# DYNAMICS AND CONTROL OF CHEMICAL REACTORS AND DISTILLATION COLUMNS

Edited by

C. McGREAVY

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# DYNAMICS AND CONTROL OF CHEMICAL REACTORS AND DISTILLATION COLUMNS

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Edited by

C. McGREAVY
*University of Leeds, Yorkshire, UK*

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# DISTILLATION CONTROL SYSTEM STRUCTURES

K. V. Waller

*Process Control Laboratory, Department of Chemical Engineering, Åbo Akademi, 20500 ÅBO, Finland*

Abstract. Much of the recent research on distillation control has been treating the question of control system configuration. Dual-composition control by controlling temperature differences and sums in a column, various ways of reducing interaction by use of flow ratios as manipulators, and use of decoupling strategies are examples on discussed structures.
In a common framework the different suggestions can be viewed as control systems of the same basic multivariable structure. The approaches then mainly differ in their ways of designing the various parts of the control system. It seems that what has been labeled as a structural problem could equally well be considered an algorithmic problem within the general multivariable structure.

Keywords. Distillation control; process control; control system analysis; decoupling; multivariable control systems; control systems synthesis.

## INTRODUCTION

It has often been stated that the most important problem in chemical process control is not the development of more sophisticated algorithms, but rather the establishment of a structural framework for selecting the manipulated and measured variables and linking them appropriately (Lau, Alvarez and Jensen, 1985).

The theoretically optimal structure where all outputs are utilized for computation of the control action, i.e. all outputs are connected to all inputs, has not so far gained much acceptance in the process industries. Instead the control system design has aimed at single input single output (SISO) control loops, and much work has been devoted to finding suitable combinations of inputs and outputs in order to decrease or eliminate the interaction between the loops.

Generally, this area of variable transformations is a field of significant potential in process control (Waller, 1980, 1982) where applications may be to

- o eliminate or decrease interaction between control loops
- o eliminate or decrease nonlinearities
- o decrease dimensionality of high-dimensional problems

Some successful applications of variable transformations have already been reported. One example outside the distillation field is the modeling and control of pH (Gustafsson and Waller, 1983) (Gustafsson, 1984). Other applications are reviewed by Waller and Mäkilä (1981).

In distillation control various transformations of variables have been shown much interest during the last decades. So far the main interest has been devoted to dual composition control, i.e. controlling both the product compositions from a continuously operating two-product distillation column. Since the aim has been to reduce detrimental interaction effects between the control loops, similar approaches can be expected to be used in the future for control of more tightly (heat) integrated trains of columns. Another field, not much explored as yet, is control of the compositions from multicomponent distillation columns with significant sidestreams.

Structural aspects are emphasized in the following review of various approaches that have been suggested for dual-composition control of distillation.

## CHOICE OF CONTROLLED VARIABLES

It has been known for a long time that the interaction between the two composition control loops in a dual-composition control system for distillation, as illustrated in Fig. 1, may degrade control quality. As a remedy Rosenbrock (1962) already in 1962 suggested the control system in Fig. 2, which according to him often can be shown to be noninteracting. The rationale behind the control scheme of Fig. 2 is expressed by Rosenbrock in the following way. "The 'top loop' now manipulates the flow of top product to control the sum of the two measured compositions. The 'bottom loop' manipulates the boil-up and (with fixed flow of top product) the reflux to control the difference between the two compositions. Thus the two loops respectively determine the vertical position of the composition curve, and its slope, by manipulating two appropriate variables (cf. Fig. 3)."

A few years later Davison (1967) extended Rosenbrock's treatment and suggested, for a column studied, the scheme in Fig. 4 for the case where pressure is constant. The control scheme suggested is obtained by Rosenbrock's modal analysis procedure. The criterion is that "the dominant time constant of the controlled plant is minimized".

The multiloop SISO (single-input single-output) scheme in Fig. 1 can be drawn as in Fig. 5. The interaction between the two loops is caused by the elements $G_{21}$ and $G_{12}$.

The interaction can be eliminated or reduced by inserting compensators, much like feedforward controllers, between the two primary feedback loops. The approach is called (external) decoupling in the distillation control literature and has been shown much interest since Luyben's (1970) early paper.

A decoupling scheme is shown in Fig. 6. To decouple the two feedback loops, the decouplers have to be chosen in such a way that they counteract the interaction caused by the two process elements $G_{12}$ and $G_{21}$. The decouplers in Fig. 6 then become $-G_{21}/G_{22}$ and $-G_{12}/G_{11}$.

The decoupling scheme of Fig. 6 has the structure of a multivariable control system where each of the two outputs are connected to each input. In standard multivariable control theory the system is treated as a whole when the controllers are designed. This has the implication that interaction in the system that might be beneficial for disturbance rejection is taken advantage of in the design. In the decoupling approach the basic idea is to eliminate all interaction, be it detrimental or not, and make the system behave as two isolated SISO-loops. It has been stated that decoupling control is the opposite to multivariable control.

Rosenbrock's and Davison's suggestions in Figs 2 and 4 can be compared with the decoupling scheme in Fig. 6. Rosenbrock's scheme can be drawn as in Fig. 7. Fig. 7 can be redrawn as in Fig. 8 to show the structural equivalence between Rosenbrock's scheme and the decoupling scheme of Fig. 6. Davison's scheme of Fig. 4 can analogously be redrawn as in Fig. 9.

A comparison between Rosenbrock's and Davison's schemes as plotted in Figs 8 and 9 and the decoupling scheme of Fig. 6 shows that the elements in Rosenbrock's and Davison's schemes that correspond to the decouplers in Fig. 6 are not directly based on the properties of the process (only indirectly through the controllers and their tuning). It therefore seems that they cannot generally be expected to decouple the loops and make the system noninteracting. Actually this was not the basic aim of Davison's system, and Figs 8 and 9 are here used only to show the structural similarity between the schemes and the decoupling scheme of Fig. 6 and to emphasize that all three schemes can be structurally viewed as general multivariable control systems where all (in this case two) outputs are connected to all inputs, as in Fig. 7.

Also Ryskamp (1982) discusses schemes where one temperature above the feed plate and one below the feed are used as the two measurements from which product composition is inferred. Ryskamp suggests a scheme where heat input is set by the sum of the temperatures and the difference between them is used to set reflux.

Structurally Ryskamp's scheme resembles Rosenbrock's and Davison's schemes. It differs, however, in two respects. Firstly, Rosenbrock and Davison use distillate flow D as a manipulator in addition to boilup V, whereas Ryskamp use reflux flow L in addition to V. Secondly, the temperature difference is used to set boilup in Rosenbrock's and Davison's schemes, whereas the sum of temperatures is used in Ryskamp's scheme.

Recently Bequette and Edgar (1986) used so called singular value analysis to design a control scheme for a simulated column. A structurally non-interacting system was obtained when distillate flow D was paired with the sum of two temperatures, and reboiler heat duty was paired with the difference in tray temperatures, i.e. the system had the same structure as has Rosenbrock's scheme in Fig. 2. Bequette and Edgar state that the pairing for their column should not be the same as suggested by Ryskamp (1982).

Different design methods to obtain non-interacting control were studied by Bequette and Edgar and they all resulted in essentially the same scheme, i.e. one using the sum and the difference between two temperature measurements as inputs to the controllers. The methods studied were (1) column profile control, (2) implicit decoupling, (3) modal control, (4) output decoupling, and (5) extensive variable control (Georgakis, 1986). It should be noted, however, that the study aimed at a control system for a column where the manipulators were chosen to be D and V.

A multivariable structure where both outputs are connected to both inputs is obtained also by other combinations of measured variables from the two ends of the column. In an attempt to get linearization in addition to non-interaction, Weber and Gaitonde (1982) use the conventional manipulators reflux flow L and vapor boilup V to control certain combinations of top and bottom compositions. The variables controlled are called

$$\text{fractionation} = x_B + K(1-x_D)$$

which is controlled by reflux L, and

$$\text{cutpoint} = (1-x_D)/x_B$$

which is controlled by boilup V.

Weber and Gaitonde calculate the constant K from the normal operating point as $x_{Bo}/(1-x_{Do})$.

McAvoy (1983) discusses Weber's and Gaitonde's scheme and states that a "better", i.e. less interacting, choice for K would be $x_F/(1-x_F)$.

McAvoy (1983) suggests a scheme where a variable $\xi$ defined as

$$\xi = x_B + \frac{x_F}{1-x_F} x_D$$

is controlled by distillate flow D.

McAvoy state that use of $\xi$ as a controlled variable results in an almost one-way steady-state decoupled system, i.e. changes in V do not significantly affect $\xi$. The relationship between the controlled and the manipulative variable is further stated to be linear (McDonald and McAvoy, 1983).

Instead of $\xi$ as a controlled variable, resulting in an almost one-way steady-state decoupled system, a similar variable could be used giving perfect one-way steady-state decoupling when the manipulators are D and V. This variable is (Häggblom and Waller, 1986)

$$\xi' = x_B + K'x_D$$

where the constant K' can be calculated from steady-state compositions or flows as

$$K' = \frac{x_{Fo} - x_{Bo}}{x_{Do} - x_{Fo}} = \frac{D_o}{B_o}$$

In McAvoy's scheme (McAvoy, 1983, McDonald and McAvoy, 1983) the second controlled variable is separation factor S, which is controlled by boilup V. The separation factor is defined as

$$S = \frac{x_D}{1-x_D} \cdot \frac{1-x_B}{x_B}$$

This loop is not decoupled from the other one, changes in D affect the separation factor S.

Separation factor control is also discussed by Shinskey (1984). It could be added that Boyd (1975) and Ya and Luyben (1984) also have discussed control schemes where temperature differences, in their schemes differences between differences, are used as controlled variables.

It is interesting to note the similarities and differences between the schemes discussed above. For symmetrical separations, i.e. $D_O = B_O$, $1-x_{DO} = x_{BO}$, and $x_{FO} = 0.5$, the controlled variables and manipulators become the ones shown in Table 1.

## CHOICE OF CONTROL VARIABLES

In the previous section were reviewed various suggestions for transformation of controlled variables mainly to make the two control loops noninteracting for dual-composition control of distillation.

At the other end of the control system there are the control variables or manipulators used to control the process. They, too, can be chosen in various ways, and this is also a subject much discussed in the recent distillation control literature.

For feedback composition control of a distillation column with two products there are the following four primary control variables: distillate flow D, reflux L, bottoms flow B, and vapor boilup V (the last one indirectly manipulated through heat input to the reboiler).

The manipulators in the so called conventional or energy balance scheme are L and V. They are the manipulators in Fig. 1, whereas D and V are the manipulators in Rosenbrock's scheme in Fig. 2 and Davison's scheme in Fig. 4. Schemes where either D or B are manipulated to control composition are usually referred to as material balance control schemes.

McDonald and McAvoy (1983) use the "material balance variable, D or B", to control a linear combination of product compositions (see previous section). The "energy balance variable", V or L, is used to control the separation factor.

Between the two base cases of energy balance control and material balance control there are a number of combinations. Many suggestions to use various ratios between flows as manipulators can be found in the literature. An early example is given by Rijnsdorp (1965), who suggests the ratio of reflux flow and top vapor flow as a manipulator for the top loop $(L/(L+D) \leftarrow x_D)$ (here the arrow pointing backwards denotes feedback). Stainthorp and Jackson (1974) experimentally studied a scheme in which the top loop manipulator was L/D. For a number of simulated columns McAvoy (1977) studied the steady-state interaction also for Rijnsdorp's suggestion, both in combination with $(V \leftarrow x_B)$ and - as a combination of Rijnsdorp's scheme and a material balance scheme - with $(B \leftarrow x_B)$. McAvoy found the smallest amount of steady-state interaction for the last scheme, $(L/(L+D) \leftarrow x_D)(B \leftarrow x_B)$. He also extended the idea in search of such functional combinations of manipulated variables as would make the loops noninteracting, the final result was degeneracy (Jafarey and McAvoy, 1978).

A list of ratio control schemes suggested in the literature is given in the book by Rademaker, Rijnsdorp, and Maarleveld (1975). The book discusses various ratio-control schemes, among them also two-ratio schemes, in which both the manipulators are flow ratios.

One of the schemes recently most discussed where a flow ratio is used as manipulator is a scheme suggested by Ryskamp (1980). The manipulators for composition control in the scheme are D/(L+D) and V.

The rationale for the scheme is expressed by Ryskamp (1982) as follows. The scheme "holds reflux ratio constant if the top AC output is constant. An increase of heat input from the bottom AC does not make top product as impure as would occur with reflux constant (conventional control) nor as overpure as would occur with distillate flow constant (material balance control)". Thus, this property of the scheme results in a certain decoupling effect and the scheme is often said to result in "implicit decoupling", in contrast to "explicit decoupling" accomplished by external decoupling elements, discussed in the previous section and later in this paper treated more in detail.

A modification of Ryskamp's scheme to a scheme where the manipulators are D/(L+D) and V/B has been suggested by Takamatsu, I. Hashimoto and Y. Hashimoto (1982) (1984) and by Shinskey (1984).

An implementation of Ryskamp's scheme can be illustrated as done in Fig. 10 for the top of the column.

An important difference between the manipulators in the scheme of Fig. 10 and the schemes previously discussed with D, L, V, and B as manipulators should be noted. In the schemes where two of the basic manipulators D, L, V, and B are used to control composition, the other two are used for level control (as illustrated e.g. by Fig. 4). These level control loops have not been considered in the discussion above, in order to simplify the treatment. However, strictly speaking, the control problem discussed is concerned with control of four outputs using four manipulators, i.e. a 4x4 problem.

In Ryskamp's (1980) scheme in Fig. 10 both the manipulators L and D at the top end of the column are simultaneously used for control of both composition and level, i.e. each output is connected to each input, as illustrated in Fig. 11, which shows the structure of Ryskamp's scheme in block diagram form.

If, in analogy with the case discussed above, the bottoms composition $x_B$ and the reboiler level are controlled by a flow ratio, like V/B, this means that both these outputs are connected to both the inputs V and B.

The various schemes using various flow ratios as manipulators have as a rule been obtained by heuristic reasoning. Obviously they have been found advantageous in industrial practice. Theoretically this is not unexpected: they have the structure of an optimal system where each output is connected to each input. However, it seems reasonable that still better control can be anticipated if other algorithms than pure division between flows were used.

Furthermore, the four outputs and four inputs have been split into two groups. Still better control can be expected if all four outputs are connected to all four inputs, i.e. if information about what happens at one end of the column is transmitted also through the control system to the other end of the column.

## EXTERNAL DECOUPLING

Inserting compensators between interacting loops, as shown in Fig. 6, is usually called (external) decoupling in the distillation control literature. This subject has attracted much interest in the literature ever since Luyben's paper in 1970 (Luyben, 1970), and it was discussed in connection with Rosenbrocks's and Davison's schemes (see Figs 6, 8, and 9). Below some complementary aspects are given.

The decoupling scheme as drawn in Fig. 6 is actually one of several possible decoupling schemes. Which one to use is usually determined by realizability aspects (Waller, 1974).

Two-way decoupling (where there are two decouplers between the two primary loops, as in Fig. 6) and one-way decoupling (only one decoupler) are compared by Fagervik, Waller, and Hammarström (1983). Results obtained in the study also indicate that, in general, the best disturbance rejection is not obtained by perfect decoupling, but that the best response is obtained by some tuning of both decouplers and feedback controllers.

We are then left with a parametric optimization problem of a considerable size. Even if the types of the feedback controllers and the form of the decouplers are decided upon, the problem of simultaneous tuning of "decouplers" and feedback controllers is still considerable. It is further desirable that various decoupling structures (such as one-way versus two-way decoupling in a 2x2 system) can be tried, as well as various forms for the decouplers.

Use of the Inverse Nyquist Array (INA) technique for simultaneous feedback controller and "decoupler" tuning is demonstrated by Waller, Wikman, and Gustafsson (1985). The paper also shows that minimizing interaction at the critical frequency often, but not always, is a good criterion for design of the decouplers. It is also shown that it may be enough to use pure gains as decouplers; adding dynamics need not significantly improve control quality.

It should further be emphasized that although the control quality, as measured e.g. by error integrals after step disturbances, is not very different for different decoupling schemes, the robustness of the scheme may significantly speak in favor of one of the schemes, as is quantitatively illustrated by Fagervik, Waller, and Hammarström (1983).

## ASPECTS ON HOLISTIC MULTIVARIABLE CONTROL

In the previous treatment it was found that many of the schemes for dual-composition control discussed in the literature and there treated as multiloop SISO systems can be viewed as MIMO (multi input multi output) systems.

An alternative would then be to start from the structure of the system (be it 2x2, 3x3, or 4x4) and use a true multivariable design method and calculate the controller by some optimization procedure, instead of determining part of the controller by more or less heuristic choices. One such method is the so-called linear quadratic (LQ) design. A number of simulation studies of LQ-design have been reported, reviews can be found in Edgar and Schwanke (1977) and Waller (1982).

The LQ-design results in a scheme where all the state variables are used for feedback. The size of the feedback coefficients may, however, differ considerably. By neglecting small feedback coefficients, Oakley and Edgar (1976) concluded for a specific example analyzed that the resulting scheme could be approximated with good accuracy by a scheme having the same structure as a one-way decoupled scheme, where changes in reboiler heat duty are fed to the top loop, not only through the column but also through the decoupler. The same conclusion is obtained in a study by Tung and Edgar (1978).

In chemical process control, the number of sensors is usually much lower than the number of state variables used to describe the process. In that case an optimal multivariable (LQ) controller contains an observer or state estimator, by which the unmeasured states are calculated before they are used for feedback.

An LQ-design can very well start from a system model consisting of simple transfer functions containing dead times. An illustration of the various steps of the design starting from experimentally obtained transfer functions is given in Hammarström, Waller, and Fagervik (1982). The paper is focused on how errors in the process models affect the control properties of the multivariable control system obtained. Connections between model structure, the performance index, the control quality, and the sensitivity are illustrated.

One further aspect on state estimation may be mentioned here, since it has to do with the structure of the state estimator. When there are disturbances with non-zero mean, such as step disturbances, estimation e.g. by a Kalman-filter results in steady-state estimation offset if a model of the deterministic disturbances is not included in the estimator. Also the resulting control quality may be drastically reduced, compared to the case when a model of the disturbances is included in the estimator. In an distillation example treated by Hammarström and Waller (1974), the control was improved by several orders of magnitude simply by including estimation of an occuring step disturbance in feed composition. It should be noted that this improvement was accomplished not by any added sensors or disturbance measurements, but by changing the structure of the estimator so that the control system was informed about the fact that there might be disturbances of step type. Estimation of more deterministic disturbances (such as steps both in feed composition and flow) than actually occured (in feed composition) did not degrade control quality. However, not more disturbances can be estimated than there are measurements on the process (Hammarström, 1980). Further illustration of LQ-control in distillation can be found in Hammarström (1980).

## NUMBER AND LOCATION OF SENSORS

The number and location of sensors are important issues directly related to the control system structures.

Waller, Gustafsson, and Hammarström (1974) illustrated, through simulation, how drastic an effect the location of a third sensor (two fixed in the product lines) may have on distillation control quality. Also when state estimation (Kalman-filter) was used (Hammarström and Waller, 1974) the location of the third sensor strongly affected control quality in LQ-design. This could easily be understood if the measurements were inaccurate, but in the study mentioned perfect measurements were assumed.

A frequent approach in the literature for sensor location is to use some kind of observability or sensitivity consideration. In recent literature so-called singular value analysis has been popular.

Already in 1974, Hammarström and Waller (1974) studied the relation between control quality and observability properties of a distillation system. No correlation was found between the observability index used and control quality. Observability considerations are probably not enough to solve the sensor location problem. This seems also to be the opinion of Mellefont and Sargent (1978) who suggest an implicit enumeration algorithm for the selection of measurements to be used in optimal feedback control of linear stochastic systems.Application of the algorithm to a distillation system gave results which were reported to be "considerably different from what would be expected for pure estimation" (Mellefont and Sargent, 1978).

The location and number of sensors are also directly related to the optimal size and complexity of the process model used for controller design. Dahlqvist (1980) investigated, both experimentally and through simulation on an 11-plate pilot column, LQ-controllers based on various model sizes. The measured states were obtained thorugh state estimation. Using two sensors, a second order model gave better results than did a sixth order model. With three sensors, a sixth order model gave better control than a 13th order model did, and also better control than a fourth order model gave.

The relation between sensor number and location and process model size and complexity in multivariable control is likely to be a function of the quality of the measurements, such as accuracy and dynamics. These relations are also functions of the properties (both static and dynamic) of the process to be controlled, as well as of the product specifications.

Another closely related problem, not much studied so far, is how to combine slow and direct (desirable) measurements (like those of a gas chromatograph) with fast and indirect ones (like temperatures).

## DISCUSSION

Dual-composition control of distillation has been treated emphasizing the structure of various control schemes. Many suggested SISO schemes have been shown to be structurally equal to a general multivariable scheme. For the problem studied, it then seems that the structural question could equally well be viewed as an algorithmic question.

So far only feedback control strategies have been treated. For distillation feedforward control is often used to cope with changes in feed flow rate. If feed composition can be measured, feedforward can be used also to compensate disturbances in feed composition. In this way the two feedback loops normally used in dual composition control could be replaced by one feedforward loop and one feedback loop, as suggested by Jafarey and McAvoy (1980).

An issue that seems to be, at least partly, open when controlling various (linear) combinations of concentrations (or temperatures) instead of the product compositions themselves is the following. Does good control of a combination of concentrations (or temperatures) also implay good control of the product concentrations which usually are the important variables to control? What about robustness? How should e.g. integral action in the control system be implemented to bring the product compositions to desired values? This last question was recently discussed by Georgakis (1986).

Among interesting problems for future research in distillation control can be mentioned the question of sensor number and location (observability considerations do not give the whole picture) and their relations to the complexity of the process models used for design. Here the combination of various types of sensors is an interesting and important subproblem.

## NOTATION

| | |
|---|---|
| B | bottoms flow |
| D | distillate flow |
| F | feed flow |
| L | reflux flow |
| o | as index denotes steady state |
| T | temperature |
| V | boilup |
| x | composition |

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TABLE 1 Controlled variables and manipulators in discussed schemes for symmetric separations

| | Controlled variable(s) | Manipulator(s) |
|---|---|---|
| Rosenbrock (1962) | $x_1 + x_2$ | D |
| | $x_1 - x_2$ | V |
| Ryskamp (1982) | $T_1 + T_2$ | V |
| | $T_1 - T_2$ | L |
| Weber and Gaitonde (1982) | $x_D - x_B$ | L |
| McAvoy (1983) | $x_D + x_B$ $(= \xi)$ | D |
| Bequette and Edgar (1986) | $T_1 + T_2$ | D |
| | $T_1 - T_2$ | V |
| Häggblom and Waller (1986) | $x_D + x_B$ $(= \xi')$ | D |

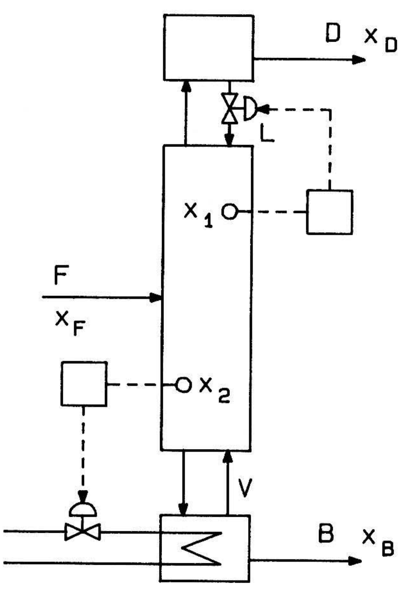


Fig. 1. Dual composition control of distillation column.

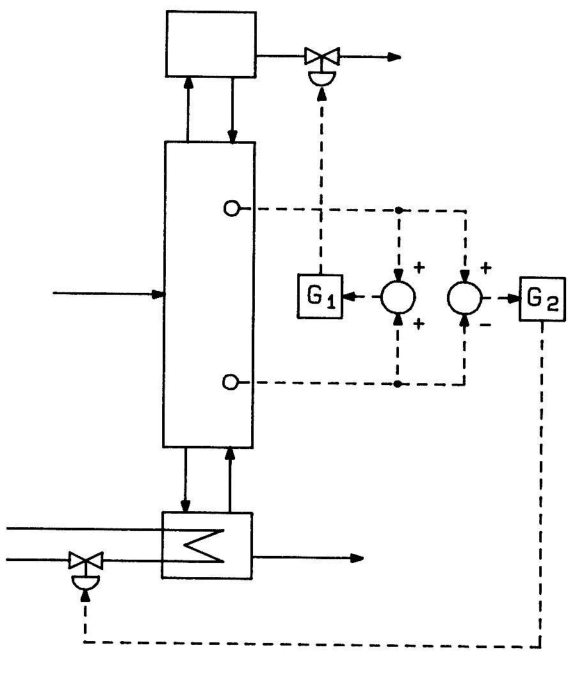


Fig. 2. An alternative scheme for dual composition control (Rosenbrock, 1962).

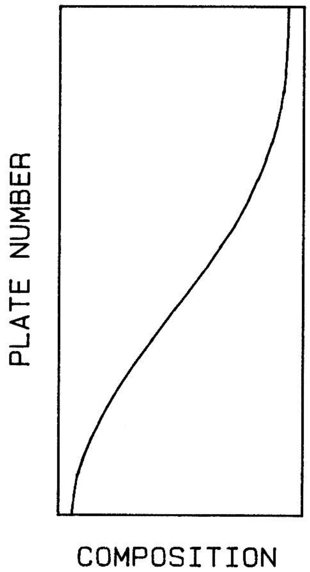


Fig. 3. Composition profile in a distillation column.

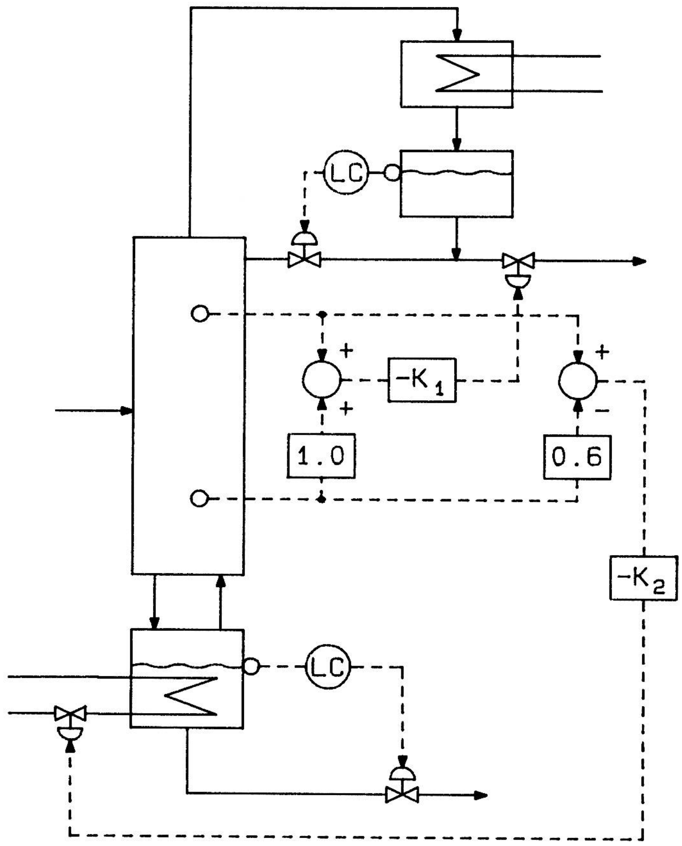


Fig. 4. Dual composition control scheme suggested by Davison (1967).

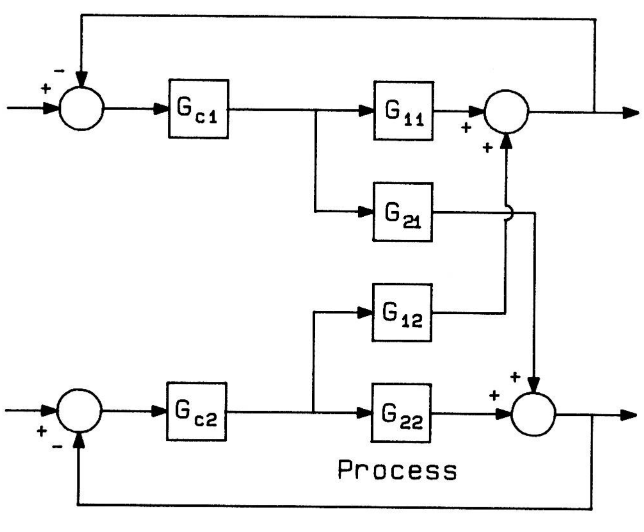


Fig. 5. Scheme of Fig. 1 in block diagram form.