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Finite time thermodynamic optimization for heat-driven binary separation processes

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ABSTRACT

The performance of heat-driven binary separation processes with linear phenomenological heat transfer law ($q \propto \Delta(T^{-1})$) is optimized by using finite time thermodynamics. Two performance indexes, the dimensionless minimum average entropy production rate and dimensionless minimum average heat consumption of the heat-driven binary separation processes, are taken as optimization objectives, respectively. The separation processes are viewed as heat engines which work between high- and low-temperature reservoirs and produce enthalpy and energy flows out of the system. The temperatures of the heat reservoirs are assumed to be time- and space-variables. The convex optimization problem is solved using numerical method, and the average optimal control problem is solved using Lagrangian function. The major influence factors on the performance of the separation process, such as the properties of different materials and various separation requirements for the separation process, are represented by dimensionless entropy production rate coefficient and dimensionless enthalpy flow rate coefficient. The dimensionless minimum average entropy production rate and dimensionless minimum average heat consumption of the heat-driven binary separation processes are obtained, respectively.

Keywords: Linear phenomenological heat transfer law; Heat-driven separation; Binary separation process; Heat consumption; Entropy production rate; Finite time thermodynamics
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1. Introduction

Separation process is one of traditional industry fields with high energy consumption. The thermodynamic study of separation process is of great importance because of world-wide overdevelopment and shortage of energy. Some thermodynamic studies have focused on the problem of decreasing the energy consumption for separation process by using thermodynamic theory, especially heat-driven separation processes.

The performance bounds of heat engines, heat pumps, and refrigerators have been studied with the development of finite time thermodynamics [1–9]. Among them, the limits on the average power output of heat engines are well known [10, 11]. The efficiency

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of a heat engine at the maximum power point is lower than or equal to $1 - \sqrt{T_L/T_H}$, where T_H and T_L ($T_H > T_L$) are the temperatures of high- and low-temperature heat reservoirs. The efficiency is less than the classical reversible limit $1 - T_L/T_H$ because of the finite rate of the process with fixed nonzero average power output. The result is also suitable for separation process. Many heat-driven separation processes can be analyzed by taking them as heat engines which work between high-temperature heat reservoir T_H and low-temperature heat reservoir T_L and produce enthalpy and energy flows out of the system (instead of power output of the conventional heat engines). For separation process, there exists an upper bound on the average enthalpy flow rate of the system for fixed entropy flow rate, or there exists a lower bound on the average entropy flow rate of the system for fixed average enthalpy flow rate. It implies that there exists an upper bound on the average feed flow rate when proper assumptions on input and output are made.

Finite time thermodynamics has been a powerful tool for researching the performance of separation processes [12]. Mullins and Berry [13] studied the minimum average entropy production of perfect separation process and imperfect separation processes. The optimal locations of intermediate heat exchangers that reduce entropy production are found. Brown et al. [14] optimized the performance of a porous plug separation system by taking ''turnpike'' (i.e., boundary-singular-boundary branch) trajectory. The minimum work required to move the plug from one equilibrium position to another in a given time period was optimized. And the lower bound for the separation work of gases by diffusion was obtained. Kazakov and Berry [15] calculated the upper bound on average productivity and efficiency and the low bounds on entropy production of an irreversible cyclic separation process with space-variable temperature and chemical-potential reservoirs via the generalized formalism of finite time thermodynamics. Tsirlin et al. [16] derived the new thermodynamic limits on the performance of irreversible separation processes, including work of separation in finite time (a generalization of Van't Hoff reversible work of separation for finite rate processes), maximum productivity of heat-driven binary separation process, the minimum average dissipation and the ideal operating line in an irreversible distillation column. The minimum dissipation level and the distillation column's maximum productivity are achieved by realizing the ideal operating line for the profiles of heat supply/removal. The total entropy production of a fully diabatic distillation column was minimized by Schaller et al. [17]. The entropy production counts the interior losses due to heat and mass flow as well as the entropy generated in the heat exchangers. The results show that a column design with consecutive interior heat exchanger and only one exterior supply for each of the two sections (stripping section and rectifying section) is appealing. Koeijer et al. [18,19] improved the model for minimization of entropy production rate in diabatic tray distillation. Equal thermal driving force distribution rule, linear with steam flow rate distribution rule, equal area distribution rule, and equal entropy production rate distribution rule for heat transfer area were studied. They found that heat exchangers had a significant effect on the entropy production rate and the minimum entropy production rate was obtained when the heat exchangers were distributed with equal thermal driving force. Jimenez et al. [20] carried out improvement on the model of the diabatic distillation column. The diabatic distillation column with fully controllable heat exchangers took place by diabatic distillation column with sequential heat exchangers. The exergy loss of diabatic distillation was significantly reduced by sequential heat exchangers. Shu et al. [21] improved the diabatic distillation model and researched the optimal allocation of the heat exchanger inventory for the sequential heat exchangers in the diabatic distillation column. The optimal allocation of the heat exchanger inventory for the sequential heat exchangers was obtained and the optimal performance of the diabatic distillation column was achieved.

Orlov and Berry's work [22] has been one of the representative studies on heat-driven separation processes by using finite time thermodynamic theory. The separation process was assumed to be weakly periodic, and simplified as a heat engine that works between high- and low-temperature heat reservoirs and produces enthalpy and energy flows out of the system (instead of power output of conventional heat engines). The analytical expressions of minimum average heat consumption and minimum average entropy production rate for the process with fixed average enthalpy flows and average entropy flows out of the system were obtained. The minimum average heat consumption problem for heat-driven separation process with time-variable feed flow, time- and space-variable temperature heat reservoirs was transformed to a convex optimization problem and was solved with numerical method.

Heat transfer law has effects on the performance of various processes and devices [23–31]. Therefore, the optimal performance of heat-driven binary separation process with linear phenomenological heat transfer law ($q \propto \Delta(T^{-1})$) is studied in this paper based on Ref. [22] by using finite time thermodynamics. Two performance indexes, the dimensionless minimum average entropy production rate and dimensionless minimum

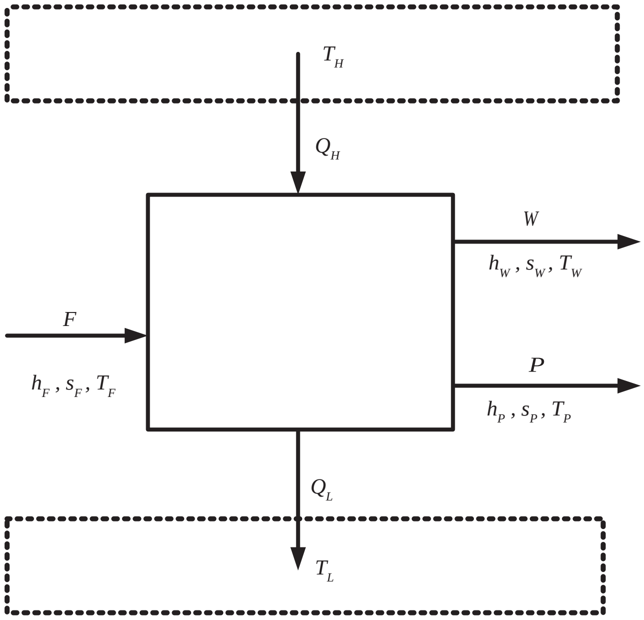

Fig. 1. Schematic diagram of a heat-driven binary separation process.

average heat consumption of the heat-driven binary separation processes, are taken as optimization objectives, respectively. The temperatures of the heat reservoirs are assumed to be time- and space-variables. The convex optimization problem is solved by numerical method and the average optimal control problem is solved by using Lagrangian function. The dimensionless entropy production rate coefficient and dimensionless enthalpy flow rate coefficient are adopted to indicate the major influence factors on the performance of the separation process, such as the properties of different materials and various separation requirements for the separation process. The analytical expressions and the numerical examples for the dimensionless minimum average entropy production rate and dimensionless minimum average heat consumption of the heat-driven binary separation processes are obtained, respectively.

2. Physical model

A binary heat-driven separation process is shown in Fig. 1. The heat transfer in the separation system obeys linear phenomenological heat transfer law ($q \propto \Delta(T^{-1})$). The flow rates of feed, product, and waste are F, P, and W, respectively. The mass balance equation of the binary separation process is

$$\frac{\mathrm{d}N}{\mathrm{d}t} = F - P - W, \frac{\mathrm{d}N_x}{\mathrm{d}t} = x_F F - x_P P - x_W W, \quad (1)$$

where N and N_x are the total mole numbers of the mass and the volatile mass in the system, x_F, x_P, and x_W are the volatile mass molar fractions in the feed, separation output, and the waste, respectively. The major assumptions made in this paper are:

(1) The changes of potential energy and kinetic energy of flows are neglected;
(2) The separation process under consideration is a binary one;
(3) The molar fractions x_F, x_P, and x_W, enthalpies h_F, h_P, and h_W, and entropies s_F, s_P, and s_W are stationary (independent of time);
(4) The process is weakly periodic in material, energy, and entropy, that is, $N(0) = N(\tau)$, $E(0) = E(\tau)$, $S(0) = S(\tau)$, where time τ is the period of the process.

Then, one can obtain the following equations:

$$\bar{P} = \bar{F}\ (x_F - x_W)/(x_P - x_W), \quad (2)$$

$$\bar{W} = \bar{F}\ (x_P - x_F)/(x_P - x_W), \quad (3)$$

where $\bar{F}$, $\bar{P}$, and $\bar{W}$ are the average molar flow rates of feed, product, and waste, respectively. The energy balance for the heat-driven binary separation process with linear phenomenological heat transfer law is

$$\frac{\mathrm{d}E}{\mathrm{d}t} = Fh_F - Ph_P - Wh_W + \int_{A_H(t)} \alpha_H \left(\frac{1}{T} - \frac{1}{T_{\mathrm{H}}}\right) \mathrm{d}a - \int_{A_L(t)} \alpha_L \left(\frac{1}{T_{\mathrm{L}}} - \frac{1}{T}\right) \mathrm{d}a, \quad (4)$$

where $E(t)$ is the total energy of the separation process, h_F, h_P, and h_W are the molar enthalpies of feed, product, and waste, respectively. $\alpha_H = \alpha_H(\xi)$ is the heat transfer coefficient between the process and the high-temperature heat reservoir, and $\alpha_L = \alpha_L(\xi)$ is the heat transfer coefficient between the process and the low-temperature heat reservoir. $T(t,\xi)$, $T_H(t,\xi)$ and $T_L(t,\xi)$ are the temperatures of the system, high-temperature heat reservoir, and low-temperature heat reservoir. $A_H(t)$ and $A_L(t)$ are the surface between the process and the high-temperature heat reservoir, and the surface between the process and the low-temperature heat reservoir, and $\xi = (\xi_1, \xi_2, \xi_3)$ is a vector of coordinates of a point in the Cartesian system. Integration in Eq. (4) is carried out over the area of the surfaces A_H and A_L.

The entropy balance of the system is as follows

$$\frac{\mathrm{d}S}{\mathrm{d}t} = Fs_F - Ps_P - Ws_W + \int_{A_H(t)} \frac{\alpha_H \left(\frac{1}{T} - \frac{1}{T_H}\right)}{T} \mathrm{d}a - \int_{A_L(t)} \frac{\alpha_L \left(\frac{1}{T_L} - \frac{1}{T}\right)}{T} \mathrm{d}a + \sigma(t), \quad (5)$$

where $S(t)$ is the total entropy production of the system, and $\sigma(t) \geq 0$ is the total entropy production rate inside the system. The separation process is not specified in this paper. They may be distillation, thermal diffusion, absorption, or something else. The most important thing is that $\sigma(t) \geq 0$ holds for any specific separation process.

The period of the process is τ. Let us now calculate the classical reversible minimum average heat assumption amount per cycle Q_H^{rev}. Temperatures T_H and T_L are considered as constants in the calculation. Let

$$\bar{f} = \frac{1}{\tau}\int_0^\tau f(t)\mathrm{d}t, \tag{6}$$

$$f_h(t) = Ph_P + Wh_W - Fh_F, \tag{7}$$

$$f_s(t) = Ps_P + Ws_W - Fs_F, \tag{8}$$

where $f_h(t)$ and $f_s(t)$ are the molar flow rates of enthalpy and entropy. From Eq. (6), one can obtain

$$\bar{f}_h = r_h\bar{F}, \quad \bar{f}_s = r_s\bar{F}, \tag{9}$$

where

$$\begin{aligned} r_h &= h_P(x_F - x_W)/(x_P - x_W) \\ &\quad + h_W(x_P - x_F)/(x_P - x_W) - h_F, \\ r_s &= s_P(x_F - x_W)/(x_P - x_W) \\ &\quad + s_W(x_P - x_F)/(x_P - x_W) - s_F \end{aligned} \tag{10}$$

According to Eq. (4), the average enthalpy flow rate for a weakly periodic process can be written as follows

$$Q_H - Q_L = \bar{f}_h, \tag{11}$$

where $Q_H = \frac{1}{\tau}\int_0^\tau\int_{A_H(t)}\alpha_H\left(\frac{1}{T} - \frac{1}{T_H}\right)\mathrm{d}a\ \mathrm{d}t$ is the average heat flow rate from high-temperature heat reservoir to the system, and $Q_L = \frac{1}{\tau}\int_0^\tau\int_{A_L(t)}\alpha_H\left(\frac{1}{T_L} - \frac{1}{T}\right)\mathrm{d}a\ \mathrm{d}t$ is the average heat flow rate from the system to the low-temperature heat reservoir. From Eq. (5), one can obtain

$$\frac{Q_H}{T_H} - \frac{Q_L}{T_L} = \bar{f}_s + \delta, \tag{12}$$

where

$$\begin{aligned} \delta = -\frac{1}{\tau}\int_0^\tau\Bigg\{\sigma(t) &+ \int_{A_H(t)}\alpha_H\left(\frac{1}{T} - \frac{1}{T_H}\right)^2\mathrm{d}a \\ &+ \int_{A_L(t)}\alpha_L\left(\frac{1}{T_L} - \frac{1}{T}\right)^2\mathrm{d}a\Bigg\}\ \mathrm{d}t. \end{aligned} \tag{13}$$

It is easy to see that $\delta \leq 0$ holds for the heat-driven separation process with linear phenomenological heat transfer law, and the equality holds for reversible process. The heat consumption can be obtained according to Eqs. (11) and (12)

$$Q_H \geq \frac{\bar{f}_h - T_L\bar{f}_s - T_L\delta}{1 - T_L/T_H}. \tag{14}$$

The following equation is obtained according to Eq. (14) and $\delta \leq 0$

$$Q_H \geq \frac{\bar{f}_h - T_L\bar{f}_s}{1 - T_L/T_H} = Q_H^{\text{rev}}. \tag{15}$$

The equality in Eq. (15) holds for a stationary process because of net work $W_n \geq \Delta B_{\text{sep}}$ [15], where $\Delta B_{\text{sep}} = \Delta H - T_0\Delta S$ is the change in exergy, $W_n = Q_H(T_H - T_0)/T_H - Q_L(T_L - T_0)/T_L$, and $\Delta H = f_h$, $\Delta S = f_s$.

The heat consumption for real separation processes is much higher than the right-hand side of inequality in Eq. (15). The more realistic higher bound of the heat consumption for heat-driven binary separation process with linear phenomenological heat transfer law is studied in this paper, and the finite time of the process, the corresponding finite flow rates of heat, and the finite thermal resistance have been taken into account.

3. Optimization

If the temperature of the heat-driven binary separation system with linear phenomenological heat transfer law is $T(t,\xi)$, the average heat consumption is

$$Q_H = \frac{1}{\tau}\int_0^\tau\int_{A_H(t)}\alpha_H\left(\frac{1}{T} - \frac{1}{T_H}\right)\mathrm{d}a\ \mathrm{d}t. \tag{16}$$

It seems that it is necessary to define the model more accurately to find the temperature $T(t,\xi)$. However, this will not be done in this paper. Instead, Eqs. (4) and (5), and the fact that $T(t,\xi) > 0$ holds for any process, are adequate for the study. The temperature $T(t,\xi)$ is taken as a control, and the following problems are solved.

Problem 1: Given functions $f_h(t)$ and $f_s(t)$, solving the maximum of $-Q_H$ with constraints $E(0) = E(\tau)$ and $S(0) = S(\tau)$.

Problem 1 is a typical average optimization control problem, Orlov and Berry solved the similar problem for heat engine [11] and heat-driven binary separation process [22] with Newtonian heat transfer law by using the same method. The difference between heat-driven separation process and heat engine is the nonzero item $f_s(t) = Ps_P + Ws_W - Fs_F$ in Eq. (5). The upper bound of criteria of problem 1 can be solved by using Lagrangian function. There exist two constraints of problem 1 that can be reduced to a two-dimensional convex optimization problem by using Lagrangian function. However, the problem will be simplified to a one-dimensional convex optimization problem after solving problem 2.

Problem 2: Given function $f_s(t)$, solving the maximum of $Q_H - Q_L$ with constraint $S(0) = S(\tau)$.

Problem 2 is also a typical average optimization control problem similar to the maximum average power output problem in Ref. [11] and the maximum enthalpy flow rate problem in Ref. [22]. The difference between heat-driven separation process and heat engine is the nonzero item $f_s(t) = Ps_P + Ws_W - Fs_F$ in Eq. (5). There exists one constraint of problem 2 that can be transformed to a one-dimensional convex optimization problem by using Lagrangian function.

3.1. Transformation to convex optimization problems

The problem in this section is problem 2. The upper bound of problem 2 can be solved by solving average unconstrained problem 2′.

Problem 2′: Solving the maximum of L_2 over the range of admissible control $T > 0$. The Lagrangian function is as follows

$$L_2 = Q_H - Q_L + \frac{\lambda}{\tau}\int_0^\tau\left\{\int_{A_H(t)}\frac{\alpha_H(1/T - 1/T_H)}{T}\mathrm{d}a - \int_{A_L(t)}\frac{\alpha_L(1/T_L - 1/T)}{T}\mathrm{d}a\right\}\mathrm{d}t - \lambda\bar{f}_s, \quad (17)$$

where $\lambda < 0$ is Lagrangian multiplier, and the nonpositive item $\lambda\bar{\sigma}$ is omitted. It is denoted that $\phi_2(T_H, T_L;\bar{f}_s, \lambda) = \max_{T>0} L_2$. The upper bound of ϕ_2 can be obtained analytically by maximization with $T > 0$ under the constraints of $\lambda < 0$ and $T > 0$. The upper bound is

$$\phi_2 = \frac{1}{\tau}\int_0^\tau\left\{-\int_{A_H(t)}\frac{\alpha_H(T_H+\lambda)^2}{4\lambda T_H{}^2}\mathrm{d}a - \int_{A_L(t)}\frac{\alpha_L(T_L+\lambda)^2}{4\lambda T_L{}^2}\mathrm{d}a\right\}\mathrm{d}t - \lambda\bar{f}_s. \quad (18)$$

The optimum upper bound is $P(T_H, T_L;\bar{f}_s) = \min_\lambda \phi_2 (T_H, T_L;\bar{f}_s, \lambda)$. Differentiating Eq. (18) with respect to λ, the expression of optimum λ, $\hat{\lambda}$ can be written as follows

$$\hat{\lambda} = -\frac{T_H T_L\sqrt{\gamma_H + \gamma_L}}{\sqrt{\gamma_H T_L{}^2 + \gamma_H T_L{}^2 + 4T_H{}^2 T_L{}^2\bar{f}_s}}, \quad (19)$$

where $a_H(t)$ is the area of the surface $A_H(t)$, $a_L(t)$ is the area of the surface $A_L(t)$, $\gamma_H = \overline{a_H\alpha_H}$, and $\gamma_L = \overline{a_L\alpha_L}$. Functions g_H and g_L are used here to define the averaging value,

$$\bar{g}_H = (1/\tau)\int_0^\tau (1/a_H)\int_{A_H(t)} g_H(t,\xi)\mathrm{d}a\mathrm{d}t,$$
$$\bar{g}_L = (1/\tau)\int_0^\tau (1/a_L)\int_{A_L(t)} g_L(t,\xi)\mathrm{d}a\mathrm{d}t. \quad (20)$$

Substituting Eq. (19) into (18), one can obtain

$$\begin{aligned}P(T_H, T_L;\bar{f}_s) &= \phi_2(T_H, T_L;\bar{f}_s, \lambda(T_H, T_L;\bar{f}_s))\\ &= \frac{\gamma_H}{4T_H}\left(\frac{T_L\sqrt{\gamma_H+\gamma_L}}{\sqrt{\gamma_H T_L{}^2 + \gamma_L T_H{}^2 + 4T_H{}^2T_L{}^2\bar{f}_s}} + \frac{\sqrt{\gamma_H T_L{}^2 + \gamma_L T_H{}^2 + 4T_H{}^2T_L{}^2\bar{f}_s}}{T_L\sqrt{\gamma_H+\gamma_L}} - 2\right)\\ &+ \frac{\gamma_L}{4T_L}\left(\frac{T_H\sqrt{\gamma_H+\gamma_L}}{\sqrt{\gamma_H T_L{}^2 + \gamma_L T_H{}^2 + 4T_H{}^2T_L{}^2\bar{f}_s}} + \frac{\sqrt{\gamma_H T_L{}^2 + \gamma_L T_H{}^2 + 4T_H{}^2T_L{}^2\bar{f}_s}}{T_H\sqrt{\gamma_H+\gamma_L}} - 2\right),\\ &+ \frac{T_H T_L\sqrt{\gamma_H+\gamma_L}}{\sqrt{\gamma_H T_L{}^2 + \gamma_L T_H{}^2 + 4T_H{}^2T_L{}^2\bar{f}_s}}\bar{f}_s\end{aligned} \quad (21)$$

where the first two arguments are functions $T_H(t,\xi)$ and $T_L(t,\xi)$, the third argument is the scalar $\bar{f}_s$. And this function solves the problem 2′ and gives the estimation under the condition of average enthalpy flow $\bar{f}_h = Q_H - Q_L$

$$\bar{f}_h \le P(T_H, T_L;\bar{f}_s). \quad (22)$$

The inequality (22) will be used to get the value of the maximum average feed flow into the system in section 3.3.

3.2. The minimum average heat consumption problem

In this section, problem 1 is under consideration. The upper bound for the criterion in this problem can be obtained by solving the unconstrained averaged problem 1′.

Problem 1′ is maximizing function L_1 over the range of the admissible control $T > 0$

$$\begin{aligned}L_1 = &-Q_H + l(Q_H - Q_L)\\ &+ \frac{\lambda}{\tau}\int_0^\tau\left\{\int_{A_H(t)}\frac{\alpha_H(1/T - 1/T_H)}{T}\mathrm{d}a - \int_{A_L(t)}\frac{\alpha_L(1/T_L - 1/T)}{T}\mathrm{d}a\right\}\mathrm{d}t - \lambda\bar{f}_s - l\bar{f}_h,\end{aligned} \quad (23)$$

where $\lambda < 0$ is Lagrangian multiplier, and the nonpositive item $\lambda\bar{\sigma}$ is omitted again. It is denoted that $\phi_1(T_H, T_L\,\bar{f}_s, \bar{f}_h, \lambda, l) = \max_{T>0} L_1$. The upper bound of L_1 can be obtained analytically by maximization with $T > 0$ under the constraints of $\lambda < 0$ and $T > 0$. The upper bound is

$$\phi_1 = \frac{1}{\tau}\int_0^\tau\left\{\int_{A_H(t)}\left(\frac{\alpha_H[(l-1)T_H+\lambda]^2}{-4T_H^2\lambda}\right)\mathrm{d}a + \int_{A_L(t)}\left(\frac{\alpha_L(lT_L+\lambda)^2}{-4T_L^2\lambda}\right)\mathrm{d}a\right\}\mathrm{d}t - \lambda\bar{f}_s - l\bar{f}_h. \quad (24)$$

The optimum (least average) upper bound of convex function ϕ_1 can be obtained by minimizing Eq. (24) with respect to variables λ and l. Firstly, minimizing ϕ_1 with respect to the variable λ, one can obtain ψ_1 $(T_H, T_L; \bar{f}_s, \bar{f}_h, l) = \min_\lambda \phi_1$. Using the expression of Eq. (21), when λ gets the optimum in the following form:

$$\hat{\lambda} = -\frac{T_H T_L \sqrt{(l-1)^2 \gamma_H + l^2 \gamma_L}}{\sqrt{\gamma_H {T_L}^2 + \gamma_L T_H^2 + 4{T_H}^2 {T_L}^2 \bar{f}_s}} \tag{25}$$

the expression of function ψ_1 can be obtained

$$\psi_1(T_H, T_L; \bar{f}_s, \bar{f}_h, l) = \\ = \frac{\gamma_H \left(l - 1 - T_L \sqrt{\frac{(l-1)^2 \gamma_H + l^2 \gamma_L}{\gamma_H T_L^2 + \gamma_L T_H^2 + 4{T_H}^2 T_L^2 \bar{f}_s}} \right)^2}{4 T_H T_L \sqrt{\frac{(l-1)^2 \gamma_H + l^2 \gamma_L}{\gamma_H {T_L}^2 + \gamma_L {T_H}^2 + 4{T_H}^2 {T_L}^2 \bar{f}_s}}} + \frac{\gamma_L \left(l - T_H \sqrt{\frac{(l-1)^2 \gamma_H + l^2 \gamma_L}{\gamma_H {T_L}^2 + \gamma_L {T_H}^2 + 4{T_H}^2 {T_L}^2 \bar{f}_s}} \right)^2}{4 T_H T_L \sqrt{\frac{(l-1)^2 \gamma_H + l^2 \gamma_L}{\gamma_H {T_L}^2 + \gamma_L {T_H}^2 + 4{T_H}^2 {T_L}^2 \bar{f}_s}}} \\ + T_H T_L \bar{f}_s \sqrt{\frac{(l-1)^2 \gamma_H + l^2 \gamma_L}{\gamma_H {T_L}^2 + \gamma_L {T_H}^2 + 4{T_H}^2 {T_L}^2 \bar{f}_s}} - l \bar{f}_h \tag{26}$$

Let $\psi_1(T_H, T_L; \bar{f}_s, \bar{f}_h, \hat{l}) \le \psi_1(T_H, T_L; \bar{f}_s, \bar{f}_h, l)$ for all $l > 1$. Then the upper bound for problem 1 is $\psi_1(T_H, T_L; \bar{f}_s, \bar{f}_h, l)$. The corresponding minimum heat consumption in the separation process is $Q_H^{\min}(T_H, T_L; \bar{f}_s, \bar{f}_h) = -\psi_1(T_H, T_L; \bar{f}_s, \bar{f}_h, \hat{l})$ and the corresponding estimate is

$$Q_H > Q_H^{\min}. \tag{27}$$

Let us now consider some problems about the heat-driven separation process obeying linear phenomenological heat transfer law ($q \propto \Delta(T^{-1})$). It is easy to see that $Q_H^{\min}(T_H, T_L; \bar{f}_s, \bar{f}_h)$ is a convex function in the variables $\bar{f}_s$ and $\bar{f}_h$, and, $\partial Q_H^{\min}/\partial \bar{f}_s = \hat{\lambda}$, $\partial Q_H^{\min}/\partial \bar{f}_h = \hat{l}$. From these equalities and the conditions $\lambda < 0$ and $l > 1$, it is found that $Q_H^{\min}$ is a strictly monotonically decreasing function in the argument $\bar{f}_s$ and a strictly monotonically increasing function in the argument $\bar{f}_h$. It is also easy to see that $\mathrm{d}\psi_1/\mathrm{d}l \to -\bar{f}_h$ when $l \to 1$. The condition $\lim_{l \to +\infty} \psi_1/l > 0$ guarantees the existence of a minimum point. Using $P(aT_H, aT_L; \bar{f}_s) = aP(T_H, T_L; \bar{f}_s)$ for $a > 0$, one can obtain the equivalent condition $P(T_H, T_L; \bar{f}_s) > \bar{f}_h$, which is the strict form of inequality (22).

It is reasonable to assume that $\bar{f}_h \ge 0$ for heat-driven separation processes, which implies that $P(T_H, T_L; \bar{f}_s) \ge \bar{f}_h$ according to Eq. (22). The inequality gives the lower bound for $\bar{f}_s$. In fact, $P(T_H, T_L; \bar{f}_s^{\min}) = 0$. Then $\bar{f}_s \ge \bar{f}_s^{\min}$ because P is a strictly monotonically increasing function in the argument $\bar{f}_s$.

From Eq. (22), one can obtain

$$\bar{f}_s^{\min} = -\frac{\gamma_H \gamma_L (T_H - T_L)^2}{4{T_H}^2 T_L^2 (\gamma_H + \gamma_L)}. \tag{28}$$

When the functions $\alpha_H(\xi)$, $T_H(t, \xi)$, $\alpha_L(\xi)$, and $T_L(t, \xi)$ of the surfaces $A_H(t)$ and $A_L(t)$, and the corresponding flows $f_s(t)$ and $f_h(t)$ are given, one can calculate the minimum heat consumption by solving a one-dimensional convex minimization problem for the function ψ_1. For constant-temperature reservoirs, this minimization is carried out analytically as follows:

The best (least) upper bound of $\psi_1(T_H, T_L; \bar{f}_s, \bar{f}_h, \hat{l})$ can be obtained by substituting $\hat{l}$ into Eq. (26).

$$Q_H^{\min}(T_H, T_L; \bar{f}_s, \bar{f}_h) = -\psi_1(T_H, T_L; \bar{f}_s, \bar{f}_h, \hat{l}) \\ = \hat{l}\bar{f}_h - \frac{\gamma_H \left(\hat{l} - 1 - T_L \sqrt{\frac{(\hat{l}-1)^2 \gamma_H + \hat{l}^2 \gamma_L}{\gamma_H {T_L}^2 + \gamma_L {T_H}^2 + 4{T_H}^2 {T_L}^2 \bar{f}_s}} \right)^2}{4 T_H T_L \sqrt{\frac{(\hat{l}-1)^2 \gamma_H + \hat{l}^2 \gamma_L}{\gamma_H {T_L}^2 + \gamma_L {T_H}^2 + 4{T_H}^2 {T_L}^2 \bar{f}_s}}} - \frac{\gamma_L \left(\hat{l} - T_H \sqrt{\frac{(\hat{l}-1)^2 \gamma_H + \hat{l}^2 \gamma_L}{\gamma_H {T_L}^2 + \gamma_L {T_H}^2 + 4{T_H}^2 {T_L}^2 \bar{f}_s}} \right)^2}{4 T_H T_L \sqrt{\frac{(\hat{l}-1)^2 \gamma_H + \hat{l}^2 \gamma_L}{\gamma_H {T_L}^2 + \gamma_L {T_H}^2 + 4{T_H}^2 {T_L}^2 \bar{f}_s}}}, \\ - T_H T_L \bar{f}_s \sqrt{\frac{(\hat{l}-1)^2 \gamma_H + \hat{l}^2 \gamma_L}{\gamma_H {T_L}^2 + \gamma_L {T_H}^2 + 4{T_H}^2 {T_L}^2 \bar{f}_s}} \tag{29}$$

where, $\hat{l}$ is as follows

$$\hat{l} = \frac{\gamma_H \{-4T_H T_L^2 [\bar{f}_h^2 T_H + \gamma_H(\bar{f}_h - \bar{f}_s T_H)] + \gamma_L [4{T_H}^2 T_L(\bar{f}_s T_L - \bar{f}_h) + \gamma_H (T_H - T_L)^2]\} + \sqrt{\frac{\gamma_H \gamma_L \{-4T_H T_L^2 [\bar{f}_h^2 T_H + \gamma_H(\bar{f}_h - \bar{f}_s T_H)] + \gamma_L [4{T_H}^2 T_L(\bar{f}_s T_L - \bar{f}_h) + \gamma_H (T_H - T_L)^2]\}}{[T_H \gamma_L + T_L(2\bar{f}_h T_H + \gamma_H)]^2}}}{(\gamma_H + \gamma_L)\{-4T_H T_L^2 [\bar{f}_h^2 T_H + \gamma_H(\bar{f}_h - \bar{f}_s T_H)] + \gamma_L [4{T_H}^2 T_L(\bar{f}_s T_L - \bar{f}_h) + \gamma_H (T_H - T_L)^2]\}}, \tag{30}$$

3.3. The maximum feed flow rate problem

According to Eqs. (12) and (14), one can obtain

$$Q_H^{\min} \geq \frac{\bar{f}_h - T_L \bar{f}_s}{1 - T_L/T_H}. \quad (31)$$

According to Ref. [22], one can get that $\frac{Q_H^{\min}(T_H, T_L; r_s\bar{F}, r_h\bar{F})}{\bar{F}} \to \frac{r_h - T_L r_s}{1 - T_L/T_H}$ when $\bar{F} \to 0$. When the heat transfer in the heat-driven separation process obeys linear phenomenological law, it is easy to see that the function $Q(\bar{F}) = Q_H^{\min}(T_H, T_L; r_s\bar{F}, r_h\bar{F})$ is a convex and strictly monotonically increasing function for $r_s < 0$ and $r_h > 0$, which means that the average heat consumption increases with the increase in the average feed flow. Inequality (22) follows that the average feed flow $\bar{F}$ could not be increased to infinity. There is an upper bound for average feed flow $\bar{F}^{\max}$, which is the solution of the following equation

$$\bar{F} r_h = P(T_H, T_L; r_s\bar{F}). \quad (32)$$

In fact, the function $P(\bar{F}) = P(T_H, T_L; r_s\bar{F})$ is a concave, a strictly monotonically decreasing concave for $r_s < 0$ and $r_h > 0$, and

$$P(0) = \frac{\gamma_H}{4T_H}\left(\frac{T_L\sqrt{\gamma_H + \gamma_L}}{\sqrt{\gamma_H {T_L}^2 + \gamma_L {T_H}^2}} + \frac{\sqrt{\gamma_H {T_L}^2 + \gamma_L {T_H}^2}}{T_L\sqrt{\gamma_H + \gamma_L}} - 2\right) + \frac{\gamma_L}{4T_L}\left(\frac{T_H\sqrt{\gamma_H + \gamma_L}}{\sqrt{\gamma_H {T_L}^2 + \gamma_L {T_H}^2}} + \frac{\sqrt{\gamma_H T_L^2 + \gamma_L {T_H}^2}}{T_H\sqrt{\gamma_H + \gamma_L}} - 2\right) > 0. \quad (33)$$

These properties guarantee the existence and the uniqueness of the solution of Eq. (32). Calculating $Q(\bar{F})$ at $\bar{F}^{\max}$, one can obtain the following equation by using Eq. (29)

$$\begin{aligned} Q(\bar{F}^{\max}) &= Q_H^{\min}(T_H, T_L; \bar{f}_s, \bar{f}_h) = -\psi_1(T_H, T_L; \bar{f}_s, \bar{f}_h, \hat{l}) \\ &= \hat{l} r_h \bar{F}^{\max} \\ &- \frac{\gamma_H\left(\hat{l} - 1 - T_L\sqrt{\frac{(\hat{l}-1)^2\gamma_H + \hat{l}^2\gamma_L}{\gamma_H T_L^2 + \gamma_L T_H^2 + 4{T_H}^2 T_L^2 r_s \bar{F}^{\max}}}\right)^2}{4T_H T_L\sqrt{\frac{(\hat{l}-1)^2\gamma_H + \hat{l}^2\gamma_L}{\gamma_H T_L^2 + \gamma_L T_H^2 + 4{T_H}^2 T_L^2 r_s \bar{F}^{\max}}}} \\ &- \frac{\gamma_L\left(\hat{l} - T_H\sqrt{\frac{(\hat{l}-1)^2\gamma_H + \hat{l}^2\gamma_L}{\gamma_H T_L^2 + \gamma_L T_H^2 + 4{T_H}^2 T_L^2 r_s \bar{F}^{\max}}}\right)^2}{4T_H T_L\sqrt{\frac{(\hat{l}-1)^2\gamma_H + \hat{l}^2\gamma_L}{\gamma_H T_L^2 + \gamma_L T_H^2 + 4{T_H}^2 T_L^2 r_s \bar{F}^{\max}}}}, \\ &- T_H T_L r_s \bar{F}^{\max}\sqrt{\frac{(\hat{l}-1)^2\gamma_H + \hat{l}^2\gamma_L}{\gamma_H T_L^2 + \gamma_L T_H^2 + 4{T_H}^2 T_L^2 r_s \bar{F}^{\max}}} \end{aligned} \quad (34)$$

where the optimum $\hat{l}$ is

$$\hat{l} = \frac{\gamma_H\{-4T_H T_L^2[(r_h\bar{F}^{\max})^2 T_H + \gamma_H(r_h\bar{F}^{\max} - r_s\bar{F}^{\max}T_H)] + \gamma_L[4{T_H}^2 T_L(r_s\bar{F}^{\max}T_L - r_h\bar{F}^{\max}) + \gamma_H(T_H - T_L)^2]\} + \sqrt{\frac{\gamma_H\gamma_L\{-4T_H T_L^2[(r_h\bar{F}^{\max})^2 T_H + \gamma_H(r_h\bar{F}^{\max} - r_s\bar{F}^{\max}T_H)] + \gamma_L[4{T_H}^2 T_L(r_s\bar{F}^{\max}T_L - r_h\bar{F}^{\max}) + \gamma_H(T_H - T_L)^2]\}}{[T_H\gamma_L + T_L(2r_h\bar{F}^{\max}T_H + \gamma_H)]^2}}}{(\gamma_H + \gamma_L)\{-4T_H T_L^2[(r_h\bar{F}^{\max})^2 T_H + \gamma_H(r_h\bar{F}^{\max} - r_s\bar{F}^{\max}T_H)] + \gamma_L[4{T_H}^2 T_L(r_s\bar{F}^{\max}T_L - r_h\bar{F}^{\max}) + \gamma_H(T_H - T_L)^2]\}}. \quad (35)$$

Eq. (34) is the analytical expression of the minimum average heat consumption when feed flow rate reaches its upper bound.

4. Numerical examples and discussions

The dimensionless minimum heat consumption $Q_H^{\min'} = Q_H^{\min}/Q_H^{\text{rev}}$ for propylene-propane distillation column is calculated. The temperatures of high- and low-temperature heat reservoirs are $T_H = 377.6$ K and $T_L = 294.3$ K. The heat transfer coefficients and contact areas for this process are appointed physically reasonable values, $\gamma_H = \alpha_H a_H = 13,000 \text{kW}/(\text{m}^2 \times \text{K})$, and $\gamma_L = \gamma_H$. The minimum entropy production rate $\bar{f}_s^{\min}$ can be calculated according to Eq. (28).

According to Ref. [22], the dimensionless entropy production rate and dimensionless enthalpy flow rate which indicate the major influence factors for the performance of the separation process, such as the

Table 1
Dimensionless minimum average heat consumption $Q_H^{\min'}$ for different $\bar{f}'_s$ and $\bar{f}'_h$

$\bar{f}'_h \backslash Q_H^{\min'} \backslash \bar{f}'_s$	1.0	0.8	0.6	0.4	0.2	0.0
0.8	1.9761	1.6533	1.5503	1.4800	1.4260	1.3819
0.6	1.9539	1.5363	1.4141	1.3337	1.2733	1.2251
0.4	1.9333	1.4557	1.3239	1.2391	1.1764	1.1270
0.2	1.9142	1.3935	1.2562	1.1691	1.1054	1.0557

properties of different material and various separation requirements for the separation process are adopted. The dimensionless entropy production rate is assumed to be $\bar{f}'_s = \bar{f}_s / \bar{f}_s^{\min}$, and the dimensionless enthalpy flow rate is assumed to be $\bar{f}'_h = \bar{f}_h / P(T_H, T_L; \bar{f}_s^{\min})$. The parameters are taken as $\bar{f}_s = \bar{f}'_s \bar{f}_s^{\min}$ and $\bar{f}_h = \bar{f}'_h P(T_H, T_L; \bar{f}_s)$. The dimensionless minimum average heat consumption $Q_H^{\min'} = Q_H^{\min}/Q_H^{\text{rev}}$ is calculated by using Eqs. (14) and (29).

Table 1 lists the dimensionless minimum heat consumption $Q_H^{\min'}$ for different $\bar{f}'_s$ and $\bar{f}'_h$. From Table 1 one can see that the dimensionless minimum average heat consumption $Q_H^{\min'}$ varies from 1.0557 to 1.9761. And the dimensionless heat consumption $Q_H^{\min'}$ increases with the increases in dimensionless entropy production rate and dimensionless enthalpy flow rate.

Fig. 2 shows the dimensionless minimum average heat consumption $Q_H^{\min'}$ versus the dimensionless enthalpy flow rate $\bar{f}'_h$ characterized by different dimensionless entropy production rate $\bar{f}'_s$. Curves 1 to 4 correspond to the dimensionless entropy production rates $\bar{f}'_s = 0.2$, 0.4, 0.6, and 0.8, respectively. One can see that dimensionless minimum average heat consumption $Q_H^{\min'}$ increases with the increase in the dimensionless enthalpy flow rate $\bar{f}'_h$. Moreover, $Q_H^{\min'}$ increases with the increase in dimensionless entropy production rate $\bar{f}'_s$.

Fig. 3 shows the dimensionless minimum average heat consumption $Q_H^{\min'}$ versus the dimensionless entropy production rate $\bar{f}'_s$ characterizes different dimensionless enthalpy flow rates $\bar{f}'_h$. Curves 1 to 6 correspond to the dimensionless enthalpy flow rate $\bar{f}'_h = 0.0$, 0.2, 0.4, 0.6, 0.8, and 1.0, respectively. It can be seen that dimensionless minimum average heat consumption $Q_H^{\min'}$ increases with the increases in dimensionless entropy production rate $\bar{f}'_s$ and the dimensionless enthalpy flow rate $\bar{f}'_h$. Because $\bar{f}_s < 0$, the increase of $\bar{f}'_s$ means the decrease of $\bar{f}_s$. This indicates that $Q_H^{\min'}$ decreases with the increase on $\bar{f}_s$.

When T_H, T_L, γ_H, and γ_L are other appointed physically reasonable values, the results are qualitatively coincide with those in Table 1, and Figs. 2 and 3. The minimum heat consumption of heat-driven binary separation process with linear phenomenological heat transfer law calculated by Eq. (29) is more realistic than that of reversible heat-driven binary separation process. For the process with time- and space-variable temperatures of the heat reservoirs, Eq. (22) may be employed to search the minimum heat consumption.

5. Conclusion

The performance optimizations of the heat-driven binary separation process are carried out in this paper by using finite time thermodynamics. Two performance indexes, the dimensionless minimum average entropy production rate and dimensionless minimum average heat consumption of the heat-driven binary separation processes, are taken as optimization objectives, respectively. The heat transfer in the

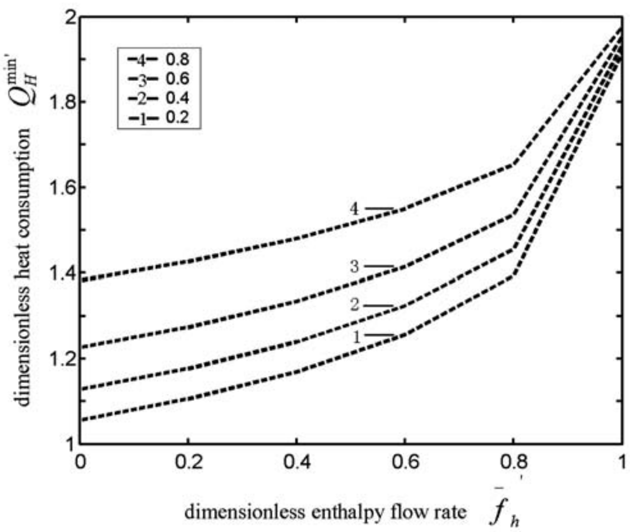

Fig. 2. Dimensionless minimum average heat consumption $Q_H^{\min'}$ versus dimensionless enthalpy flow rate $\bar{f}'_h$.

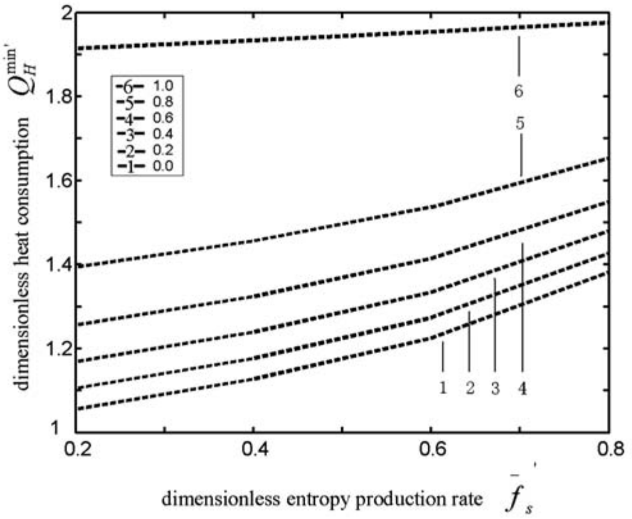

Fig. 3. Dimensionless minimum average heat consumption $Q_H^{min'}$ versus dimensionless entropy production rate $\bar{f}'_s$.

separation process obeys linear phenomenological law ($q \propto \Delta(T^{-1})$) and the temperatures of the heat reservoirs are assumed to be time- and space-variable. The analytical expressions of minimum average heat consumption and minimum average entropy production rate of the separation process with given average enthalpy flow rate and entropy flow rate are obtained. The analytical expression of minimum average heat consumption of the binary separation process with fixed average flow rate is also obtained. The minimum heat consumption problem of the heat-driven separation process with time- and space-variable temperature heat reservoirs is transformed to a convex optimization problem by using numerical method. The dimensionless entropy production rate and dimensionless enthalpy flow rate which indicate the major influence factors for the performance of the separation process, such as the properties of different material and various separation requirements for the separation process, are adopted. As a special example, in the case of constant temperature heat reservoirs, the analytical expressions of dimensionless entropy production rate and dimensionless minimum average heat consumption of separation processes are obtained. The numerical results indicate that dimensionless minimum average heat consumption $Q_H^{min'}$ increases with the increases in dimensionless enthalpy flow rate $\bar{f}'_h$ and the dimensionless entropy production rate $\bar{f}'_s$. $Q_H^{min'}$ increases with the decrease in $\bar{f}_s$ because of $\bar{f}_s < 0$. The purity of reactants and feed is not taken as a constraint in this theoretical optimization study. How to obtain more practical results including purity constraint will be a future subject.

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