

## Optimal Safe Layouts with Heat Exchanger Networks Synthesis Having Isothermal Process Streams

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This paper proposes a new MINLP model for heat exchanger network synthesis considering streams with phase change and their geographical allocation based on safety. For heat exchanging, the model includes streams with latent heat, streams with sensible heat, and streams with both latent and sensible heat. Streams may be generated in either an already installed facility or in a new facility for siting, and their point of generation inside the facility is given. For safety, the model considers the possibility of having toxic releases in either installed or for siting facilities. Hence the facilities layout becomes a part of the HEN synthesis optimization problem. A grid layout is adopted to allocate facilities in the available land and a new strategy is developed to solve the non-overlapping facilities constraint. This strategy also reduces the numerical difficulties appearing when Euclidian distances are required when calculating safety affectations.

### 1. Introduction

The design and synthesis of heat exchanger networks (HEN) has been substantially improved along last decades due to the high economical savings in the chemical and process industry. The design and synthesis of HEN has been largely explored and a broad research has been published in the chemical engineering literature. An early method to obtain HEN with minimum area, proposed by Hohmann (1972) and described in (Gundepesen and Naess, 1988), called the attention of several researchers. This work included a strategy to assess feasibility of streams assuming suitable approach temperature and given utility supplies. The underdeveloped technology eventually evolved into what became known as the pinch design method (Linnhoff and Hindmarsh, 1983). From a mathematical programming point of view, Grossmann and Sargent (1978) gave the first step into the MINLP developments by using an algorithm for discrete variables to solve the HEN problem with incorporated integer variables in the mathematical model. This algorithm was in fact a clever extension of the method developed by Ponton and Donaldson (1974). In particular, the concept of superstructure gave a graphical understanding of the HEN problem (Yee and Grossmann, 1990; Yee *et al.*, 1990). An interesting work has increased stages in previous superstructures by calculating the number of stages based on the inlet temperatures of the hot and cold streams as well as on the exchanger minimum approach temperature (Zamora and Grossmann, 1997). An excellent review on HEN has been elaborated by Furman and Sahinidis (2002). Besides numerical improvements to solve the optimization problem, HEN research and their applications have been evolved in several directions. The operation of heat exchangers have been also included in the optimization model to provide flexibility and resilience in HEN designs (Jäschke and Skogestad, 2014). Some of the difficulties to solve during operations due to bad designs have been explored recently (Jensen and Skogestad, 2008). A mixed-integer linear model to detect the optimal set of units to be cleaned during plant maintenance has been recently developed (Assis *et al.*, 2013). In general, the main purpose of HEN synthesis became the finding of optimal solutions in an efficient way, and several models were proposed to solve different conditions or scenarios. The proposed approaches have ended up in

large mixed integer optimization problems. However, safety has been aside the main goals. More recently, the interest in incorporating safety analysis during this stage of process design has increased. The conventional HEN synthesis, as expressed in (Zamora and Grossmann, 1997), has been combined with the layout problem (Inchaurregui-Méndez *et al.*, 2015; Vázquez-Román *et al.*, 2015). The hypothesis of optimizing the layout to improve safety in the plants has been already explored by the authors in previous works (Díaz-Ovalle *et al.*, 2010; Vázquez-Román *et al.*, 2010). The problem consists in allocating a given number of facilities in a given land to optimize an objective function, which typically depends on the separation distance among facilities. In this work, the HEN synthesis where phase change, i.e. isothermal streams, is included as indicated in Ponce-Ortega *et al.* (2008). The geographical unit location is then incorporated into the HEN synthesis to account for the preference of a possible match between two streams to prevent matches among highly separated streams. Given are coordinates inside facilities where streams for heat exchange are produced and facilities that could release toxic gas are identified. Then a grid-plan is assumed for allocating facilities.

## 2. Problem statement

The HEN problem is established as having a set of hot streams, HPS, to cool down and a set of cold streams, CPS, to be heated. Some streams may exchange latent or sensible heat to have fixed or varying temperatures, respectively. Thus, HPS1, HPS2 and HPS3 are subsets of HPS to contain the hot process streams that exchange sensible heat in the network, the hot process isothermal streams and the hot process streams that exchange both latent and sensible heat, respectively. Similarly, CPS1, CPS2 and CPS3 are subsets of CPS that are nonisothermal, isothermal and a combination of latent and sensible heat, respectively. In a given stage, any stream can exchange energy only once and several stages are required to include all possible combinations. Figure 1 shows the typical superstructure for 2 hot-2 cold streams arrangement. This representation has included in red the coordinates where the streams are generated though they could belong to a different facility. A facility is a rectangular area surrounded by streets where some process units are kept together due to the convenience in the process. Emergency response plans and access requirements suggests that any vehicle going into a plant should be able to cross the plant without maneuvering. This naturally results in a grid-type of layout where facilities footprints are rather rectangular. For the layout problem, a set of facilities could be already installed in part of the available land but some others are to be allocated. In addition, it is assumed that some facilities, either installed or to install, may release some toxic material. Releasing coordinates are already detected via appropriate risk analysis. Thus the HEN problem and the safety layout become interdependent through the geographical allocation of streams generation and safety layout.

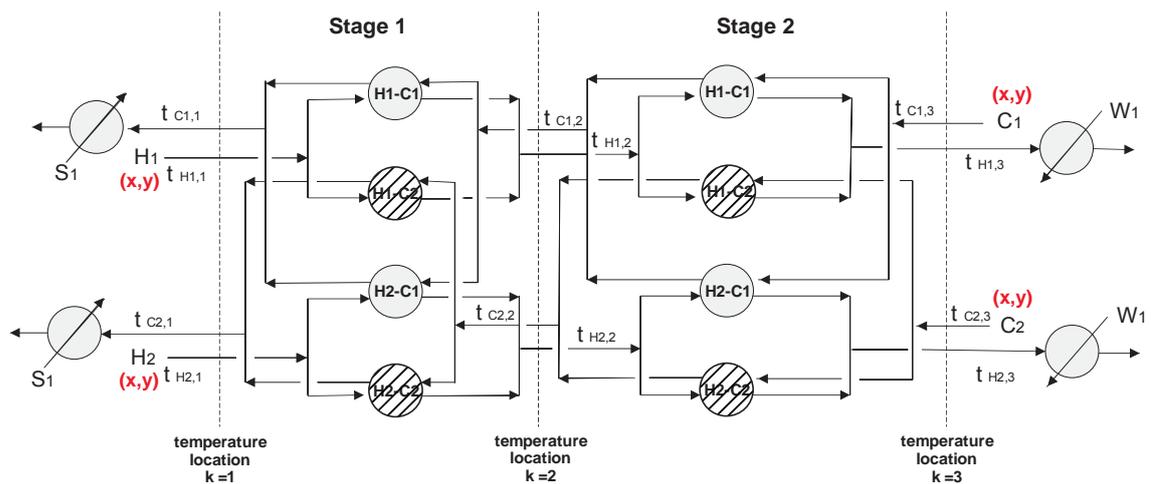


Figure 1: Superstructure for 2 cold streams and 2 hot streams

### 3. The mathematical model

Table 1 contains part of the model related to the pure HEN synthesis-Layout problem: Equations 1-6 shows the overall energy balance for each hot or cold stream, energy balance in each k-stage are covered in Equations 7-10, Equation 11 assign known inlet temperatures, Equations 12-17 provide temperatures feasibility, Equations 18-21 are used to estimate heating and cooling duties, and Equations 22-23 incorporate latent heat balance. Several disjunctions are included to, among others, model feasibility of latent heat exchange and to model the logarithmic mean temperature differences. Disjunctions are typically modelled using the convex hull but this and more options have been improved recently (Trespalcios and Grossmann, 2015b; Trespalcios and Grossmann, 2015a). Additional equations are required to include some other features in the HEN problem; for details, readers should address the work by Ponce-Ortega *et al.* (2008). For details of the mathematical model related to the layout problem, readers are suggested to consult (Vázquez-Román *et al.*, 2010; Vázquez-Román *et al.*, 2015).

For the layout problem, it is considered that a set of facilities  $f^i$  have been already installed but another set contain facilities  $f^s$  to be sited. The available land is represented by a rectangular shape-grid, Figure 2. A facility, surrounded by streets, is allocated in a single grid. A binary variable is used to indicate if a facility for sitting is allocated in a g-grid whereas a binary parameter is used to indicate if an already installed facility is occupying the g-grid. Thus, Equation (24) prevents using more than one g-grid to allocate a sitting facility. The non-overlapping constraint is imposed with Equation (25). It is then assumed that specific facilities, either already sited or to be sited, could release a toxic material. To reduce effects of potential releases, worst-case scenarios have been considered to estimate mass concentration around the releasing facilities. These concentrations are converted into probability of death via probit functions and then fitted to an exponential decay as suggested in (Vázquez-Román *et al.*, 2010). Equation (26) is the type of equation to estimate probability of death. The grid allocation approach allows the estimation of separation facilities via parameters once facilities have a grid assigned. Thus the only involved variables to estimate separation distances among facilities are the already mentioned binary variables. When separation distances are used to estimate risk, the Euclidian distance is used as indicated in Equation (27) but the Manhattan distance is preferred for estimating pipe lengths to interconnect streams in the HEN, Equation (28). Separation distances become relevant when the HEN problem is simultaneously solved with the safety layout for toxic releases. The combined objective function becomes,

$$\begin{aligned}
 \min \quad & \sum_{(f_1, f_2) \in M_{f_1, f_2}} C_p d_{f_1, f_2}^M + C_p \sum_h \sum_c \sum_{f_1} \sum_{f_2} d_{f_1, f_2}^M B_{h, f_1} B_{c, f_2} B_{h, c} + c_l A_{land} + c_{pp} t_l \sum_{f_2} \sum_{f_1} f_{1,r} p_{f_2} P_{r, f_1, f_2} \\
 & + \sum_{i \in HPS} CCU q c u_i + \sum_{i \in CPS} CHU q h u_j + \sum_{i \in HPS} \sum_{j \in CPS} \sum_{k \in ST} C F_{i,j} z_{i,j,k} \\
 & + \sum_{i \in HPS} C F_{i,cu} z c u_i + \sum_{j \in CPS} C F_{cu,j} z h u_j \\
 & + \sum_{i \in HPS} \sum_{j \in CPS} \sum_{k \in ST} C_{i,j} \left\{ \frac{q_{i,j,k} \left( \frac{1}{h_{i,k}} + \frac{1}{h_{j,k}} \right)}{l m t d_{i,j,k} + \delta} \right\}^\beta \\
 & + \sum_{i \in HPS} C_{i,cu} \left\{ \frac{q c u_i \left( \frac{1}{h_{i,cu}} + \frac{1}{h_{cu}} \right)}{\left[ (d t_{i,cu}) (T O U T_i - T I N_{cu}) (d t_{i,cu} + T O U T_i - T I N_{cu}) / 2 + \delta \right]^{1/3}} \right\}^\beta \\
 & + \sum_{j \in CPS} C_{hu,j} \left\{ \frac{q h u_j \left( \frac{1}{h_{hu}} + \frac{1}{h_{j,hu}} \right)}{\left[ (d t_{hu,j}) (T I N_{hu} - T O U T_j) (d t_{hu,j} + T I N_{hu} - T O U T_j) / 2 + \delta \right]^{1/3}} \right\}^\beta
 \end{aligned} \tag{30}$$

where the first term contains the piping cost due to natural process interconnectivity, the second term is piping cost due to the HEN synthesis, the third term is the cost of occupied land where the occupied area is estimated using equation (29), the fourth term is the compensation risk cost, and the following terms are related to the HEN synthesis problem. The resulting problem is a MINLP where the main nonlinearities come from the HEN problem which has been broadly solved in the chemical engineering area.

Table 1: The HEN synthesis-Layout mathematical model.

Equation	
$(TIN_i - TOUT_i)FCp_i = \sum_{k \in ST} \sum_{j \in CPS} q_{ijk} + qcu_i, \quad i \in HPS1$	(1)
$F\lambda_i^{cond} = \sum_{k \in ST} \sum_{j \in CPS} q_{ijk} + qcu_i, \quad i \in HPS2$	(2)
$(TIN_i - TOUT_i)FCp_i + F\lambda_i^{cond} + (T_i^{cond} - TOUT_i)FCp_i = \sum_{k \in ST} \sum_{j \in CPS} q_{ijk} + qcu_i, \quad i \in HPS3$	(3)
$(TOUT_j - TIN_j)FCp_j = \sum_{k \in ST} \sum_{i \in HPS} q_{ijk} + qhu_j, \quad j \in CPS1$	(4)
$F\lambda_j^{evap} = \sum_{k \in ST} \sum_{i \in HPS} q_{ijk} + qhu_j, \quad j \in CPS2$	(5)
$(TOUT_j - T_j^{evap})FCp_j + F\lambda_j^{evap} + (T_j^{evap} - TIN_j)FCp_j = \sum_{k \in ST} \sum_{i \in HPS} q_{ijk} + qhu_j, \quad j \in CPS3$	(6)
$(t_{i,k} - t_{i,k+1})FCp_i = \sum_{j \in CPS} q_{ijk}, \quad k \in ST, \quad i \in HPS1$	(7)
$(t_{i,k} - t_{i,k+1})FCp_i + q_{i,k}^{\Delta} = \sum_{j \in CPS} q_{ijk}, \quad k \in ST, \quad i \in HPS3$	(8)
$(t_{j,k} - t_{j,k+1})FCp_j = \sum_{i \in HPS} q_{ijk}, \quad k \in ST, \quad j \in CPS1$	(9)
$(t_{j,k} - t_{j,k+1})FCp_j + q_{j,k}^{\Delta} = \sum_{i \in HPS} q_{ijk}, \quad k \in ST, \quad j \in CPS3$	(10)
$TIN_i = t_{i,1}, \quad i \in HPS; \quad TIN_j = t_{j,NOK+1}, \quad j \in CPS$	(11)
$t_{i,k} \geq t_{i,k+1}, \quad k \in ST, \quad i \in HPS1 \text{ or } i \in HPS3$	(12)
$t_{i,k} = TIN_i, \quad k \in ST, \quad i \in HPS2$	(13)
$t_{j,k} \geq t_{j,k+1}, \quad k \in ST, \quad j \in CPS1 \text{ or } j \in CPS3$	(14)
$t_{j,k} = TIN_j, \quad k \in ST, \quad j \in CPS2$	(15)
$TOUT_i \leq t_{i,NOK+1}, \quad i \in HPS1 \text{ or } i \in HPS3$	(16)
$TOUT_j \geq t_{j,1}, \quad j \in CPS1 \text{ or } j \in CPS3$	(17)
$(t_{i,NOK+1} - TOUT_i)FCp_i = qcu_i, \quad i \in HPS1$	(18)
$(t_{i,NOK+1} - TOUT_i)FCp_i + q_i^{\Delta, cu} = qcu_i, \quad i \in HPS3$	(19)
$(TOUT_j - t_{j,1})FCp_j = qhu_j, \quad j \in CPS1$	(20)
$(TOUT_j - t_{j,1})FCp_j + q_i^{\Delta, hu} = qhu_j, \quad j \in CPS3$	(21)
$F\lambda_i^{cond} = \sum_{k \in ST} q_{i,k}^{\Delta} + q_i^{\Delta, cu}, \quad i \in HPS2 \text{ or } i \in HPS3$	(22)
$F\lambda_j^{evap} = \sum_{k \in ST} q_{j,k}^{\Delta} + q_j^{\Delta, hu}, \quad j \in CPS2 \text{ or } j \in CPS3$	(23)
$\sum_{g \in G} B_{f^s, g} = 1, \forall f^s \in F^s$	(24)
$\sum_{f^s \in F^s} B_{f^s, g} + \sum_{f^i \in F^i} B_{f^i, g} \leq 1, \forall g \in G$	(25)
$P_{r, f_1, f_2} = a_{r, f_1} e^{-b_{r, f_1} d_{f_1, f_2}}$	(26)
$d_{f_1, f_2}^E = \sum_{g_1} \sum_{g_2} D_{g_1, g_2}^E B_{g_1, f_1} B_{g_2, f_2}, \quad \forall g_1 > g_2, \in G$	(27)
$d_{f_1, f_2}^M = \sum_{g_1} \sum_{g_2} D_{g_1, g_2}^M B_{g_1, f_1} B_{g_2, f_2}, \quad \forall g_1 > g_2, \in G$	(28)
$A_{land} \geq A_g \sum_f B_{f, g}, \quad \forall g \in G$	(29)

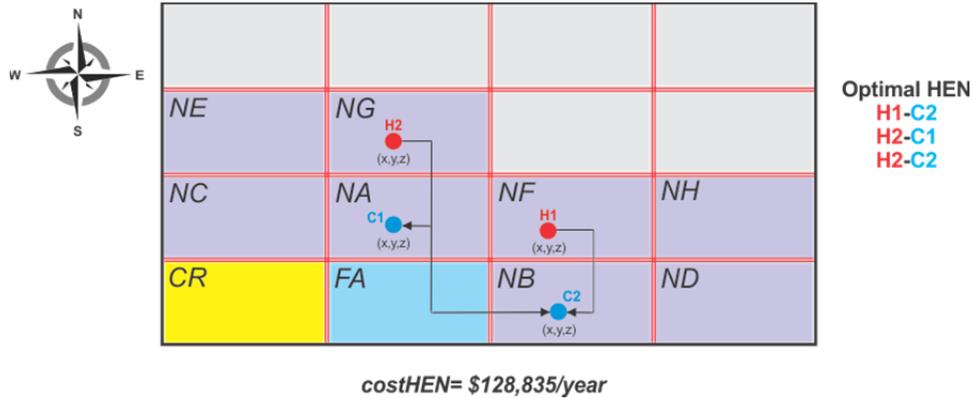


Figure 2: The grid-layout

4. Case Study and Results

The GAMS package has been used to solve the MINLP problem in a PC with processor x64, Intel® Core™ i7-4500U CPU @ 1.80 GHz. This case study is the rather simple but motivational case study used in (Ponce-Ortega *et al.*, 2008), where only isothermal streams are considered: 2 hot and 2 cold streams. The capital cost for heat exchangers is given by  $\$1650 A^{0.65}$  where  $A$  is in  $m^2$ , the annuity factor is 0.23/year, and the  $\Delta T_{min} = 5K$ . Data for the two condensing streams are: 400K and 425K for temperature, 4,000 and 3,000 kW for flow-heat capacity, 1.8 and 1.9  $kW/m^2-K$  for the film heat transfer coefficients, respectively. Data for the two evaporating streams are: 410K and 390K for temperature, 4,000 and 3,000 kW for flow-heat capacity, 1.7 and 1.85  $kW/m^2-K$  for the film heat transfer coefficients, respectively. Two facilities, the control room “CR” and facility “FA”, have been already installed and 8 new facilities will be sited “NA”-“NH”. Chlorine releases could occur in facilities “ND”, “NG” and “NH”. The first hot and condensing stream is produced in “NF” and the second one in “NG”. The first cold and evaporating stream is produced in “NA” and “NB”. The costs considered are:  $\$196.8/m$  of pipe,  $\$6.00/m^2$  of occupied land, and  $\$10^6/injured$  individual. The expected life of the plant is 15 years and a maximum of 4 facilities are installed in each row where sizes of facilities are  $30m \times 20m$ . Parameters to estimate the exponential decay of the probability of death, Equation (26), are 0.235 and 0.02, respectively. The frequency of release is 0.0001 and the expected population in the control room is 10.

Results for the pure HEN synthesis problem indicates exchanges between H1-C2, H2-C1 and H2-C2 with a total cost of  $\$128,835/year$ , Figure 2. By solving the combined safe-HEN model, the HEN cost increases slightly to  $\$128,840/year$  and the suggested heat exchanges are H1-C2 and H2-C1. Due to the separation distance, using local utility service became a better solution than including a H2-C2 heat exchanger. Since utilities are assumed to exist in all facilities, no extra cost has been included for piping.

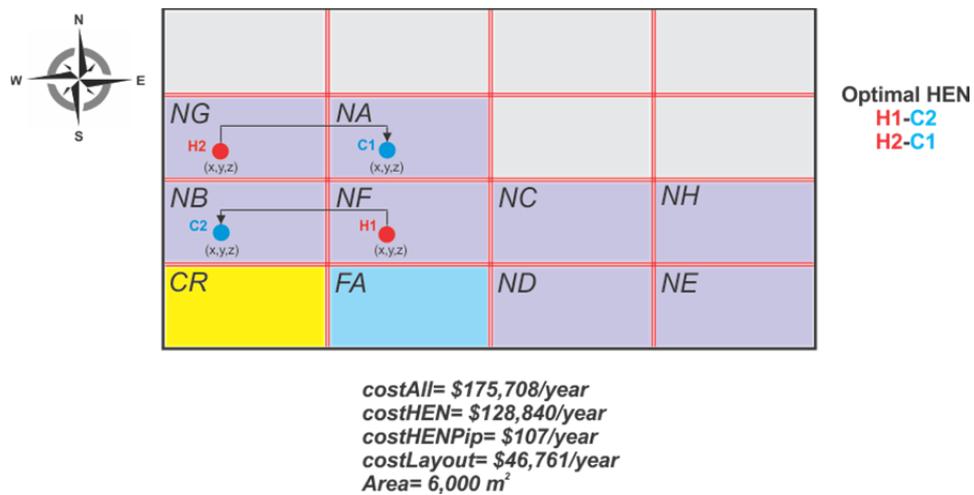


Figure 3: Optimal Safe HEN

## 5. Conclusions

This paper demonstrates that HEN synthesis can be linked to safety layout via separation distances among facilities and cost objective functions. The traditional optimality in HEN faces another challenge since facilities could be allocated far apart due to safety issues. The number of equations when including isothermal streams increases considerably due to the amount of disjunctions (not shown due to space limitations). However, combining both problems have not introduce any extra numerical difficulties to the traditional HEN problem and it can be solved with conventional codes contained in packages such as GAMS. Currently HEN synthesis may be modified when safety issues are included in the optimization procedure. It has resulted in producing optimal safe HEN.

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