DEGREES OF FREEDOM
IN THE CONTROL OF DISTILLATION COLUMNS, I.

GENERAL CONSIDERATIONS

By

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1. Introduction

Most of the up-to-date distillation plants are automated and quite a number of papers deal with the various questions of their control. The most important feature of this problem is the correct definition of aims, and in order to find this definition the degree of freedom for control in a given apparatus must be known. Of course, in the control of an apparatus the values of only a certain number of variables can be changed at will, the other parameters are then unequivocally fixed and are not amenable to independent regulation, otherwise the functioning of the apparatus would be over-defined. This is important especially in cases involving complex automation, computer techniques, and optimization.

In the running and controlling of an existing plant the number of parameters variable at will is termed the degree of freedom for control. This notion must be distinguished from the general degree of freedom which allows e.g. to choose from the variables those to be fixed in the course of design work.

2. Survey of the literature

The first known mention of this problem is to be found in a paper by GILLILAND and REED [1] who compare the different methods of distillation column calculation. According to them the chief difficulty is that in the course of design work more parameters are generally fixed than there are independent variables available. This pioneering paper deals with this problem in its general aspect, also covering the point of view of design, and presents the fundamental theory for further work in this field. However, it does not take into account the simplifications actually effective in the operation of distillation columns, therefore it cannot be used directly for the solution of problems of their control.

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MORSE [2], investigating the degree of freedom in flow systems, amplifies his method to embrace the questions referring to distillation columns as well. By introducing definitions valid also for chemical reactions he endeavoured to generalize, therefore his approach grew to be too complicated and difficult to survey. A paper by LARIAN [3] deals with points of view touching control, but no final conclusions are drawn. More recently, BENEDEK and LÁSZLÓ [4] investigated the question of degrees of freedom in a general formulation where the question of control is mentioned but not discussed. A thorough treatment by KWAUK [5] gives a reasonable system for the definition of the degree of freedom and for its construction from elements. A tabulated list of degrees of freedom for simple and for complex units is presented; his aim is to furnish an adequate basis for computer work on processes of separation. He introduces the notion of repetitive units as a new variable. In his analysis, feed, pressure, and heat loss to surroundings are regarded as fixed. With the introduction of the idea of a complex unit he made the first step towards the circumferential method.

SMITH [6] in essence follows the method of KWAUK. Among the limitation formulae he puts the inherent constraints into a separate group but remarks that this is, to a certain measure, a matter of arbitrary decisions. Anyhow, one should be warned against over-definition. Directives are given for the choosing of variables to be fixed.

Another group of works on the determination of controllable variables is found in the introductory parts of papers on the automation of distillation columns. Most of the authors do not use the expression degree of freedom, and give no justification but enumerate the number of controllable variables and discuss on this basis the question of regulation. A communication of RADEMAKER and RIJNSDORP [7] is worth mentioning, therein the variables are counted, and after their grouping it is stated that 24 variants of control are possible. Among these, phases and boundary conditions constitute simplifications, so, according to these authors, five variants remain. BLAUHUT [8] deduces the degree of freedom from the number of variables and the number of equations, taking the phase rule into account. In his investigations some variables and equations having no purpose, are introduced and the final result is not explicitly stated. The paper of BERTRAND and JONES [9] is very interesting. There the variables are grouped as the independent, the prescribed, and the dependent variables, and on this basis the degree of freedom for an important special case of the distillation of binary mixtures is calculated.

At their starting point, and proposing some simplifying conditions, AN'ISIMOV and KRIVSUNOV [10] also touch upon the question, in connexion with the calculation of correlations between static characteristics.

3. General, theoretical method for the determination of the degree of freedom for control and regulation

3.1 General considerations

In a general sense, the number of the freely determinable parameters of stationary physical systems, i.e. its degree of freedom F is

$$F = N - M \tag{1}$$

meaning that the degree of freedom of the system can be found by subtracting from the number N of the variables the number M of the equations which express the correlations between these variables. In establishing N, the several restrictions, the number of characteristics fixed from the outset, must be taken into account. In most of the cases an exhaustive, all-embracing description of a process is impossible, but it always suffices when the variables essential from the point of view of the problem dealt with are considered.

The regularities which describe the distillation process can be grouped as follows.

1. Material balances, on the basis of the principle of conservation of mass;

2. Energy balances, on the basis of the principle of conservation of energy;

3. Correlations of thermodynamics and chemical physics for the description of the laws of phase equilibria;

4. Correlations of plant operation and of inherent restrictions.

Of course, also when fixing the value of the parameters to be freely chosen at the expense of the degree of freedom, the physical limits set by the process and by the apparatus ought to be considered. Thus, for instance, vapour velocity cannot be made to exceed a certain critical value because of the carry-over of droplets, and flooding; reflux ratio must be greater than the minimum value; etc.

In design work, a number of data, corresponding to the degree of freedom, can be fixed at values required for successful operation. The remaining data can be calculated, but their value must not be fixed beforehand otherwise the problem is over-defined. For the regulation of a process as many control loops or final control elements can be installed as are allowed by the degree of freedom.

Further, we may point out that *at least one of the parameters to be controlled must be of an extensive quantity because for the unequivocal description of a process some absolute quantity (mass, enthalpy, etc.) must be fixed.* On this basis one cannot regulate the functioning of a system through ratio controllers alone, even when the number of regulated characteristics (quantity ratios) equal the degree of freedom. To illustrate this the following example may serve.

Figure 1 presents the simple case of two fluid streams to be mixed.

The number of variables is three; in the stationary phase one correlation between them holds: $L_1 + L_2 = L_3$. On this basis, as immediately perceivable, only two of the three quantities can be chosen at will, i.e. the degree of freedom is two. This means e.g. that by fixing L_1 and L_2 through regulation, L_3 is also set. The regulation of L_3 and L_2 would, of course, also be feasible. The question which of the variables to prefer for regulating must be decided after an analysis of the remaining parameters and the sources of disturbances of the system. However, the two possibilities of control cannot be used for the regulation at
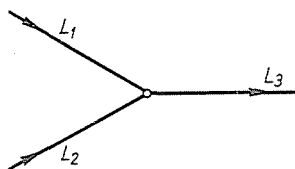

Fig. 1

will of one or the other of the ratios, since these are not independent of each other; but even if values are set in conformity with the material balance, functioning may become indefinite because the quantities L_1, L_2 and L_3 are not fixed.

This means that if only the flow ratios are to be regulated and the absolute mass is allowed to vary, then the degree of freedom for control is not fully utilized, i.e. the parameters to be regulated have been chosen incorrectly (see § 3.3). With the control of one quantity and one ratio the process is unequivocally defined.

3.2. The role of phase boundaries; control of levels

From the point of view of the degree of freedom for control, phase boundaries are of special importance. On the example of a steam heated heat exchanger (Fig. 2) this can be easily demonstrated.

In the heating section there is a change of phase (steam condenses) and, independently of the construction of the apparatus, a variable phase level forms between certain spatial boundaries. Here there are four mass streams as variables, and two equations expressing the correlations between them, i.e.

$$L_1 = L_3 , \tag{2}$$

$$L_2 = L_4 . \tag{2a}$$

To simplify the picture, its caloric side is left out of consideration. Accordingly, since the number of the degrees of freedom is $4 - 2 = 2$, it seems that the process in the given apparatus can be defined unequivocally by the regulation of two quantities.

In practice, however, one of the material balances Equation (2) cannot be ensured without the control of levels, and this means that the duty of this controller is the physical realization of the equation that expresses the material
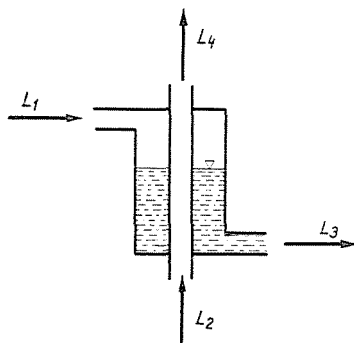

Fig. 2

calance term, i.e. the necessary stationary condition. Let a vessel with a bonstant cross-section A be considered, holding a liquid of constant density s^* to a variable level H. The material balance is generally the following

$$\Sigma L_i = \frac{dG}{dt} = \frac{dH}{dt} A s \tag{3}$$

where L_i = mass streams (with a $+$ sign for the inflows, and a $-$ sign for the outflows); G = the mass of the liquid in the vessel, t = time.

In our discussion we use the equation of the stationary material balance, thus the variations of mass within the vessel are to be disregarded and

$$\Sigma L_i = 0 . \tag{3a}$$

This condition, i.e. that $\dfrac{dG}{dt} = \dfrac{dH}{dt} = 0$, or that $H = $ const., can be fulfilled by a control of the level of the fluid. If this condition is not fulfilled we

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* If, as in the case of gases or vapours, density cannot be regarded as constant because pressures vary, then the regulation of this density must be provided for even if no other consideration suggested it.

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take a smaller number of correlations into consideration, or, in the non-stationary case, we take more variables (H), consequently the number of degrees of freedom grows.

In other words, *any phase boundary, and level-control involved by it, adds one more degree of freedom to the number calculated according to Equation (1) and adds another possibility for control* which must be taken into account. Thus the degree of freedom for control F' is

$$F' = N - M + \text{level controls} . \qquad (4)$$

This does not mean that the installation of an additional control device is imperative since by a proper construction of the apparatus, e.g. provision for overflow, self-regulation can be ensured.

In order to give a more generalised exposition of the importance of phase boundaries, and to throw light upon the foregoing from another side, the following might be pointed out. Any physical system has spatial extension and in design work it is possible to choose the geometrical data which define it. This circumstance must be considered in connexion with the degree of freedom when prescribing the dimensions of an apparatus. On the other hand, control is concerned with an apparatus already in existence. in this case geometrical degrees of freedom play no role since spatial extensions are already defined by rigid walls. However, if several phases are present the volume and mass of each are determined by non-rigid phase boundaries not depending on the structure enclosing the space involved and these add one degree of freedom each. It follows from the relationship between the general degree of freedom and the degree of freedom for control.

3.3. Limits of choice

Among the variables characteristic for the process, the parameters, limited in number by the degree of freedom, cannot be chosen arbitrarily. Due note must be taken of the fact that there are restrictive correlations, therefore, the independently variable controllable parameters should be fixed in such a way that the following criteria are complied with. *If among all the M equations describing the system any smaller i number of correlations (M > i), and k number of variables contained in them are investigated, the maximum number of the independent variables allowed is only k − i* even in the case when, for the whole of the system, the number of degrees of freedom is greater. Otherwise expressed, within the range set by the degree of freedom further variables can be chosen arbitrarily only from variables which had not been considered yet in one of the i number of equations. If the i number of equations considered deal with all the variables, then further correlations mean only

further limitations, consequently the degree of freedom of the system will become less than $k - i$.

To illustrate the foregoing general argument by an easily appreciable example we might mention that it is not feasible to fix arbitrarily the feed rate B, the rate D of distillate flow, and the rate W of residue draining simultaneously, even if the number of characteristics arbitrarily to be chosen is not less than three, because with the material balance $B = W + D$ forming a correlation between them the system would be over-defined. In the case of what has been stated above, the number of quantities to be fixed is $k - i = = 3 - 1 = 2$. Extending this investigation to the material balance comprising also the volatile component, it can be said that among the rate of feed B, that of distillate flow D, and that of residue or bottom draining W, and the concentrations x_B, x_D and x_W of the more volatile component in them, not more than four variables can be chosen arbitrarily, since we have to deal with $k = 6$ parameters, and $i = 2$ equations (that for the overall, and that for the partial, material balance).

On the basis of similar considerations it is not feasible simultaneously to control concentration x, pressure p and temperature t, at a certain point in the column. In the case of a binary mixture only two of these values can be independent variables since t is a function of x and p.

3.4. Controllable variables allowed for choice at the expense of the degree of freedom

In the literature mention is made of directly affected, indirectly affected, and independent variables. From the point of view of the degree of freedom for control, independent variables do not enter the picture, these must be discounted when the number of controls is being determined. The distinction made between directly and indirectly affected variables is only noteworthy from the point of view of the design of control loops and has no bearing upon the determination of the degree of freedom. Characteristics given in advance and not depending on our decisions must be regarded, from the point of view of control, as variables fixed at the expense of the degree of freedom, as must those be regarded the regulation of which is precluded by features of technology. Generally, the aim of control is just the elimination of disturbing effects that originate with independent variables outside our control.

Variables that remain constant at a fixed, or convenient, value without any regulation, are also left to themselves. Accordingly, the number of degrees of freedom for control might be higher than the number of parameters in fact controlled. Generally, the degree of freedom is the sum of the degree of freedom for control and the number of independent variables.

Finally, it should be noted that multi-parameter control, cascade control, and ratio control count as one each, since, though several characteristics are measured, only one final control element is arranged for.

The conclusions arrived at in the foregoing (§ 3) are generally valid and do not refer to distillation alone, so should be considered when solving any similar problem.
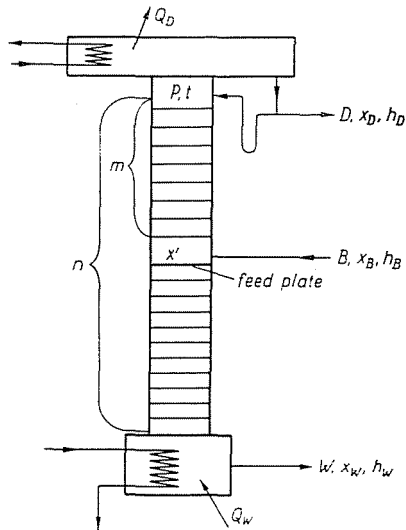

Fig. 3

4. The most general case of a distillation column for the separation of binary mixtures, with one feed-point and two product streams

The process (Fig. 3) is characterized by the parameters listed in Table I.

Table I

1. Flow rate of feed, B .... kilomoles per hour
2. Flow rate of bottom product, W .... kilomoles per hour
3. Flow rate of distillate, D .... kilomoles per hour
4. Composition of the feed, x_B .... mole fraction of the more volatile component
5. Composition of the bottom product, x_W .... „
6. Composition of the distillate, x_D .... „
7. Composition of the liquid at feed-plate, x'; in general this is not necessarily the same as the composition of the feed .... „
8. Enthalpy of the feed, h_B .... Kcal per Kmol
9. Enthalpy of the residue, or bottoms, h_W .... „
10. Enthalpy of the distillate, h_D .... „
11. Heat input, from steam to reboiler, Q_W .... Kcal per hour
12. Heat carried off by coolant in condenser, Q_D .... „
13. Number of plates, n ....
14. Number of plates in the upper section of the column; this defines the location of the feed point, m ....
15. A parameter, e.g. relative volatility, characterizing the conditions of phase equilibrium, α ....
16. Pressure at the top of the column, P .... Kponds per cm²
17. Temperature at the top of the column, t .... °C

An adiabatic column is assumed, i.e. there is no heat loss. Our discussion refers to the most frequent case when all the products are liquids. The concentrations on the plates are definite functions of those concentrations and other variables which are listed in *Table I*, therefore these are not enumerated here. Should we have given the concentration at each plate, as many limiting equations might be written for those not listed as the number of plates in the column. Consequently these cannot be fixed at will as dependent variables and do not count in the determination of the degree of freedom. Similar considerations are valid for the pressures at various points in the column since these also are definite functions of the pressure at the top of the column, and of the other parameters named. The pressure drop over the column is determined by the conditions of its operation, the physical properties of the phases, and the construction of the column.

The concentrations in the liquid, and not also those in the vapour phase, are mentioned since the latter are definitely determined at each of the plates by the former and the equilibrium curve $y_i = f(x_i, \alpha)$.

The parameters listed are interconnected by the following limiting correlations:

overall material balance,

$$B = W + D \tag{5}$$

partial material balance, (6)

$$B \cdot x_B = W \cdot x_W + D \cdot x_D$$

heat balance, (7)

$$B \cdot h_B + Q_W = W \cdot h_W + D \cdot h_D + Q_D .$$

Between temperature and pressure, both at the top of the column, and the composition of the distillate there is a definite thermodynamic relationship

$$t = f(P, x_D) . \tag{8}$$

The same is true for the temperature at whichever of the plates, $t_i = f(P_i, x_i)$, therefore the various values t_i do not figure in our list.

The enthalpy of the bottom product cannot be set arbitrarily because this product is kept at its boiling point, i.e. its enthalpy is defined by

$$h_W = f(x_W , t) . \tag{9}$$

Here it should be noted that a correlation of a similar type can be written for h_D when the reflux and the distillate are liquids at their boiling point, i.e. when there is no undercooling of liquid in the condenser. In such instances there is a further limiting factor, the number of the degrees of freedom is smaller by one; in a general case, however, this does not arise.

There is an operating function determined by the number of plates in the upper column section co-ordinating the composition of the distillate to the composition of the liquid at the feed plate:

$$x_D = f\left(x', \ m, \ \frac{L}{V}, \alpha\right). \tag{10}$$

A similar relationship exists between the composition of the liquid at the feed plate and that of the bottom product:

$$x_W = f\left[x', \ (n-m), \ \frac{L'}{V'}, \ \alpha\right] \tag{11}$$

L, L', V, V' representing the mass velocities, in kilomoles per hour, of the liquid and vapour streams, in the upper and the heating-section of the column, respectively. These so-called internal variables are also functions of the characteristics listed; for the present, let this assertion be accepted without verification, in the Second Part of this paper we propose to deal with this question in detail.

The conditions of a phase equilibrium are definite thermodynamic functions of pressure, consequently with a given mixture

$$\alpha = f(P). \tag{12}$$

Since we deal with the control of an apparatus already installed, the total number of plates, n, in the column is fixed and is a further limiting factor. It should be noted that in a general case the number of plates, m, in the upper section of the column, i.e. the location of the feed point, is not given a priori, and with specific methods of control it is possible to counteract disturbances just by changing this location, i.e. to choose the best place for it.

Here we might point out that the plate number is constant only in a structural sense since the number of theoretical plates (plate efficiency, measure of mass transfer) which characterizes the separation effect is a function of various operating factors of the column. A similar statement is valid for the efficiency of a packed column in so far as the height corresponding to one transfer unit also depends on various parameters (incidentally, also the separating efficiency of a packed column can be characterized by a number of

theoretical plates).* This does not introduce a new independent variable degree of freedom as the separating efficiency of column is unequivocally determined by the factors named in our list, and this means that e.g. if plate efficiency (E) is taken into account as a further parameter then a further limiting equation can be written for it

$$E = f(\dots).\tag{13}$$

Thus, in a most general case the degree of freedom F in the work of a distillation column with one feed for the separation of a binary mixture into two liquid product streams is given by

$$F = 17 - 9 = 8.\tag{14}$$

Between the 17 variables listed in Table I there were found to exist 8 correlations, a further limiting factor, the ninth one, was found to be the fixed number of the plates.

Due to the phase boundaries in the reflux collector and in the reboiler, two level controls are required in addition

$$F' = F + 2 = 10.\tag{15}$$

From this figure the number of the independent variables must be subtracted.

In this analysis the control of the several heat fluxes is considered as a single variable. Should the method of heating render it necessary more than one control device can be installed, e.g. a level control for a change of phases, or a pressure regulator if steam pressure fluctuates, etc.

Of course, circumstances like these must be considered separately and the problem, i.e. the determination of the degree of freedom for control, extended accordingly.

On the basis of this most general case, characterized by 8 as its degree of freedom, some special problems can be investigated where various limiting factors can be considered.

Summary

A general method for the determination of the degrees of freedom is given. The special role of the level control is shown; some points of view and limitations for choosing the controllable variables are discussed. The degree of freedom $(F = 8)$ for the most general case of a binary distillation with one feed and two products is determined.

* Our discussion refers to any kind of column, whatever its construction.

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