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An Algorithm for Optimal Design of Chemical Process Equipments and Its Application to Design of Shell-and-Tube Heat Exchangers

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A computer-oriented algorithm is presented for design of chemical process equipments, incorporating both optimality and realizability into the design. A table, which consists of all the physically realizable designs, is prepared for the equipment to be designed under a given specification. The designs in the table are arranged in order of the cost of the equipment that is to be made according to each design. Successive ratings of each design in the table (case studies) give the optimal one which meets the specification. An application of this algorithm to thermal design of shell-and-tube heat exchangers is described briefly.

1. Introduction

With recent development of digital computer systems, their ability to handle large quantities of information in a short time has been used extensively in design of chemical processes and equipments,[1,2] and use of digital computers now has become more than economy of man-hours for design calculations.

In design of chemical processes and equipments, certain optimality and realizability of the result are always required for a given specification. Various analytical and numerical techniques for optimization have been developed and applied to a variety of engineering problems.[3,4] In design of chemical process equipments, however, there is an inherent large number of independent variables to be considered, and this makes it laborious and even impossible for many cases to solve the design equations for an optimality both analytically and numerically. If an optimal design is obtained by any one of the conventional optimization techniques, its realizability is not always assured, since the size standardizations of the various constructing materials make it possible for the dimensions of a equipment to take only discrete values.[5,6,7] Incorporation of this limitation into the constraints for the optimal design equations will make it prohibitively difficult futher to solve them.

By conventional design methods with hand calculations, diagrams, tables and approximative equations are used with the aid of designer's intuitions and experiences, and over-designs far from the optimum are usually obtained.

In this paper, a computer-oriented algorithm is proposed for design of chemical process equipments, which incorporates both optimality and realizability into the design. An application of this algorithm to design of shell-and-tube heat exchangers is also demonstrated.

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2. Algorithm

Suppose that one has an equipment in a service and is to test whether it can be used for another service or not. This process is usually called "rating"[8] and consists of calculating the performance of the existing equipment in the specified conditions. If the evaluated performance is favorably comparable with that required, the equipment can be used for the new service. The "rating" is essential to the algorithm to be described now:

(1) All the designs, $\boldsymbol{S}_i$ $(i=1, 2, \cdots, n)$, which are regarded as physically realizable in accordance with a variety of the regulations and the codes, machinery conditions in a workshop and so on, are prepared for the equipment to be designed for a given specification. For example, in a shell-and-tube heat exchanger design, $\boldsymbol{S}_i$ is a set of; inner diameter of shell, outer diameter and length of tube, number of tubes, number of tube paths, tube arrangement, and baffle spacing, etc.

(2) A function $\mathrm{m}(\boldsymbol{S}_i)$ is defined as a measure of the cost of the equipment that is to be made according to the design $\boldsymbol{S}_i$. An example of such a measure is heat transfer area available in case of an exchanger design.

(3) All the $\boldsymbol{S}_i$'s listed in the step (1) are rearranged and numbered according to the relation

$$\begin{aligned} &\mathrm{m}(\boldsymbol{S}_1) \leqq \mathrm{m}(\boldsymbol{S}_2) \leqq \cdots \leqq \mathrm{m}(\boldsymbol{S}_n), \\ &(\text{if } j<k, \text{ then } \mathrm{m}(\boldsymbol{S}_j) \leqq \mathrm{m}(\boldsymbol{S}_k)). \end{aligned} \tag{1}$$

The set of all the $\boldsymbol{S}_i$'s thus obtained will be called the table **D**.

(4) A decision criterion for acceptance or rejection of a design $\boldsymbol{S}_j$ selected arbitrarily will now be defined: A design specification $\mathbf{P}_A$ may be regarded as the performance required of the service that the equipment should offer. The performance of a design $\boldsymbol{S}_j$, $\mathbf{P}(\boldsymbol{S}_j; \boldsymbol{p})$, can be calculated by the usual design equations for the equipment to be designed, where $\boldsymbol{p}$ is a set of parameters for the equations. $\boldsymbol{p}$ can be considered as a condition under which the equipment should be operated. $\mathbf{P}(\boldsymbol{S}_j; \boldsymbol{p})$ is compared with $\mathbf{P}_A$, and if $\mathbf{P}$ is equal or superior to $\mathbf{P}_A$, i.e., if the relation

$$\mathbf{P}(\boldsymbol{S}_j; \boldsymbol{p}) \geqq \mathbf{P}_A \tag{2}$$

holds, the design $\boldsymbol{S}_j$ is acceptable for the service.

Now, the algorithm for optimal design of physically realizable equipments can be best stated by the flow chart shown in Fig. 1. Successive rating of each design $\boldsymbol{S}_j$ in the table **D** for a given specification (case studies) could find the best one which meets the specification, and the design calculation finished. The design thus obtained, say $\boldsymbol{S}_q$, can offer the service required under the condition $\boldsymbol{p}$, is optimum in the sense that $\mathrm{m}(\boldsymbol{S}_q)$ is minimum, and is physically realizable.

This algorithm expects *a priori* the capability of modern digital computers to handle large quantities of data in a short time so that its implementation should be done by a digital computer program. Otherwise, the present algorithm may become substantially useless.

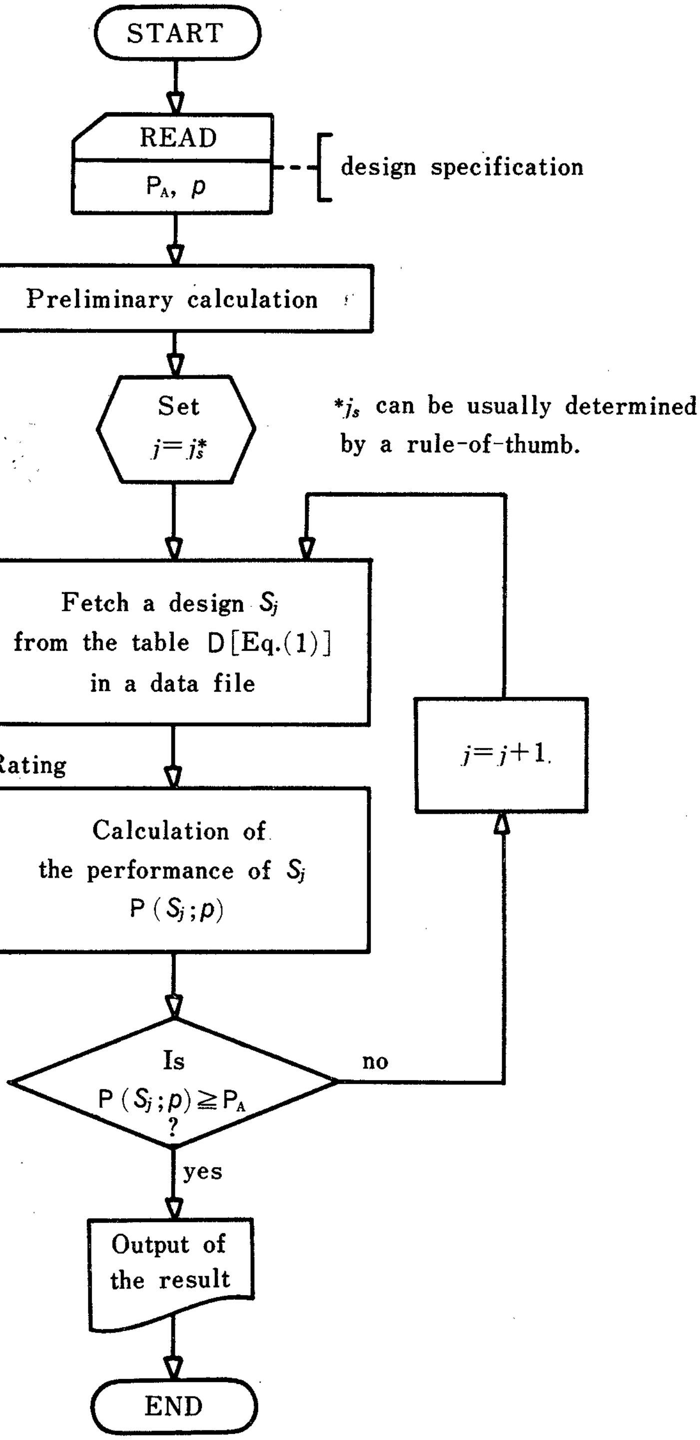

Fig. 1 Flow chart of an algorithm for optimal design of chemical process equipments

3. Application to thermal design of shell-and-tube heat exchanger

As an example of applications of the present algorithm, an optimal thermal design of shell-and-tube heat exchangers will be considered. Heat exchangers of this type find very wide applications in many of chemical plants and are well suitable to design by the present algorithm, because the size standardizations of various parts of the unit have been promoted strongly. For example, one can find the authorized standards for the exchanger in the JIS code and the JPI code.[6,7]

A fictious table of realizable designs for the exchangers is assembled by referring to the JIS code "B8249"[7] and the JPI code "7B-30-64",[6] as is shown partly in Table 1. Heat transfer area available of each exchanger design ($\boldsymbol{S}_j$) is chosen as the function $m(\boldsymbol{S}_j)$ in Eq. (1). Therefore, smaller number in Table 1 means smaller transfer area. The design specification is given in the form as shown in Table 2. The required performance

Table 1 A part of the table **D** for design of shell-and-tube heat exchangers

SHELL AND TUBE HEAT EXCHANGER						Page 1
Tube O.D. 25.4 mm Pitch 32.0 mm DELT STAT T-SHEET						
No.	Shell dia.	Tube-Length	L/D	Pass	Tubes	Area (m²)
1	199.9	1500	7.5	4	16	1.92
2	199.9	1500	7.5	2	18	2.15
3	199.9	1500	7.5	1	20	2.39
4	248.8	1500	6.0	4	24	2.87
5	248.8	1500	6.0	4	28	3.35
6	248.8	1500	6.0	2	32	3.83
7	248.8	1500	6.0	1	32	3.83
8	297.9	1500	5.0	4	38	4.55
9	248.8	2500	10.0	4	24	4.79
10	297.9	1500	5.0	6	42	5.03

↑ j ↑ heat transfer area

Table 2 Design Specification

		shell	tube
fluid flow rate	[kg/hr]	w_s	w_t
density	[kg/m³]	ρ_s	ρ_t
viscosity	[kg/m·hr]	μ_s	μ_t
heat capacity	[kcal/kg·°C]	C_s	C_t
thermal conductivity	[kcal/m·hr·°C]	k_s	k_t
inlet temperature	[°C]	t_{si}	t_{ti}
outlet temperature	[°C]	t_{so}	t_{to}
fouling factor allowable	[m²·hr·°C/kcal]	r_{dA}	
pressure drop allowable	[kg/cm²]	Δp_{sA}	Δp_{tA}

$\mathbf{P}_{\Delta}$ is a sef of $-\Delta p_{s\Delta}$, $-\Delta p_{t\Delta}$ and $r_{d\Delta}$ in this table and the others correspond to $\boldsymbol{p}$.

The performance of a design $\boldsymbol{S}_j$ can be calculated simply by using various equations given in the standard textbooks for exchanger design,[8,9,10] as

$$\mathbf{P}=\mathbf{P}(\boldsymbol{S}_j;\ \boldsymbol{p}), \tag{3}$$

where

$$\mathbf{P}=\{-\Delta p_s,\ -\Delta p_t,\ r_d\}.$$

In the present case, the condition of Eq. (2) is equivalent to the simultaneous equations

$$\left.\begin{array}{l}\Delta p_s \leqq \Delta p_{s\Delta} \\ \Delta p_t \leqq \Delta p_{t\Delta} \\ r_d \geqq r_{d\Delta}\end{array}\right\}, \tag{4}$$

and if Eq. (4) holds, the design $\boldsymbol{S}_j$ is for the realizable exchanger which can offer the

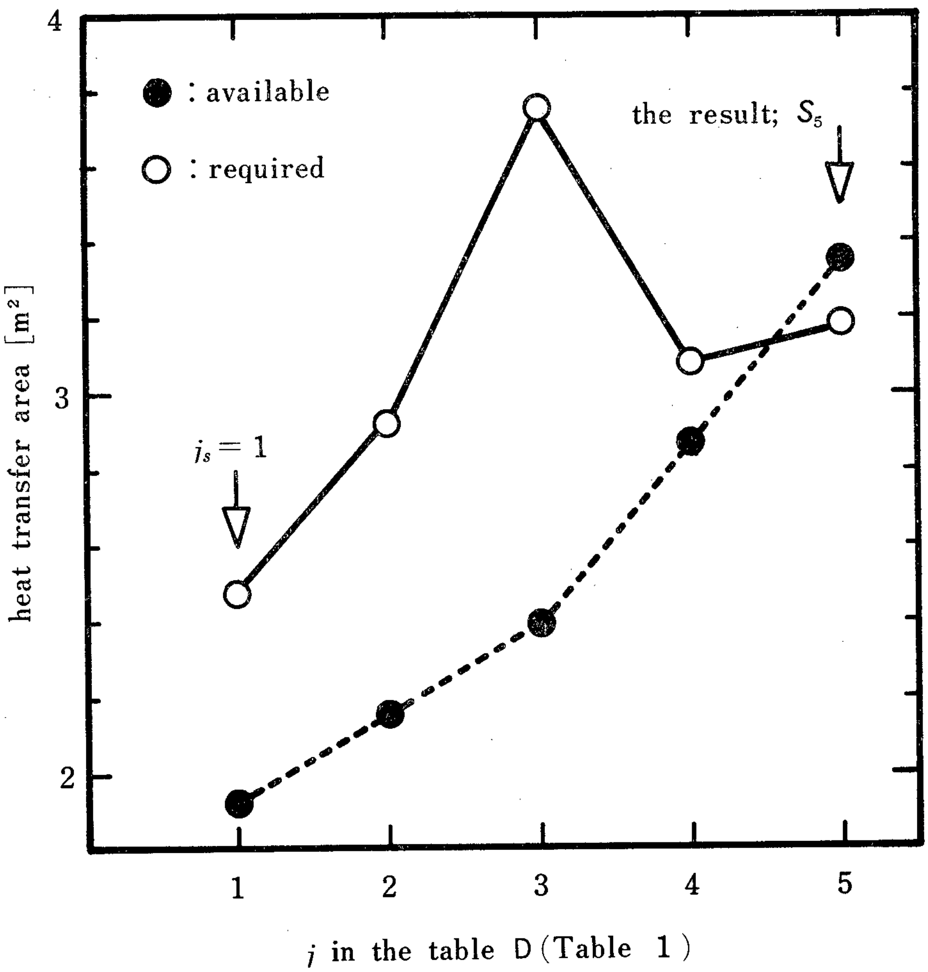

Fig. 2 A design process of a shell-and-tube heat exchanger for a certain specification by the present algorithm

required service with minimum heat transfer area. If any one of the relations in Eq. (4) does not hold, next design S_{j+1} should be rated untill Eq. (4) holds.

Fig. 2 shows an example of the design processes by the present algorithm for a certain specification. Rating does not always begin at the minimum of heat transfer areas in the table **D** (Table 1). The number of trials required to reach an optimal design, however, changes widely ranging from a few times to about 50 times according to the specification given. This may not be critical since the machine time necessary for one trial (a rating) is very short (about 200 milliseconds/rating with TOSBAC-3400-41).

Although the present program considers only the pressure drops in both shell and tube sides and the fouling factor as the performance of exchanger, the limitations on the dimensions of the unit can be easily taken into account if required by the customer. Application of the present algorithm to the mechanical design of shell-and-tube heat exchangers is also possible and described in detail elsewhere.[11]

4. Conclusion

An algorithm for optimal design of chemical process equipments which incorporates the realizability of the design is presented, and its application to shell-and-tube heat exchanger design is described briefly.

Possible applications of the present algorithm to other process equipments are also clear. Once the design could be obtained for a given specification by the algorithm, it might be always optimal in the sense that m is minimum. It is noted, however, that the design could not always exist for some specifications, since the table **D** prepared may be rather limited in the capacity, or physical realizability requires that n in Eq. (1) be finite. If the present algorithm is to be effective, the table **D** should be carefully organized.

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