N	= number of cells in pneu-escalator	[—]		pneu-escalator	[°]
$P(N, m)$	= fraction of particles experiencing mixing m times through N cells	[—]	θ_p	= inclination angle of sectionalizing plate	[°]
S	= cross-sectional area of sampling case	[cm ²]	ρ_b	= bulk density of particles	[g/cc]
t	= discharge time	[sec]	σ^2	= variance of residence time of particles within pneu-escalator	[—]
$\bar{t}$	= average residence time of particles within pneu-escalator	[sec]	ϕ	= dimensionless time defined by Eq.(10)	[—]
t_c	= average residence time of particles within one cell	[sec]			
θ	= dimensionless time defined by Eq.(5)	[—]			
θ_f	= inclination angle of the filter of	[—]			

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ON DESIGN MARGIN FOR PROCESS SYSTEM WITH PARAMETER UNCERTAINTY*

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A method of determining rational design margin of unit operation in a process is developed by taking account of parameter uncertainties usually involved in actual process system design. Since decision variables which are to be determined in process system design consist of design variables and manipulating variables, design may be estimated rationally by considering admissible ranges of manipulating variables. The method proposed in this paper is applied to design of a simple chemical reaction process with recycle, and the result obtained by this method is compared with that obtained by the method proposed previously by the authors.

Introduction

In usual process system design, the nominal design value is enlarged by a design margin or safety factor for compensation of undesirable effects of many uncertainties included in design procedure and in system operation. Quantitative and rational evaluation of design margin, however, has not been discussed sufficiently, especially for a large, complex process system.

The authors have proposed a method to estimate quantitative design margin taking account of parameter uncertainty^{4,5)}. In this paper a method is developed to determine design margin in concert with manipulating variable. Since decision variables consist of design variables and manipulating variables design margin may be determined rationally by considering ranges of the manipulating variables. The method proposed in this report is simpler in calculation than the other method^{2,3)}, and also can give some important information in design procedure, such as which manipulating variable strongly affects output variables and

performance index. At the end of this paper, the design of a chemical reaction process with recycle is described as a numerical example of the proposed method.

Design Margin in Concert with Control of Manipulating Variable

Description of problem

The system equations of a process system can be described by

$$f_1(x, u, M, P) = 0 \quad (1)$$

where, x , u , M , P , f_1 denote n -dim. vector of state variables, r -dim. vector of manipulating variables, m -dim. vector of design variables, p -dim. vector of parameters and n -dim. vector function, respectively.

Here, design and manipulating variables are defined as follows; Design variable M represents the variable which cannot be altered after being determined. On the other hand, manipulating variable u represents the variable which can be changed after the process is constructed.

Output variables from the process l -dim. vector Z is given by

$$Z = f_2(x, u, M, P) \quad (2)$$

where f_2 represents l -dim. vector function ($l < r$).

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Output vector Z is desired to be a certain specified value, C .

$$Z = C \quad (3)$$

where C is l -dim. constant vector. Nominal optimum design means that decision variables u and M are determined so that the value of a performance index J given by Eq.(4) takes the minimum value under the conditions of given parameter value $\bar{P}$ and output value C .

$$J = g(x, u, M) \quad (4)$$

If the true value of parameter $\bar{P}$ is given a priori, it may be enough for practical design to calculate the nominal optimum decision values $\bar{u}$, $\bar{M}$ based on the nominal parameter value $\bar{P}$. Value of parameter P included in Eq.(1) and Eq.(2), however, involves an inevitable error of estimation, and also frequently deviates from the nominal value $\bar{P}$ during operating period. Usually, a design margin or safety factor is applied to the nominal design value for compensation of undesirable deviation of output variable or system performance caused by such parameter uncertainties. The problem investigated in this paper is to estimate a reasonable design margin ΔM which must be added to the nominal design value $\bar{M}$.

Determination of reasonable design margin

It is assumed that only the range of parameter deviation, that is, upper and lower limit of parameter deviation, is known, and that the probability density function of parameter deviation is not given a priori. If the probability density function is given, a different method from that proposed here, such as the statistical decision method, may be applied. The equality constraint Eq.(3) means practically an inequality constraint, that is, the output Z is allowed to deviate only in a specified direction or range. Moreover the direction of deviation of output Z which has a bad effect on the performance index may usually be known. These assumptions might be reasonable in practical process design.

Then the problem investigated here is to determine the value of design variable, $M (= \bar{M} + \Delta M)$, so as to fulfill a specified performance under the condition of parameter deviation in a given range. The principle of determining design variable $M (= \bar{M} + \Delta M)$ is to minimize the performance index which is evaluated when the process is designed so as to satisfy a specified performance under any given conditions of parameter deviation.

This problem can be solved as follows by using a first-order approximation which is convenient to evaluate the effect of parameter deviation on the performance index and the output variables. The first-order approximation is evaluated at nominal value of parameter, $\bar{P}$ and design margin ΔM is determined as below based on $\bar{P}$.

When parameter deviates by ΔP from the nominal value $\bar{P}$, and decision variables u and M are also moved by Δu and ΔM respectively from the nominal opti-

mum values $\bar{u}$ and $\bar{M}$, the deviation of state variable Δx is given from Eq.(1) as

$$\Delta x = - \left(\frac{\partial f_1}{\partial x} \right)^{-1} \left\{ \frac{\partial f_1}{\partial u} \Delta u + \frac{\partial f_1}{\partial M} \Delta M + \frac{\partial f_1}{\partial P} \Delta P \right\} \quad (5)$$

where $\partial f_1 / \partial x$ represents $n \times n$ nonsingular matrix and $\partial f_1 / \partial u$, $\partial f_1 / \partial M$, $\partial f_1 / \partial P$ represent $n \times r$, $n \times m$, $n \times p$ matrices, respectively. Superscript -1 indicates the inverse matrix. These matrices are evaluated at $\bar{P}$, $\bar{u}$, $\bar{M}$. Substituting Eq.(5) into the equation for small perturbation of Eq.(2), the deviation of output vector ΔZ is given by the equation

$$\begin{aligned} \Delta Z = & \left\{ \frac{\partial f_2}{\partial u} - \frac{\partial f_2}{\partial x} \left(\frac{\partial f_1}{\partial x} \right)^{-1} \frac{\partial f_1}{\partial u} \right\} \Delta u \\ & + \left\{ \frac{\partial f_2}{\partial M} - \frac{\partial f_2}{\partial x} \left(\frac{\partial f_1}{\partial x} \right)^{-1} \frac{\partial f_1}{\partial M} \right\} \Delta M \\ & + \left\{ \frac{\partial f_2}{\partial P} - \frac{\partial f_2}{\partial x} \left(\frac{\partial f_1}{\partial x} \right)^{-1} \frac{\partial f_1}{\partial P} \right\} \Delta P \end{aligned} \quad (6)$$

where $\partial f_2 / \partial x$, $\partial f_2 / \partial u$, $\partial f_2 / \partial M$ and $\partial f_2 / \partial P$ are $l \times n$, $l \times r$, $l \times m$, $l \times p$ matrices evaluated at $\bar{P}$, $\bar{u}$, $\bar{M}$, respectively. The range of parameter deviation ΔP is assumed to be given by p -dim. constant vector η from experience or experiment. Moreover, the allowable range of output deviation ΔZ is assumed to be given by $\Delta C_L \leq \Delta Z \leq \Delta C_U$, where ΔC_L and ΔC_U express the lower and the upper limits for an allowable range of ΔZ . Therefore the rational design margin can be determined based on the relation

$$\begin{aligned} \text{Min}_{\Delta M, \Delta u} \{ \Phi = \Phi(\Delta M, \Delta u) \mid \Delta C_L \leq \Delta Z \leq \Delta C_U, \Delta M \geq 0, \\ \Delta P_k = \pm \eta_k, \Delta u \in U \} \quad k = 1, 2, \dots, p \end{aligned} \quad (7)$$

where U represents a domain of admissible control Δu , and ΔZ must be subjected to Eq.(6).

The sign of ΔP_k which is a component of ΔP should be chosen so that the deviation of ΔP_k causes an undesirable effect on ΔZ_i . For example, let us consider the case where the following equations can be written for Eq.(6),

$$\begin{aligned} \Delta Z_1 &= a_1 \Delta u + b_1 \Delta M + d_1 \Delta P_1 + e_1 \Delta P_2 \\ \Delta Z_2 &= a_2 \Delta u + b_2 \Delta M + d_2 \Delta P_1 + e_2 \Delta P_2 \end{aligned} \quad (6)'$$

and where the allowable ranges of ΔZ_1 and ΔZ_2 are given by

$$\begin{aligned} \Delta C_{L1} &\leq \Delta Z_1 \leq \Delta C_{U1} \\ \Delta C_{L2} &\leq \Delta Z_2 \leq \Delta C_{U2} \end{aligned} \quad (7)'$$

ΔC_L may usually take negative value for many cases. Moreover, the constraint for ΔZ sometimes needs either the upper or the lower bound only. The sign of ΔP is uncertain, and it cannot generally be known whether ΔP takes negative or positive value. Only the absolute value of ΔP can be estimated. In some cases, it may be clear that P changes dynamically in one direction from the nominal value of $\bar{P}$.

Assuming that d_1 and e_1 take positive values and that ΔZ_1 must not be over the positive value of ΔC_{U1} , the sign of ΔP_1 or ΔP_2 must be positive. Assuming that d_2

and e_2 take negative value and positive value, respectively, and that ΔZ_2 must be greater than the negative value of ΔC_{L2} , the sign of ΔP_1 and ΔP_2 must be positive and negative, respectively. Practically it does not happen that ΔP_2 takes simultaneously positive value for ΔZ_1 and negative value for ΔZ_2 , but the above treatment gives a result in the direction of safety. In general, Φ represents a negative effect for adding some margin to the nominal design values. Here, Φ is defined as the first variation of the performance index J due to Δu and ΔM . The physical meaning of this definition is to determine the margins of design and manipulating variables so that the deviation of J caused by ΔM and Δu becomes as small as possible. Then Φ is defined by

$$\Phi = \left\{ \frac{\partial g}{\partial M} - \frac{\partial g}{\partial x} \left(\frac{\partial f_1}{\partial x} \right)^{-1} \frac{\partial f_1}{\partial M} \right\} \Delta M + \left\{ \frac{\partial g}{\partial u} - \frac{\partial g}{\partial x} \left(\frac{\partial f_1}{\partial x} \right)^{-1} \frac{\partial f_1}{\partial u} \right\} \Delta u \quad (8)$$

where $\partial g/\partial x$, $\partial g/\partial M$ and $\partial g/\partial u$ are n -dim., m -dim. and r -dim. row vectors evaluated at $\bar{u}$, $\bar{M}$ and $\bar{P}$. In Eq.(8) the coefficients multiplied to ΔM and Δu are not in general equal to zero. Eq.(7) subjected to Eq.(8) is reduced to a linear programming (L.P.) problem because Φ is a linear function of ΔM and Δu . Hereafter, a solution of the L.P. problem is assumed to exist. After all, a reasonable design margin ΔM may be determined from the solution of the L.P. problem given by Eqs. (6)–(8). The design margin obtained by this method (denoted by Method I) may be more rational than that by the method proposed previously by the authors^{4,5)} (denoted by Method II) because the manipulating variables admissible in a certain specified range are considered. In fact, if the deviation Δu of a manipulating variable is sufficient to compensate for the undesirable parameter uncertainties and also minimizes Φ , the addition of a design margin to the nominal design variable is not always necessary. Moreover, it is also shown from this consideration which manipulating variable has a strong effect on the values of output variable and performance index.

Application to Design of a Simple Chemical Reaction Process with Recycle

Nominal optimum design at steady state

Let us consider the design margin of the reactor in a simple chemical process with recycle shown in Fig. 1 as an example of the method proposed in this paper. The reactor is assumed to be a single C.S.T.R. with perfect mixing and the type of reaction is assumed to be Denbigh's reaction, which comprises first order elementary reactions as shown in Fig. 2. R is the desired product, and this is produced from fresh feed containing only A (molar concentration C_{A0} [gmol/l]). The effluent flow from the reactor containing A , B , R , X and Y is assumed to be separated into a product flow containing only R and another flow containing A , B , X and Y . X and Y are undesired products. A and B are

Fig. 1 A simple chemical reaction process with recycle

Fig. 2 Denbigh's reaction

Table 1 Given parameter values and boundary conditions

$F_{A0} = 100$ mol/hr,	$C_{A0} = 0.1$ mol/l,	$k_B = 0.4$ hr ⁻¹
$k_R = 0.1$ hr ⁻¹ ,	$k_X = 0.02$ hr ⁻¹ ,	$k_Y = 0.01$ hr ⁻¹
$C_1 = 70$ mol/hr,	$C_2 = 0.005$ mol/l,	
$\$b = 0.01$ \$/l,	$\$r = 0.125$ \$/mol/hr	

Table 2 Nominal optimum design

$\bar{F}_i = 320$,	$\bar{V} = 1.27 \times 014$,	$\bar{\alpha} = 0.921$,	$\bar{\beta} = 0.278$
$\bar{x}_A = 0.179$,	$\bar{x}_B = 0.552$,	$\bar{x}_X = 0.020$,	$\bar{x}_Y = 0.030$
$\bar{x}_R = 0.219$,	$\bar{J} = 154\$$		

partially recycled at the ratio of α to the amount of A and B in the inlet flow to the separator, and X and Y are also recycled at the ratio of β . Denoting the fraction of molar concentration C_i [gmol/l] of each component i to C_{A0} ($C_i = C_{A0}x_i$, $i = A, B, R, X, Y$) by x_i , the hourly molar flow rate of fresh feed by F_{A0} [mol/hr], the flow rate of the inlet flow into the reactor which consists of fresh feed and recycle flow by F_i [mol/hr] ((volumetric flow rate) $\times C_{A0} = F_i$), and the volume of the reactor by V , the process equations for steady state are given by

$$\begin{aligned} F_{A0} + \alpha F_i x_A - F_i x_A - V(k_B + k_X)C_{A0} x_A &= 0 \\ \alpha F_i x_B - F_i x_B + VC_{A0} \{k_B x_A - (k_R + k_Y)x_B\} &= 0 \\ \beta F_i x_X - F_i x_X + VC_{A0} k_X x_A &= 0 \\ \beta F_i x_Y - F_i x_Y + VC_{A0} k_Y x_B &= 0 \\ -F_i x_R + VC_{A0} k_R x_B &= 0 \\ x_A + x_B + x_R + x_X + x_Y &= 1 \end{aligned} \quad (9)$$

where k_i ($i = B, R, X, Y$) [1/hr] shows the reaction rate constant for each elementary reaction. These equations correspond to Eq.(1) for general expression.

Output state Z_1 and Z_2 are defined as

$$\begin{aligned} Z_1 &= F_i x_R \\ Z_2 &= (x_X + x_Y)C_{A0} \end{aligned} \quad (10)$$

Z_1 is the amount of R produced hourly and Z_2 is the molar concentration of undesired products X and Y . It is assumed that the values of Z_1 and Z_2 are desirable to be maintained as

Table 3 Rational design margin for parameter uncertainty

Allowable ranges of $\Delta Z_1, \Delta Z_2$				Design margin						
case	ξ_1	ξ_2	ξ_3	by the method proposed here				by the previous method		
				ΔV	$\Delta\alpha$	$\Delta\beta$	ΔJ	ΔV	worst ΔZ_2	ΔJ
1	1.0	2×10^{-4}	10.75×10^{-4}	1097	-0.018	-0.278	1.26	565	7.94×10^{-4}	3.36
2	1.0	2×10^{-4}	20×10^{-4}	233	0.0022	-0.278	0.0095	565	7.94×10^{-4}	3.36
3	1.0	2×10^{-4}	22.5×10^{-4}	0	0.0076	-0.278	-0.326	565	7.94×10^{-4}	3.36
4	1.0	4×10^{-4}	20×10^{-4}	233	0.0022	-0.278	0.0095	565	7.94×10^{-4}	3.36
5	1.5	2×10^{-4}	20×10^{-4}	150	-0.0008	-0.278	-1.01	365	6.68×10^{-4}	2.17

where $|\Delta k_B| \leq 0.08, |\Delta k_X| \leq 0.04, \Delta Z_1 \geq -\xi_1, \xi_2 \geq \Delta Z_2 \geq -\xi_3$

$$\begin{aligned} Z_1 &= C_1 \\ Z_2 &= C_2 \end{aligned} \quad (11)$$

Eqs.(10) and (11) correspond to Eqs.(2) and (3), respectively. For simplicity the following objective function is assumed for the numerical calculation.

$$\begin{aligned} J &= \left(\text{volume of reactor} \right) \left(\text{unit cost of reactor} \right) + \left\{ \left(\text{recycle rate of } A \text{ and } B \right) \right. \\ &\quad \left. + \left(\text{recycle rate of } X \text{ and } Y \right) \right\} \left(\text{unit cost for recycle} \right) \\ &= V\$_b + \{ \alpha F_i(x_A + x_B) + \beta F_i(x_X + x_Y) \} \$_r \end{aligned} \quad (12)$$

Practical performance index J might be more complex, but the above simplification may be enough to illustrate a numerical example of design margin problem. This form of J is referred to in the literature¹⁾.

Nominal optimum design is to determine the values of design variable V and operating variables α and β which minimize the value of performance index J given by Eq.(12), subjected to Eqs.(9), (10) and (11) under the specified values of F_{A0}, C_{A0}, C_1 and C_2 . The values of parameters and the boundary conditions used in the numerical calculation are given in **Table 1**. The results of numerical calculation are shown in **Table 2**. The following can be recognized from the results; i) β is not equal to zero. Partial recycle of X and Y is more effective than no recycle of X and Y because the output molar concentration of X and Y , that is, Z_2 , is specified. ii) The optimum recycle rate is 320 moles/hr in this example, and the optimum retention time in the reactor is about 4 hr based on C_{A0} .

Design margin for parameter uncertainty

For simplicity, the rate constants k_B and k_X are assumed to involve the maximum estimation error of $\eta^\circ\%$ for absolute values of the nominal values $\bar{k}_B$ and $\bar{k}_X$, respectively.

$$|\Delta k_B| \leq \frac{\eta^\circ}{100} \bar{k}_B, \quad |\Delta k_X| \leq \frac{\eta^\circ}{100} \bar{k}_X \quad (13)$$

The value of η° is taken as 20 in this example. It is assumed that the allowable ranges for deviation of output variables Z_1 and Z_2 are given by

$$\Delta Z_1 \geq -\xi_1, \quad \xi_2 \geq \Delta Z_2 \geq -\xi_3 \quad (14)$$

The movable ranges of $\Delta\alpha, \Delta\beta$ (deviation of manipulating variables α and β) and ΔV (margin for design variable V) are constrained by

$$-\bar{\alpha} \leq \Delta\alpha \leq (1-\bar{\alpha}), \quad -\bar{\beta} \leq \Delta\beta \leq (1-\bar{\beta}), \quad \Delta V \geq 0 \quad (15)$$

The design margin ΔV can be determined by solving the L.P. problem, which is composed of Eqs.(6)–(8) and Eqs.(13)–(15). The result is shown in **Table 3** for various allowable ranges of ΔZ_1 and ΔZ_2 . The design margin calculated by the method presented in the literature⁴⁾ (Method II) which does not take account of operation of manipulating variables, are also shown in the right column of Table 3. In the case by Method II, design margin ΔV cannot compensate for undesirable deviation ΔZ_2 because the coefficient multiplied to ΔV in the equation of ΔZ_2 is positive and ΔZ_2 is greater than ξ_2 even if ΔV is equal to zero. That is, by Method II, there is no feasible solution of the L. P. problem composed of Eqs.(6)–(8) and Eqs.(13)–(15). Then the design margin ΔV by Method II is determined so as to satisfy only the constraint of ΔZ_1 .

From this calculated result the following points are concluded. i) Comparing the method proposed in this paper (Method I) with Method II, the design margin ΔV and the increment ΔJ of performance index J by Method I are smaller than those by Method II in each case except for case 1. For example, in case 2, ΔV by Method I is 233 l, which corresponds to about 2% of nominal value $\bar{V}$. On the other hand, ΔV by Method II is 565 l, which corresponds to about 4.5% of nominal value. ΔJ by Method II is about 350 times as much as that by Method I. In case 1, ΔJ by Method II is about 3 times that by Method I, in spite of the fact that ΔV by Method II is smaller than that by Method I. Moreover, the deviation of output Z_2 due to uncertainty of k_B, k_X cannot be compensated by Method II, and the deviation ΔZ_2 is about 3 times ξ_2 . These results suggest that Method I is more reasonable than Method II. ii) It becomes clear by comparing case 2 and case 3 that manipulating variable β can sufficiently compensate for the effect of Δk_B and Δk_X so that ΔZ_2 is smaller than ξ_2 . It also becomes clear by comparing case 2 and case 5 that the estimated design margin ΔV decreases if ξ_1 becomes smaller. iii) If ξ_3 is greater than or equal to 22.5×10^{-4} , the design margin ΔV is zero, as shown in case 3. That is, α and β can sufficiently control ΔZ_2 within the specified allowable ranges of ΔZ_2 .

Conclusion

A method to determine rational design margin taking account of parameter uncertainty is developed for practical process system design. The design margin is determined by minimizing the deviation of a performance index under the allowable limitation of the deviation of output variables. An altered form of the performance index, however, may have to be considered in the future. The method proposed here is applied to design of a simple chemical reaction process with recycle. Numerical calculation shows that this method is more rational and practical.

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Nomenclature

A	= reactant	
B	= intermediate product	
ΔC_L	= allowable lower limit of the deviation of output vector	
ΔC_U	= allowable upper limit of the deviation of output vector	
C_i	= molar concentration of i -th component ($i=A, B, R, X, Y$)	[mol/l]
F_{A0}	= mole flow rate of fresh feed	[mol/hr]
F_i	= output flow rate from reactor	[mol/hr]
k_i	= reaction rate constant ($i=B, X, Y, R$)	[1/hr]
M	= m -dim. column vector of design variable	
$\bar{M}$	= nominal optimum value of M	
ΔM	= deviation of design variable from $\bar{M}$	
P	= p -dim. column vector of parameter	
$\bar{P}$	= nominal value of P	
ΔP	= deviation of parameter from $\bar{P}$	
R	= desired product	

u	= r -dim. column vector of manipulating variable	
$\bar{u}$	= nominal optimum value of u	
Δu	= deviation of u from $\bar{u}$	
V	= tank volume	[l]
$\bar{V}$	= nominal optimum value of V	[l]
ΔV	= design margin of V	[l]
x_i	= mol fraction of each component i to C_{A0} [$i=A, B, X, Y, R$]	[—]
X	= undesired product	
Y	= undesired product	
$\$b$	= hourly unit cost of reactor	[\$/l/hr]
$\$r$	= unit cost of recycle of A, B, X and Y	[\$/mol]
α	= recycle ratio of A and B	[—]
β	= recycle ratio of X and Y	[—]
ξ_i	= allowable upper or lower limit of output variable in Eq.(14) ($i=1, 2, 3$)	
η	= p -dim. vector of the range of parameter deviation	
η°	= relative range of parameter deviation in Eq.(13)	
η_k	= k -th element of vector η	
<Subscript>		
A	= reactant	
B	= intermediate product	
R	= desired product	
X	= undesired product	
Y	= undesired product	
<Superscript>		
-1	= inverse matrix	

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SHORT COMMUNICATIONS

A NOTE ON THIN FILM EVAPORATION — PREDICTION OF HEAT TRANSFER RATES* —

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Introduction and Analysis

Chun and Seban²⁾ experimentally investigated the falling-film evaporator under turbulent flow conditions of the liquid film. The data obtained are correlated by the following non-dimensional equation for the turbulent flow of the film.

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$$h \left(\frac{\nu_L^2}{gk^3} \right)^{1/3} = 3.8 \times 10^{-3} Re_L^{0.4} Pr_L^{0.65} \quad (1)$$

The data obtained are also compared to the analysis of Dukler³⁾ and it is observed that the deviation between the experimental results and the theoretical analysis is considerable. Dukler³⁾ obtained heat transfer rates in falling films by numerical integration, and the analysis did not offer any straightforward equation to facilitate ready computation. The present note attempts to establish an equation for heat transfer coefficient in explicit form making use of some of the available hydrodynamic aspects of falling liquid films. The