Heat and mass exchange and feasible mode sets of irreversible separation processes

Alexandr I. Balunov, Anatoliy M. Tsirlin *

Yaroslavl State Technical University, Yaroslavl, Russia
Program Systems Institute Russian Academy of Sciences, Pereslavl-Zalesskiy, Russia

ARTICLE INFO

ABSTRACT

The article deals with the separation systems' mean boundary from the perspectives of finite-time thermodynamics. We obtained the lower-bound estimates of the minimum energy input for the separation systems that have a specified separation. It is shown that these inputs do not tend toward zero while the concentration of one of the separated mixture's components tends to one. Separation systems using heat power have ultimate performance. The article provides examples of the obtained estimates' application.

© 2017 Elsevier Ltd. All rights reserved.

1. Introduction

Industry spends a significant part of the world's energy consumption on separation processes. Such processes are very diverse by the nature of the energy used and their design. The absorption-desorption and adsorption-desorption cycles, distillation, stripping, drying, etc. use heat energy (they are called thermal systems of separation); centrifuging, membrane separation use mechanical energy (such systems are called mechanical). Boshnyakovich noted that most non-production energy losses in the industry are associated with chemical and metallurgical processes [1]. For example, oil separation uses only about 6% of the energy contained in it.

The energy loss analysis in these industries is an important component of their exergy analysis (see [2]). The exergy approach allows identifying the losses caused by the irreversibility in an engineered or operating system. However, this approach says nothing about the limit, to which these losses can be reduced with account of the limited dimensions of the apparatuses and their performance. The minimum energy required to separate the mixture of a certain composition can be estimated by reversible thermodynamics methods.

However, such estimates are insufficiently precise and do not take into account kinetic factors (the regularities and coefficients of the heat and mass transfer, system performance, etc.).

The purpose of the article is to obtain a lower-bound estimate for the separation work, which would take into account the listed

factors and to identify the difference between the shape of the boundary between the feasible modes for the separation systems that use mechanical and heat power.

We keep to the general finite-time thermodynamics methodology in this article (see [3–18]). The sequence of such tasks' solution comprises two stages:

– finding the minimum possible entropy production σ_{min} as a function of the flux intensity at specified limits (for the surfaces of the heat and mass transfer, for the intensity of certain fluxes, etc.);
– expressing the sought estimates through the entropy production or increase using equations of the thermodynamic balances by substance, energy, and entropy.

Thermodynamic balances of separation systems using mechanical and heat energy (mechanical and heat systems) are different.

In the first case, the flux of the energy used is not associated with the entropy flux and is not part of the entropy balance. Usually, processes in mechanical systems can be treated as isothermal. In the second case, the energy flux is supplied to the system at one temperature and removed from it at a different temperature and is conjugated with the entropy supply and removal. The irreversible estimates obtained below differ from the reversible ones not only by quantity, but also by quality. For example, for lean mixtures, in which the concentration of one of the components is close to 1, the irreversible estimate unlike the reversible one tends to a finite margin dependent on kinetic coefficients, but not to zero. This fact is confirmed in real apparatuses, in which the actual energy input is hundreds of thousands of times higher than their reversible estimates [19].

* Corresponding author.
    E-mail addresses: balunovai@ystu.ru (A.I. Balunov), tsirlin@sarc.botik.ru (A.M. Tsirlin).

For thermal separation processes, the accounting the irreversibility factors allows not only obtaining an estimate for the minimum heat input, but also finding the thermodynamic margin of the process rate, which it cannot exceed at any heat input. The dependence of the maximum systems performance on the energy input or minimum energy input on the performance is the thermodynamic boundary of the feasible process mode set (the feasible set).

The article deals with building a feasible set boundary for mechanical separation systems in the first part, and for thermal ones in the second part.

2. The feasible set of mechanical separation systems

Assumptions and task statement. Consider an initially reversible isothermal separation process and assume that the mixture and its components' properties are close to those of ideal gases or ideal solutions, so the chemical potential of the ith component can formulated as:

$$\mu_i(T, P, C_i) = \mu_{0i}(T, P) + RT \ln C_i, \quad i = 1, \dots, n, \quad (1)$$

where C_i – is the i-th component concentration, R – universal gas constant, T and P – are the temperature and pressure in the system. Ideal solutions differ from ideal gases by the form of $\mu_{0i}(T, P)$ in expression (1).

Let's assume that the temperature and pressure in the system before and after the separation process have not changed and the system is adiabatically isolated (the heat is neither supplied nor removed). The separation work in such a system at as low process rate as can be is equal to the change in its Gibbs energy, i.e. for one mole of the mixture to the aggregate increment of the chemical potentials [1]. This work can be expressed through the initial concentration vector $\mathbf{C_0} = (C_{01}, \dots, C_{0i}, \dots, C_{0n})$ and the mixture concentration vectors in m separation products $\mathbf{C_j} = (C_{j1}, \dots, C_{ji}, \dots, C_{jn})$, $(j = 1, \dots, m)$.

Under mixture separation on two products the energy change is equal to:

$$\Delta A_0 = \sum_{i=1}^{n} \left[\gamma C_{1i} \mu_i(T, P, C_{1i}) + (1 - \gamma) C_{2i} \mu_i(T, P, C_{2i}) - C_{0i} \mu_i(T, P, C_{0i}) \right]. \quad (2)$$

In this case, the share of the mixture supplied to the first product be denoted through γ, and to the second one through $(1 - \gamma)$.

If we substitute expressions for chemical potentials in (2) and take into account that for any component the mass balance conditions are true:

$$\gamma C_{1i} + (1 - \gamma) C_{2i} = C_{0i}, \quad i = 1, \dots, n, \quad (3)$$

then terms μ_{0i} will be reduced and expression (2) will be formulated as follows:

$$\Delta A_0 = RT \sum_{i=1}^{n} [\gamma C_{1i} \ln C_{1i} + (1 - \gamma) C_{2i} \ln C_{2i} - C_{0i} \ln C_{0i}]. \quad (4)$$

Separating the mixture into n rather than two parts results in a similar expression. In case of complete separation, when one component is taken to each product, its share $\gamma_i = C_{0i}$, concentration $C_{ii} = 1$ by formula (4) we obtain the work of mixture separation into pure components in a reversible process:

$$A_0 = -RT \sum_{i=1}^{n} C_{0i} \ln C_{0i}. \quad (5)$$

From comparison (4), (5) it follows that the reversible work of incomplete separation is equal to the difference between the reversible work of the source mixture separation and the mean reversible work of the mixture separation with weights γ and $(1 - \gamma)$ in products 1 and 2:

$$\Delta A_0 = A_0 - \gamma A_{01} - (1 - \gamma) A_{02}. \quad (6)$$

The energy inputs for the separation, found by this method, are the lower-bound estimate of the actual inputs. At the separation of a two-component (binary) mixture, this estimate depends on the $\mathbf{C_0}$ concentration of one of them in the source mixture as is shown in Fig. 1 (curve A_0).

However estimates obtained do not take into account kinetic factors. They depend only on the mixture composition before and after the separation. At the same time, taking these factors into account results in the irreversibility of the processes, and, subsequently, to a rise in the energy input.

The separation work in an isothermal process for an adiabatically isolated system can be expressed by the Stodola's formula [1] through reversible work A_0 and the system's entropy increment ΔS, as:

$$A_r = A_0 + T\Delta S = A_0 + \delta A, \quad (7)$$

where T is the ambient temperature in K.

To estimate the energy input in the separation, we need to find the minimum entropy increment at the given process duration, heat and mass exchange coefficients, and use formula (7).

Consider the calculation diagram (Fig. 2) consisting of a container with the source mixture, m subsystems, where the fluxes are directed to after being separated, and the apparatus, which performs the separation process (hereinafter referred to as the "working body").

The working body receives energy from outside and creates the substance fluxes. Assume that the source mixture composition $\mathbf{C_0}$ and the mixture composition in every j-th subsystem $\mathbf{C_j}$, the total quantity of moles N_0, subject to separation, and the quantity of moles N_j, supplied to each subsystem, as well as the process duration τ are given and meet the mass balance conditions (3). The driving force creating the substance fluxes is the chemical potential difference between the working body and the source mixture container and between the subsystems and working body. In an isothermal process, the chemical potential value can be controlled by changing the pressure.
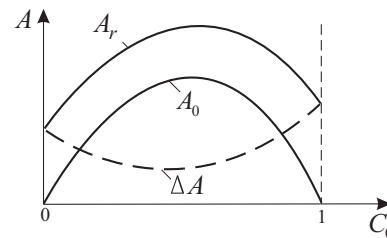

Fig. 1. The dependence of the reversible A_0 and irreversible A_r estimates of the minimum work of a binary system separation on the concentration of one of the components.
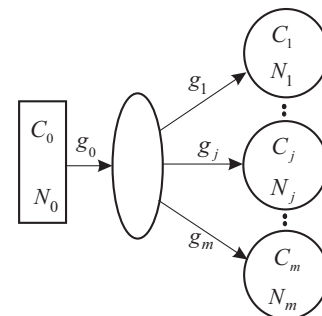

Fig. 2. The diagram of the mixture separation into m subsystems.