generated for the selection of direct and indirect heat transfer between hot and cold streams and different types of heat exchangers (HEs). Both individual HE and overall HEN risks were analysed and different risk limits have been imposed during the synthesis of HEN, considering toxicity, flammability and explosiveness, accounting for the most important aspects of risk. The results indicate that significantly safer HEN designs exhibiting similar economic efficiency can be obtained.

1. Introduction

External utility consumption reduction via Heat Integration is a well-developed field of chemical engineering; however, obtaining realistic results still presents a great challenge. HENs should be reliable, energy efficient and present low harm to the environment. Therefore, considering safety when performing Heat Integration is a significant step towards improving HENs design. The application of safety metrics as a part of the design of several unit operation and chemical processes is still at an early stage of development (Roy et al., 2016), despite continuously increasing public interest in safer and more reliable processes (Marhavilas et al., 2011). Risk assessments are still performed mostly via qualitative assessments, while quantitative methods comprise a smaller part of the developed methodology. Furthermore, most of the quantitative methods are adopted for retrofitting already existing plants with the aim of increasing safety. There are some examples of considering safety in the early stage of planning, however. Jung et al. (2010) optimised the placement of a hazardous process unit and other facilities using mixed-integer nonlinear programming considering a risk map in the plant area. Kim et al. (2011) presented an index-based approach to qualitative risk assessment for a hydrogen infrastructure comparing different infrastructure scenarios. Shariff et al. (2012) presented the process stream index (PSI) that enables designers to identify critical streams with high explosion potential in order to indicate critical points in a network regarding explosiveness. Later, a similar study was conducted for toxic release (Shariff and Zaini, 2013).

Chan et al. (2014) combined the inherent safety index with Stream Temperature vs. Enthalpy Plot (STEP) analysis, developed for HEN design resulting in a graphical approach based on heuristics. Liu et al. (2015) presented a step-by-step procedure for risk assessment of heat transfer between different processes in Total Sites, considering direct or indirect heat transfer. Vázquez-Román et al. (2015) presented a mathematical programming approach to determine the optimal layout of facilities considering toxic releases using a cause-effect analysis. Similarly, Inchaurregui-Méndez et al. (2015) presented a HEN synthesis approach based on inherent safety, where a HEN layout with allocations of hot/cold streams was considered.

Safety analysis is usually performed sequentially: i) either before the final HEN design or ii) after the HEN design is set. This strategy of performing a risk assessment before HEN synthesis can prohibit potentially unsafe matches before optimisation. In this case, some heat transfer with high Heat Integration potential and medium

risk can be cut off. In the second case, when risk assessment is performed on an already selected HEN design, increasing safety can be achieved by higher control of potential risks; however, the options for inherent safety increases are here rather limited.

The aim of this study is to propose inherently safer HEN designs, where safety analysis is performed simultaneously during HEN synthesis. For this purpose, a superstructure approach for HEN synthesis was upgraded with additional safer alternatives in the superstructure and embedded risk assessment in the mathematical model formulation.

2. Methodology

The mixed-integer nonlinear programming (MINLP) model of HEN is based on the stage-wise optimisation model by Yee and Grossmann (1990), upgraded by: i) considering different types of HE, similarly as described in Soršak and Kravanja (2002), ii) including risk assessment for each heat transfer, iii) considering different modes of heat transfer in the superstructure (Figure 1), and iv) enabling parallel heaters and coolers. The different modes of heat transfer include direct heat transfer between hot and cold process streams and indirect transfer using an intermediate utility that presents a penalty in cases of high risk in order to avoid the selection of those matches as much as possible, while still enabling heat transfer at higher cost. The heaters and coolers have upper size limits that can be reached either by area upper limits or risk tolerance; therefore, additional coolers and heaters are allowed in a parallel arrangement.

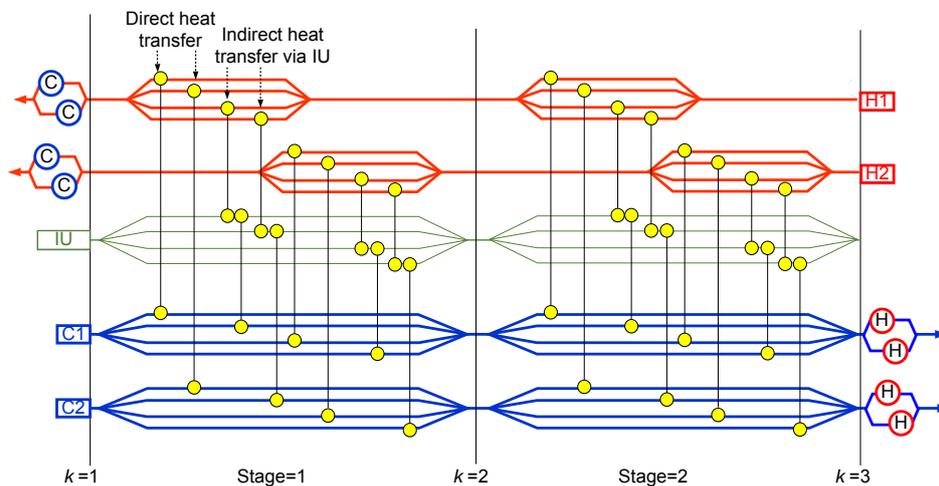


Figure 1: Superstructure for HEN synthesis for two hot and two cold process streams within two stages considering also indirect heat transfer via intermediate utilities

Risk assessment considers the mass of the substance present in the HE. Different types of HEs have different ratios between areas of heat transfer and the volumes of the HEs, leading to significantly different masses in HEs. Moreover, the area of heat transfer for the same amount of heat can vary based on the different geometries of different types of HE. Therefore, it is evident that different types of HE must be considered in order to perform the risk assessment. In our model formulation, a convex hull for different types of HEs was introduced.

Risk assessment measures failure frequency and the severity of the consequences. Failure frequency is a function of the quality of the equipment and the severity of consequences to the substance present in the HE. Failure frequency is usually determined based on historical data. Different approaches can be used to determine the severity of the consequences. In this study, an indication number of intrinsic hazard is determined as described in Uijt de Haag and Ale (2005), who considered toxicity, flammability, and explosiveness. The indication number depends on the mass present in the HE Eq(1).

$$AI_{s,hx,risk} = \frac{m_{s,hx} \cdot f_{hx}^1 \cdot f_{hx}^2 \cdot f_s^3}{G_{risk}} \quad \forall s \in S, hx \in HX, risk \in RISK \quad (1)$$

where $m_{s,hx}$ represents the quantity (mass) of substance s present in the installation, f^1 , f^2 and f^3 present the process conditions, and G is the mass limiting value. f^1 is a factor that accounts for process installation versus storage installation, f^2 is a factor for the position of the installation, whether it is an outdoor or indoor installation, and f^3 accounts for process conditions, whether the substance is in gas (different range accounting for pressure),

liquid or solid phase. For gases, different pressure ranges are defined related to different β factor. The limiting value G for toxicity depends on LC_{50} (rat, inh, 1h) value and phase state of the substance, while the limiting value for flammable materials is 10,000 kg. The limiting value for explosive substances is the amount of substance (in kg) that releases an amount of energy equivalent to 1,000 kg TNT (explosion energy 4,600 GJ). The mass of substance in the HE is determined from the area of the HE, area density β_{hx} and density of the substance ρ_s Eq(2). The area density is a ratio between heat transfer area and volume on one side of the HE and depends on the geometry of each type of HE.

$$m_{s,hx} = \frac{A_{hx}}{\beta_{hx}} \cdot \rho_s \quad \forall s \in S, hx \in HX \quad (2)$$

Substituting Eq(2) into Eq(1) the risk of a substance $R_{s,hx,risk}$ on one side of the HE can be determined from Eq(3).

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

The risk of heat transfer $R_{hx,m,risk}^{HX}$ is then determined as a sum of all substances in the HE, originating from the hot process and cold process stream. The direct heat transfer occurs in one HE. The risk calculated is presented in Eq(4).

$$R_{hx,m=DIRECT,risk}^{HX} = f_{hx}^{fail} \cdot \frac{A_{hx,m=DIRECT} \cdot \rho_{hp} \cdot f_{hx}^1 \cdot f_{hx}^2 \cdot f_{hp}^3}{\beta_{hx} \cdot G_{hp,risk}} + f_{hx}^{fail} \cdot \frac{A_{hx,m=DIRECT} \cdot \rho_{cp} \cdot f_{hx}^1 \cdot f_{hx}^2 \cdot f_{cp}^3}{\beta_{hx} \cdot G_{cp,risk}} \quad \forall hx \in H, risk \in RISK \quad (4)$$

The indirect heat transfer in a match between hot and cold streams is performed via two HEs with an intermediate utility in between, each HE having its own area of heat transfer. In this study, the area of HEs was determined for heat transfer from hot process stream to intermediate utility A^{hot} and from intermediate utility to the cold process stream A^{cold} . The heat losses during indirect heat transfer are neglected Eq(7).

$$A_{hp,iucold,k,hx,m=INDIRECT}^{hot} = \frac{Q_{hp,iucold,k,hx,m=INDIRECT} \cdot \left((1/hh_{hp}) + (1/h_m^{iu}) \right)}{f_{hx} \cdot \left(\left(\Delta T_{hp,iu,k} \cdot \Delta T_{hp,iu,k+1} \cdot \frac{(\Delta T_{hp,iu,k} + \Delta T_{hp,iu,k+1})^{1/3}}{2} \right) \right)} \quad \forall hp \in HP, iu \in IU^{cold}, k \in K \quad (5)$$

$$A_{iuhot,cp,k,hx,m=INDIRECT}^{cold} = \frac{Q_{iuhot,cp,k,hx,m=INDIRECT} \cdot \left((1/hh_m^{iu}) + (1/hc_{cp}) \right)}{f_{hx} \cdot \left(\left(\Delta T_{iu,cp,k} \cdot \Delta T_{iu,cp,k+1} \cdot \frac{(\Delta T_{iu,cp,k} + \Delta T_{iu,cp,k+1})^{1/3}}{2} \right) \right)} \quad \forall iu \in IU^{hot}, cp \in CP, k \in K \quad (6)$$

$$Q_{hp,cp,k,hx,m=INDIRECT} = Q_{hp,iucold,k,hx,m=INDIRECT} = Q_{iuhot,cp,k,hx,m=INDIRECT} \quad (7)$$

The risk of this indirect transfer is then calculated as a sum risk of the hot process stream in A^{hot} and risk of the cold process stream in A^{cold} , while the risk of intermediate utility is not considered as the water or vapour is not toxic, nor flammable or explosive.

$$R_{hp,iucold,hx,m=INDIRECT,risk}^{HX,hot} = f_{hx}^{fail} \cdot \frac{A_{hp,iucold,k,hx,m=INDIRECT}^{hot} \cdot \rho_{hp} \cdot f_{hx}^1 \cdot f_{hx}^2 \cdot f_{hp}^3}{\beta_{hx} \cdot G_{hp,risk}} \quad \forall hp \in HP, iu \in IU^{cold}, hx \in HX, risk \in RISK \quad (8)$$

$$R_{iu,cp,hx,m=INDIRECT,risk}^{HX,cold} = f_{hx}^{fail} \cdot \frac{A_{iu,cp,k,hx,m=INDIRECT}^{cold} \cdot \rho_{cp} \cdot f_{hx}^1 \cdot f_{hx}^2 \cdot f_{cp}^3}{\beta_{hx} \cdot G_{cp,risk}} \quad \forall iu \in IU^{hot}, cp \in CP, hx \in HX, risk \in RISK \quad (9)$$

The overall risk R_{risk}^{HEN} is determined as a sum of risk of all HEs

$$R_{risk}^{HEN} = \sum_{hp} \sum_{cp} \sum_{hx} R_{hp,cp,hx,m=DIRECT,risk}^{HX} + \sum_{hp} \sum_{iucold} \sum_{hx} R_{hp,iucold,hx,m=INDIRECT,risk}^{HX,hot} + \sum_{iuhot} \sum_{cp} \sum_{hx} R_{iuhot,cp,hx,m=INDIRECT,risk}^{HX,cold} \quad \forall risk \in RISK \quad (10)$$

The objective function is defined as incremental expected net present value ΔW_{ENPV} of savings as a result of performing Heat Integration, where the additional investment for Heat Integration is considered:

$$\Delta W_{ENPV} = W_{ENPV}^{HI} - W_{ENPV}^{NoHI} = -\Delta I + \Delta F_C \cdot \frac{(1+r^{disc})^{LT} - 1}{r^{disc} \cdot (1+r^{disc})^{LT}} = -\Delta I + \left((1-r_T) \left(c_{n,v}^{tot} - c_{n,v}^{OP} \right) + r_T \frac{\Delta I}{I_{LT}} \right) \cdot \frac{(1+r^{disc})^{LT} - 1}{r^{disc} \cdot (1+r^{disc})^{LT}} \quad (11)$$

3. Case study

3.1 Input data

The case study consisted of two hot and two cold process streams as presented in Table 1. It should be noted that besides the usual data for heat integration - supply T^S and target T^T temperature, heat capacity flow rate FC , heat flow Q and h heat transfer coefficient - additional data are required for risk assessment, including the

boiling temperature at atmospheric pressure, phase of media in the stream, lethal concentration LC_{50} (rat, 1h, inh), information, whether the substance is flammable Flam and explosion energy Q^{expl} for explosive substances. Those additional data are used to determine the limiting value G separately for each substance in each HE for toxicity, flammability and explosiveness. In this case study, all media are assumed to be in a liquid phase (having the density of water) with boiling temperature 330 °C. The properties of the different types of HEs are presented in Table 2, including coefficients lower T_{hx}^{LO} and upper T_{hx}^{UP} temperature limits, the upper limit on the area A_{hx}^{UP} , fixed cf_{hx} and variable cost cv_{hx} , the ft_{hx} correction factor for temperature driving force, β_{hx} area density, and f^{fail} failure frequency of HE in one year.

Table 1: Input data of process and utility streams

Stream	$T^S/$ °C	$T^T/$ °C	$FC/$ kW °C ⁻¹	$Q/$ kW	$h/$ (kW/(m ² °C))	$LC_{50}(\text{rat,1h,inh})/$ mg	Flammability	$Q^{expl}/$ (kJ/ kg)
H1	500	400	150	15,000	0.8	100	No	0
H2	450	390	125	7,500	0.9	200	Yes	500
C1	330	390	240	14,400	0.6	5,000	Yes	10
C2	380	500	50	6,000	0.9	500	Yes	100
HU	510	510			5	-	Yes	∞
CU	300	321			1	-	Yes	∞

Table 2: Input data for different type of heat exchangers

HE type	T_{hx}^{LO} /K	T_{hx}^{UP} /K	A_{hx}^{UP} /m ²	$cf_{hx}/$ k€	cv_{hx}/k € m ⁻²	ft_{hx}	$\beta_{hx}/$ m ² m ⁻³	$f^{fail}/$ (HX y) ⁻¹
Double pipe	173.15	873.15	200	46	2.742	1	80	0.009929
Plate and frame	248.15	523.15	1,200	129.8	0.347	1	1,300	0.010908
Fixed plate shell and tube	73.15	1,123.15	1,000	121.4	0.193	1	720	0.009929
Shell and tube with U-tubes	73.15	1,123.15	1,000	100.9	0.272	0.8	80	0.009929

3.2 Solutions and discussion

Different risk limits were considered when calculating solutions. First, a reference solution was obtained at no risk limit corresponding to the economically optimal solution (Table 3, optimisation a). The risk for the reference case study was recalculated after optimisation. In the following optimisation, the overall risk limit was set to one-half of that calculated in the reference case (Table 3, optimisation b). As can be seen in Table 3, the NPV was decreased by 276.6 k€ (0.03 %) when the overall risk limit was halved, or in other words, the safety increased two times, while the NPV change was negligible. It is a consequence of increased investment by 314.88 k€ presenting a 32.3 % increase in investment. It should be noted that the heat integration rate was not changed. When observing the highest individual risk, it can be seen there are significant individual risks in case b). In the case of toxicity, one individual HE presents 38.6 % of overall risk; for flammability, this ratio is 38 %, while for explosivity the ratio is 56 %. This shows the need for a limit on individual HE risk as well. In case c), the overall risk limit was set as one-half of that of the reference case, while the individual HE risk was set as one-third when indirect heat transfer is used and one-sixth when direct heat transfer is used. The solution is presented in Table 3 as optimisation ad c).

It can be seen that NPV decreased in case c) slightly more by 4,129.3 k€, resulting in a 0.5 % decrease, which can still be considered a small change. Now, the NPV decrease is twofold, because of the increased investment by 45.4 %, and the heat integration rate is somewhat reduced, resulting in higher utility consumption. When observing overall risk, it can be seen that the same level of risk is achieved as in case b). When analysing the highest individual risk, it can be concluded that it is approximately halved compared to case b) and nearly quartered compared to the reference case.

In Figure 2, different HENs are presented for the previously described cases. The reference case with no risk assessment is presented in Figure 2(a). It consists of four process stream to process stream HEs, either fixed plate shell-and-tube HE or a small U-tube shell-and-tube HE. An additional cooler is needed with a U-tube shell-and-tube HE type and a double-pipe heater in order to obtain a feasible HEN. When the overall risk is halved (safety is increased two times), the arrangement of the HEs is different, as hot stream H2 is split and the HE

Table 3: Comparison of solutions considering a) no risk assessment, b) overall risk assessment limit halved compared to a), and c) overall risk assessment halved and initial risk assessment is set as one-third of overall risk limit

Optimisation	NPV/k€	Q^{HU}/kW	Q^{CU}/kW	I/k€	R^{HEN}/y^{-1}	R^{HXI}/y^{-1}
a) No safety	817,672.9	2,150.0	50.0	976.0	$R^{HEN,tox} = 0.0427$ $R^{HEN,flam} = 0.0007$ $R^{HEN,expl} = 8.881 \cdot 10^{-6}$	$R^{HXI,tox} = 0.0142$ $R^{HXI,flam} = 0.0002$ $R^{HXI,expl} = 7.77 \cdot 10^{-6}$
b) R^{HEN} limited	817,396.3	2,150.0	50.0	1,290.9	$R^{HEN,tox} = 0.021$ $R^{HEN,flam} = 2.63 \cdot 10^{-4}$ $R^{HEN,expl} = 1.71 \cdot 10^{-6}$	$R^{HXI,tox} = 0.0081$ $R^{HXI,flam} = 0.0001$ $R^{HXI,expl} = 9.65 \cdot 10^{-7}$
c) both R^{HEN} and R^{HE} are limited	813,267.0	2,250.0	150	1,419.6	$R^{HEN,tox} = 0.021$ $R^{HEN,flam} = 2.64 \cdot 10^{-4}$ $R^{HEN,expl} = 6.121 \cdot 10^{-7}$	$R^{HXI,tox} = 0.00354$ $R^{HXI,flam} = 5.14 \cdot 10^{-5}$ $R^{HXI,expl} = 4.02 \cdot 10^{-7}$
b)/a)	99.97%	100 %	100 %	132.3 %	Tox: 49.2 % Flam: 37.5 % Expl: 19.3 %	Tox: 57.0 % Flam: 50 % Expl: 12.4 %
c)/a)	99.46%	104.6 %	300 %	145.4 %	Tox: 49.2 % Flam: 37.7 % Expl: 6.89 %	Tox: 28.1 % Flam: 25.7 % Expl: 5.17 %

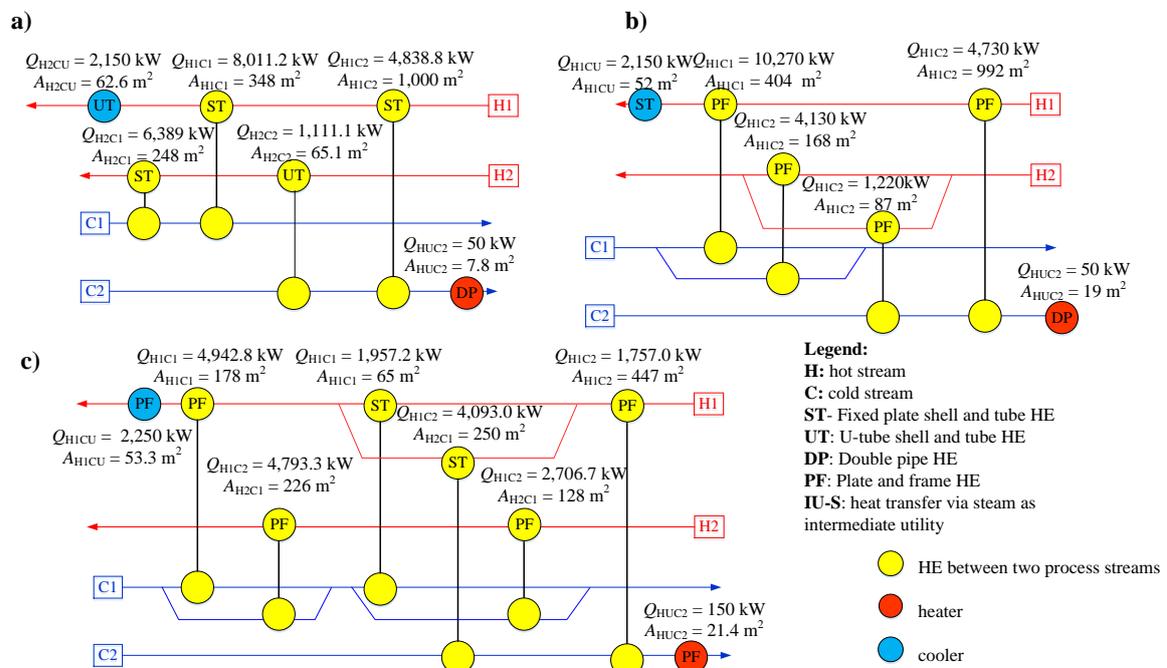


Figure 2: HEN design considering (a) no risk assessment, (b) overall risk assessment limit halved compared to (a), and (c) overall risk assessment halved and initial risk assessment set as one-third of overall risk limit

types selected are plate and frame between process streams. It should be noted that the number of HEs remains the same at six. This selection can be related to a much higher area density of plate and frame type of HE, resulting in much lower volume and consequently mass being present in the HEs for a similar rate of heat transfer. Further, limiting the individual risk of each smaller HE, while keeping the overall risk limit, results in more complex HEs. The trend is still that for higher heat transfer, plate and frame HEs are used, while for smaller heat transfer, fixed plate shell-and-tube HEs are used. The number of HEs is increased to eight HEs; however, the HEs are smaller, leading to smaller individual HE risks. Even with an increased number of HEs, the rate of Heat Integration is decreased. Any further decrease in risk limits would eventually lead to additional HEs and even indirect heat transfer.

4. Conclusions

An MINLP model for HEN synthesis upgraded with simultaneous risk assessment accounting during optimisation has been developed considering different types of HEs and different modes of heat transfer. The solutions indicate that a significant enhancement of safety can be achieved with only a minor economic expense. A further important observation is that setting individual risk for each HE can lead to significantly different designs and that both individual and overall risk limits should be considered.

In future studies, a composed objective, including economic and safety aspects factored directly into the objective function, is planned. This will enable more appropriate trade-offs and offer a single solution, taking into account all the trade-offs presented in this study. The methodology presented here will be extended to other process subsystems as well as to overall process systems.

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