Coupled heat and resource allocation network design considering multi-contaminants, properties and non-isothermal mixing

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Abstract:

This paper introduces a new approach for the design of heat-integrated resource allocation network with a minimum total annualized cost. In a first step, a MILP model determines the minimum fresh resource flow rate necessary to satisfy all mass-related constraints. The model takes into account multicontaminants and multiproperties cases. It also includes the possibility to use several fresh resources (with different characteristics) and several waste sinks (with different limitations). Then, a second MILP model is used to design an optimal heat integrated resource allocation network. The objective function includes fresh resource, waste discharge and utilities costs. The fresh resource flow rate search space is restrained thanks to the first model results. The heat integration is realized with a modified transshipment model, where the temperature scale is discretized in order to account for non-isothermal mixing. Technical constraints, expressing real on site industrial restrictions, are introduced to lead the optimal solution towards a more realistic network. The methodology is demonstrated on a literature case study. It shows the interest of simultaneous optimization of both heat and resource compared to a sequential approach.

Keywords:

Energy integration, Mass integration, Process integration, MILP, Non-isothermal mixing, Multicontaminants, Multiproperties.

1. Introduction

As environmental and quality regulations gets more restrictive, resource recovery becomes an effective way to reduce raw material requirements, waste generation and overall operating cost. The design of a relevant mass allocation network needs to characterize the process streams properly, considering their physical and chemical properties, such as, but not limited to, their temperature and their composition of multiple contaminants [5]. Temperature will allow quantifying the energy requirements created by the mass allocation network. Most of previous works focused on sequential optimization where the minimum fresh resources is targeted first, and then the minimum energy requirements (MER) [3]. These methodologies elude the fact that it is not only the minimization of few parameters but the overall cost that will determine whether a solution will be implemented on-site or not. Few works developed methodologies that minimize the overall operating cost [4], but these methodologies are often non-linear when they consider non-isothermal mixing, which cannot guarantee a global optimum. Moreover, these methodologies do not integer technical restrictions that can occur on-site, such as limitations on fresh supplies, on waste treatment units or on certain allocations due to available space, security or operability. The proposed optimization model includes a more accurate characterization of mass and heat streams and allows constraining the solution search space so that it is more likely to be implemented on site. The methodology is formulated as two sequential mixed integer linear programming (MILP) models. It determines a heat-integrated mass allocation network with a minimum annual operating cost, giving all technical constraints imposed by the designer.

2. Problem Statement

The basic problem to be dealt with is how to reuse process sources into process sinks, in order to minimize the global fresh resource and the energy requirements (Fig. 1). This optimization takes into account the constraints generated by the composition and other properties of the sources (fresh and process), and the requirements and limitations on the sinks (waste and process).

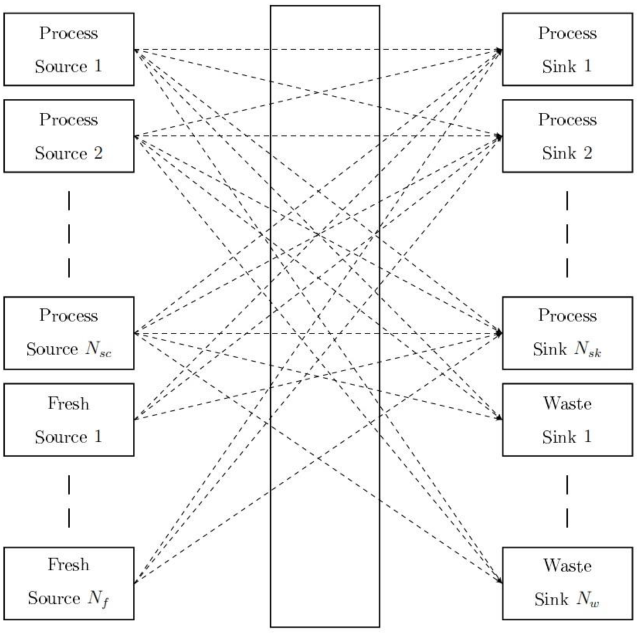

Fig. 1. Schematic representation of heat-integrated resource allocation network.

Process sources ($J_p = \{1..N_{sc}\}$) are characterized by a flow rate (L), temperature (T), heat capacity (cp), composition (y_k) and properties (p_m). Process sinks ($I_p = \{1..N_{sk}\}$) are characterized by requirements in terms of flow rate (G, maximum allowable composition ($z_k^{\max}$) and acceptable ranges for each property ($p_m^{\min}; p_m^{\max}$). Several Fresh Sources ($J_f = \{1..N_f\}$) and Waste Sinks ($I_w = \{1..N_w\}$) can be considered. They have the same characterization as the process sources and process sinks, respectively, except for their flow rate which is a variable of the model (Fig. 2).

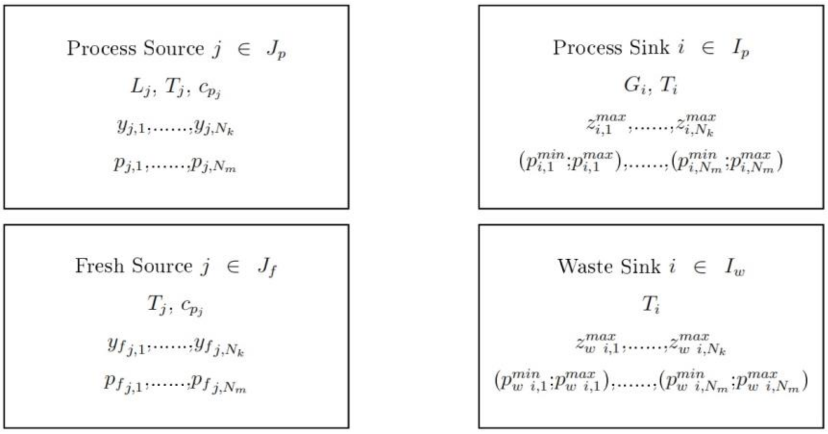

Fig. 2. Sources and sinks initial characterization.

The aim of this methodology is to design an optimal direct reuse network while minimizing the total operating cost of such network, considering the annual cost of fresh resources, hot and cold utilities (given the total operating hours per year).

3. Mathematical formulation

The methodology consists of the resolution of two consecutive MILP models. The objective of the first model is to determine the minimum global fresh resources required to meet all the mass-related constraints (thermodynamic and technical). The results of this model show if a solution exists and what is the minimum global fresh resource requirements. Once the existence of a solution is established, the second model will optimize the annual operating cost (AOC), taking into account mass and energy aspects simultaneously.

3.1. 1st MILP: Mass Integration under technical constraints

The objective of this first model is to determine the minimum global fresh resources required considering all the mass-related constraints.

3.1.1. Mass related equations (multi fresh source and waste sink included)

Let L_{ij} be the variable mass flow rate that goes from source j to sink i.

For each process sink $i \in I_p$, the mass flow rate requirement (G_i) has to be met by a linear combination of all sources mass flow rates, while never exceeding the maximum allowable mass load for each contaminant k ($z_{i,k}^{\max}$):

$$\sum_{j \in J_p} L_{ij} + \sum_{j \in J_f} L_{ij} = G_i , \qquad (1)$$

$$\forall k,\ \sum_{j \in J_p} L_{ij} \times y_{j,k} + \sum_{j \in J_f} L_{ij} \times y_{f\,j,k} \le G_i \times z_{i,k}^{\max} , \qquad (2)$$

For each waste sink $i \in I_w$, the total mass flow rate ($G_{w\,i}$) treated by each waste unit, which is a result of the optimization, is equal to a linear combination of all process source mass flow rates. Fresh resources cannot be allocated to a waste unit sink. Limitations on the maximum allowable mass load for each contaminant k can be imposed by the user for these particular sinks, but there are not mandatory. If no value is given to $z_{w\,i,k}^{\max}$ by the user, then it is automatically set to $\max_{j \in J_p}(y_{j,k})$.

$$\sum_{j \in J_p} L_{ij} = G_{w\,i} , \qquad (3)$$

$$\forall k \in \{1..\mathrm{N}_k\},\ \sum_{j \in J_p} L_{ij} \times y_{j,k} \le G_{w\,i} \times z_{w\,i,k}^{\max} , \qquad (4)$$

Finally, for each process source $j \in J_p$, the sum of stream mass flow rates allocated to each sink must be equal to its total mass flow rate:

$$\sum_{i \in I_p} L_{ij} + \sum_{i \in I_w} L_{ij} = L_j , \qquad (5)$$

3.1.2. Property related equations (multi fresh source and waste sink included)

Similar equations are used for properties that can be used to characterize sources and sinks. Each property p_m is characterized by a mixing rule defined by a function ϕ_m [2] [5][6]. For each sink i, the resulting value of the property p_m must be within the range defined by the user, similarly to the max allowable concentration included between 0 and $z_{i,k}^{\max}$ or $z_{w,i,k}^{\max}$ (if $i \in I_p$ or $i \in I_w$).

Assuming that ϕ_m is an increasing function, for each sink $i \in I_p$:

$$\forall m \in \{1..\mathrm{N}_m\},\ G_i \times \phi_m(p_{i,m}^{\min}) \le G_i \times \phi_m(p_{i,m}) = \sum_{j \in J_p} L_{ij} \times \phi_m(p_{j,m}) + \sum_{j \in J_f} L_{ij} \times \phi_m(p_{f\,j,m}) \le G_i \times \phi_m(p_{i,m}^{\max}) , \qquad (6)$$

Similarly, for each sink i $\in I_W$:

$$\forall m \in \{1..\mathrm{N}_{\mathrm{m}}\}, G_{w\,i} \times \phi_m(p^{\min}_{w\,i,m}) \le G_{w\,i} \times \phi_m(p_{w\,i,m}) = \sum_{j \in J_p} L_{ij} \times \phi_m(p_{j,m}) \le G_{w\,i} \times \phi_m(p^{\max}_{w\,i,m})\,, \quad (7)$$

Similarly to contaminant composition, limitations on properties can be imposed by the user for each sink i $\in I_W$, but there are not mandatory. If no value is given to ($p^{\min}_{w\,i,m}$; $p^{\max}_{w\,i,m}$) by the user, then it is set to ($\min_{j \in J_p}(p_{j,m})\,; \max_{j \in J_p}(p_{j,m})$).

For this case study the properties that characterize the streams are the pH and the vapor pressure (p_v). Their specific mixing rules are defined by a function ϕ_{pH} and ϕ_{p_v}, respectively [1]:

$$\phi_{pH}(p_{j,pH}) = 10^{p_{j,pH}} \text{ and } \phi_{p_v}(p_{j,p_v}) = p_{j,p_v}$$

3.1.3. Technical constraints related to mass allocation

Due to restrictions on site, allocations can be limited, forbidden or imposed.

Binary variables (γ_{ij}) are introduced to establish the existence of an allocation between sink i and source j, and define the acceptable range for the mass flow rate that transits between them:

$$L_{ij} - \gamma_{ij} \times L^{\min}_j \ge 0\,, \qquad (9)$$

$$L_{ij} - \gamma_{ij} \times L^{\max}_j \le 0\,, \qquad (10)$$

In case the user does not want to define a lower or an upper bound for a given allocation, extreme values are given to $L^{\min}_j$ or $L^{\max}_j$, respectively 0 and $\sum_{i \in I_p} G_i$ (if $j \in J_f$) or L_j (if $j \in J_p$).

If the connection is imposed, then the value of L_{ij} is set to a specific value L^{exist}_{ij} defined by the user:

$$L_{ij} = L^{exist}_{ij}\,, \qquad (11)$$

If the connection is forbidden, then the value of L_{ij} is set to 0:

$$L_{ij} = 0\,, \qquad (12)$$

Restrictions on the total available mass flow rate of a particular fresh resource can be imposed:

$$j \in J_f\,,\ \sum_{i \in I_p} L_{ij} \le L^{\max,\ total}_j\,, \qquad (13)$$

Similar restrictions can be imposed to a particular waste unit:

$$i \in I_w\,,\ \sum_{j \in J_p} L_{ij} \le G^{\max,\ total}_{w\,i}\,, \qquad (14)$$

Finally, the number of connections for each source can be limited:

$$\forall j \in J_p\,,\ \sum_{i \in I_p} \gamma_{ij} + \sum_{i \in I_w} \gamma_{ij} \le N^{\max}_j\,, \qquad (15a)$$

$$\forall j \in J_f\,,\ \sum_{i \in I_p} \gamma_{ij} \le N^{\max}_j\,, \qquad (15b)$$

Note that $N^{\max}_j$ has to be superior to 1 if $j \in J_p$.

3.2.1.4. Objective function

The objective of the introduced MILP model is to minimize the global fresh resources consumption:

$$\min\ L^{\min}_{fresh} = \sum_{j \in J_f} \sum_{i \in I_p} L_{ij}\,, \qquad (16)$$

3.2. 2nd MILP: Mass and Heat Integration under technical constraints

The second MILP model optimizes the global fresh resource and the energy consumption simultaneously. It will take into account non-isothermal mixing. The first MILP is not necessary to do a total cost optimization, however it gives useful insights on preferential allocations considering only mass integration. Moreover, it allows the user to reduce the search space for the global fresh resource consumption, which can speed up the resolution.

The equations (1) to (15b) are used again in this model.

3.2.1. Fresh resource search space

The first MILP gives the value of the lower bound for the global fresh resource search space $L_{fresh}^{\min}$:

$$\sum_{j\in J_f}\sum_{i\in I_p} L_{ij} \ge L_{fresh}^{\min}, \tag{17}$$

An upper bound $L_{fresh}^{\max}$ is defined by the user relatively to $L_{fresh}^{\min}$ thanks to a parameter $\Delta L_{fresh}^{\max}$:

$$\sum_{j\in J_f}\sum_{i\in I_p} L_{ij} \le L_{fresh}^{\max} = L_{fresh}^{\min} \times (1+\Delta L_{fresh}^{\max}), \tag{18}$$

Note that the equation (10) is slightly changed here for the fresh sources. If the user does not want to define an upper bound for a given allocation, then $L_j^{\max}$ is set to $L_{fresh}^{\max}$ in (10).

3.2.2. Heat integration

The heat integration model used is based on the classic transshipment model. To remain linear while considering non-isothermal mixing, a temperature scale is built where the intermediate temperature levels are predefined.

An initial temperature scale $\{T_n^*\}_{n\in[1,N]}$ is built, assuming that all sources and sinks are connected, and that all heat streams, which are created by the connections between sources and sinks, take part in the Heat Exchange Network (HEN) (Fig. 4). N represents the number of distinct shifted temperatures obtained with equations (19) and (20).

For hot streams ($T_j \ge T_i$):	*For cold streams*($T_j < T_i$):
$T_j^{h*} = T_j - \Delta T_{\min}/2,$ (19a)	$T_j^{c*} = T_j + \Delta T_{\min}/2,$ (20a)
$T_i^{h*} = T_i - \Delta T_{\min}/2,$ (19b)	$T_i^{c*} = T_i + \Delta T_{\min}/2,$ (20b)

The final temperature scale $\{T_n^{'*}\}_{n\in[1,N']}$ is obtained by dividing the previous temperature scale $\{T_n^*\}_{n\in[1,N]}$ so that the difference between two consecutive temperatures is smaller than $\Delta T_{step}^{\max}$ (Fig.4). N' is the number of temperature levels in the final scale . If two consecutive temperatures on the initial temperature scale $\{T_n^*\}_{n\in[1,N]}$ are separated by an interval strictly greater than $\Delta T_{step}^{\max}$, then this interval is divided into smaller ones, such as they all are shorter than $\Delta T_{step}^{\max}$:

$$\forall n \in [1, N'-1],\ T_{n+1}^{'*} - T_n^{'*} \le \Delta T_{step}^{\max} \quad , \tag{21}$$

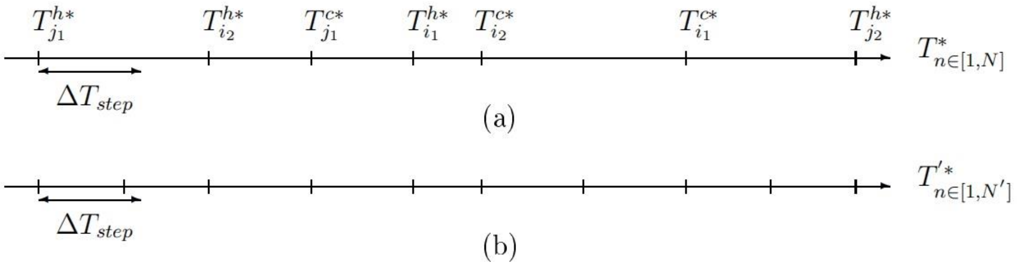

Fig. 4. Temperature Scale: (a) Initial scale (b) Final scale.

The following temperatures indicate the level, on the temperature scale $\{T_n^{'*}\}_{n\in[1,N']}$, at which begins and finishes a heat stream, depending on its nature(hot or cold).

Let $n \in [1, N' - 1]$,

For hot streams:

$n = N_j^h,\ T_n^{'*} = T_j^{h*}$, (22a)

$n = N_i^h,\ T_n^{'*} = T_i^{h*}$, (22b)

For cold streams:

$n = N_j^c,\ T_n^{'*} = T_j^{c*}$, (23a)

$n = N_i^c,\ T_n^{'*} = T_i^{c*}$, (23b)

The amount of matter extracted from a stream, going from source j to sink i, at a temperature level $T_n^{'*}$ is defined by the variable $L_{ij,n}$.

Let's consider a stream going from source j to sink i. This stream will be referred to as the main stream. At each temperature level $T_n^{'*}$ (between T_j^{c*} and T_i^{c*}, for cold streams, or, between T_j^{h*} and T_i^{h*}, for hot streams), the main stream can be split. Part of the main stream $L_{ij,n}$, which can be the entire stream, is extracted at a temperature level $T_n^{'*}$ and is directly sent to sink i, to be mixed with the other streams allocated to it. The remaining part of the main stream, if there is still one, exchanges heat through the HEN (indirect heat transfer) between $T_n^{'*}$ and $T_{n-1}^{'*}$ for a hot stream (descending order), or between $T_n^{'*}$ and $T_{n+1}^{'*}$ for a cold stream (ascending order).

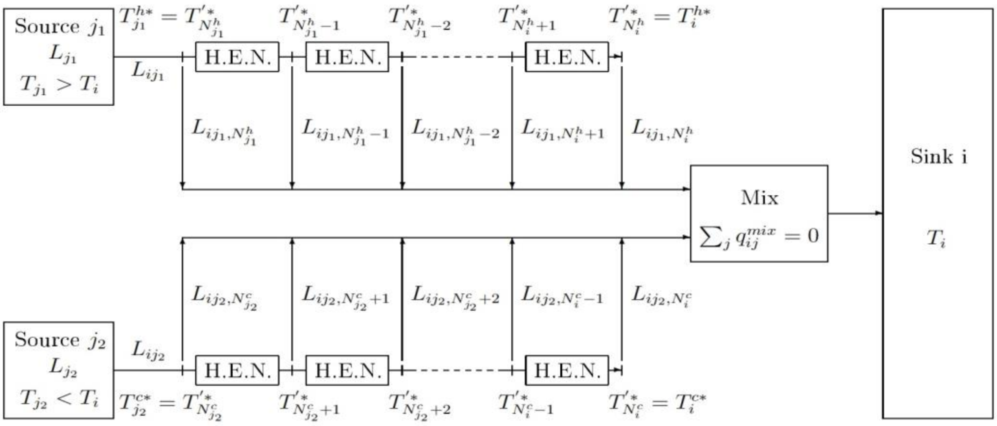

Fig. 5. Superstructure for heat integration through non-isothermal mixing.

The amount of matter coming from source j to sink i, and extracted at $T_n^{'*}$, cannot exceed the total amount allocated to sink i from source j:

$L_{ij,n} \le L_{ij}$, (24)

The sum of all extractions is equal to the amount of matter allocated from source j to sink i:

$\sum_n L_{ij,n} = L_{ij}$, (25)

Each extraction is sent to sink i from the extraction point and, within the mixing, its temperature varies from $T_n^{'*}$ to T_i^{h*} for hot streams, or to T_i^{c*} for cold streams. Hence, the amount of heat provided from each extraction to the mix $q_{ij,n}^{mix}$ can be calculated as follows:

For hot streams:

$\forall n \in [N_i^h, N_j^h],\ q_{ij,n}^{mix} = L_{ij,n} \times c_{pj} \times (T_n^{'*} - T_i^{h*}) \le 0$, (26)

The global heat provided by the source j to the mix before sink i: $q_{ij}^{mix} = \sum_{N_i^h}^{N_j^h} q_{ij,n}^{mix} \le 0$, (27) *For cold streams:*

$$\forall n \in [N_j^c, N_i^c],\; q_{ij,n}^{mix} = L_{ij,n} \times c_{pj} \times (T_n^{'*} - T_i^{c*}) \geq 0, \qquad (28)$$

The global heat provided by the source j to the mix before sink i: $q_{ij}^{mix} = \sum_{N_j^c}^{N_i^c} q_{ij,n}^{mix} \geq 0$, (29)

For each sink $i \in I_p$, heat provided by hot streams must be equal to heat required by cold streams:

$$\sum_{j \in J_p} q_{ij}^{mix} + \sum_{j \in J_f} q_{ij}^{mix} = 0, \quad (30)$$

For each sink $i \in I_w$, heat provided by hot streams must be equal to heat required by cold streams:

$$\sum_{j \in J_p} q_{ij}^{mix} = 0, \qquad (31)$$

As for the heat transferred through the HEN, matter extracted at each previous temperature level has to be subtracted (Fig. 5):

For hot streams:

$$\forall n \in [N_i^h, N_j^h - 1],\; q_{ij,n}^{HEN,h} = (L_{ij} - \sum_{k=n+1}^{N_j^h} L_{ij,k}) \times c_{pj} \times (T_{n+1}^{'*} - T_n^{'*}) \leq 0, \qquad (32)$$

The total heat entering the nth temperature interval ($n \in [1, N' - 1]$) is:

$$q_n^h = \sum_{j \in J_p} \sum_{i \in I_p} q_{ij,n}^{HEN,h} + \sum_{j \in J_p} \sum_{i \in I_w} q_{ij,n}^{HEN,h} + \sum_{j \in J_f} \sum_{i \in I_p} q_{ij,n}^{HEN,h} \leq 0, \qquad (33)$$

For cold streams:

$$\forall n \in [N_j^c, N_i^c - 1],\; q_{ij,n}^{HEN,c} = (L_{ij} - \sum_{k=N_j^c}^{n} L_{ij,k}) \times c_{pj} \times (T_n^{'*} - T_{n+1}^{'*}) \geq 0, \qquad (34)$$

The total heat exiting the nth temperature interval ($n \in [1, N' - 1]$) is:

$$q_n^c = \sum_{j \in J_p} \sum_{i \in I_p} q_{ij,n}^{HEN,c} + \sum_{j \in J_p} \sum_{i \in I_w} q_{ij,n}^{HEN,c} + \sum_{j \in J_f} \sum_{i \in I_p} q_{ij,n}^{HEN,c} \geq 0, \qquad (35)$$

The model formulation also allows the analysis of isothermal cases. In this particular case, the extractions can only occur at the sink temperature level.

From this point, the steps are identical to the classic transshipment model to calculate the minimum energy requirements (MER) (Fig. 6).

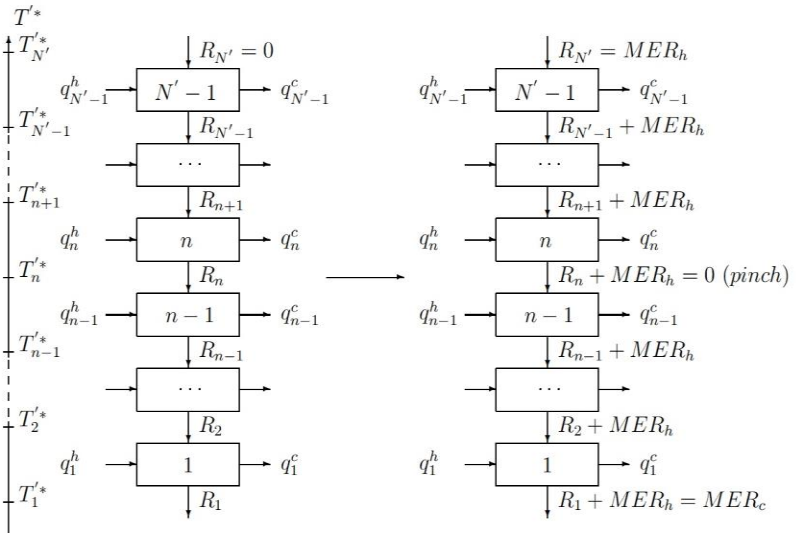

Fig. 6. Heat Cascade Diagram.

The energy balance at the n^{th} temperature interval is:

$$R_n = q_n^h + q_n^c + R_{n+1}, \quad (36)$$

where R_n represents the residual heat provided by the n^{th} temperature interval. Note that $R_{N'} = 0$, granted that no heat can come from outside the temperature scale.

Finally, the hot and cold minimum energy requirement, respectively MER_h and MER_c, are defined as follow:

$$MER_h = -\min_{R_n \le 0} R_n, \quad (37)$$

$$MER_c = R_1 + MER_h, \quad (38)$$

3.2.3. Technical constraints related to non-isothermal mixing

Restrictions can be considered to control how non-isothermal mixing is done.

Binary variables ($\lambda_{ij,n}$) are introduced to establish the existence of a stream split at the n^{th} temperature level for a given connection:

$$L_{ij,n} - \lambda_{ij,n} \times L_j^{\max} \le 0, \quad (39)$$

The number of extractions can be restrained to manage the complexity of the optimal configuration:

$$\sum_n \lambda_{ij,n} \le N_{ij}^{split\max}, \quad (40)$$

Note that $N_{ij}^{split\max}$ has to be superior to 1 because it is assumed that the entire stream has to go through mixing before entering the sink.

3.2.4. Objective function

The objective of the second MILP model is to minimize the annual operating cost (AOC):

$$\min\ AOC = h_{op} \times [\sum_{j \in J_f} (C_j \times \sum_{i \in I_p} L_{ij}) + C_{hot} \times MER_h + C_{cold} \times MER_c], \quad (41)$$

where C_j is the unit cost of fresh source $j \in J_f$, C_{hot} is the unit cost for hot utility, C_{cold} is the unit cost for cold utility and h_{op} is the annual operating hours.

4. Case Study

4.1. Process Data for the case study

To illustrate the methodology, a case study [1] is used. It is the process used to produce phenol from cumene hydroperoxide (CHP) (Fig. 7). The use and reuse of water as the main component is studied. Only one contaminant is considered, which is phenol. Streams are characterized by two properties in addition to temperature: pH and the vapor pressure in phenol.

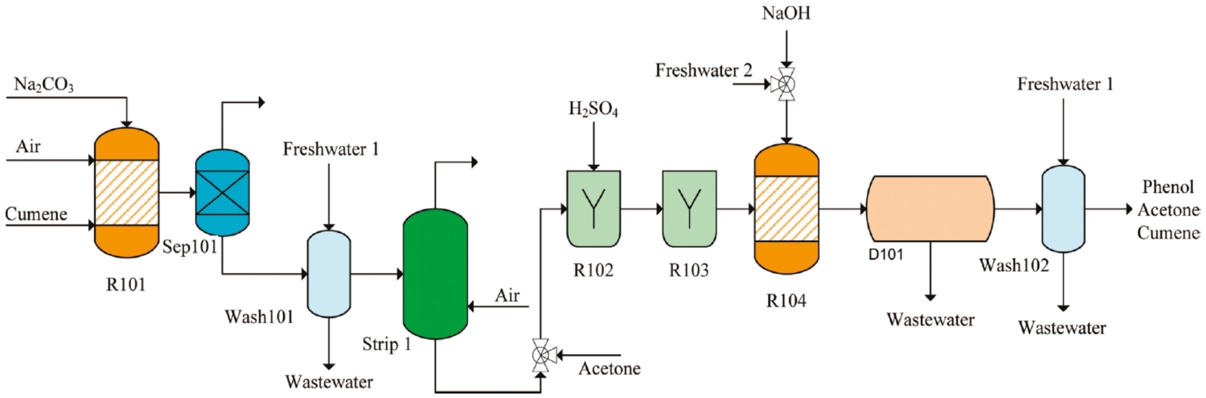

Fig. 7. Process Flowsheet of the production of phenol from cumene [1].

Table 1. Data for the Process Sources and Fresh Sources [1].

Source	*Flow rate,* kg/h	*Composition,* mass fraction	*Temperature,* °C	*Vapor pressure,* kPa	*pH*
Washer 101	3661	0.016	85	38	5.4
Decanter 101	1766	0.024	65	25	5.1
Washer 102	1485	0.220	40	7	4.8
Freshwater 1		0.000	25	3	7
Freshwater 2		0.012	35	6	6.8

Table 2. Data for the Process Sinks and Waste Sinks [1].

Sink	*Flow rate,* kg/h	*Composition,* mass fraction	*Temperature,* °C	*Vapor pressure,* kPa	*pH*
Washer 101	2718	0.013	60	20-47	4.5-7.0
Washer 102	1993	0.013	78	4-38	4.0-8.0
R104	1127	0.100	40	3-25	4.5-7.0
Waste		0.15	30		5.0-9.0

4.2. Results for the case study

4.2.1. Global fresh resource consumption minimization - 1st MILP

Several sets of constraints are tested to show their impact on the minimum global fresh resource consumption and waste generation (Table 3).

The theoretical minimum global fresh resource consumption and waste to be treated is obtained when no constraints are set (case 1). The results are 973.0 kg/h and 2047.0 kg/h, respectively.

If one tries to limit the use of the fresh resource *Fresh1* by limiting the maximum flow rate that can be allocated from this source to each sink (case 2), the resulting global consumption and waste production will increase to 1733.3 kg/h and 2807.3 kg/h. However, one can note that a solution will still exist.

Limiting the use of one fresh resource can be done in other way. For instance, if the total use of the fresh resource *Fresh2* is limited to 200kg/h (case 3), one can observe that this particular constraint has no influence on the optimal global fresh resource consumption because this source is not used in case 1.

Table 3. Minimum Fresh Resources and Waste for different technical constraints

Case n°	Constraints	Solution Exists	L_{Fresh1}, kg/h	L_{Fresh2}, kg/h	$L^{\min}_{fresh}$, kg/h	$G^{\min}_{waste}$, kg/h
1	No Constraints	Yes	973.0	0.0	973.0	2047.0
2	$L^{\max}_{Fresh1} = 300\,\text{kg/h}$	Yes	600.0	1133.3	1733.3	2807.3
3	$L^{\max,\ total}_{Fresh2} = 200\ \text{kg/h}$	Yes	973.0	0.0	973.0	2047.0
4	$L^{exist}_{R104/Fresh2} = 500\ \text{kg/h}$	Yes	938.9	500.0	1438.9	2512.9
5	$L_{Washer2/Fresh1} = 0\ \text{kg/h}$	Yes	509.6	1494.8	2004.4	3078.4
6	$G^{\max,\ total}_{Waste} = 2000\ \text{kg/h}$	No	-	-	-	-
7	$N^{\max}_{Decanter1} \le 2$	Yes	1100.4	0.0	1100.4	2174.4

The process flowsheet shows that the fresh resource *Fresh2* is used to feed the reactor *R104*. A pipeline connecting those two points of the process may exist already. Therefore, one may want to keep using this line. If one imposes that *Fresh2* sends 500 kg/h to *R104* (case 4), then the optimization results in an increase in the global fresh resource consumption (1438.9 kg/h).

The process flowsheet also shows that the fresh resource *Fresh1* is used to feed the sink *Washer2*. If this allocation is forbidden (case 5), it will cause a strong increase in fresh resource consumption (2004.4 kg/h); consequently it will cause a strong increase in waste generation (3078.4 kg/h).

One can face specific limitations on site, such as limited capacity of the waste treatment unit (for instance, limited to 2000 kg/h (case 6)), or limitations on the number of pipes that can be installed at one place in the process (for instance, the number of allocations of the source Decanter1 cannot exceed 2 (case 7)). In the first case, the limitation cannot comply with the mass balances. In the second case, the limitation generates an increase in fresh resource use compared to the initial case.

The results of this first study show the influence of technical constraints on the optimal solution and the necessity to consider them at an early stage of the network design. Certain constraints result in doubling the fresh resource consumption, which can direct the user towards other solutions early on in the design process. The second model optimizes the AOC of the network, and shows the influence of heat integration and the technical constraints on the performances of the optimal solution.

4.2.2. Annual Operating Cost minimization - 2nd MILP

The economic data and chosen parameters for this study are shown in Table 4. Technical constraints are the same as the ones used with the first model. The methodology allows comparing two strategies of optimization: sequential and simultaneous.

Table 4. Economic data and Parameters

C_{Fresh1}, x10^{-3}\$/kg	C_{Fresh2}, x10^{-3}\$/kg	C_{hot}, \$/kWh	C_{cold}, \$/kWh	h_{op}, h	ΔT_{step}, °C	ΔT_{pinch}, °C	$N_{ij}^{split\max}$	cp_j, kJ/(kg K)
3.0	1.0	0.1	0.025	8000	1.0	10.0	2	4.2

By setting $\Delta L_{fresh}^{\max} = 0\%$, the global fresh resource is forced to its minimum found with the 1st MILP model (Table 3). The cost optimization will target the minimum energy consumption, as the global fresh resource target is fixed and set to its minimum value.

By setting $\Delta L_{fresh}^{\max} = 900\%$, the global fresh resource mass flow rate can go up to 10 times its minimum value. The model will calculate the optimal mass and energy targets simultaneously, within the defined search space for the global fresh resource consumption.

Table 5 and Table 6 show the results of the sequential and simultaneous strategy, respectively.

Table 5. Results for different technical constraints - $\Delta L_{fresh}^{\max} = 0\%$ (sequential strategy)

Case n°	Constraints	L_{Fresh1}, kg/h	L_{Fresh2}, kg/h	$L_{fresh}^{\min}$, kg/h	$G_{waste}^{\min}$, kg/h	MER_h, kW	MER_c, kW	AOC, x10^3\$
1	No Constraints	973.0	0.0	973.0	2047.0	0.0	98.8	43.1
2	$L_{Fresh1}^{\max} = 300\,\text{kg/h}$	600.0	1133.3	1733.3	2807.3	0.0	107.6	45.0
3	$L_{Fresh2}^{\max,\,total} = 200\ \text{kg/h}$	973.0	0.0	973.0	2047.0	0.0	98.8	43.1
4	$L_{R104/Fresh2}^{exist} = 500\ \text{kg/h}$	938.9	500	1438.9	2512.9	0.0	101.9	46.9
5	$L_{Washer2/Fresh1} = 0\ \text{kg/h}$	509.6	1494.8	2004.4	3078.4	1.2	111.4	47.4
6	$N_{Decanter1}^{\max} \le 2$	1100.4	0.0	1100.4	2174.4	0.0	98.0	46.0

Table 6. Results for different technical constraints - $\Delta L_{fresh}^{\max} = 900\%$ *(simultaneous strategy)*

Case n°	Constraints	L_{Fresh1}, kg/h	L_{Fresh2}, kg/h	$L_{fresh}^{\min}$, kg/h	$G_{waste}^{\min}$, kg/h	MER_h, kW	MER_c, kW	AOC, x10^3\$
1	No Constraints	803.9	317.6	1121.5	2195.5	0.0	101.6	42.2
2	$L_{Fresh1}^{\max} = 300\,\text{kg/h}$	600.0	1133.3	1733.3	2807.3	0.0	107.6	45.0
3	$L_{Fresh2}^{\max,\ total} = 200\ \text{kg/h}$	866.5	200.0	1066.5	2140.5	0.0	100.6	42.5
4	$L_{R104/Fresh2}^{exist} = 500\ \text{kg/h}$	827.8	722.7	1550.0	2624.0	0.0	103.8	46.4
5	$L_{Washer2/Fresh1} = 0\ \text{kg/h}$	509.6	1494.8	2004.4	3078.4	1.2	111.4	47.4
6	$N_{Decanter1}^{\max} \leq 2$	803.9	317.6	1121.5	2195.5	0.0	101.6	42.2

The first thing to note is that simultaneous optimization gives in general better results than sequential optimization in terms of AOC. In the cases where the results are better (cases 1, 3, 4 and 6), the global fresh resource consumption increases compared to its minimum value found with the first model. It highlights the coupling between mass and heat integration. Optimal mass integration can lead to poor heat integration. Therefore, their optimization should be considered at the same time.

Moreover, the technical constraints for mass integration can result, but not all the time, in constraints for heat integration (for instance in cases 2 and 6). Note that in case 5, the minimum hot utility is not equal to 0.0kW contrary to the other cases. In this case, the constraint limits the possibilities for optimal heat integration, because not enough heat (at the right temperature) can be found within the process. If a subsequent analysis is led on the capital investments, the solution may not be deemed profitable enough. Thus, another solution may need to be found.

Overall, the optimization of the mass allocation network requires considering the influence of heat integration and technical constraints early in the design process. The proposed methodology allows testing several sets of constraints and several optimization strategies. The set of solutions found can then be analyzed more precisely to determine its economic and technical feasibility on-site.

4. Conclusion

The introduced methodology is using two MILP problems to generate heat integrated mass allocation network by optimizing mass and energy related operating costs simultaneously.

The proposed methodology allows the user to characterize more precisely the industrial process and design several optimized heat integrated mass allocation network taking into account real on-site constraints.

This two steps methodology allows the user to have a better understanding of the influence of certain parameters on mass integration and the influence of heat integration on the network design.

Nomenclature

L	source mass flow rate, kg/s
G	sink mass flow rate requirement, kg/s
cp	specific heat, kJ/(kg K)
T	temperature, °C
q	heat stream, kW
y	source composition
z	sink acceptable composition
p	property

$N_j^{\max}$	maximum number of allocation for a given source j
$N_{ij}^{split\max}$	maximum number of stream split
R_n	residual heat provided by the nth temperature interval, kW

Greek symbols

γ	binary variable establishing the existence of an allocation
λ	binary variable establishing the existence of a split
$\Delta L_{fresh}^{\max}$	maximum relative variation of L_{fresh} compare to $L_{fresh}^{\min}$, %
$\Delta T_{step}^{\max}$	maximum gap between two consecutive temperature level on temperature scale, °C
ΔT_{pinch}	minimum temperature approach in heat exchanger, °C

Subscripts and superscripts

c	cold
h	hot
i	sink
j	source
f	fresh
w	waste
k	kth contaminant
m	mth property
HEN	indirect heat transfer
mix	direct heat transfer
*	shifted temperature

References

- **Journals**:

[1] Kheireddine H., Dadmohammadi Y., Deng C., Feng X., El-Halwagi MM., Optimization of direct recycle networks with simultaneous consideration of property, mass and thermal effects. Ind. Eng. Chem. Res. 2011;50:3754-3762.

[2] Nápoles-Riviera F., Ponce-Ortega J., El Halwagi MM., Jimenez-Gutierrez A., Global Optimization of mass and property integration networks with in-plant property interceptors. Chem.Eng. Sci. 2010;65:4363-4377.

[3] Sahu G., Bandyopadhyay S., Energy optimization in heat integrated water allocation networks. Chem. Eng. Sci. 2012;69:352-364.

[4] Tan Y., Ng D., El Halwagi MM., Foo D., Samyudia Y., Heat integrated resource conservation networks without mixing prior to heat exchanger networks. Journal of Cleaner Production 2014.

[5] Hortua, A., El Halwagi, M., Ng, D., Foo, D., 2013. Integrated approach for simultaneous mass and property integration for resource conservation. ACS Sustain. Chem. Eng. 1, 29_38.

- **Chapter in a book**:

[6] El Halwagi MM., Sustainable Design Through Process Integration - Fundamentals and Applications to Industrial Pollution Prevention, Resource Conservation, and Profitability Enhancement. Elsevier. 2012. p.201-222