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MATHEMATICAL MODEL OF THERMAL REACTION PROCESS FOR EXTERNAL HEATING EQUIPMENT IN THE MANUFACTURE OF SEMICONDUCTORS (PART II)

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Abstract. *This paper proposes a mathematical model that is derived from bilinear partial differential equations (BPDs) in order to configure a control system including the external heat equipment (EHE) proposed in Part1. It is widely recognized that the mathematical model of the heat exchange unit has been reported. The target control system can be configured using the control parameter of the overall heat exchange coefficient (OHEC), which is given using a linear approximation from BPDs to an ordinary differential equation (ODE). The numerical simulation results are also represented for the optimal control system, and the gradient method is used in this simulation. Our findings show that this study is suitable for possible practical systems.*
Keywords: Semiconductor manufacturing equipment, Thermal reaction process, Bilinear partial differential equation, Distributed parameter system

1. **Introduction.** Previously, many studies on the optimal control system of a distributed parameter system (DPS) have been reported. With regard to the DPS, these studies have been reported and incorporate advanced mathematics such as the semigroup theory. The models in the previous studies focus on hyperbolic partial differential equations and the variable parameters depending on time and spatial parameters [1].

In such DPS studies, the derivation of optimal control systems is proposed using a bilinear partial differential equation (BPD). The DPS with time delay is proposed for a feedback control system [3]. With regard to the DPS, the target model is described by a hyperbolic partial differential equation. This mathematical model includes a diffusion term and an advection term, and it has been reported that the control system can be configured in a more realistic manner [4].

With regard to nonlinear DPS, this study focuses on an optimal control system. The analytical process uses a linearization method that approximates from an infinite-dimensional space to a finite-dimensional space. This method uses the single-network adaptive-type neural network, and is considered to be a very interesting area of research [5].

With regard to the optimal control system for heat exchange, a previous study obtains the optimal solution that approximates from BPDs to ODE along characteristic curves

[6]. This paper obtains the optimal configuration and optimal strategy for semiconductor manufacturing equipments by applying the idea proposed by Shima et al. Our proposed system was constructed using the control parameter of the overall heat exchange coefficient (OHEC). This approach is suitable for constructing a relatively practical system. The numerical simulation results are also reported for an optimal control solution. The gradient method is used in this simulation. The findings show that this study is suitable for possible practical system.

2. **Modeling for Heat Reaction Process.** Figure 1 shows the schematic diagram of a heat reaction unit.

Let the parameters used in this study define as follows:

Definition 2.1. *Definitions for various variables*
$v_b = V_b + L_b S$: *Substantial volume of the reaction process unit* $[m^3]$
$v_h = V_h + L_h S$: *Substantial volume of the heater unit* $[m^3]$
V_b: *Substantial volume of the heater unit* $[m^3]$
V_h: *Substantial volume of the heater unit* $[m^3]$
L_b: *Effective length of the reaction process side* $[m]$
L_h: *Effective length of the heater unit* $[m]$
S: *Cross-sectional area of the pipe* $[m^2]$
Θ_b: *Internal temperature of the reaction process* $[K]$
Θ_h: *Internal temperature of the heat unit* $[K]$
q: *Flow rate* $[m^3 \cdot s^{-1}]$
ρ: *Density of the reaction mixture* $[kg \cdot m^{-3}]$
c: *Heat capacity of the reaction mixture* $[Cal \cdot Kg^{-1} \cdot K]$
P: *Input power of the reaction process* $[W]$
H: *Input power of the heat unit* $[W]$
Θ_0: *Ambient temperature of the reaction process* $[K]$
P_b: *Exothermic reaction of the reaction process* $[W]$
κ_0: *Coefficient of heat dissipation to the outside* $[s^{-1}]$
$1/R$: *External radiation coefficient of the reaction mixture* $[s^{-1}]$
C_M: *Heat capacity of the heat unit* $[Cal \cdot Kg^{-1} \cdot K]$
Θ_c: *Ambient temperature from the outside* $[K]$
$U(t)$: *Overall heat transfer function (control parameter)*

As a method of heating films in the reaction process, the following two methods are considered.

The heat unit is installed directly into the reaction process unit as the built-in type in Figure 2(a), and the thermal model can be derived by

$$v_b \rho c \frac{d\Theta_b}{dt} = \kappa_0 v_b \rho c(\Theta_0 - \Theta_b) + P_b + P \tag{1}$$

where, let $\Theta_b(0) = \Theta_{b_0}$.

To realize semiconductor miniaturization processes, such systems that are widely used conventional methods were used until a few years ago. However, their usage is again increasing.

Figure 2(b) shows that the system is capable of heating the reaction liquid indirectly, instead of requiring that the heat exchange unit be installed directly into the reaction process.

The above system model as Figure 2(b) can be shown as Figure 3.

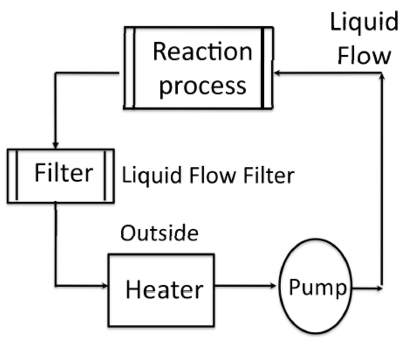

FIGURE 1. Schematic of reaction process

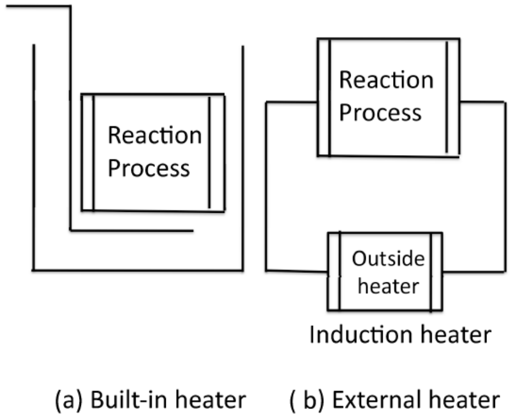

FIGURE 2. (a) Buit-in heater, (b) outside heater

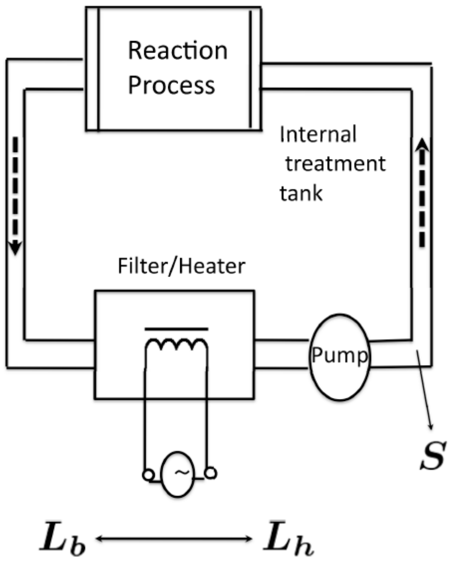

FIGURE 3. Detailed model of the external heat system

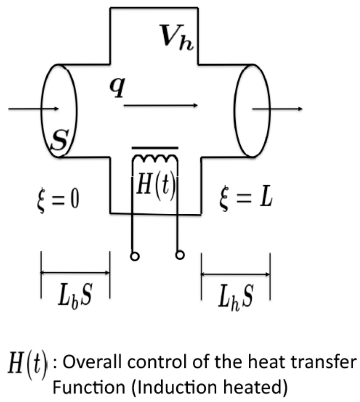

FIGURE 4. Conceptual model of the external heat

With regard to the external heat unit, Figure 4 shows the schematic diagram of this model. In this case, the model including the external heating equipment (EHE) is expressed as

$$v_b \rho c \frac{d\Theta_b}{dt} = \{-\Theta_b + \Theta_h(t, L))\} q \rho c + (\Theta_0 - \Theta_c)\kappa_0 v_0 \rho c + P_b \tag{2}$$

$$\frac{\partial \Theta_h(t,\xi)}{\partial t} + q(t)\frac{\partial \Theta_h(t,\xi)}{\partial \xi} = \frac{\hat{U}(t)}{RC_M}\{R\Theta_c(t) - \Theta_h(t.\xi)\} \tag{3}$$

$$\hat{U}(t) \equiv U(q, H, t : \xi) \tag{4}$$

where, let $U(t)$ be an OHEC, let ξ be a spatial variable at this time, and let $0 \leq \xi \leq L$, $L \cong L_b + L_h$.

Figure 5 shows the schematic diagram used to construct the control system configuration obtained using the exact linearization method. As shown in Figure 5, it can be described by BPDs including EHD. The control parameter is to use the OHEC.

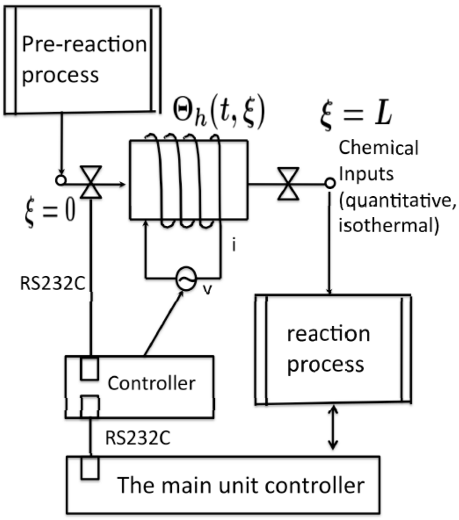

FIGURE 5. Reaction process control system equipment

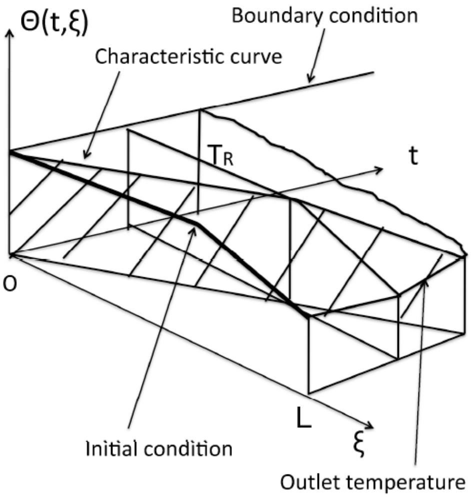

FIGURE 6. Temperature distribution $Theta(t, \xi)$

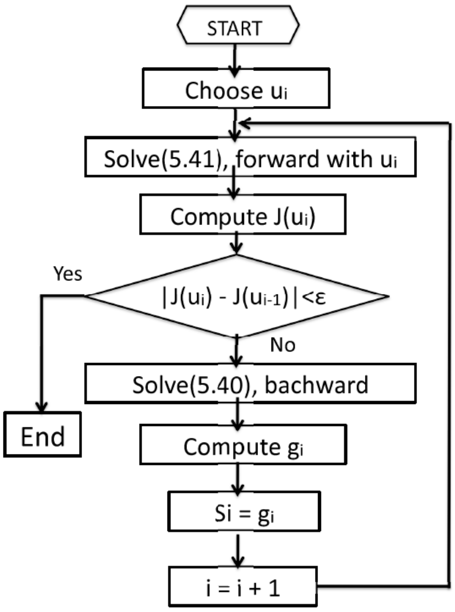

FIGURE 7. Computational procedure

As EHE is generally heat exchanger, EHE can be described by

$$\frac{\partial \Theta_h(t,\xi)}{\partial t} + q(t)\frac{\partial \Theta_h(t,\xi)}{\partial \xi} = \frac{1}{RC_M}\hat{U}(t,\xi)\left\{R\Theta_c(t) - \frac{A}{(V_h + L_h s)\rho_c}\Theta_h(t,\xi)\right\}$$
$$= \frac{\hat{U}(t,\xi)}{RC_M}\{k_0\Theta_c(t) - k_1\Theta_h(t,\xi)\} \quad (5)$$

where, the parameter A denotes a heat exchange effective area $[m^2]$, let $v_b = V_h + L_h s$, and $q(t)$ denotes the advection velocity of liquid.

3. **Flow Control on the Model Derived Using the BPDs-OHEC as the Control Parameter-.** This section discusses the optimal control problem derived by the BPDs.

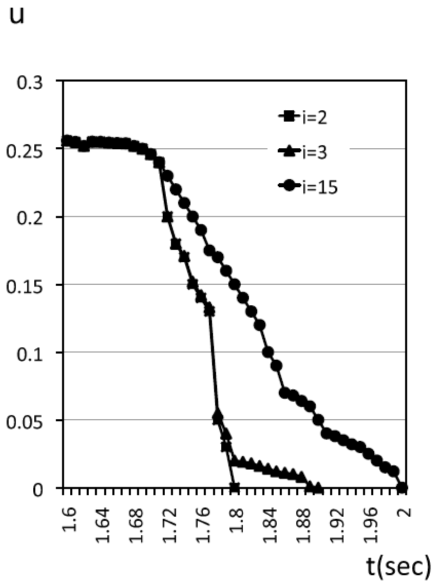

FIGURE 8. Computed control

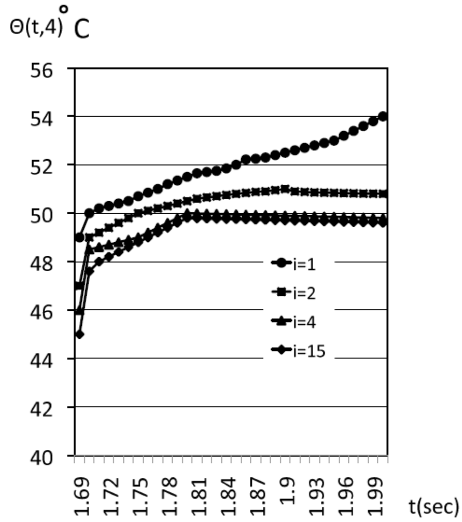

FIGURE 9. Behavior of temperature distribution

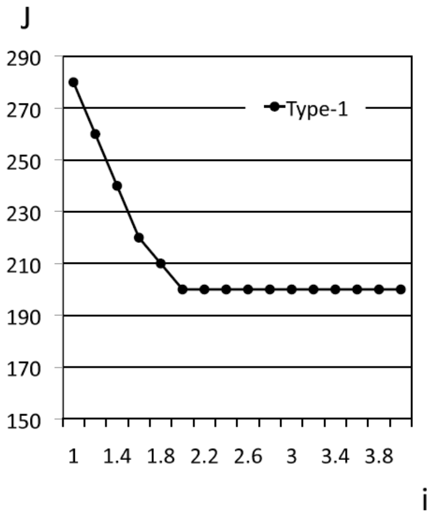

FIGURE 10. Behavior of performance index

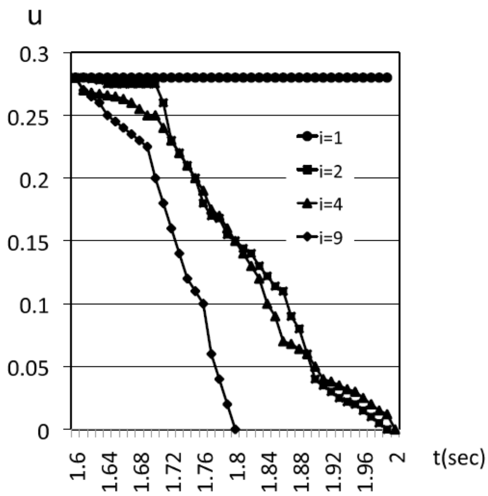

FIGURE 11. Computed control

Because Equation (5) is suitable for the target model system, it is obtained by

$$\frac{\partial \Theta_h(t,\xi)}{\partial t} + q(t)\frac{\partial \Theta_h(t,\xi)}{\partial \xi} = \frac{\hat{U}(t,\xi)}{RC_M}\{k_0\Theta_c(t) - k_1\Theta_h(t,\xi)\} \tag{6}$$

where, it assumes that $\Theta_c(t)$ is derived as follows:

Assumption 1.

$$\Theta_c(t) \equiv \Theta_c \ \ (const.) \tag{7}$$

From this assumption, Equation (6) can be rewritten by

$$\frac{\partial \Theta_h(t,\xi)}{\partial t} + q(t)\frac{\partial \Theta_h(t,\xi)}{\partial \xi} = \frac{\hat{U}(t,\xi)}{RC_M}\{k_0 - k_1\Theta_h(t,\xi)\} \tag{8}$$

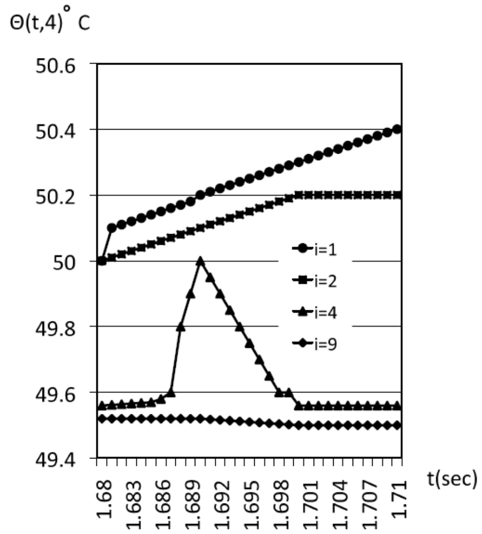

FIGURE 12. Behavior of temperature distribution

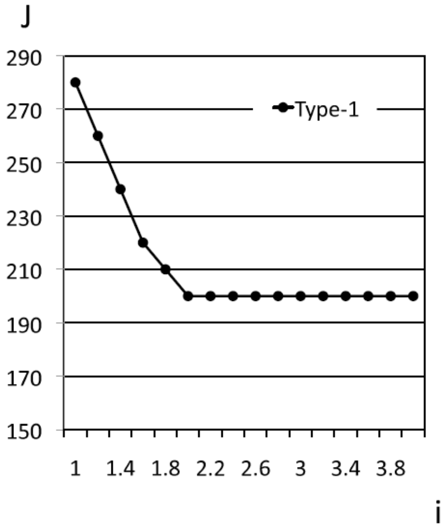

FIGURE 13. Behavior of performance index

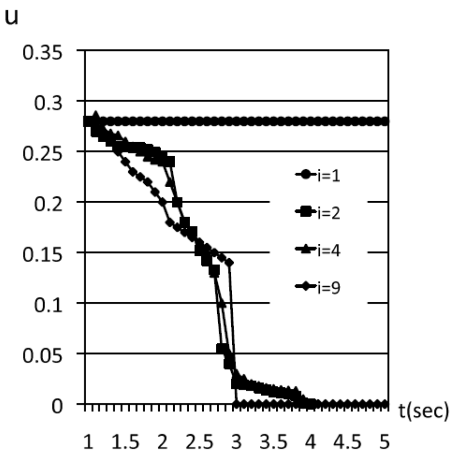

FIGURE 14. Computed control

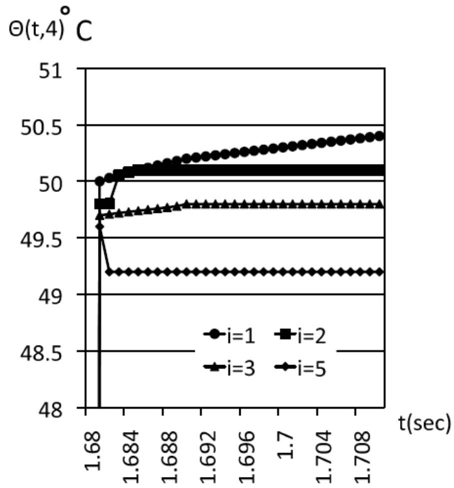

FIGURE 15. Behavior of temperature distribution

Let $w(t) = \hat{U}(\bullet)/RC_M$, Equation (8) is obtained by

$$\frac{\partial \Theta_h(t,\xi)}{\partial t} + q(t)\frac{\partial \Theta_h(t,\xi)}{\partial \xi} = w(t)\{k_0 - k_1\Theta_h(t,\xi)\} \tag{9}$$

The particular solution exists in Equation (9) as follows [7]:

1. $T \leq T_R$: T_R Residence time in the heat exchanger. The switching time T_0 is derived by

$$T_0 = -\frac{1}{M}\ln\frac{\Theta^* - k_0}{\Theta(t_f) - k_0} \tag{10}$$

(a) $\frac{\Theta - k_0}{\Theta(t_f) - k_0} < 1$,

$$u^* = M, \ {}^{\forall}t \leq T \tag{11}$$

$$u^* = \begin{cases} M: & 0 \leq t \leq T_0 \\ 0: & T_0 \leq t \leq T \end{cases} \tag{12}$$

(b) $\frac{\Theta - k_0}{\Theta(t_f) - k_0} > 1$,

$$u^* = m, \ {}^{\forall}t \leq T_0 \tag{13}$$

$$u^* = \begin{cases} m: & 0 \leq t \leq T_0 \\ 0: & T_0 \leq t \leq T \end{cases} \tag{14}$$

2. $T > T_R$

In the case of $T_R \leq t \leq T$, the desired temperature is maintained. In this case, the optimal control strategy can be determined by the dynamic characteristics of this system, and is derived by

$$u(t) - u(t - T_R) = 0, \ \ t \geq T_R \tag{15}$$

The optimal control strategy $u^*(t)$ within the residence time T_R is derived by

$$u^* = M \text{ or } m, \ {}^{\forall}t \leq T_0 \tag{16}$$

$$u^* = \begin{cases} m: & 0 \leq t \leq T_0 \\ 0: & T_0 \leq t \leq T \end{cases} \tag{17}$$

In the case where the residence time is exceeded, e.g., $u(t) = u(t - T_R)$, it is recommended that the process should be carried out repeatedly using the optimal control strategy $u^*(t)$. Let $u(t)$, $m \leq u(t) \leq M$ $(m < 0, M > 0)$.

If the residence time $0 \leq t \leq T_R$, the optimal control strategy $u^*(t)$ equals M (or m) uniformly. If the temperature does not reach the desired temperature, it is derived by

$$T_0 = -\frac{1}{M} \ln \frac{\Theta^* - k_0}{\Theta(t_f) - k_0} > T_R \tag{18}$$

As described above, the new desired temperature Θ^* exceeds the given limit, and it is physically impossible to satisfy such a change request.

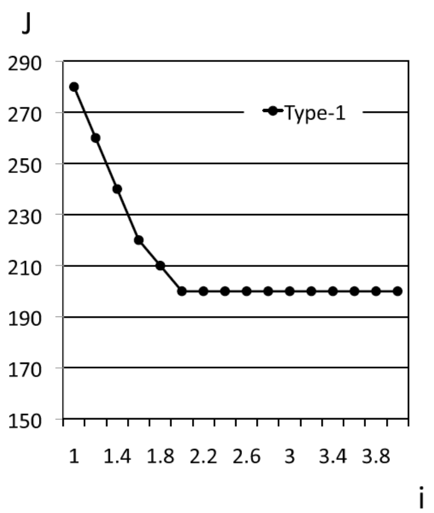

FIGURE 16. Behavior of performance index

4. **Numerical Example.** The purpose of this numerical examples indicates that the optimal control strategy and performance index varies when several parameters fluctuates. According to the parameter setting status, the convergence to the optimal control and the desired temperature is different respectively. However, the values of the evaluation function for all case of parameters obtain the similar results.

Here, in the numerical simulation, the target range of the residence time, we examine the case that it is the residence time (T) $T \leq T_R$. If the control parameter is designed according to the OHEC, the evaluation function, initial condition, and boundary condition are derived by

$$J = \int_0^T [\Theta_h(t, L) - \Theta^*]^2 dt \to \min_{w(t)} \tag{19}$$

$$\Theta_h(0, \xi) = \Theta_{h_0}(\xi) \tag{20}$$

$$\Theta_h(t, 0) = \Theta_{h_0}(t) \tag{21}$$

where, $\Theta_{h_0}(t)$ denotes the temperature at the entrance through which the object moves into the drying oven.

Here, to minimize Equation (19) given by Equations (20) and (21), it is to find the control parameter $w(t)$.

The theory of the first-order partial differential equation indicates that the ODE can be obtained from a first-order partial differential equation using the approximation method. To minimize Equation (19), ODE should be solved as follows [7]:

$$\frac{dt}{1} = \frac{d\xi}{q(t)} = \frac{d\Theta}{w(t)(k_0 - \Theta} \tag{22}$$

The characteristic curves can be obtained by integrating Equation (22). However, there are two cases for which the control time T is within the residence time T_R and exceeds it. Both the initial and boundary conditions need to be considered. For the initial condition, the characteristic curves are derived as follows (See Figure 6):

$$\Theta(t, \xi) = k_0 + \left\{ \Theta_0 \left(\xi - \int_0^t q(\tau) d\tau \right) - k_0 \right\} \times \exp \left(\int_0^t w(\tau) d\tau \right) \tag{23}$$

The temperature of the way out at $\xi = L$ in the drying oven is given by

$$\Theta(t, L) = k_0 + \left\{ \Theta_0 \left(L - \int_0^t q(\tau) d\tau \right) - k_0 \right\} \times \exp \left(\int_0^t w(\tau) d\tau \right) \tag{24}$$

To consider the control strategy used by the OHEC, let $q(t) = q_0$, and the control function is rewritten by

$$u(t) = w(t) - w_0 \tag{25}$$

$$z(t) = \Theta(t, L) - k_0 \tag{26}$$

Substituting into the above equation, the optimal control function $u(t)$ must be

$$\dot{z}(t) = -u(t) z(t) \tag{27}$$

From Equation (27), the control problem requires us to identify a control method that minimizes Equation (19) by the gradient method under the control parameter limitation of $m \leq u(t) \leq M$ $(m < 0, M > 0)$. The Hamiltonian on this problem is as follows [8]:

$$H = -\frac{1}{2}(z - \Theta^* + k_0) \tag{28}$$

The differential equation that should satisfy the optimal trajectory is obtained by

$$\dot{\varphi} = -\frac{\partial H}{\partial z} = u\varphi + (z - \Theta^* + k_0) \tag{29}$$

$$\dot{z} = -\frac{\partial H}{\partial \varphi} = -uz \tag{30}$$

where, $\varphi(t)$ denotes the conjugate condition variable.

Let the initial condition be $z(0) = \Theta_0(L) - k_0$, the final condition $z(T)$ is no constraint, and let $\varphi(T) = 0$.

According to the previous study, the gradient function that is used to search for the optimal solution is as follows [8]:

$$g(t) = -\left(\frac{\partial H}{\partial u}\right)_{z(t),u(t),\varphi(t)} = \varphi(t) \cdot z(t) \tag{31}$$

We now discuss the computational algorithm. The discrete control function u_{i+1} is derived by

$$u_{i+1} = u_i - \alpha \left(\frac{\partial H}{\partial u}\right)_{z_i,u_i,\varphi_i} \tag{32}$$

where, α denotes a gradient coefficient.

Because the control function u_{i+1} is constrained, this control function is determined using the following method.

It has been already known that the optimal control strategy is the bang-bang control and singular control. It is sufficient to discuss the constraints of the control function, and its constraints of the control function are derived by

$$u^* = \begin{cases} M \text{ or } m: & 0 \le t \le T_0 \\ 0: & T_0 \le t \le T_R \end{cases} \tag{33}$$

With regard to the calculation algorithm, see Figure 7.

Table 1. Set parameter values

Figure 8, Figure 9	Figure 11, Figure 12	Figure 14, Figure 15
Time step $= 1 \times 10^{-1}$	Time step $= 1 \times 10^{-2}$	Time step $= 1 \times 10^{-3}$
Slope coefficient $= 1 \times 10^{-3}$	Slope coefficient $= 1 \times 10^{-2}$	Slope coefficient $= 1 \times 10^{-1}$
$\epsilon = 1 \times 10^{-9}$	$\epsilon = 1 \times 10^{-9}$	$\epsilon = 1 \times 10^{-9}$

The various values used in the numerical simulation here are as follows. $\Theta^* = 50$°C, $k_0 = 100$°C, $\Theta_0(0) = \Theta_0(L) = 20$°C, $q_0 = 1$m/sec, $L = 4$m, $T_R = 4$sec, $T = 3$sec, $u = w(t) - w_0 = 0.40 - 0.1z = 0.28$.

5. **Conclusion.** As described above, by transforming the BPDs along the characteristic curves, we were able to obtain the exact mathematical model. Note that the translated ODE was given by the finite-dimensional optimal control problem. We were able to find the optimal solution by solving the optimal problem that controls the parameter as the OHEC under ODE. It is theoretically easy to understand the concept that approximates from BPDs to ODE using the characteristic curves.

Therefore, we confirmed that the control strategy became a bang-bang control by taking a specific fixed value, and another strategy that was called the singular control had a value of zero.

This paper also presented the simulation results that were used to calculate the ODE for the evaluation of the outlet side temperature using the gradient method. However, our simulation results were not compared with those of other methods, because the approach used in this paper has been used for optimal problems with conventional heat exchange. Therefore, this approach is useful for engineering techniques.

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