Optimal Heat Exchanger Network Design for Rapid Start-up Operation of Fuel Cell System

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[Abstract]

A new synthesis technique is proposed for a problem of a heat exchanger network design taking account of a rapid start-up operation of a fuel cell system. The proposed method consists of two optimization steps. First, the structure of the heat exchanger network which minimizes total utility consumption is derived assuming that main devices in the process follow the pre-defined temperature profiles. The transshipment model for the conventional heat integration approach is extended to the dynamic transshipment model, which can handle the heat accumulation in the devices during the transitional operation. Second, the flow rate of each stream is optimized as a function of time using more detailed dynamic physical models of the process obtained at the first step. Effective use of the proposed two-step optimization method is demonstrated through a case study of a fuel cell system. This two-step optimization method can be applied to not only fuel cell systems but also many processes where non-steady state operation is inevitable.

[Key words]

Fuel cell system, Heat exchanger network, Process synthesis, Non-steady state operation

1. INTRODUCTION

A fuel cell system needs to be designed taking account of frequent start-up, shutdown and load change operations, since it is generally operated on demand manner. Though the conventional design approach such as a pinch technology gives us the optimal structure of a heat exchanger network (HEN) of a fuel cell system during the steady state operation, the extra devices need to be added in the derived structure later for transitional operations.

Since the 1980s, several authors have investigated HENs with regard to flexibility and controllability. Papoulias and Grosmann (1983) and Yee and Grossmann (1990) proposed a design method for HEN, that yields a reasonable trade-off between capital and operating cost through both sequential and simultaneous approaches. Kotjabasakis and Linnhoff (1986) introduced sensitivity tables to find the heat exchanger areas that should be increased in order to make a nominal design sufficiently flexible. Glemmestad and Skogestad (1999) considered the optimal operation of HEN with a given structure, heat exchanger areas and stream data including pre-defined disturbances. Furman and Sahinidis (2002) provided a critical review of the literature on the synthesis of HEN. Aaltola (2002) developed a multi-period optimization model for a flexible HEN based on the MINLP formulation of Yee and Grossmann. These studies, however, only focus on the flexibility and controllability of HEN around a certain steady state condition.

This paper is organized as follows: First, a rapid start-up problem of the fuel cell system is outlined as a case study which requires us a simultaneous optimization of design and operation. Then, the new heat exchange model which can handle the dynamic operation of a process is proposed by extending the conventional heat exchange model used in the pinch technology. Finally, the proposed method is applied to the case study and some conclusions are drawn in the last section.

2. OPTIMAL DESIGN AND OPERATION PROBLEM OF SOFC SYSTEM

Solid Oxide Fuel Cell (SOFC) is considered to be more energy efficient compared to the other commercialized fuel cells due to its high operating temperature. In the operation of the SOFC system, frequent start-up, shutdown and load change are required by nature because the SOFC system is generally operated on demand manner. In the SOFC system, there are a lot of operational constraints. For example, the maximum heat-up rate of an SOFC membrane is limited to a certain value to avoid the membrane destruction, since the membrane is mainly made of ceramics. Therefore, it is very important to optimize the design and operation of the SOFC system so as to satisfy those operational constraints.

Figure 1 illustrates the schematic diagram of the SOFC system, which mainly consists of SOFC membrane, SOFC stack and external case. During the steady state operation, the feed fuel and air are heated by some heat exchangers and heaters and fed into the SOFC membrane where reforming and electrochemical reactions occur. The SOFC stack connects the parallelized SOFC membranes to supply the specified power output. The external case covers the SOFC system for insulation.

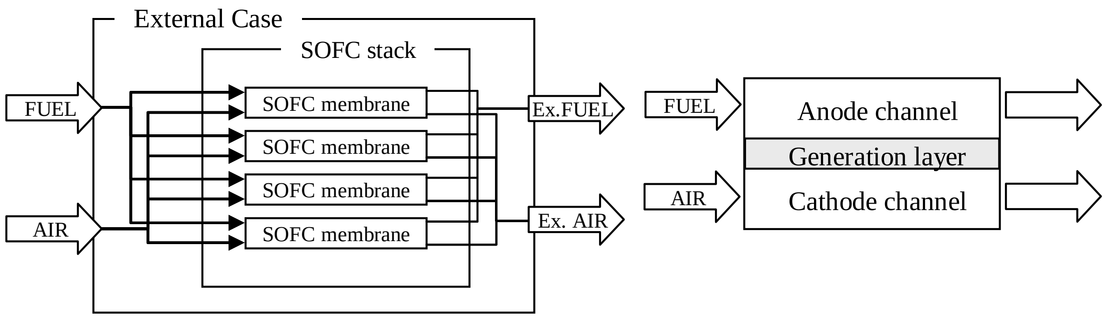

Fig. 1 Schematic Diagram of SOFC system (Left) and SOFC Membrane (Right)

The start-up operation of the SOFC system is to heat up the SOFC membrane, the SOFC stack and the external case from the initial temperature to the steady state temperatures. The fuel and air flows are used as thermal mediums after being heated up by heat exchangers and/or heaters during the start-up operation. The heater is assumed to be able to heat up the fluid to 1200 K. In order to avoid the membrane destruction, the maximum heating up rate of the SOFC membrane is restricted. Using this information, the theoretical minimum start-up time t_{min} of the SOFC system can be calculated by Eq. (1).

$$t_{\min} = (T_f - T_i) / R_{\max} \tag{1}$$

Here, R_{max} is the maximum heating-up rate of the SOFC membrane, T_f and T_i are the final and the initial temperatures of the SOFC membrane.

In this paper, the optimal design and operation problem of the SOFC system considering rapid start-up is defined as follows: The objective function of the problem is to minimize the total utility cost during the start-up operation. The total time for start-up operation is fixed at the theoretical minimum start-up time t_{min} calculated by Eq. (1). The heat exchanger network including the sizes of them is derived so as to minimize the objective function. The flow rates of the fuel and the air are also optimized as a function of time. The heat capacities and surface areas of the SOFC membrane, SOFC stack and external case are given and utilized to develop their dynamic models. The initial temperatures and the steady state temperatures of basic units are also given.

3. SYNTHESIS OF HEAT EXCHANGER NETWORK

Heat integration techniques have been widely applied in the chemical industry. The conventional synthesis problem is to determine HEN that minimizes the utility cost while assuming that the following design conditions are given in advance (Biegler et al., 1997).

(1) A set of hot process streams to be cooled and a set of cold streams to be heated
(2) Flow rates and inlet and outlet temperatures of all these process streams
(3) Available utilities and their temperatures

On the other hand, the synthesis problem discussed in this paper is to design not only HEN and heat transfer area of each heat exchanger in the network but also operation condition during the start-up period. The operation condition includes the flow rates of process and utility streams and temperature profiles of process streams and main devices. Here, a main device is defined as the dominant facility which must be installed to perform the function of the process properly. The objective function of this problem is to minimize the total utility cost required for dynamically transferring the state of process streams and main devices in a process from an initial condition to the specified final condition. Heat exchangers, heaters and coolers are not included in the set of the main devices. In this problem, the following information needs to be supplied.

(1) Heat capacities, heat transfer areas, initial and final temperatures of main devices
(2) Specific heat, inlet and outlet temperatures of process streams
(3) Network of process streams
(4) Available utilities and their temperatures

The characteristics of this problem are summarized as follows: The accumulation of heat into main devices in the system is considered, and the flow rates of process streams can be optimized as functions of time. The operational constraints, such as the maximum heat-up rate of a main device, are also considered.

4. OPTIMIZATION APPROACH FOR DESIGN AND OPERATION PROBLEM OF HEN

4.1 Synthesis of Steady State HEN

The extended transshipment model shown in Fig. 2 is an algorithmic optimization model that can automatically synthesize the optimal HEN (Papoulias and Grossmann, 1983). The extended transshipment model can be formulated as follows. First, K temperature intervals are generated based on the inlet and outlet temperatures of the process streams, and temperatures of the utilities. At interval k, the following heat balance equations (1) – (6) must be satisfied. The numbers in Fig. 2 represents points where each heat balance equation is defined.

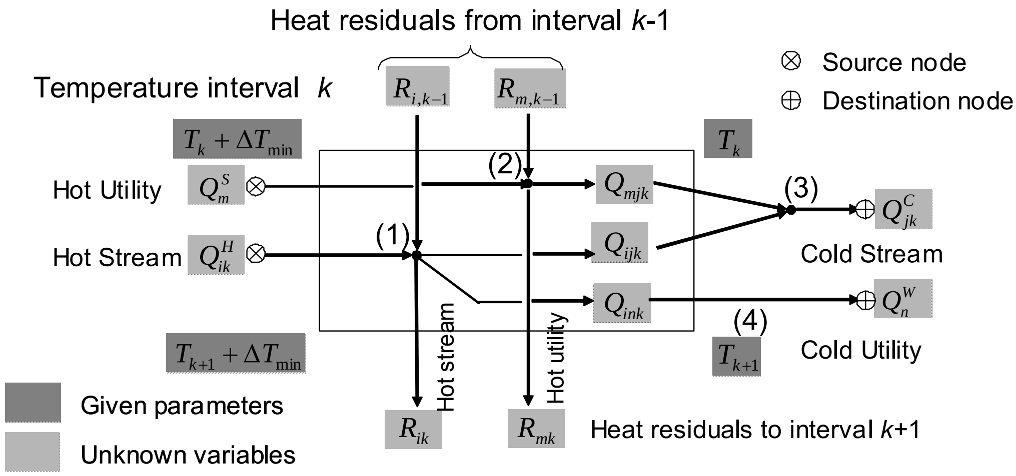

Fig. 2 Extended transshipment model at temperature interval *k*

$$R_{ik} + \sum_{j \in C_k} Q_{ijk} + \sum_{n \in W_k} Q_{ink} = R_{i,k-1} + Q_{ik}^H, \; i \in H_k \tag{1}$$

$$R_{mk} + \sum_{j \in C_k} Q_{mjk} = R_{m,k-1} + Q_m^S, \quad m \in S_k \tag{2}$$

$$\sum_{m \in S_k} Q_{mjk} + \sum_{i \in H_k} Q_{ijk} = Q_{jk}^C, \quad j \in C_k \tag{3}$$

$$\sum_{i \in H_k} Q_{ink} = Q_n^W, \quad n \in W_k \tag{4}$$

$$R_{ik}, R_{mk}, Q_{ijk}, Q_{mjk}, Q_{ink}, Q_n^S, Q_n^W \geq 0 \tag{5}$$

$$R_{i1} = R_{iK} = 0 \tag{6}$$

In Eqs. (1)-(6), the following given parameters and unknown variables exist.

Given parameters:

- Q^H_{ik} : Available heat content of hot stream *i* at interval *k*
- Q^C_{jk} : Available heat content of cold stream *j* at interval *k*
- c_m : Utility cost of hot utility *m*
- c_n : Utility cost of cold utility *n*
- T_k : Interval temperature at interval *k*
- T_{min} : Minimum temperature difference

Unknown variables:

- Q^S_m : Heat load of hot utility *m*
- Q^W_n : Heat load of cold utility *n*
- Q_{mjk} : Heat content transferred from hot utility *m* to cold stream *j* at interval *k*
- Q_{ijk} : Heat content transferred from hot stream *i* to cold stream *j* at interval *k*
- Q_{ink} : Heat content transferred from hot stream *i* to cold utility *n* at interval *k*
- R_{ik} : Heat residual of hot stream *i* exiting interval *k*
- R_{mk} : Heat residual of hot utility *m* exiting interval *k*

Index sets:

S_k = {*m* | hot utility *m* is present at or above interval *k*}

W_k = {n | cold utility n extracts heat from interval k}
H_k = { i | hot stream i is present at or above interval k}
C_k = { j | cold stream j demands heat from interval k}

The minimum utility cost problem for a given set of hot and cold streams can then be formulated as the following LP problem (Biegler et al., 1997).

[Extended transshipment model]

$$\text{Min} \quad \sum_{m \in S} c_m Q_m^S + \sum_{n \in W} c_n Q_n^W \quad \text{s.t. Equations (1)-(6)}$$

4.2 Dynamic Transshipment Model

The extended transshipment model is a powerful tool for designing the optimal HEN because the model includes all the possibilities of heat transfer between streams. However, this model does not take into account any transitional behavior of the process, which is very important for the optimal design problem considering non-steady state operations. In this section, we develop a novel dynamic transshipment model by modifying the extended transshipment model. The biggest difference between the design problems of steady state and non-steady state HENs is that heat accumulation into main devices in the process needs to be taken into account in the non-steady state design.

We develop the dynamic transshipment model by modifying the extended transshipment model via following steps. First, the whole period of the non-steady state operation is divided into a set of sub-periods, and in each sub-period, the process is assumed to be in a pseudo steady state. By introducing this assumption, the dynamic model of the process can be transformed to the discrete model. Second, for each main device q, the ideal temperature profile $T_q(t)$ is defined as a function of sub-period number t to calculate the amount of heat accumulated in the main device during each sub-period. The ideal temperature profiles of main devices are usually obtained at the preliminary process design stage without considering HEN structure. In this research, we adopt the simple linear temperature profile, given by Eq. (7).

$$T_q(t) = \frac{t}{T_f}(T_q(T_f) - T_q(0)) + T_q(0) \tag{7}$$

where $T_q(0)$ and $T_q(T_f)$ are respectively the initial and final temperatures of main device q. The amount of the heat accumulated in main device q in sub-period t is calculated by Eq. (8). Here, Cp and M are the heat capacity and weight of main device q, respectively.

$$Q_q(t) = MCp(T_q(t+1) - T_q(t)) \tag{8}$$

Third, the interval temperatures $T_k(t)$ ($k = 1,\ldots,K$) are defined as a function of sub-period t based on the inlet and outlet temperatures of streams, temperatures of available utilities, and ideal temperature profiles of main devices. To solve the defined problem, the following information needs to be supplied.

(1) A set of hot process streams and a set of cold process streams that can be used

as the heating and cooling medium
(2) Inlet and outlet temperatures of all process streams
(3) Initial and final temperatures of the main devices in the process
(4) Heat transfer areas and heat capacities of the main devices in the process
(5) Available utilities and their temperatures

Figure 3 shows a schematic diagram of the dynamic transshipment model at interval *k* and sub-period *t*. In this example, the main device is assumed to be a heat sink, since it needs to be heated up during the operation. When the main device's temperature is between $T_k(t)$ and $T_{k+1}(t)$, $Q_{qk}(t)$ is located at interval *k*.

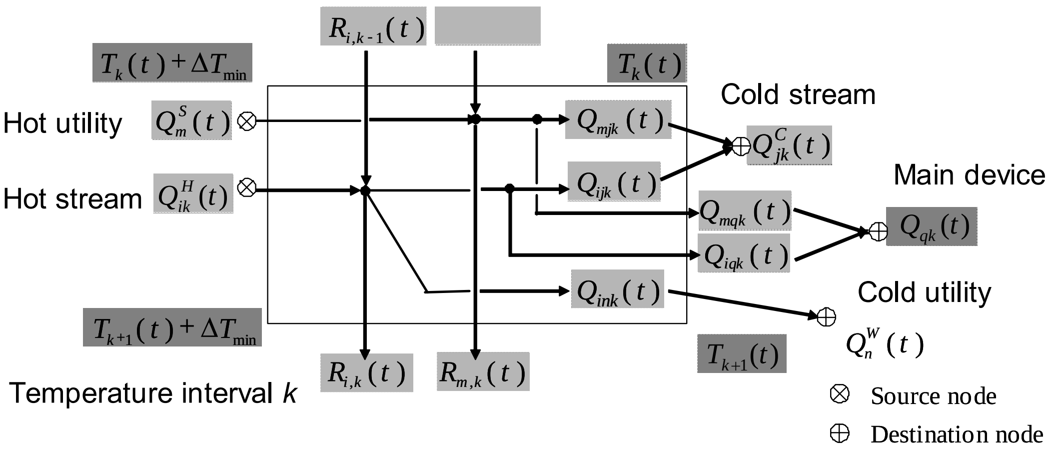

Fig. 3 Dynamic transshipment model at temperature interval *k*

The dynamic transshipment model is formulated as follows. The definition of variables in the dynamic transshipment model is the same as those of the extended transshipment model except that all variables are functions of sub-period *t*. Some new variables are also introduced in this model. Since this model is formulated as an LP model, the optimal solution can be obtained relatively easily.

[Dynamic transshipment model]

$$Min \quad \sum_{t=1}^{T_f}\left(\sum_{m\in S} c_m Q_m^S(t) + \sum_{n\in W} c_n Q_n^W(t)\right)$$

$$s.t. \quad R_{ik}(t) + \sum_{j\in C_k} Q_{ijk}(t) + \sum_{n\in W_k} Q_{ink}(t) + \sum_{q\in E_k} Q_{iqk}(t) = R_{i,k-1}(t) + Q_{ik}^H(t), \;\; i\in H_k$$

$$R_{mk}(t) + \sum_{j\in C_k} Q_{mjk}(t) + \sum_{q\in E_k} Q_{mqk}(t) = R_{m,k-1}(t) + Q_m^S(t), \quad m\in S_k$$

$$\sum_{m\in S_k} Q_{mjk}(t) + \sum_{i\in H_k} Q_{ijk}(t) = Q_{jk}^C(t), \quad j\in C_k$$

$$\sum_{i\in H_k} Q_{ink}(t) = Q_n^W(t), \quad n\in W_k$$

$$Q_{qk}(t) = \sum_{m \in S_k} Q_{mqk}(t) + \sum_{i \in H_k} Q_{iqk}(t)$$

$$R_{ik}(t), R_{mk}(t), Q_{ijk}(t), Q_{mjk}(t) \geq 0, \quad Q_{ink}(t), Q_n^S(t), Q_n^W(t) \geq 0$$

$$R_{i1}(t) = R_{iK}(t) = 0, \quad t = 1,...,T_f, \quad k = 1,...,K$$

Given parameter:

Q_{qk} : The amount of the heat accumulated in main device *q* at interval *k*

Unknown variables:

Q_{iqk} : Heat transfer from hot stream *i* to main device *q* at interval *k*

Q_{mqk} : Heat transfer from hot utility *m* to main device *q* at interval *k*

Index set:

E_k = {*q* | main device *q* existing at interval *k*}

The dynamic transshipment model provides the optimal HEN structure and heat contents transferred between process streams and main devices, and between process streams. The heat transfer area $A_{ijk}(t)$ of each heat exchanger at temperature interval *k* and sub-period *t* can be calculated by Eq. (9).

$$A_{ijk}(t) = Q_{ijk}(t) / U\Delta T_{ijk}^{lm}(t) \tag{9}$$

Here, ΔT^{lm} represents the logarithmic mean temperature difference between hot stream and cold stream. Aaltora (2002) proposed a multi-period optimization model with a bypass flow. In this model, for the case of sub-periods with a smaller heat transfer area $A_{ijk}(t)$ than the maximum heat transfer area $A^{max}{}_{ijk}$ defined by Eq.(10), the bypass flow is used to maintain the amount of the heat transfer between hot and cold streams at the optimal level.

$$A_{ijk}^{\max} = \max\{A_{ijk}(t) : t = 1,...,T_f\} \tag{10}$$

In the proposed approach, $A^{max}{}_{ijk}$, is also selected as the heat transfer area of each heat exchanger, but the bypass flow model is not adopted. Though this assumption may lead to infeasible situations into the obtained network structure and operational profiles, the conflict will be resolved in a two step optimization explained in the next section.

4.3 Two Step Optimization Approach

In this study, we take the two-step optimization approach to solve a synthesis problem of HEN considering non-steady state operation. In the first step, the optimal HEN is derived by solving the optimization problem based on the dynamic transshipment model. In the second step, the optimal operation profile is derived by solving the dynamic optimization problem, where the structure of HEN obtained in the first step is fixed. The dynamic optimization problem using the detailed process model can be solved by a simultaneous approach proposed by Alkaya et al. (1999). In this approach, the dynamic model of the process, which consists of differential algebraic equations (DAEs), is converted to a set of algebraic equations by using orthogonal collocation on finite elements. Then, the problem of finding the optimal operation profiles is formulated as a nonlinear programming problem with inequality constraints on state and manipulated variables. The resulting nonlinear programming problem is solved by applying the reduced SQP technique. In this paper, we focus on the first optimization step and do not discuss the detail of the second step, which is described in another paper (Ono et al., 2003). In the next section, we explain the first step of the proposed approach in detail through a case study.

5. CASE STUDY

In this section, the proposed approach is applied to the optimal design problem of the SOFC system considering rapid start-up operation. In the SOFC system, three basic units, i.e. SOFC membrane, SOFC stack and external case are required at least for the generation of electricity. In this case study, these units need to be heated up from the initial temperature to the final temperature. The data related to these basic units are summarized in Table 1.

Table 1 Design Conditions on SOFC system

	Initial temp. [°C]	Final temp. [°C]	Heat capacity [kJ/K]	Heat transfer coefficient [J/(s K)]
SOFC membrane	50	950	5	10
SOFC stack	30	900	50	10
External case	30	300	100	10

One of the operational constraints related to the SOFC membrane is that the maximum heating-up rate of the SOFC membrane must be less than 50 ◦C/ h. Thus, the theoretical minimum start-up time is 18 hours. The ideal temperature profiles of basic units are defined by Eqs. (11) to (13).

$$\text{SOFC membrane} \quad : T_s(t) = 50 + 50t \tag{11}$$

$$\text{SOFC stack} \quad : T_a(t) = 30 + 48t \tag{12}$$

$$\text{External case} \quad : T_b(t) = 30 + 15t \tag{13}$$

In order to define the synthesis problem of heat exchanger network considering non-steady state operation, a set of hot and cold streams and those inlet and outlet temperatures, location of basic units in the network need to be supplied by a designer. Figure 4 shows the basic structure of the SOFC system taken up in the case study. The cold stream C1 and C2 need to be heated up from 20◦C to $T_s(t)$ and $T_s(t)$ - ΔT_{min}, respectively by time period *t.* On the other hand, the hot stream H1 and H2 need to be cooled down from $T_s(t)$ and $T_s(t)$ - ΔT_{min} to 20◦C, respectively by time period *t*. The amount of heat which must be transferred from H1 and H2 to the SOFC membrane is calculated by Eq.(8) according to the ideal temperature profile of the SOFC membrane. The cold stream C2 also supplies the heat to the SOFC stack and the external case so that temperatures of those units follow the ideal temperature profiles defined by Eqs. (12) and (13).

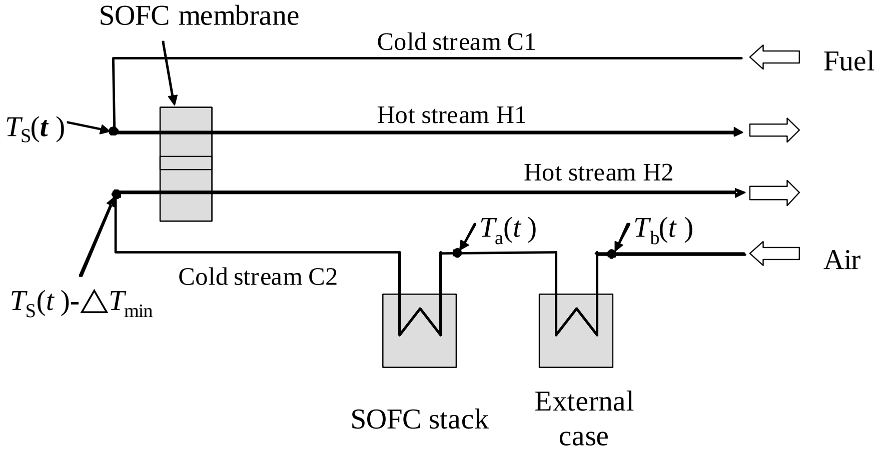

Fig. 4 Basic Structure of SOFC System

Figure 5 shows the dynamic transshipment model of the basic structure. A heater unit, which can supply any amount of heat at any temperature level, is allocated to each temperature interval as shown in Fig. 5.

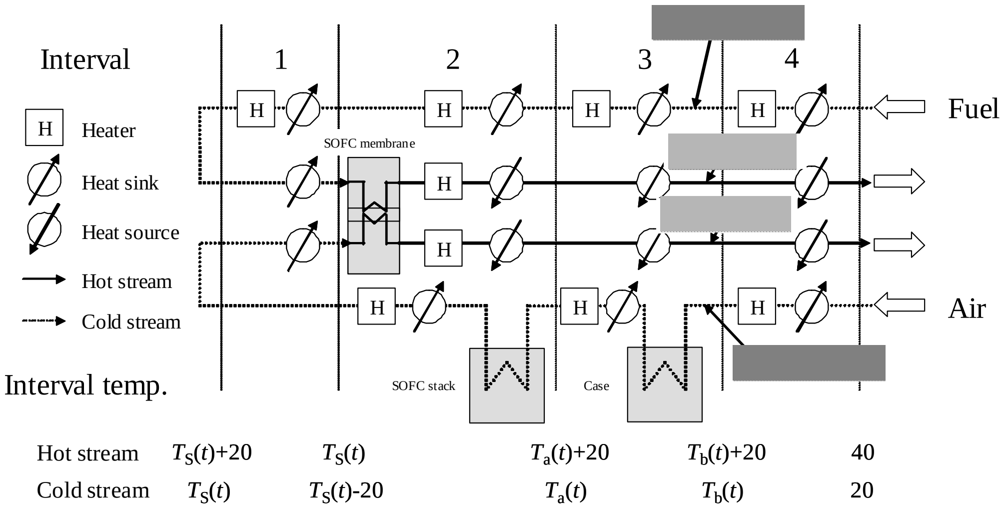

Fig. 5 Dynamic transshipment model of basic structure

In the start-up operation of the SOFC system, a constraint on the maximum temperature difference ΔT_{smin} between inlet temperature T_{in} and outlet temperature T_{out} of the SOFC membrane exists and is given by Eq. (14).

$$T_{in} - T_{out} \leq \Delta T_{s\min} \tag{14}$$

However, temperature variables do not appear in the dynamic transshipment model explicitly, since the dynamic transshipment model is formulated as non-linear equations when temperature variables are included in the model. Therefore, in this study, Eq.(14) is transformed to Eq.(15), where H_{in} and H_{out} is enthalpies of inlet and outlet streams.

$$\frac{T_{in} - T_{out}}{T_{in}} = \frac{H_{in} - H_{out}}{H_{in}} \leq \frac{\Delta T_{s\min}}{T_s(t)} \tag{15}$$

Figure 6 shows the optimal heat exchanger network obtained by the proposed approach. In Fig. 6, an arrow connecting two points illustrates the heat exchange between two streams. By solving the optimal design problem considering the start-up operation, the structure having two heaters just after the SOFC membrane and eight heat exchangers is obtained. Four heat exchangers in the fuel line can be replaced by one heat exchanger, since these heat exchangers are connected in series, and there is no unit between them. The number attached to each arrow shows the heat exchange area which is calculated by Eq.(16) for each heat exchanger.

$$A = \max_t (Q(t) / \Delta T_{\min}) \tag{16}$$

Here, *Q*(*t*) is the amount of heat transferred through a heat exchanger at sub-period *t*. This result is used as an initial guess for the second step optimization problem.

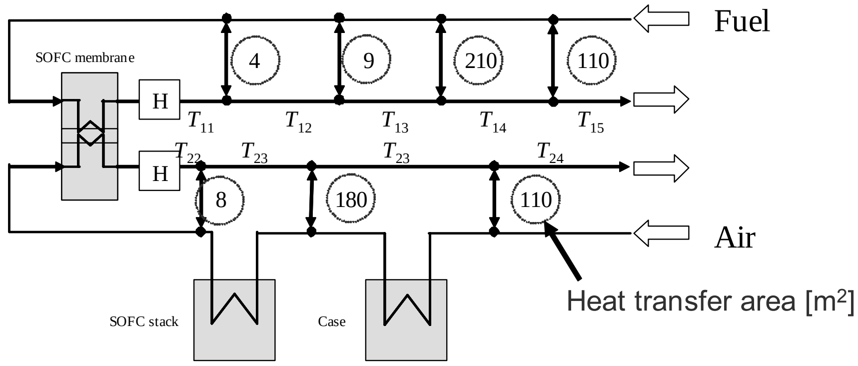

Fig. 6 Optimal heat exchanger network and heat transfer area of each heat exchanger

Figure 7 illustrates the optimal operation profiles. The outputs of two heaters at fuel and air lines are plotted in terms of flow rate of ethane consumed in heaters. As shown in Fig. 7, fuel and air flows are almost kept constant during the start-up operation.

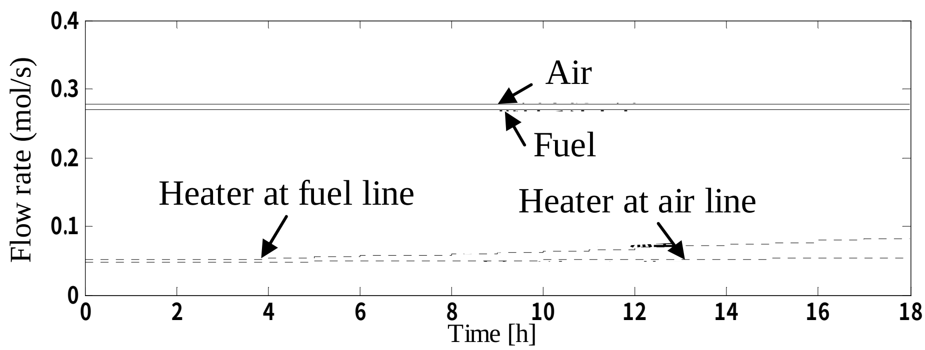

Fig. 7 Operation profiles of SOFC system

Figure 8 shows the temperature profiles in the SOFC system when the optimal start-up operation is applied to the system. The legend in the graph corresponds to the temperature in Fig. 6. As seen in Fig. 7, the air inlet temperature of the SOFC membrane increases at maximum heat-up rate and achieves the final temperature in the theoretical minimum start-up time (18 hours). These results can be used as the initial solution for the second step optimization.

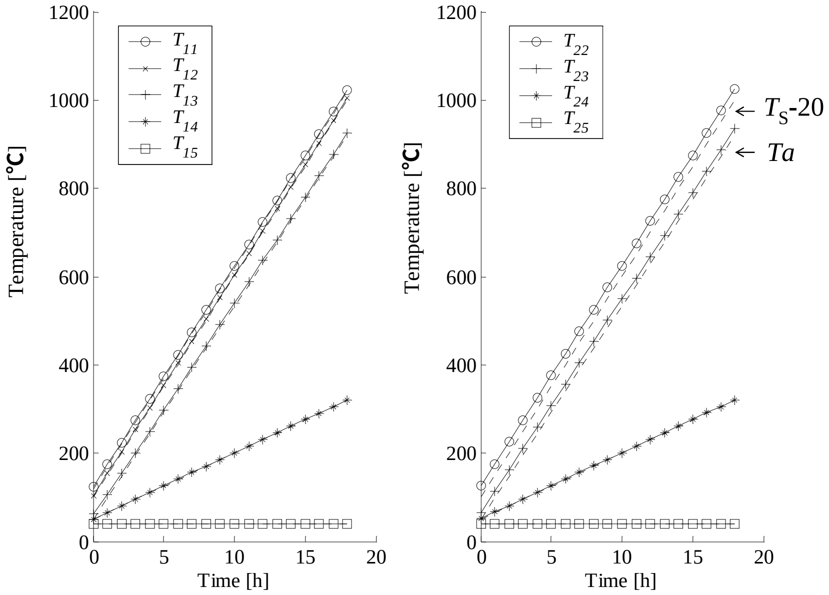

Fig. 8 Temperature profiles of SOFC system

6. CONCLUSION

We propose the process synthesis method which considers non-steady state operation for chemical processes. Furthermore, we developed a dynamic transshipment model to describe heat accumulation to main devices during the transitional operation, which is not included in the conventional extended transshipment model.

Effective use of the proposed two-step optimization method is demonstrated through a case study of a fuel cell system. The proposed method only requires information related to temperature profiles of process streams and heat capacities and heat transfer areas of main devices to derive the optimal heat exchanger network considering non-steady state operations, and those design specifications can usually be obtained at an early stage of the process design. The obtained design result can be used as the initial design for more precise optimization step. The proposed two-step optimization method that considers the non-steady state operation can also be applied to other chemical processes where the transitional operation is essential.

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