OPTIMUM CRITERION OF EXTRACTOR DESIGN AND OPERATION

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For optimizing a production plant an objective function, "optimum criterion", was formulated and an optimum criterion of a part of the plant, an apparatus, consistent with that of the plant was proposed. This was specified for a counter-current extraction column with mechanical agitation and various sets of constraints were discussed. An optimization algorithm of complex system based on alternating minimization of individual parts and of the whole system was suggested.

Nowadays systematic research is going on in developing mathematical models of various chemical engineering processes and the respective equipment with the aim of their rational design and operation. The models are, as a rule, of physical nature and do not directly refer to the economy of the process. Generally, however, the notion of "optimum design and operation" implies a link between the physical parameters of the process and its economy. Obviously this link should be a properly selected objective function called here the "optimum criterion".

The present work is focussed on a single chemical engineering operation, the liquid–liquid extraction and on the search for optimum design and operation of an extraction column, in particular of the vibrating plate extractor VPE (ref.[1]). Usually, however, extraction is only a single step in a technological process and its optimum performance is subject to the condition of optimum performance of the technological process as a whole. This is true about any step of a process and therefore the analysis of the particular problem of seeking an optimum criterion of extractor design and operation is to be started with establishing the optimum criterion of a production plant – the system – and of the respective criteria of the individual units – the elements of the system.

Optimum Criterion of a System

In a plant, in which a technological process is performed, entering streams of raw materials and energy and exit streams of products and wastes can be distinguished. The amounts and compositions of some material streams are defined by technical conditions or standards and similarly some energy and enthalpy streams may be prescribed. The conditions, constraints, may be of the form $p_i \in \langle a_i; b_i \rangle$, $p_i \geqq a_i$; $p_i \leqq b_i$; $p_i = a_i = b_i$, where p_i is the parameter in question, a_i, b_i its lower and upper limit, respectively. Of course, in a numerical procedure the equality type of constraints has to be replaced by $p_i \in (a_i; b_i)$; $b_i - a_i = \delta$; $\delta/a_i \ll 1$.

The aim of optimum design of a plant is to reach maximum profit per unit of product, P_{max}. The optimum criterion of the system is

$$P_{max} = \max\{P\} = \max\{PP - C\} = \max\{PP - MC - EC - W - O - D\}\,. \quad (1)$$

Here PP denotes the price of products, C total costs, MC material costs, EC energy costs, W wages, O overhead, D investment depreciation. The price of products may be a function of quality (composition) but here it is asumed, that the quality is prescribed by standards ($p_i = a_i = b_i$) and therefore PP is constant during optimization. The ratio of amounts of individual products is supposed to be constant, too. Also the wages and overhead are assumed constant, unless principally different variants of the plant design are considered. (The depreciation term is here separated from overhead as its variable part). Accordingly the criterion (1) may be simplified to

$$\max\{P\} \rightarrow \min\{C\} \rightarrow \min\{MC + EC + D\}\,. \quad (2)$$

The losses do not enter explicitly the relations (1) and (2), they are concealed in the increased material and energy costs caused by them.

Optimum Criterion of an Element of the System

Any part of the plant contributes to the total costs by its own consumption of raw materials, energy and its own part of wages, overhead and depreciation. Accordingly, the parts of total costs consumed by the j-th element of the system are

$$C_j = MC_j + EC_j + W_j + O_j + D_j\,; \quad j = 1, 2, \ldots, n \quad (3)$$

and

$$C = \sum_j C_j\,. \quad (4)$$

A complete economic balance of the element j includes also the costs of intermediate streams – entering the element $IM_{j,i}$ and leaving it, $IM_{j,o}$ so that the costs of intermediates and products from element j are

$$IM_{j,o} = C_j + IM_{j,i}\,. \quad (5)$$

The intermediates entering the element are those leaving other elements of the system, among the intermediates leaving the element may also be some recycles or some final products. A problem may arise, how to distribute the costs on individual leaving streams, but in particular cases it can be solved consistently regarding the nature of the system. The advantage of Eq. (5) over Eq. (3) when seeking for the optimum criterion of an element lies in the fact that it contains all terms which can be influenced by an optimum design and operation of the part of the plant represented by the element j. When summing up over all elements the intermediate terms cancel, so that

$$\sum_j (IM_{j,o} - IM_{j,i}) = C\,. \tag{6}$$

In general, it is certainly not true, that minimum of the sum of costs produced in individual elements according to Eq. (4) can be reached by minimizing separately the individual terms C_j. The influence of the amounts and compositions of the streams leaving one element on the costs produced in elements which they enter may be highly nonlinear because of nonlinearity of the mathematical models of the elements in question. Nevertheless if these amounts and compositions are fixed by equality constraints, a minimum of the depreciation term D_j characterized by the corresponding values of design and operation parameters of the element should always exist. Accordingly partial optimization of individual elements in this sense should always bring about a decrease of the optimum criterion of the system. In particular systems the constraints of the element may not be so severe and some streams, e.g. the losses, may enter the partial optimization procedure. Some examples are discussed below. Accordingly introducing the "optimum criterion of the element" in analogy to that of the system, together with properly chosen constraints, is meaningful.

The optimum criterion of the element is

$$\min \{IM_{j,o}\} \doteq \min \{(C_j + IM_{j,i})\} \tag{7}$$

and is subject to the constraints

$$p_{j,k} = a_{j,k} = b_{j,k}\,, \quad \text{or} \quad p_{j,k} \geqq a_{j,k}\,, \quad \text{or} \quad p_{j,k} \leqq b_{j,k}\,,$$
$$\text{or} \quad p_{j,k} \in \langle a_{j,k};\, b_{j,k}\rangle\,; \quad k = 1, 2, \ldots, m\,. \tag{8}$$

The input streams of material and energy can be split into the theoretically necessary or net amount for producing the respective amount and quality of output intermediates and products and the losses. Similarly the costs of net amounts and losses are introduced

$$MC_j = NMC_j + ML_j; \quad EC_j = NEC_j + EL_j;$$
$$IM_{j,i} = NIM_{j,i} + IML_{j,i}$$

and after dropping the constant terms of wages and overhead the optimum criterion of element j becomes

$$\min \{NMC_j + NEC_j + ML_j + EL_j + NIM_{j,i} + IML_{j,i} + D_j\} . \quad (9)$$

Sometimes some of the loss streams may be partially or fully valorized. The respective costs will then appear among the intermediate or product costs $IM_{j,o}$.

The streams of intermediates are the cause of interdependence among the elements of the system. At global optimum of the system their amount and quality (composition), as well as the amount and quality of raw materials, energy inputs and products are fixed. These conditions form a part of the equality relations in constraints (*8*). The mathematical models of the individual parts of the plant have then, as a rule, unique solutions for their parameters which fulfil the conditional optimum according to the criterion (*9*) and the constraints (*8*). For calculating the general optimum of the system some of the constraints concerning the amount and quality of intermediates and other streams are relaxed and the respective parameters enter the vector of variable parameters which have to be optimized.

The introduction of the optimum criterion of an element makes it possible to divide the search of optimum of a system into two steps: optimization of the system and optimization of individual elements. These two steps can be a part of an iterative algorithm. The vector of parameters to be optimized, $\mathbf{r} = \{r_k\}$ can be divided into a vector containing the variable amounts and qualities of the material and energy streams with exception of losses, $\mathbf{t} = \{s_k\}$, and n vectors containing the variable parameters of individual elements, e.g. their operational and design parameters, $\mathbf{e}_j = \{e_{j,k}\}$. In the first step of the algorithm material and energy balances of the system are solved, so that estimates of all amounts and quality parameters of the streams among elements can be taken as fixed. Then in the second step the individual elements are optimized and new estimates of losses and operational and design parameters are obtained. In the second step the mathematical models of elements are used for computation. In special cases the constraints of an element may be sufficient for separate calculation of its optimum. Examples will be given below.

Optimum Criterion of an Extraction Column with Reciprocating Plates

The results obtained for an arbitrary part of a plant will be now applied to the particular case of a countercurrent reciprocating plate extraction column. Most conclusions, however, will be applicable to other types of extraction equipment as well. First the extraction of one solute only and the case of extract being the product stream are considered.

The cost of extract per unit amount of solute (product), CE, equals the sum of costs of net feed, NCF, solvent, CS, raffinate, CR, energy, EC, wages, overhead and depreciation

$$CE = NCF + CS + CR + EC + W + O + D\,. \qquad (10)$$

The mechanical energy costs are usually negligible, the costs of heating or cooling are included in the terms *NCF*, *CS*, *CR*. The amount and composition of the net feed do not enter the vector of optimization variables, NCF = const. Hence the optimization criterion is

$$\min\{CS + CR + D\}\,. \qquad (11)$$

The depreciation term relates only to the investment costs of the extractor and the initial costs of its liquid content. The costs of auxiliary equipment, buildings, etc. are not involved, because they are not expected to vary with the extractor size within some limits of variation of column length or diameter.

The cost of regenerated solvent per unit of product is assumed to be proportional to its amount S, the costs of feed and raffinate to the amount of solute in them, x_FF, x_RR. The depreciation term is proportional to the mass of the extractor related to unit mass of product, G, corrected on the effect of the design parameters of the set of plates

$$G = K_1Ld^2(1 + K_2h^{-1})\,.\,\Phi(l_1, l_2, \ldots)\,, \qquad (12)$$

where K_1, K_2 are proportionality constants, L, d the length and diameter of column, h plate spacing and l_i geometrical parameters of plates. The optimum criterion expressed in terms of physical variables and per unit solute in the feed is

$$\min\{n_SS/n_xx_FF + x_RR/x_FF + n_GG/n_xx_FF\}\,, \qquad (13)$$

where n_S, n_x, n_G are the costs per unit of solvent, solute and mass of extractor, respectively. This formulation tacitly implies, that the feed is an aqueous soution.

Optimum Criterion for Various Sets of Constraints

The optimum criterion of extraction column (*13*) has to be applied together with a set of constraints. If there are constraints of the type of equality, the respective terms of the criterion (*13*) become constant and can be omitted. In what follows some typical examples are discussed.

A) Limited concentrations of extract and raffinate: Some design parameters may be limited as well:

$$S/F \geqq a_{S/F}\,; \quad x_R \leqq b_{x_R}\,; \quad L \leqq b_L\,; \quad d \leqq b_d\,; \quad h \geqq a_h\,; \qquad (14)$$

$$\min\{n_SS/n_xx_FF + x_RR/x_FF + n_GG/n_xx_FD\}\,.$$

The reason for an upper limit of extract concentration may be the increasing solubility of impurities in extract, i.e. the decreasing selectivity of extraction. The upper limit of solute concentration in the raffinate may reflect the hygienic standards. The height of the column may be limited by the height of the factory building. An example of the limitation of the column diameter is the criticality condition in nuclear technology. The lower limit for the plate spacing in a sieve plate pulsed column may depend on the pulse amplitude. Below this limit a rapid increase of axial mixing will take place and the column efficiency will deteriorate. The constraints of the design parameters may occur in some of the following examples, too, but they will not be repeated there.

B) Prescribed concentration in raffinate:

$$x_R = a_R = b_R\,;$$
$$\min\{n_S S/n_x x_F F + n_G G/n_x x_F F\}\,. \qquad (15)$$

This case may arise when the solute is not very expensive and the hygienic standard severe. Even with expensive solutes it may happen, that the ecologically admissible concentration of the solute in wastes is far below the range of economical importance of its losses.

C) Fixed solvent to feed ratio:

$$S/F = a_{S/F} = b_{S/F}\,;$$
$$\min\{x_R R/x_F F + n_G G/n_x x_F F\}\,. \qquad (16)$$

This case may reflect the situation when the available facility for solvent regeneration has a limited capacity, apparently below the optimum of S/F. A more general situation is that the absolute optimum value of S/F is not known at the start of calculation. Then the first period of optimization corresponds to the case *A*) and can be described by the form of constraint

$$S/F \in \langle a_{S/F};\, b_{S/F}\rangle\,. \qquad (17)$$

After the upper limit has been reached, the criterion (*16*) is applied. An analogous reasoning may be applied to any case of constraint of the type of inequality, because almost always a plausible second limit of the parameter can be technically substantiated. Therefore all the constraints in the case *A*) can be reduced to the type (*17*) without loss of generality.

D) Fixed design parameters of the extractor:

$$L = a_L = b_L\,;\quad d = a_d = b_d\,;\quad h = a_c = b_c\,;\quad l_i \doteq a_{l_i} = b_{l_i}\,; \qquad (18)$$
$$\min\{n_S S/n_x x_F F + x_R R/x_F F\}\,.$$

This case relates to the optimization of the extractor operation. Such situation is typical for optimizing an existing plant under operation. Generally the amount and composition of net feed are no longer fixed but optima may be sought for a set of these parameters. For any item of this set the vector of optimized parameters contains e.g. the solvent to feed ratio, the raffinate concentration and the mixing intensity parameters of a mechanically agitated column.

E) Fixed solvent to feed ratio and raffinate concentration:

$$S/F = a_{S/F} = b_{S/F}\ ; \quad x_R = a_{xR} = b_{xR}\ ;$$
$$\min\{n_G G/n_x x_F F\} \rightarrow \min\{G/x_F F\}\ . \qquad (19)$$

This case corresponds to the problem of optimizing the extractor design and the intensity of mechanical agitation. The optimum criterion reduces to the minimum of the extractor costs.

DISCUSSION

A more detailed discussion of case *E*) may throw light on the complexity of the optimization problems *A*), *B*) and *C*), of which *E*) may be considered to be a particular case. The particular type of extraction column, the vibrating plate extractor VPE (ref.[1]), will be considered. The plates of this extractor have small circular perforations for the dispersed phase and large downcomers for the flow of continuous phase. The main effect of the reciprocating motion of plates may be expressed by the amplitude-frequency product $a\,.f$, but separate effects of these parameters on the column performance are not negligible. The variable design parameters of the plates are the diameter of the perforations d_c, the specific free area of the perforations e_d and the ratio of specific free areas of perforations and downcomers e_d/e_c. Accordingly together with the plate spacing and the column length and diameter the vector of optimized parameters may contain up to 8 elements. Moreover in the case of systems with large solute concentration changes stepwise variation of some design parameters along the extractor may substantially improve its performance and reduce its cost. Therefore a well structured mathematical model of the extractor and an effective optimization algorithm are quite important.

In the criterion (*14*) the product $n_G G$ represents the investment cost per unit of product of an extractor of optimum size and construction with respect to a particular extraction task. In the above types of problems this task is expressed by the respective constraints, in which the capacity required is represented by the quantities F, S/F and the extraction efficiency by x_F and x_R. From these quantities and a stagewise or differential model of countercurrent extraction the number of theoretical stages or transfer units $N = NTS$, NTU can be calculated. There the requirements on the extractor performance can be generalized in the form

$$N \,.\, F(1 + S/F)\,; \quad |\text{kg/kg of product}|\,. \tag{20}$$

This may be called the extractor performance. In the cases *A*) to *D*) the value of extractor performance varies during optimization, in the case *E*) it remains constant. For a given liquid system and fixed amount and composition of feed the value of performance is equivalent to the constraints in Eq. (*19*). It may be noticed that in the case *D*) maximizing the column performance would not be equivalent to the minimization of the criterion (*18*), as the weighing factor of costs does not enter the performance. Nevertheless the criterion

$$\max \{N \,.\, F(1 + S/F)\} \tag{21}$$

may be considered in comparative studies.

Often[1] the so called volumetric efficiency

$$\max \{\eta_{\text{vol}}\} = \max \{(U_c + U_d)/H\}\,; \quad |\text{h}^{-1}| \tag{22}$$

has been recommended as an optimization criterion, where U_c, U_d are the superficial velocities of continuous and dispersed phases and H is the height of transfer unit or of theoretical stage $H = L/N = HETS, HTU$. When average densities of phases ρ_c, ρ_d are considered, one can write

$$U_c = 4F \,.\, P/\pi d^2 \rho_c\,; \quad U_d = 4S \,.\, P/\pi d^2 \rho_d\,; \quad |\text{m h}^{-1}|\,;$$
$$P\,|\text{kg of product/h}^{-1}| \tag{23}$$

Then Eq. (*22*) becomes

$$\max \{\eta_{\text{vol}}\} = \max \{4P \,.\, N(F/\rho_c + S/\rho_d)/\pi L d^2\} \tag{24}$$

According for a given system and extractor performance (*20*) (which corresponds to the case *E*)) optimization of the column design according to the volumetric efficiency leads to

$$\min \{Ld^2\}\,; \quad |\text{m}^3| \tag{25}$$

the minimum of column volume, which is an approximation of the criterion (*19*).

As mentioned above, the problem of optimizing an extraction column has been discussed for the case of single solute and for the extract as the product containing stream, whereas the solute in the raffinate was considered as losses. Often, however, the raffinate represents the intermediate or product stream and the extract represents losses. Extraction refining, i.e. separation of impurities from an intermediate of product stream, is an example. In analogy to Eq. (*10*) minimization of the costs or raffinate will be required

$$CR = NCF + CE + EC + W + O + D\,. \qquad (26)$$

For aqueous feed and neglecting the cost of impurities the cost of extract is

$$CE = CS + n_x y_E E \doteq (n_S + n_x y_E)\, S\,, \qquad (27)$$

where y_E, E are the mass fraction of the product species and the mass of extract per unit of product, respectively. Under the assumptions made earlier the optimum criterion is

$$\min \{(n_S + n_x y_E)\, S/n_x x_F F + n_G G/n_x x_F F\}\,. \qquad (28)$$

Many extraction problems of practical interest involve separation of two or more solutes and sometimes also partial solubility of solvents must be taken into account. Dual solvent systems and extraction with various reflux streams are well known examples. In comparison with single systems the equation of cost balance and the respective optimum criterion will contain more terms corresponding to additional streams entering and leaving the extractor. The economic effect of the degree of separation of valuable solutes will be reflected as losses of the raffinate key component in the extract stream and losses of the extract key component in the raffinate stream. On the other hand both streams will also play the role of product streams. In the optimum criterion this ambiguity may be expressed e.g. by splitting these streams into fictitious product and loss streams. Also a larger number of constraints and their possible combinations will be encountered. Nevertheless it is believed that the approach to the formulation of an appropriate optimum criterion of the extractor and the corresponding constraints is applicable to the cases of higher complexity as well.

CONCLUSIONS

At the optimum of a complex system – production plant – conditional optima of its elements – individual production units – can be defined. The corresponding optimum criteria of these units represent minimum costs of these elements under constraints specifying the amount and quality of inputs and outputs of the particular element fulfilling the overall material and energy balances of the system in its optimum.

The optimum criterion of the element has been applied to a countercurrent extraction column with mechanical agitation and the respective cost terms have been expressed by its design and operation parameters.

By means of appropriate sets of constraints typical situations, e.g. the optimization of extractor design, or optimization of operation of an existing column, have been represented. The relation between the optimization criterion and the volumetric efficiency of an extraction column often proposed in literature has been discussed.

Based on the notion of constrained optima of elements of the system an iterative optimization procedure of the system has been suggested in which the vector of optimized variables is split into the variables of streams and the design and operation parameters of the equipment.

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SYMBOLS

a	amplitude of reciprocating motion, m
a_i	lower limit of parameter p_i
b_i	upper limit of parameter p_i
C	costs, unit of currency/kg of product
CE	cost of extract, unit of currency/kg of product
CR	cost of raffinate, unit of currency/kg of product
CS	cost of solvent, unit of currency/kg of product
d	column diameter, m
d_h	diameter of holes of plate perforation, m
D	depretiation of investment, unit of currency/kg of product
e	specific free area
$\mathbf{e}$	vector of optimized design and operation parameters of element
E	extract stream, kg/kg of product
EC	energy cost, unit of currency/kg of product
EL	energy losses, unit of currency/kg of product
f	frequency of reciprocating motion, Hz
F	feed, kg/kg of product
G	effective mass of column, kg/kg of product
h	plate spacing, m
H	*HETS* or *HTU*, m
IM	intermediate stream cost, unit of currency/kg of product
IML	intermediate stream losses, unit of currency/kg of product
l	design parameter of plate
L	column length, m
m	number of constraints of element
MC	material costs, unit of currency/kg of product
ML	material losses, unit of currency/kg of product
n	number of elements
N	*NTS* or *NTU*
NCF	net feed cost, unit of currency/kg of product
NEC	net energy cost, unit of currency/kg of product
NIM	net intermediate stream cost, unit of currency/kg of product
NMC	net material costs, unit of currency/kg of product
O	overhead, unit of currency/kg of product

p	parameter of system
P	profit, unit of currency/kg of product
P	production rate, kg of product/h
PP	price of product, unit of currency/kg of product
$\mathbf{r}$	vector of optimized parameters
R	raffinate stream, kg/kg of product
$\mathbf{s}$	vector of optimized stream parameters
S	solvent, kg/kg of product
U	superficial velocity of phase, m/h
W	wages, unit of currency/kg of product
x	mass fraction of solute in feed or raffinate
y	mass fraction of solute in extract;
η	volumetric efficiency of extractor, 1/h
Φ	correction of column investment cost on work invested in special plate geometry
ϱ	density, kg/m^3

Subscripts

c	continuous phase
d	dispersed phase
i	inlet stream
j	related to element j
k	related to constraint k
o	outlet stream

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