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Research Article

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Evaluation of Irreversibility and Optimal Organization of an Integrated Multi-Stream Heat Exchange System

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Abstract: This work proposes a structure synthesis and surface distribution algorithm in a heat exchange system for the case when all heat capacity rates and inlet temperatures of the hot streams are constant, while cold streams also have outlet temperatures set. The algorithm includes the possibility of changing the phase state of the contacting streams. The synthesis is based on minimization of dissipation for a given total heat load in the form of minimum total contact surface area, which again correlates with the cost of the heat exchange system. The proposed algorithm can be considered to follow a thermodynamic rationale and as development of pinch analysis.

Keywords: multi-stream heat exchange, optimization thermodynamics, heat exchange system synthesis

1 Introduction

The problem of multi-stream heat exchange system synthesis is to organize the thermal contacts between the hot and cold streams (i. e., to choose the system structure), to distribute the heat load between the countercurrent heat exchange units, and to calculate the heat exchange coefficients (essentially heat exchanger areas), for example to minimize a certain optimality criterion while satisfying the constraints imposed. In most cases, heat exchange systems are integrated with a certain technological process (metallurgy, distillation processes, etc.) [1], in which the flows entering the technological systems, as well as outgoing hot streams, must have certain temperatures. Heat consumed by the technology is minimized due to the heat exchange.

In most papers (see [2]) the optimality criterion is techno-economic in nature, considering a total of chosen weights, capital, and operating costs, while the constraints are defined by the characteristics of the synthesized system. Thus, during the process of multi-column distillation the technological requirements dictate certain temperatures and heat capacity rates (specific heat of the fluid multiplied mass flow rate of the fluid, typically measured in W/K), and the heat exchange system may include the heat exchange column units (a boiler and a reflux condenser). The authors of the paper [3] consider the possibility of multi-stage contact of heat streams, searching through the structures and conducting numerical optimization of parameters according to economic criteria.

The synthesis of such a system with numerous flows in contact with each other is a complex combinatorial problem, usually solved numerically, in some cases using heuristic methods [4].

The use of feasibility criteria is associated with the liberty of choosing the evaluation factors of operational and capital costs depending on the cost of materials, installation, etc. Moreover, such a criterion as-

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sumes a numerical procedure and makes it impossible to use common thermodynamic principles. For simplicity of calculations, we assume the heat exchange to be single-staged, i. e., each hot stream is in contact with only one cold stream.

The book [5] used an exergy criterion, which is equivalent to exergy (useful energy) loss minimization. This approach allowed the authors to compare several systems based on their actual exergy losses. No optimization or system synthesis procedure with the chosen criterion was offered in this case.

Exergy loss is equal to the product of entropy production in the system and the absolute ambient temperature. Therefore minimum entropy production (irreversibility) corresponds to minimum loss of exergy. This fact was used in the methods of optimization thermodynamics [6–11] among others. Using these methods, the problems of optimal thermodynamic system synthesis based on the minimum entropy production criterion are solved in the present paper.

Pinch analysis is widely used in designing industrial process systems (see [12, 13], etc.). To conduct pinch analysis, the dependencies of the temperatures of contacting streams on their enthalpy are found, and consequently a zone with the closest temperatures (pinch temperatures) is determined. Further, graphs are based on the most common qualitative considerations about the nature of contacts for temperatures above and below the pinch.

This approach is justified by the fact that the entropy production for a given total heat exchange surface and system structure increases monotonically with the increase of heat load when the system structure is chosen so that the production of entropy is minimal [8, 10, 14, 15]. Conversely, for a given heat load it decreases monotonically with the increase of heat exchange surface. This means that for a structure with minimum irreversibility it is possible to ensure maximum heat load for a given surface or alternatively minimum total contact surface for a constant load, which correlates with the minimum cost of a system. Note that the monotonicity is for a given system structure and transfer coefficients while the minimum contact surface area is for a given heat load while changing the system structure and/or varying the stream distributions between the heat exchangers.

2 Optimal heat exchange

The work [14] considers the problem of the highest achievable performance of a heat exchange system ("optimal" heat exchange) among streams which do not change phase. The nomenclature of temperatures T_i and heat capacity rates W_i (heat capacity multiplied flow rate) around a given heat exchanger is shown in Fig. 1. The hot streams are labeled +, the cold streams −. The authors found the least possible entropy production rate σ^* in a system with given values of input heat capacity rates and input temperatures of hot and cold streams. Further conditions were the required heat flux density, q, for a given temperature difference in a

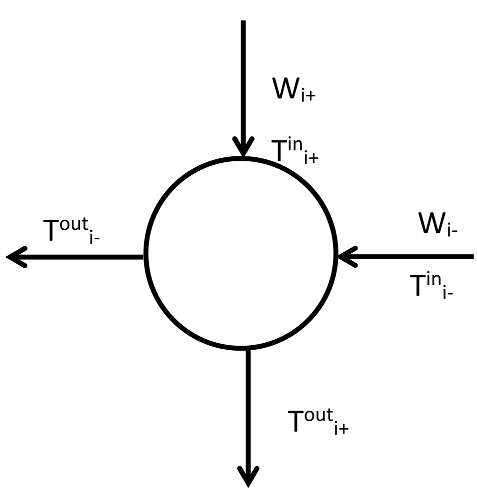

Figure 1: Definition of nomenclature around counter-current heat exchangers.

given point and total heat flux, Q, for all temperatures from the starting point to the current point. They show that in the case when the heat flow is proportional to the temperature difference (Newtonian kinetics), this optimal irreversibility limit can be achieved if the ratio of absolute flow temperatures, T_-/T_+, stays the same at each contact point along the heat exchanger, and if the system outlet temperatures T_{i+}^{out} are the same for all flows, while the inlet temperatures are constant (hot or cold) over time.

The conditions for optimal heat exchange impose very strict requirements on the system characteristics [14]:

- each heat exchange unit must be a counter-current heat exchanger;
- the ratio of heat capacity rates of hot and cold streams in it must be equal to the ratio of the absolute temperatures of the cold stream exiting the heat exchange unit to the hot stream inlet temperature ("temperature consistency conditions"), $W_{i+}/W_{i-} = T_{i-}^{\text{out}}/T_{i+}^{\text{in}}$.

Under these conditions, the system load is equal to the total energy required to heat all cold streams and is determined by the equation

$$\bar{q} = \sum_j q_j = \sum_j W_{j-}(T_{j-}^{\text{out}} - T_{j-}^{\text{in}}). \tag{1}$$

We further define the relative temperature gradient for constant outlet temperatures and heat capacity rates of the hot streams T_+^{out} related to their inlet temperatures T_{i+}^{in}, heat capacity rates W_i, and the total heat exchange rate K as [14]

$$m = 1 - \frac{1}{K}\sum_{i=1}^{n} W_{i+}(\ln T_{i+}^{\text{in}} - \ln T_+^{\text{out}}),$$

where the summation over i is over all streams and the outlet heat stream temperatures T_+^{out} must be the same and, as follows from the energy balance conditions, be equal to

$$T_+^{\text{out}} = \frac{\sum_{i=1}^{k} T_{i+}^{\text{in}} W_{i+} - Q}{\sum_{i=1}^{k} W_{i+}}, \tag{2}$$

where the summation only runs to k instead of the full n streams, because hot streams with initial temperatures less than T_+^{out} are not involved in the heat exchange system [14].

The least possible entropy production rate for this system is then

$$\sigma^* = K\frac{(1-m)^2}{m}. \tag{3}$$

These relations are valid for the optimal operation of the heat exchange network, e. g., the heat capacity rates W_{i+}.

Next, let us expand our universe of heat exchange possibilities and allow streams which change phase, i. e., either condense or evaporate. If any flow changes its phase state, in addition to its heat capacity rates, the flow (by weight) g_i and the heat of vaporization (condensation) r_i are constant. Then, if part of the hot streams is condensed during heat exchange, the heat capacity rate of the corresponding summand in (1) tends to infinity. Let us assign the index c to the condensing stream and find the limit of

$$W_c(\ln T_c^{\text{in}} - \ln T_c^{\text{out}}) = W_c\left(\ln T_c^{\text{in}} - \ln\left(T_c^{\text{in}} - \frac{q_c}{W_c}\right)\right)$$

when W_c tends to infinity. Using l'Hôpital's rule, we find

$$\lim_{W_c\to\infty} W_c\left(\ln T_c^{\text{in}} - \ln\left(T_c^{\text{in}} - \frac{q_c}{W_c}\right)\right) = \frac{q_c}{T_c^{\text{in}}} = \frac{g_c r_c}{T_c}.$$

It is assumed that temperature T_c^{in} equals the condensation temperature and the heat load equals the product of the flow rate and the hidden vaporization rate.

Therefore, the expression for m when condensing streams are involved will change to the following form:

$$m = 1 - \frac{1}{K}\left(\sum_{i \neq c} W_{i+}(\ln T_{i+}^{\text{in}} - \ln T_{+}^{\text{out}}) + \sum_{c} \frac{g_c r_c}{T_c}\right). \tag{4}$$

Regardless of whether we are considering condensing streams or not, when deriving the expressions above it was assumed that all parameters of the cold streams are chosen for a given load and total heat exchange rate K according to the minimum irreversibility condition. However, in many cases there is no possibility of such a choice.

In a multi-stream system integrated with the workflow there are values given for heat capacity rates of both hot and cold streams, and their outlet temperatures are also often set. Therefore, it is usually impossible to reach the results of an optimal heat exchange system. Instead, it is natural to pose the problem of heat exchange system synthesis with minimum irreversibility under more stringent constraints on the specifications of the flows. In this case, the optimal heat exchange conditions can only serve as a guide similar to the Carnot efficiency for heat engines, and the value of the ratio $\overline{Q} = \sum_j q_{j-} = \sum_j W_{j-}(T_{j-}^{\text{out}} - T_{j-}^{\text{in}})$ to the entropy production in a designed system can only be a measure of its thermodynamic perfection.

In the following we present the calculated ratios to evaluate the minimum dissipation from below in a system with the aforementioned restrictions and the synthesis of a hypothetical system in which such an evaluation is implemented.

3 Formulation and conditions of optimality of the heat exchange system synthesis problem

The difference in conditions imposed on the hot and cold streams is due to the fact that the cold streams leaving the heat exchange system subsequently enter the processes of the plant where specific temperatures are specified and thus require additional heating. The hot streams, on the other hand, leave the system and therefore are under no temperature restrictions, only the requirement to achieve maximum thermal efficiency.

Entropy production equals the difference between the total entropy of the outgoing flows and the total entropy of the incoming flows. Let us consider initially that all flows enter and exit the system in the same phase state, the pressure change in the system is small, and all the heat capacities are constant. Then the entropy change of each flow is equal to the product of its heat capacity rate and the logarithm of the ratio of the absolute temperatures at the inlet and the outlet [15]. Therefore, considering the thermodynamic balance condition, it results in

$$\sigma = \sigma_+ + \sigma_- = \sum_i W_{i+}(\ln T_{i+}^{\text{out}} - \ln T_{i+}^{\text{in}}) + \sum_j W_{j-}(\ln T_{j-}^{\text{out}} - \ln T_{j-}^{\text{in}}). \tag{5}$$

The first item (from absorbed heat) in this sum is negative and the second (from discharged heat) is positive, and their sum is always larger than $\sigma^* > 0$. The expression to calculate the entropy production when changing the phase state of a stream will be given below.

Note that all variables that determine the amount of gain of entropy of the cold streams, σ_-, are set through the problem conditions (fixed exit temperatures and heat capacity rates). Therefore the minimum of the first item corresponds to the minimum of entropy production at temperature T_{i+}^{out}.

A formal definition of the optimization will look as follows: Maximize the total heat exchange rate

$$K = \frac{\bar{q}}{T_+^{\text{in}} - T_-^{\text{in}} - \frac{\bar{q}}{\overline{W}}},$$

where

$$\overline{W} = \frac{W_- W_+}{W_+ + W_-}.$$

The Lagrangian of this problem is

$$L = \sum_i W_{i+}(\ln T_{i+}^{\text{out}} - \ln T_{i+}^{\text{in}}) - \lambda \sum_i W_{i+}(T_{i+}^{\text{out}} - T_{i+}^{\text{in}}). \tag{6}$$

Its stationary conditions in T_{i+}^{out} lead to

$$T_{i+}^{\text{out}} = \frac{1}{\lambda}. \tag{7}$$

Let us formulate the optimality conditions: *For any heat capacity rates W_i and inlet temperatures of the hot streams T_{i+}^{in}, there is a minimal dissipation corresponding to a heat exchange setup in which the outlet temperatures of the hot streams are the same.*

Similarly, we can show that in the case where the inlet temperatures of the cold streams are free: *For any heat capacity rates W_{j-} and outlet temperatures T_{j-}^{in} of the cold streams, the heat exchange structure for which the inlet temperatures of the hot streams stay the same corresponds to minimal dissipation.*

Let us call this outlet temperature T_{+}^{out}. It is determined by the condition of energy balance of the system (see eq. (2)). Substitution of this value of the outlet temperature of the hot streams allows us to rewrite expression (5) and find the entropy production in the system that is being designed. With this, for hot streams condensing at temperatures T_{ci+} and cold streams evaporating at temperatures T_{ej-}, the right part of eq. (5) acquires additional summands, corresponding to the decrease of entropy of a stream during condensation, $-\frac{g_i r_i}{T_{ci+}}$, and its increase during evaporation, $\frac{g_j r_j}{T_{ej-}}$. We get

$$\sigma^0 = \sigma_+ + \sigma_- = \sum_i W_{i+}(\ln T_{i+}^{\text{out}} - \ln T_{i+}^{\text{in}}) - \sum_{ci} \frac{g_i r_i}{T_{ci+}} + \sum_j W_{j-}(\ln T_{j-}^{\text{out}} - \ln T_{j-}^{\text{in}}) + \sum_{ej} \frac{g_j r_j}{T_{ej-}}. \tag{8}$$

To compare this value with the lowest possible value corresponding to an optimal heat exchange, we need to know the total heat exchange rate in the system, which, in turn, implies the choice of contacting streams, their temperatures, and the nature of hydrodynamics in the counter-current heat exchange units making this contact.

Knowing the temperature T_{+}^{out} makes it possible to find the "available heat" for each hot stream q_i and total "available heat" $\overline{Q}_+$:

$$Q_{i+} = W_{i+}(T_{i+}^{\text{in}} - T_{+}^{\text{out}}),$$
$$\overline{Q}_+ = \sum_i Q_{i+}.$$

If $T_{+}^{\text{out}} < T_0$, it is necessary to introduce an additional hot stream in such a manner as to even out this inequality. It is easy to see that for the outlet temperature determined by expression (2), $Q_+ = Q_- = \overline{Q}$.

4 The dependence of heat exchange rates on temperatures

After the structure of the heat exchange system and the heat loads of the counter-current units are determined, it is required to find the corresponding heat transfer rates, which the necessary surface areas of contact depend on. Here we present the formulas of heat exchange rates corresponding to various hydrodynamic modes of these units [4, 9], leaving out the derivation of these formulas. They are labeled by the types of flow for the hot/cold streams. Mixing means a well-stirred container, and displacement means a pipe flow. Since in this case there are only two streams, we will be using index + for hot and index – for cold streams for temperatures and heat capacity rates.

1. *Mixing–mixing*

   In this case we have

$$K = \frac{\bar{q}}{T_{+}^{\text{in}} - T_{-}^{\text{in}} - \frac{\bar{q}}{\overline{W}}}. \tag{9}$$

This value never exceeds the values of each heat capacity rate. If any stream changes its phase state (its heat capacity rate is arbitrarily large), the value $\overline{W}$ is equal to the heat capacity rate of the second contacting stream. If both streams change their phase state (one evaporates and the other condenses), then the total heat exchange rate K is

$$K = \frac{\bar{q}}{T_+^c - T_-^c}. \tag{10}$$

2. *Displacement–displacement* (*co-current flow*)
   In this case we have

$$K = \overline{W} \ln \frac{T_+^{\text{in}} - T_-^{\text{in}}}{T_+^{\text{out}} - T_-^{\text{out}}}. \tag{11}$$

3. *Mixing–displacement* (*in either order*)
   When a hot stream is in displacement mode, then

$$K = W_+ \ln \frac{T_+^{\text{in}} - T_-^{\text{in}} - \frac{\bar{q}}{W_-}}{T_+^{\text{in}} - T_-^{\text{in}} - \frac{\bar{q}}{\overline{W}}}. \tag{12}$$

   If a cold stream evaporates at temperature T_-^e at the same time, then

$$K = W_+ \ln \frac{T_+^{\text{in}} - T_-^e}{T_+^{\text{in}} - T_-^e - \frac{g_- r_-}{W_+}}. \tag{13}$$

   When a cold stream is in displacement mode, then

$$K = W_- \ln \frac{T_+^{\text{in}} - T_-^{\text{in}} - \frac{\bar{q}}{W_+}}{T_+^{\text{in}} - T_-^{\text{in}} - \frac{\bar{q}}{\overline{W}}}. \tag{14}$$

   If during this a hot stream condenses at temperature T_+^c, then

$$K = W_- \ln \frac{T_+^c - T_-^{\text{in}}}{T_+^c - T_-^{\text{in}} - \frac{g_+ r_+}{W_-}}. \tag{15}$$

4. *Displacement–displacement* (*counter-current*)
   In this case we have

$$K = \frac{1}{A} \ln \frac{T_+^{\text{in}} - T_-^{\text{out}}}{T_+^{\text{out}} - T_-^{\text{in}}}. \tag{16}$$

   Here A is defined as

$$A = \frac{W_- - W_+}{W_- W_+}. \tag{17}$$

5 Preparation of source data in systems with changing phase states of streams

Generally the streams of heat transfer agents entering the system may have different phase states: vapor (V), liquid (L), or liquid–vapor mixture (LV). The same conditions may apply when exiting the system.

If a stream k does not change its phase state and only changes its temperature, we will assume that we know its inlet temperature T_k^{in}, the heat capacity rate W_k, and for cold streams its outlet temperature T_+^{out}. The outlet temperatures of hot streams T_+^{out} are subject to choice (see eq. (2)).

If a cold stream j changes its phase state so that it is liquid at the boiling point when entering the system or saturated vapor (LV) when exiting the system, it has its own mass rate g_j, boiling point T^e_{j-}, and heat of vaporization r_j. The same is true for hot "condensing" streams. They are in the form of saturated vapor when entering the system and in the liquid form at the boiling point (LV) on exit.

Let the cold stream at the entrance to the system be an LV mixture with a given weight fraction of vapor $d^{\text{in}}_{j-} \geq 0$, and with a weight fraction of vapor $d^{\text{out}}_{j-} \geq d^{\text{in}}_{j-}$ at the exit of LV. The mass flow rate g_j, the boiling point T^c_{j-}, and the heat of vaporization r_j are known. For calculation it is convenient to divide it into three streams: an evaporating stream with the flow rate $g^c_j = g_j(d^{\text{out}}_{j-} - d^{\text{in}}_{j-})$ and two unchanging streams, vapor and liquid, with flow rates $g_j d^{\text{in}}_{j-}$ and $g_j(1 - d^{\text{out}}_{j-})$, respectively. Both these latter streams do not change their temperature and phase state and may be disregarded in calculating the increase in entropy and the heat load.

A hot stream can be considered in the same way, with the difference that its outlet vapor weight fraction is less than that of the inlet vapor. It can be represented as a condensing stream and two unchanging streams which are not included in the calculations.

When a cold stream is supplied to the system inlet in liquid form with initial temperature of $T^{\text{in}}_{j-} < T^c_{j-}$, it is heated to its boiling point T^c_{j-} and then completely or partially evaporated, and it may further be heated to a superheated vapor temperature. It can be represented by three streams: two "heating" and one "evaporating." Moreover, the "heated" streams have different heat capacity rates due to the difference in heat capacity of vapor and liquid. If it does not evaporate completely, the last stream is also broken down into two: "evaporating" and "unchanging," and the latter does not participate in the calculations.

Similarly, the hot stream in the form of superheated vapor can be represented as cooling to the boiling point T^c_{i+}, fully or partially condensing, and finally a cooling stream from the boiling point to the final liquid state. If the stream does not condense completely, an unchanging stream, which does not change its enthalpy and entropy, is released from it. There is no liquid cooling stream.

Thus, the first step is the preparation of the initial data in which we move from the actual streams and their characteristics to the estimated streams. They can be of two types: not changing their phase state (heated and cooled) and changing it at the boiling point (evaporating and condensing). The unchanging streams are not included in the calculation. To calculate the total heat load we use the expression

$$\sum_{jh} W_{jh-}(T^{\text{out}}_{jh-} - T^{\text{in}}_{jh-}) + \sum_{cj} g_{cj-} r_{cj-} = \overline{Q}. \tag{18}$$

Here the first sum in the left part of the equation is taken for all "heated" calculated flows, and the second sum is taken for all "evaporating" flows.

6 Equivalent streams and the relation between the temperatures of their contacts and the heat loads

In this section we will show that the problem of designing a multi-component heat exchanging system can be reduced to the problem with two-component heat exchangers with streams of variable heat capacity rates.

Hot streams are arranged so that index 1 corresponds to the stream with the highest input temperature. Cold streams are analogously arranged by their output temperatures. This means that the first stream has the maximum temperature.

As the hot streams transfer heat to the cold ones, the hot temperatures drop to the value T^{out}_{+}. This decrease in temperature corresponds to the transfer of some of their inherent heat q. For temperature T^{out}_{+}, the corresponding flux is equal to the heat load of the system Q. Let us denote the given heat load as Q for some intermediate temperature of the hot streams. As hot streams are cooling down, this value changes from zero to $\overline{Q}$.

We will call this Q the *current heat load*. For each intermediate value of the current heat load, temperatures of the hot streams that transferred heat and temperatures of the cold streams that received this heat in order to reach the required output temperatures can be found as shown below.

Definition. We call a cold/hot stream having at each temperature T a heat capacity rate equal to the sum of the heat capacity rates of all cold/hot flows contained in the system having this temperature an *equivalent stream* (Fig. 2).

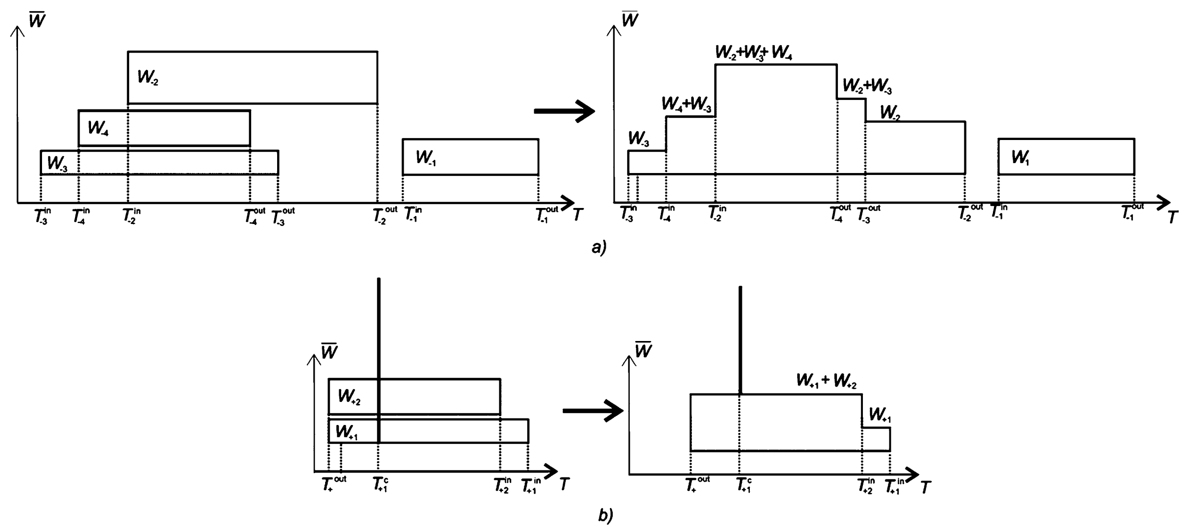

Figure 2: Dependence of the heat capacity rates of an equivalent stream on the contact temperature (a) for a cold equivalent stream, (b) for a hot equivalent stream with condensation.

We denote the temperature of the hot equivalent stream by $T_+(Q)$ and the temperature of the cold one by $T_-(Q)$. We call these values the *contact temperatures of the equivalent streams for the given heat loads.*

Thus, the heat capacity rate of the equivalent cold stream depends on which cold streams are included in it at a given temperature. For example, the first cold stream has the highest output temperature T_{1-} compared to the others, so at this temperature the heat capacity rate of the equivalent cold stream is W_{1-}.

As the temperature decreases, the equivalent cold stream begins to include the second, third, etc., cold streams and its heat capacity rate increases correspondingly. This happens until the temperature drops to a value equal to the temperature of one of the cold streams at the input. At this point, the number of cold streams entering the equivalent one decreases, and hence does its heat capacity rate. The lowest temperature of the equivalent cold stream is the lowest of the T_{j-}^{in} temperatures. Its heat capacity rate at this temperature is equal to the heat capacity rate of the cold stream with a minimal input temperature.

Similarly, for the equivalent hot stream, the highest temperature T_+ is T_{1-}^{in} and the lowest is T_+^{out}. In contrast to the cold stream, the heat capacity rate of the equivalent hot stream increases as the temperature decreases, as it includes streams with a lower initial temperature.

The dependencies of current contact temperatures of equivalent streams can be calculated from energy balance conditions similar to expression (2). For the equivalent hot stream,

$$T_+(Q) = \frac{\sum_{i=1}^{i_m} W_{i+} T_{i+}^{\text{in}} - Q}{\sum_{i=1}^{i_m} W_{i+}}, \tag{19}$$

where i_m is the set of hot stream indices for which the input temperature is higher than the current contact temperature ($T_{i+}^{\text{in}} > T_+(Q)$).

Similarly, for the contact temperature of the equivalent cold stream, we have

$$T_-(Q) = \frac{\sum_{j \in S_-(T_-)} W_{j-} T_{j-}^{\text{out}} - Q}{\sum_{j \in S_-(T_-)} W_{j-}}, \tag{20}$$

where $S_-(T_-)$ is the set of cold stream indices for which the contact temperature T_- satisfies the inequality $T_{j-}^{out} > T_-(Q) > T_{j-}^{in}$.

It follows from the above expressions that contact temperatures are piecewise linear functions with a negative slope. The value of this slope is inverse to the current heat capacity rate of the corresponding equivalent stream. This heat capacity rate changes discretely as the composition from the stream changes or at the boiling/condensation temperature of one of them.

The contact temperature curves of our subsequent examples are shown in Figs. 3 and 5. They decrease monotonically with the increase of the heat load Q, and $T_+(Q) > T_-(Q)$. On each of these curves two points (nodes) are selected where either the composition of streams included in the equivalent stream changes or the process of condensation/evaporation occurs. In the latter case, horizontal sections appear on the curves (Fig. 5). In these intervals, only the stream that changes the phase state is in contact. The slope of the cooling and heating intervals is $\frac{1}{\sum_k W_k}$, where k are indices of streams included in the equivalent stream at the current heat load. Thus, approaching the final total value $\overline{Q}$ the slope of the dependence $T_+(Q)$ in the cooling intervals is always negative. There will be vertical jumps on the $T_-(Q)$ curve if the stream temperature is $T_j^{in} > \bar{T}_{j-1}$, which means that there is a temperature gap in the equivalent stream.

The temperature dependencies of the equivalent streams on the current heat load determine the entropy production in the full system. It is equal to

$$\sigma(q) = \int_0^q \left(\frac{1}{T_-(q)} - \frac{1}{T_+(q)} \right) dq.$$

For optimal heat transfer, the heat capacity rate of the equivalent streams can vary, but always such that their ratio remains constant and inversely proportional to the ratio of the absolute temperatures of the contacting streams. This ratio is determined by the heat load and the heat transfer coefficient in accordance with expressions (2) and (3). The dependence of their temperatures on the heat load, Q, given by the hot streams to reach the current temperature, is piecewise linear.

In real systems, the input and output temperatures of part of the streams are given, as well as their heat capacities and evaporation and condensation temperatures. Therefore, the optimal dependence cannot be implemented. In the proposed method of synthesis of the implemented heat exchange system, the temperature dependence of equivalent streams on the current heat load is close to the case of the optimal countercurrent heat transfer, which means that the irreversibility of the system approaches its lower limit.

7 Calculation of the heat exchange rate for each homogeneity interval – the “model” heat exchangers

The interval δQ_ν from one of the nodes on any of the contact curves to the nearest node on the same or another curve is characterized by the same composition and phase states of the contact streams. Let us call it the *homogeneity interval*.

We now change our focus from the abstract contact temperatures of equivalent streams (the “model” heat exchangers) to the real physical system of heat exchangers. Implementing these temperature relations requires that we

1. select pairs of contacting streams,
2. select the type of fluid dynamics of each stream, and
3. calculate the heat transfer coefficient for each contact.

We will make this transition in two steps. *First*, we will determine the fluid dynamics governing each stream and calculate the heat transfer coefficients in the “model” heat exchangers in which the equivalent streams are in contact. There is only one such “model” heat exchanger in each homogeneity interval. This step allows us to select the hydrodynamic mode and find the heat transfer coefficient for each homogeneity interval.

Second, we break each "model" heat exchanger into separate real heat exchangers connected in parallel in such a way that the properties of this connection are the same as those of the single "model" heat exchanger. This implies distributing the "model" heat transfer coefficient in such a way that the change in temperature for all real contacting streams will equal the value for the equivalent stream. These dependencies in turn determine the production of entropy.

For each such interval δQ_ν three combinations of contacting streams are possible:
1. Both equivalent streams change their phase states.
2. The hot equivalent stream is cooled and the cold stream is heated.
3. One of the streams changes its phase state, while the other cools down or heats up.

The contact temperature curves provide all the data to calculate the heat exchange rate of the unit in which the contact is made. Indeed:
– heat capacity rates W_+, W_- are equal to the sum of heat capacity rates of streams which are part of the equivalent contact streams;
– temperatures of equivalent streams at the inlet and outlet of the homogeneity interval are known;
– the heat load of this calculated unit is δQ_ν.

Depending on which of the listed combinations of the contact is implemented, we can choose the type of hydrodynamics of the unit and find K_ν from (10) when both streams change their phase state, from (13) and (15) when the phase state changes in one of the equivalent streams, and, finally, from (16) and (17) when neither stream changes its phase state. The heat exchange rate when one stream condenses or evaporates and the other is in mixing mode is greater than when the second stream is in displacement mode, so this heat exchange rate value is used only when the mixing mode is dictated by technological considerations. Thus, we let the heat transfer requirements determine the types of heat exchangers. Prices and sizes of the equipment are not considered here.

Having found the heat exchange rate K_ν for each of the ν homogeneity intervals and having summed up these rates on all intervals, we end up with the total heat exchange rate K, which can be found by organizing counter-current heat exchange of equivalent streams. In turn, knowing the total heat exchange rate $\overline{Q}$ allows us to calculate the least possible entropy production σ^* with (3) and evaluate the degree of thermodynamic perfection of the constructed system as $\eta = \frac{\sigma^*}{\sigma^0}$, where σ^0 is found from (8).

8 On the physical implementation of the calculated system

In "model" heat exchangers equivalent streams are in contact. Real streams have the same temperatures as the equivalent ones. Only one hot or one cold stream can involve a phase transition on any homogeneity interval. Thus, a real heat exchanger with both streams changing their states is a condenser-vaporizer with two streams in contact. When one of the streams (let us take the hot one) changes its state, the "model" heat exchanger can be split into several two-stream heat exchangers in which the part of the hot stream proportional to the heat capacity rate of the cold one condenses. The latter satisfies the displacement condition. The heat transfer coefficient K needs to be distributed between these heat exchangers also proportionally to the heat capacity rate of the cold stream. This set of two-stream heat exchangers has the same characteristics as the "model" one.

In the case when no stream changes its state, the "model" heat exchanger implements the optimal displacement with counter-current streams and corresponding heat capacities W_+ and W_-. Such heat exchanger can be implemented as the parallel connection of heat exchangers with the same fluid dynamics. The number of these heat exchangers is equal to the number of cold streams. If the cold stream has the heat capacity rate W_{j-}, then there must be a hot stream in the corresponding heat exchanger with the heat capacity rate $W_{i+} = W_{j-}\frac{W_+}{W_-}$.

Because all the hot streams have the same temperature on the left-hand side of a homogeneity interval, every heat exchanger must include a stream with such a heat capacity rate that the total heat capacity rate will be equal to W_+. The heat transfer coefficient in this case is $K_{ij} = K_v \frac{W_j}{W_-}$. The set of such two-stream heat exchangers implements the "model" one for the corresponding homogeneity interval.

In pseudocode the heat exchanger synthesis algorithm has the following steps, as also illustrated by the examples in the next section:

1. Calculate all flows based on the source data table.
2. Order the hot streams according to their inlet temperatures and the cold streams according to their outlet temperatures.
3. Transition to equivalent flows.
4. Calculate each equivalent flow dependence on its temperature, heat capacity rate, and current heat load.
5. Determine the boundaries of the intervals of homogeneity.
6. Determine the hydrodynamic regime and calculate the heat transfer coefficients for the dual-flow "model" heat exchangers for each interval of homogeneity.
7. Calculate the total heat transfer coefficient.
8. Calculate the actual and minimally possible entropy production and, based on them, the coefficient of thermodynamic perfection of the system.
9. Turn to a physically feasible heat exchanger system.

The following examples clarify this algorithm.

9 Examples

Example 1 (Quadruple-flow heat exchanger). Let us consider a system with two hot and two cold streams. Source data are presented in Table 1.

Table 1: Source data for the two heating streams of Fig. 4 (vertical).

No.	T_{i+}^{in} K	W_i W/K	T_{j-}^{in} K	T_{j-}^{out} K	W_j W/K	q_j W
1	460	100	350	400	200	10000
2	360	150	300	340	150	6000

Since all flows do not change their phase state, the table of estimated flows will be similar.

1. The *required heat* is

$$q_- = \bar{q} = W_{1-}(T_{1-}^{out} - T_{1-}^{in}) + W_{2-}(T_{2-}^{out} - T_{2-}^{in}) = 200 \cdot 50 + 150 \cdot 40 = 16000\,\text{W}.$$

2. The *outlet temperature of hot streams*, according to expression (2), is

$$T_+^{out} = \frac{100 \cdot 460 + 150 \cdot 360 - 16000}{100 + 150} = 336\,\text{K}. \tag{21}$$

3. The *entropy production* in a system with no streams that change their phase state is (see eq. (8))

$$\begin{aligned}\sigma^0 &= \sum_i W_{i+}(\ln T_+^{out} - \ln T_{i+}^{in}) + \sum_j W_{j-}(\ln T_{j-}^{out} - \ln T_{j-}^{in}) \\ &= 100 \ln \frac{336}{460} + 150 \ln \frac{336}{360} + 200 \ln \frac{400}{350} + 150 \ln \frac{340}{300} = 3.76\,\text{W/K}\end{aligned} \tag{22}$$

4. Next, we consider the *calculation of the nodes and intervals of homogeneity on the curves of temperatures of equivalent streams*.

Consider the value $T_+(0) = T_{1+}^{in} = 460\,K$. The closest node on this curve is temperature T_{2+}^{in}, equal to 360 K, and the amount of corresponding heat transferred with the first hot stream (only this stream is involved in heat exchange) is $Q = Q_1 = W_1(460 - 360)100 \cdot 100 = 10000\,W$. The final value of temperature $T_+^{out}(\overline{Q})$ in accordance with eq. (21) is 336 K. After the first node both hot streams are involved in heat exchange with total heat capacity rate $W_{2+} = 100 + 150 = 250\,W/K$.

The initial value of the curve $T_-(0) = T_{1-}^{out}$. The closest node corresponds to the highest temperature between T_{1-}^{in} and T_{2-}^{out}. In our example this temperature is $T_{1-}^{in} = 350\,K$. The corresponding value of heat load is $Q_2 = W_{1-}(T_{1-}^{out} - T_{1-}^{in}) = 200 \cdot 50 = 10000\,W$. After this point the first cold stream is not involved in the heat exchange anymore. The curve $T_-(Q)$ jumps vertically to 340 K.

The next node is the temperature $T_{2-}^{out} = 340\,K$. In the interval from $q = 10000\,W$ to $q = 16000\,W$ only the second cold stream is involved in the heat exchange.

The dependencies $T_+(Q)$, $T_-(Q)$ are shown in Fig. 3.

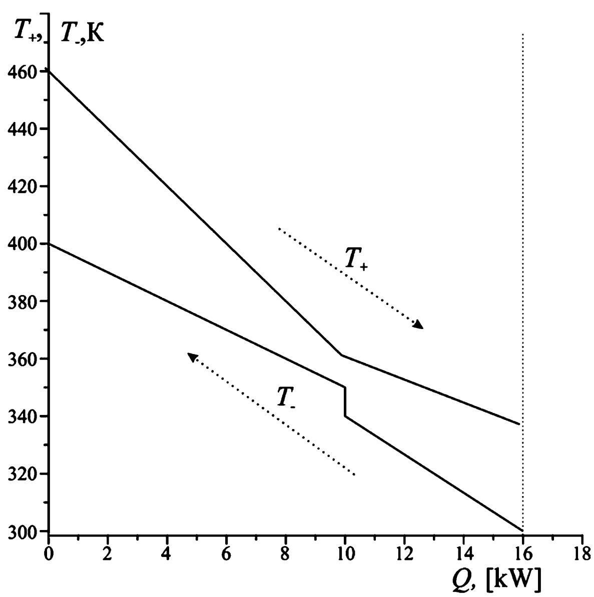

Figure 3: Combined heating temperature $T_+(Q)$ and cooling temperature $T_-(Q)$ for the non-condensing heat exchanger setup of Fig. 4 versus heat load Q. The vertical discontinuity of T_-^{out} indicates no heat requirement in that temperature interval. The dotted arrows imply that the cold (–) flow gets heated while the hot (+) flow gets cooled during the process.

Thus, we can distinguish two homogeneity intervals on the horizontal axis: from 0 to $Q = 10000\,W$ and from $Q = 10000\,W$ to $Q = 16000\,W$. The first hot and the first cold streams contact each other in the first interval, while the second streams contact each other in the second interval. A possible heat exchange structure is shown in Fig. 4.

5. Let us find the *heat exchange rates for each homogeneity interval* under the assumption of counter-current heat exchange based on (16) and (17).
For the first interval,

$$A = \frac{200 - 100}{100 \cdot 200} = 0,005, \quad K_1 = 200 \ln \frac{460 - 400}{360 - 350} = 358\,W/K.$$

For the second interval,

$$A = \frac{150 - 250}{150 \cdot 250} = -\frac{1}{375}, \quad K_2 = -375 \ln \frac{360 - 340}{336 - 300} = 220\,W/K.$$

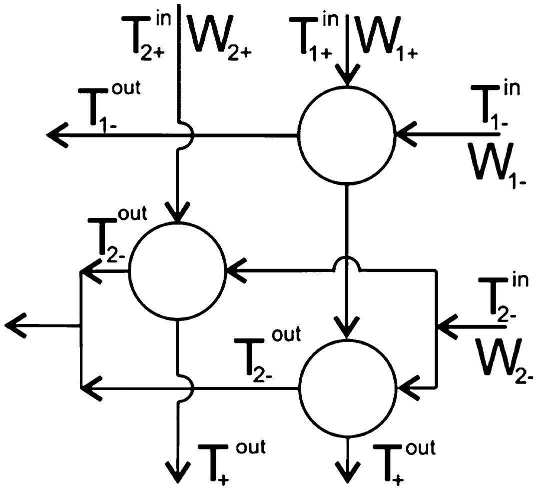

Figure 4: The heat exchange system structure without condensation offering optimal operation, i. e., with least possible entropy production.

6. Knowing the total heat exchange rate $K = K_1 + K_2 = 578$ W/K allows us to calculate the *least possible entropy production* σ^* with eq. (3) and evaluate the degree of thermodynamic perfection of the constructed system. We have

$$m = 1 - \frac{1}{578}\left(100 \ln \frac{460}{336} + 150 \ln \frac{360}{336}\right) = 0.928,$$
$$\sigma^* = 578 \frac{(1 - 0.928)^2}{0.928} = 3.22, \quad \eta = \frac{3.22}{3.76} = 0.86.$$

The system consists of three counter-current units. The first hot stream goes through two units in succession, and the second only goes through the third. The second cold stream is branched between the second and the third units so that the relationships of heat capacity rates of hot and cold streams in each of these units stay the same such that

$$W_{21} = W_{2-} \frac{W_{1+}}{W_{1+} + W_{2+}} = 150 \frac{100}{100 + 150} = 60 \text{ W/K}, \tag{23}$$
$$W_{22} = W_{2-} \frac{W_{2+}}{W_{1+} + W_{2+}} = 150 \frac{150}{100 + 150} = 90 \text{ W/K}.$$

Each unit has its own counter-current heat exchanger.

Example 2 (Quadruple-flow heat exchanger with condensation). Let us consider the system from Example 1 with one modification, i. e., the first hot stream enters the system in the form of saturated vapor at the temperature of condensation, and with the following parameters:

$$T_{1+}^{in} = 460 \text{ K}, \quad r_{1+} = 833 \text{ kJ/g}, \quad g_{1+} = 0.012 \text{ kg/s}, \quad W_{1+} = 36.2 \text{ W/K}.$$

Since one stream condenses in the heat exchange process, estimated hot streams will be as shown in Table 2.

Table 2: Estimated optimal cooling streams of Fig. 4 (horizontal).

No.	T_{j+}^{in}, K	W, W/K	g_{i+}, kg/s	r_{i+}, kJ/kg
1	460	–	0.012	833
2	460	36.2	–	–
3	360	150	–	–

Calculations will be carried out in the same sequence as in Example 1.

1. The *required heat* is

$$Q_- = \overline{Q} = W_{1-}(T_{1-}^{\text{out}} - T_{1-}^{\text{in}}) + W_{2-}(T_{2-}^{\text{out}} - T_{2-}^{\text{in}}) = 200 \cdot 50 + 150 \cdot 40 = 16000\,\text{W}.$$

2. The *outlet temperature of hot streams*, according to expression (2), is

$$T_+^{\text{out}} = -\frac{833 \cdot 12 + 36.2 \cdot 460 + 150 \cdot 360 - 16000}{36.2 + 150} = 347.6\,\text{K}. \tag{24}$$

3. The *entropy production* in a system considering the condensing stream (see eq. (8)) is

$$\begin{aligned}\sigma^0 &= -\frac{g_1 r_1}{T_{1+}^{\text{in}}} + \sum_i W_{i+}(\ln T_+^{\text{out}} - \ln T_{i+}^{\text{in}}) + \sum_j W_{j-}(\ln T_{j-}^{\text{out}} - \ln T_{j-}^{\text{in}}) \\ &= -\frac{10000}{460} + 36.2 \ln \frac{347.6}{460} + 150 \ln \frac{347.6}{360} + 200 \ln \frac{400}{350} + 150 \ln \frac{340}{300} = 8.04\,\text{W/K}. \end{aligned} \tag{25}$$

4. Next, we consider the *calculation of the nodes and intervals of homogeneity on the curves of temperatures of equivalent streams*.

Consider the value $T_+(0) = T_{1+}^{\text{in}} = 460$ K. The closest node on this curve corresponds to the end of a horizontal condensation interval, and the associated point on the horizontal axis is 10000 W. Only the condensing stream and the first cold stream are involved in the heat exchange.

In the next interval, the condensate with heat capacity rate $W_{1+} = 36.2$ contacts the cold stream until the condensate temperature drops to 360 K. At the same time, it transfers heat equal to $\delta Q = 3620$ W, heating the cold stream 24.1 K, from 315.9 to 340 K.

In the last interval, hot streams are combined, so that their total heat capacity rate is equal to $W_+ = 36.2 + 150 = 186.2$ W/K. They are cooled to $T_+^{\text{out}} = 347.6$ K while heating the cold stream from 300 to 315.9 K.

The initial value of the curve $T_-(0) = T_{1-}^{\text{out}}$. The closest node corresponds to the starting temperature of one of the cold streams, 350 K. At $q = 10000$ the cold stream contact temperature is reduced to 340 K and then the second cold stream contacts in the second interval one, and in the last interval, the third one, two hot streams. Its heat capacity rates are in accordance with eq. (23), i. e.,

$$W_{21} = 150\frac{36.2}{186.2} = 29.2\,\text{W/K}, \quad W_{22} = 150\frac{150}{186.2} = 120.8\,\text{W/K}.$$

The dependencies $T_+(Q)$, $T_-(Q)$ are shown in Fig. 5. The structure of the heat exchange system is shown in Fig. 6. In the first heat exchanger the condensation mode for the hot stream and the displacement mode for the cold streams are implemented, while in the following units the displacement mode with counter-current flow is implemented throughout.

5. Let us find the *heat exchange rates for each of the homogeneity intervals* taking into account condensation at the first and counter-current heat exchange rates at the second and third intervals of homogeneity with Eqs. (15), (16), and (17).
   For the first interval,

$$K_1 = 200 \ln \frac{460 - 350}{460 - 350 - \frac{10000}{200}} = 121\,\text{W/K}.$$

   For the second interval,

$$A = \frac{150 - 36.2}{36.2 \cdot 150} = \frac{1}{48}, \quad K_2 = 48 \ln \frac{460 - 340}{360 - 315.9} = 48.05\,\text{W/K}.$$

   For the third interval,

$$A = \frac{150 - 186.2}{186.2 \cdot 150} = -\frac{1}{772}, \quad K_3 = -772 \ln \frac{360 - 315.9}{347.6 - 300} = 59\,\text{W/K}.$$

   The dependence on contacting temperatures of the heat load is shown in Fig. 5.

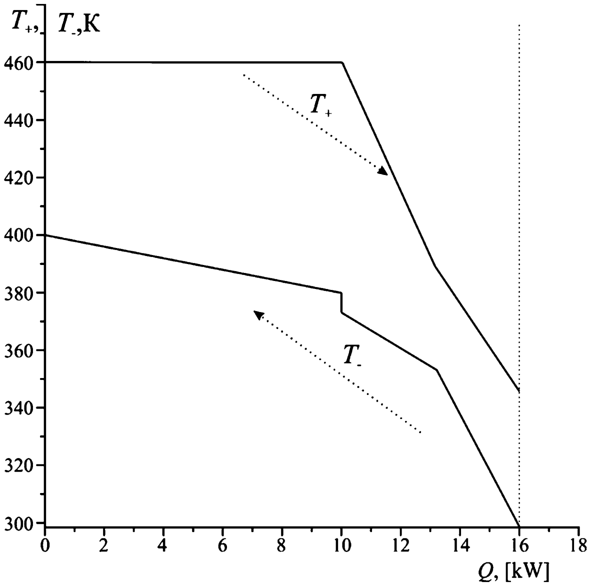

Figure 5: Combined heating temperature $T_+(Q)$ and cooling temperature $T_-(Q)$ for the condensing heat exchanger setup of Fig. 6 versus heat load Q. The horizontal section of T_+^{out} represents condensation while the vertical step of T_-^{out} indicates no heat requirement in that temperature interval. The dotted arrows imply that the cold (–) flow gets heated while the hot (+) flow gets cooled during the process.

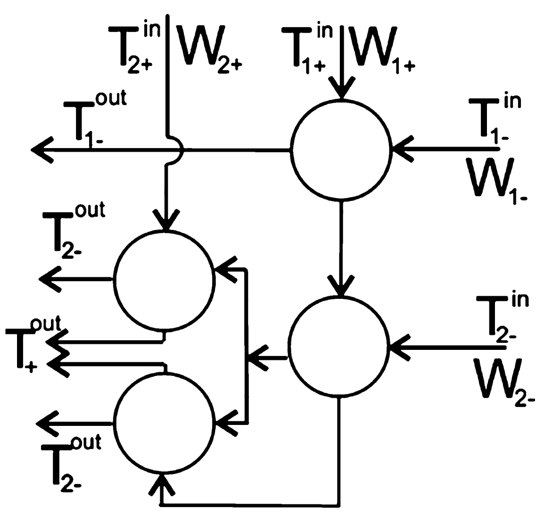

Figure 6: The heat exchange system structure with condensation of the hot stream offering optimal operation, i. e., with the least possible entropy production.

6. Knowing the total heat exchange rate $K = K_1+K_2+K_3 = 228$ W/K allows us to calculate the *least possible entropy production* σ^* with eq. (3) and evaluate the degree of thermodynamic perfection of the constructed system:

$$m = 1 - \frac{1}{228}\left(36.2\ln\frac{460}{347.6} + 150\ln\frac{360}{347.6} + \frac{12\cdot 833}{460}\right) = 0.84,$$

$$\sigma^* = 228\frac{(1-0.84)^2}{0.84} = 6.95, \quad \eta = \frac{6.95}{8.04} = 0.86.$$

10 Pinch analysis comparison

The aforementioned dependencies of temperatures of contacting streams on the current heat load are very close to the dependencies of temperatures of equivalent hot and cold streams on their enthalpy used in pinch analysis. The difference is not only the fact that all calculations in this work are based on the thermodynamic criterion of minimum dissipative losses (entropy production), but also that the external heating and cooling sources are not specified directly. This is because they are the additional streams equal to all other streams in the system, and they affect its optimal organization not only at the end temperatures but also at all intermediate temperatures. Thus, the additional heat stream in the form of vapor condenses and participates in the further heat exchange in accordance with the general algorithm.

The homogeneous intervals not only define which hot streams contact which cold streams at these temperatures, but also the hydrodynamics of counter-current heat exchangers, their heat transfer rates, and their heat capacity rates of streams during their splitting. Streams of different temperatures do not mix.

In many cases, the output temperatures of all or some hot streams are not identical (T_+). Therefore, by requiring the equality of these free temperatures obtained under the conditions of minimal dissipation, the temperatures of the hot streams suitable for the system achieve their lower limit.

The ratios we obtained in the works related to optimal heat exchange allow us to evaluate qualitatively the perfection of the synthesized system and draw up general guidelines that are recommended to follow during the synthesis:

1. The ratio of absolute temperatures of equivalent streams should be as constant as possible. This means that the minimal temperature difference (pitch zone) should be reached near the cold end of the heat exchange system.
2. The ratio of heat capacity rates of the hot and cold streams should be close to the inverse of the ratio of their temperatures in the homogeneity zone with no change in the phase states of any of the streams, i. e., W_- should be greater than W_+. In this case, the ratio of temperatures in a counter-current heat exchanger will be constant during the contact.

11 Conclusion

This paper proposes an algorithm for calculation of minimum irreversibility for heat exchange systems with constant temperatures, heat capacity rates of inlet streams, and given heat load. The algorithm leads to a solution in a finite number of steps. With this algorithm it is possible to find the structure and the distribution of heat loads and surfaces of the heat exchange between counter-current units in the given system. Each flow can contact multiple flows. The proposed algorithm can be considered to follow a thermodynamic rationale and as development of pinch analysis.

Identifiers

q heat flux density, W/K
Q heat flux, W
T temperature, K
g the refrigerant use rate, kg/s
σ entropy production, J/K
W heat capacity rate, W/K
K total heat exchange rate, W/K
s contact surface, m^2
r vaporization heat, J/kg
C specific heat capacity, J/kg K

References

[1] G. M. Ostrovskii, N. N. Ziyatdinov and I. I. Emel'yanov, Synthesis of optimal systems of simple distillation columns with heat recovery, *Dokl., Chem.* **461**, Part 1 (2015), 89–92.

[2] N. N. Ziyatdinov, G. M. Ostrovskii and I. I. Emel'yanov, Designing a heat exchange system upon the reconstruction and synthesis of optimal systems of distillation columns, *Theoretical Foundations of Chemical Engineering* **50** (2016), no. 2, 178–187.

[3] N. N. Ziyatdinov, I. I. Emel'yanov and Tuen Le Quang, Method for the synthesis of optimum multistage heat exchange systems, *Theor. Found. Chem. Eng.* **52** (2018), no. 6, 943–955. DOI: 10.1134/S0040579518060167.

[4] V. V. Kafarov, V. P. Meshalkin and V. L. Perov, Mathematical Foundations of Computer Aided Design of Chemical Plants, Ximiya, 1979.

[5] V. M. Brodjanskiy, V. Fratsher and K. Mikhalek, *Exergy Methods and Its Applications*, Energoatomizdat, Moscow, 1988.

[6] R. S. Berry, V. A. Kasakov, S. Sieniutycz, Z. Szwast and A. M. Tsirlin, *Thermodynamic Optimization of Finite Time Processes*, Wiley, Chichester, 1999.

[7] A. M. Tsirlin, W. A. Mironova, S. A. Amelkin and V. A. Kazakov, Finite-time thermodynamics: Conditions of minimal dissipation for thermodynamic processes with given rate, *Phys. Rev. E* **58** (1998).

[8] A. M. Tsirlin, Optimal control of the irreversible processes of heat and mass transfer, *Sov. J. Comput. Syst. Sci.* **2** (1991), 171–179.

[9] A. M. Tsirlin, V. Kazakov, A. A. Akhremenkov and N. A. Alimova, Thermodynamic constraints on temperature distribution in a stationary system with heat engine or refrigerator, *J. Phys. D, Appl. Phys.* **39** (2006), 4269–4277.

[10] B. Andresen and J. M. Gordon, Optimal heating and cooling strategies for heat exchangers design, *J. Appl. Phys.* **1** (1992), 71–78.

[11] P. Salamon, A. Nitzan, B. Andresen and R. S. Berry, Minimum entropy production and the optimization of heat engines, *Phys. Rev.* **21** (1980), 2115.

[12] B. Linnhoff, Pinch analysis – a state-of-the-art overview, *Trans I Chem E. Part A.* **71** (1993), no. 9. 503–522.

[13] B. Linnhoff and D. R. Vredeveld, Pinch technology has come of age, *Chem. Eng. Prog.*, **88**, (1984), no. 7, 33–40.

[14] A. M. Tsirlin, A. A. Akhremenkov and I. N. Grigorevskii, Minimum irreversibility and optimal distributions of heat transfer surface area and heat load in heat transfer systems, *Theor. Found. Chem. Eng.* **42** (2008), 203–210.

[15] A. M. Tsirlin, Ideal heat exchange systems, *J. Eng. Phys. Thermophys.*, **90** (2017), no. 5.