MODELING, IDENTIFICATION AND CONTROL, 1986, VOL. 7, NO. 2, 57–70
doi:10.4173/mic.1986.2.1

The significance of modeling and simulation in process design†

J. D. PERKINS, J. M. HOWELL and
M. P. F. WONG‡

Keywords: *Process dynamics, controllability, switchability, simulation*

Reasons for considering the dynamics of a new or existing plant are illustrated through a number of industrial examples. Recent work aimed at assessing the effects of process dynamics on plant operability is presented. Two aspects are considered—the ability to maintain a given steady state in the face of disturbances (controllability) and the ability to move between steady states (switchability). Case studies are used to illustrate these concepts, and to demonstrate what is possible with a modern simulation system.

1. Introduction

The study of process dynamics has a long history in chemical engineering. However, in recent years there has been an upsurge in interest both from academics and industrialists. There are several reasons for this. First, the economic climate within which the chemical industry operates has undergone large changes following the oil crisis, forcing design to much tighter margins, and the recent recession, forcing a more reticent approach to new plants and modifications to existing ones. Increased concern about plant operability, of which dynamics is an important part, has resulted therefore from pressures to reduce costs, and to get things right since the penalties for failure are greater. Another factor is the advance in computing capability, both in hardware and in numerical methods, which now permits systems to be simulated which were very difficult or impossible to deal with previously.

In spite of these factors however, progress in the consideration of process dynamics in industry can seem depressingly slow. Reasons for this include questions about the value of studies of the dynamics of processes, and about the high costs associated with studies that are undertaken. In the remainder of this paper, the first of these two factors will be discussed. Some examples where dynamics of industrial processes have been considered are presented and some recent academic work aimed at identifying potential control problems as early as possible will be described.

A second paper (Perkins 1985) will discuss the second aspect and review tools available to help to reduce the costs of dynamic simulation.

2. Process dynamics—Why bother?

In a now classic paper, Anderson (1966) discusses problems ICI experienced in commissioning an autothermal reactor. The reactor operated quite satisfactorily

Received 20 February 1986.

† This paper was presented at the International Seminar on Modern Methods in Dynamic simulation of Industrial Processes, Trondheim, Norway, May 1985.

‡ Department of Chemical Engineering, Imperial College, London SW7 2BY.

during the early stage of commissioning, when the throughput was about half the design rate. However, attempts to run at full rate led to uncontrollable surges in pressure and temperature in the reactor loop. The system was run at reduced throughput while the problem was investigated. This involved building a dynamic simulation of the system. Eventually, it was found to be necessary to modify both the heat exchange system for the reactor and the control system in order to cure the problem.

This case offers a counter example to the conjecture that energy integration never causes operability problems, which some advocates seem to want us to believe. However it also should concern those who say that energy integration always causes difficulties, since it was possible to cure the problem by careful analysis. The important point is that such analysis should be timely: it is rather embarrassing, stressful and costly to have to sort these problems out while trying to commission the plant. Open loop instability is not a fundamental problem in itself; it can be a worry if the first time anyone knows about it is when the plant starts oscillating violently! By analysing the dynamics of the process early enough a considered decision as to the best way to proceed can be made. Needless to say, it seems better to find these things out on a simulation rather than on the plant.

Lest it be felt that the Anderson example is an isolated case of something that does not arise anymore, an example we recently came across should be of interest, (Wong (1985)). An energy integration study of a new plant had suggested that some of the boiler heat for a distillation column be provided by cooling the product stream from an exothermic reactor in the process. The feed stream to the reactor was formed from the overheads from the same column, so the situation is exactly analogous to the Anderson case, but this particular heat exchange was only one match in a large and complex network, so it was much more difficult to isolate the cause of plant instability. Of course, with a plant like this, there are many alternative schemes of energy integration, many of which have similar economic characteristics (comparable capital costs, and energy requirements). It would be sensible to screen out those alternatives having a deleterious effect on the process dynamics, in order to try to avoid the kind of unpleasant surprises exemplified above at commissioning time.

The reduction of nasty surprises is only one aspect of normal operation of a plant which consideration of dynamics can facilitate. Recent academic work has shown how to assess the ease of control of a plant from a dynamic model (see the excellent review of Grossman and Morari (1983), and the papers at the recent PSE '85 Conference for an introduction to these ideas). One objective is to be able to rank process alternatives on the basis of ease of control without having to design control systems and perform lots of dynamic simulations. Our own work at Imperial College (Perkins and Wong (1985)) is but one example showing the practicality of this. The ideas are readily implementable, and have been implemented as an addition to our SPEEDUP system (Perkins, Sargent and Thomas (1982)). In the next section, these ideas will be described in more detail.

The above discussion has been concerned with aspects of holding the plant at one steady state operating point. Nowadays, it is becoming increasingly common to have that operating point chosen as the solution to an optimisation problem, and to update it as conditions change. One factor which has been largely neglected in setting out this strategy of plant operation is the costs associated with switching from one steady-state to the next. Typically, once new set points have been chosen for the controllers they are ramped at a rate fixed 'so as to avoid upsets'. A study by Sargent and Sullivan (1979) on a crude oil column with changing feedstock indicates that this policy is rather conservative, and that there is significant mileage for reduction in operating costs by looking for an optimal switching policy. Recent work by Howell (1984) on a similar system confirms that switching costs can be significant, and can be reduced considerably by carefully chosen operating procedures. § 5 gives more details of this study.

The above examples are all concerned with the 'normal' operation of a plant. There is obvious scope for application of dynamic simulations for the study of operability of plants in face of upsets, and for the identification of potential hazards. In the former category, one may cite the problem of an oil production platform being fed with slugs of gas and liquid in sequence (Tsitsouras (1984)). Since the cost of shutdown of such a system has recently been estimated at £125,000 per hour (Van den Buelk (1984)), it is important to try to guarantee integrity of operation in the face of such an upset!

An interesting example of the potential importance of dynamics in safety studies is given by Perris and Grogan (1981). They discuss the simulation of a plant during transition from one steady-state operating point to another. Previous studies had shown the plant to be safe at both conditions, but the dynamic simulation highlighted a potentially hazardous situation during the transient.

Summing up these examples, it is clear that there are many potential applications of dynamic simulation beyond the obvious area of control system design. Indeed, it seems that study of dynamics could pervade many phases of design and operation of a plant. In the sections which follow, some of our own work aimed at assessing the impact of process dynamics on plant operability will be described. The reasons for presenting this work are twofold: first, to describe some of the latest ideas on the importance of considering process dynamics during design, and second, to demonstrate the kinds of study that are possible using an up-to-date process simulation package.

3. Assessing controllability of chemical plant

The concept of controllability is fundamental in mathematical systems theory (Rosenbrock (1970)). Nevertheless, despite the fact that controllability assessment is a potentially important aspect of chemical process design, little use has been made of the ideas of systems theorists by chemical engineers. The reason for this is not too difficult to find, and was well presented by Rosenbrock in his book: the usual notion of state controllability is unappropriate as a basis for assessment of chemical process controllability (Rosenbrock 1970).

Nevertheless, all is not lost. Rosenbrock himself (following a proposal of Brockett and Mesarovic (1965)) put forward a definition of controllability which is more appropriate for the purposes of process control. To investigate the *functional controllability* of a plant, a desired trajectory for the outputs is formulated, and the conditions under which an input trajectory exists which generates the desired outputs exactly are investigated. Thus, in contrast to the more common state controllability, interest is focused not only on guaranteeing the performance of the plant at one particular time (when the desired state is achieved), but over an entire time interval.

The conditions necessary and sufficient for a linear plant to be functionally controllable are stated in the following Theorem: (This is the discrete time version. Similar results exist for continuous time systems).

Theorem (Rosenbrock 1970)

Given a plant, with a square transfer function matrix $G(z)$ whose McMillan degree is p, and a sequence of outputs 0, 0, 0 . . . 0, y_p, $y_{p+1}, \ldots$ then there exists a sequence of inputs $u_0, u_1, \ldots$ which generates the output sequence if and only if

$$\det [G(z)] \not\equiv 0 \tag{1}$$

The conditions for functional controllability are of two kinds. First, there are restrictions on the desired outputs. In continuous time, these amount to smoothness requirements, but in the above theorem the concept of a delay time appears. It is not allowed to move the plant output before p units of time have elapsed. We shall return to this concept later. The second class of condition is a condition on the process transfer function: functional controllability is guaranteed if and only if the transfer function is invertible. This is clearly a sufficient condition since given

$$y(z) = G(z)u(z) \tag{2}$$

and $\det [G(z)] \not\equiv 0$, it follows that

$$u(z) = G^{-1}(z)y(z) \tag{3}$$

whence the required input sequence is determined.

The concept of invertibility is fundamental to functional controllability, and it seems from the above theorem that it is all that is required. However, there are several practical limitations which need to be considered. The first was pointed out by Rosenbrock: under some circumstances the input trajectory determined from eqn. (3) will be unbounded. This will be the case if the system possesses right half-plane zeroes, since those will appear in the denominator of $u(z)$ leading to unstable modes. Thus, in practice, invertibility and absence of right half plane zeroes are both important. An obvious extension of the above argument leads to the identification of bounds on control action as of potential significance.

The second practical limitation is concerned with the delay time p in the theorem. From a practical point of view, the longer this time, the less 'controllable' the system is, since a greater restriction is placed on the desired outputs. Time delays are all too common in process systems. A statement that time delays reduce controllability is not very helpful; what is required is a means of ranking alternative designs on the basis of the effect of time delays on plant controllability. The quantity p in the Theorem would seem to offer such a means: the higher p, the less controllable the plant will be. However, in using this concept, we should use the *smallest* delay which allows independent specification of each component of the output. The McMillan-degree is the degree of the monic least common denominator of all minors of all orders of the matrix. In general, this quantity will give a gross overestimate of the minimum delay necessary, as the following example (taken from Perkins and Wong (1985)) illustrates

Example

$$G(z) = \begin{bmatrix} z^{-5} & z^{-4} \\ z^{-7} & z^{-2} \end{bmatrix}$$

For this case, $p = 11$, but feasible input sequences can be found for all output sequences commencing after a delay of 5 units.

Algorithms for computing the correct minimum delay are given by Wong (1985) and by Perkins and Wong (1985).

The final practical limitation arises from our inability to provide an exact model of any system. Different plants will show different sensitivity to modeling error in terms of performance under control. Within the framework of functional controllability, a natural measure of sensitivity arises from numerical analysis. It is necessary to solve eqn. (2), a system of linear equations, for u given G and y. The sensitivity of the solution to errors in G is given by the unequality:—

$$\frac{\|\delta u\|}{\|u\|} \leqslant \|G\| \, \|G^{-1}\| \frac{\|\delta G\|}{\|G\|} \tag{4}$$

The *condition number*

$$k(G) = \|G\| \, \|G^{-1}\| \tag{5}$$

gives the relationship between relative errors in G, and the induced errors in u. The lower the value of $k(G)$, the less sensitive the system is to modeling error.

The above theory is concerned with linear plants, and it is not obvious that it can be used to assess the controllability of real processes, where non-linear effects can be important. To examine this issue, several case studies have been performed, of which the following, taken from Perkins and Wong (1985), is a typical example.

4. A case study in controllability of chemical plants

This case study is based on the double-effect distillation of a mixture of methanol and water to pure components, a technique proposed by Tyreus and Luyben (1975) for this system. Flowsheets for three possible configurations are shown in Fig. 1.

For simulation purposes, the columns were modeled using lumped sections, and the models were matched to the slowest eigenvalues of more rigorous models. A simple dynamic model was used for the heat exchanger, also devised based on matching of eigenvalues. For full details of the models consult Howell (1984). It should be noted that no time delays were included in these models, so that controllability will be assessed on the basis of the presence or absence of right-half plane zeroes, and on the sensitivity to modelling error.

Since the analysis is based on properties of the process transfer function, it is necessary to choose inputs and outputs. Because the outputs should be related to control objectives, we have chosen the compositions of both product streams for all cases. For illustrative purposes, we present results for each configuration with the reflux flow to each column as inputs. In addition, we give the results for configuration A with the reflux to the high pressure column replaced by the split ratio of the feed. This case is labelled Configuration A′ in all the results. Wong (1985) presents results for many other choices of inputs.

The non-linear models described above were used in conjunction with the SPEEDUP flowsheeting system (Perkins and Sargent 1982) to perform steady-state and dynamic simulations of the various designs. A separate package, interfaced to SPEEDUP, was developed to linearize the non-linear dynamic models, and to

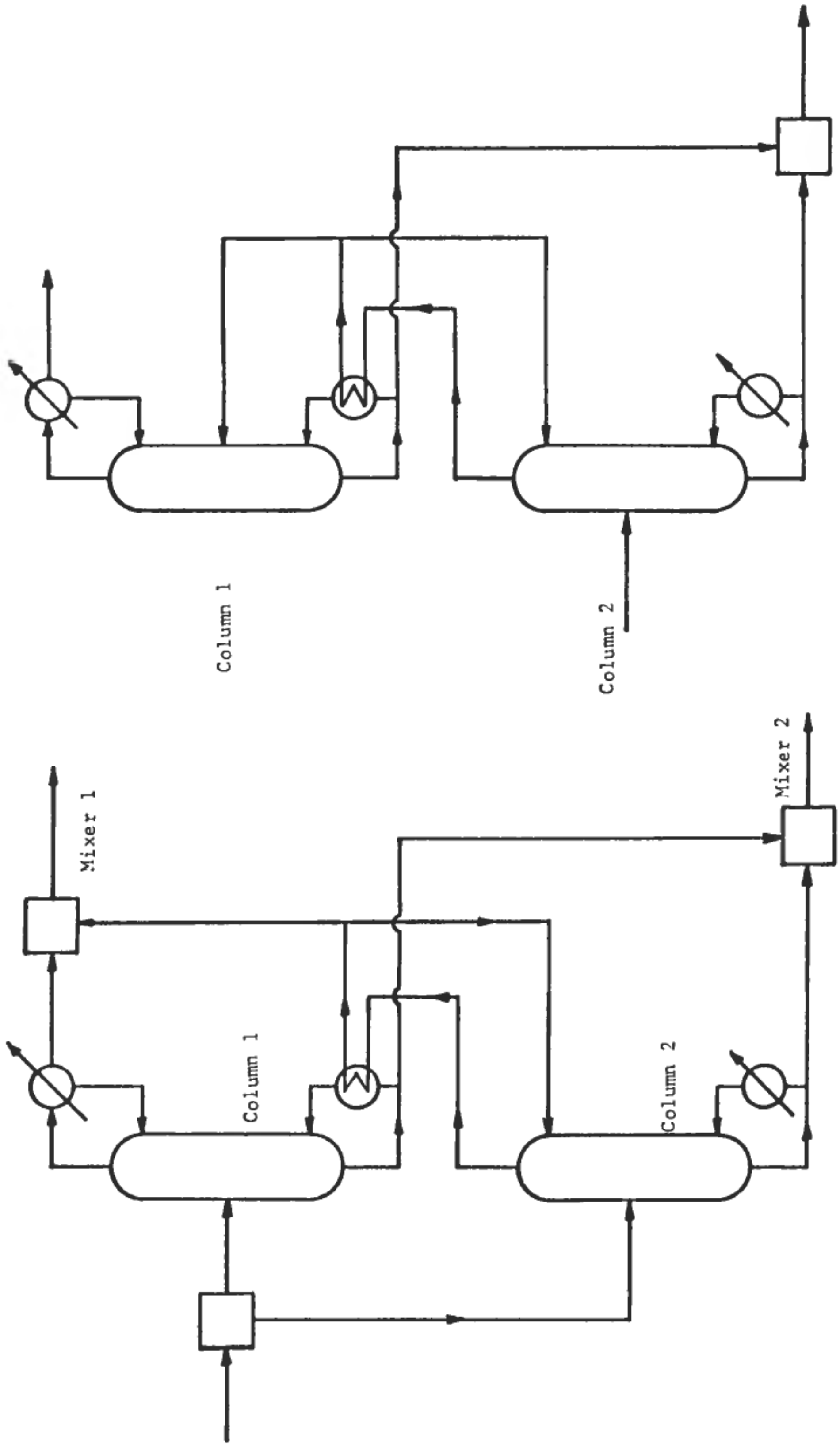
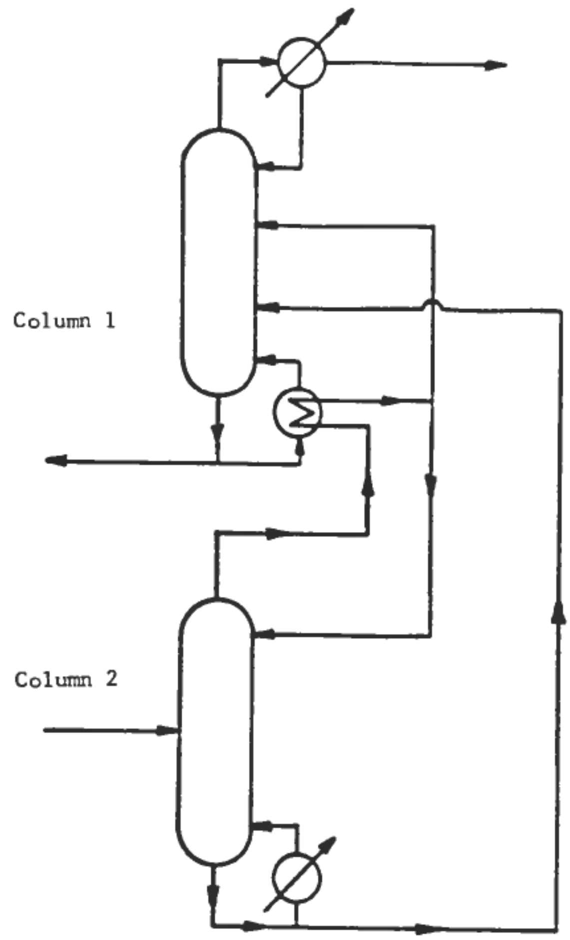


Figure 1. (*a*) Configuration A. (*b*) Configuration B.



(*c*) Configuration C.

compute the transfer function matrix and its properties at various frequencies. The package, called SPEECON, is fully described by Wong (1985).

Of the four configurations, A is the only one exhibiting a right-half plane zero, though at $s = 445$ it may be far enough into the right half plane to have a negligible effect on control performance (Holt and Morari 1984).

Table 1 gives the condition number for each configuration evaluated at zero frequency. Values at other frequencies show the same trend, and may be found in Perkins and Wong (1985).

Configuration	Condition number
A	1·85
A′	1·90
B	1·05
C	1·08

Table 1. Steady-state values of process condition number

The first feature we notice is that there is less than a factor of 2 differences between the best and the worst cases. The ranking implied by these values is first B, followed closely by C, then A, followed closely by A′. The difference between the two sets {B, C} on the one hand and {A, A′} on the other is larger than differences within the sets. Of course, the performance of A should be influenced by the presence of a zero.

To check whether the ranking implied by the analysis was borne out by performance of the designs under closed-loop control, two kinds of optimal controller were designed for each configuration, using linearized models. A quadratic performance index using output and input deviations from the desired steady-state was used in both cases. First, this performance index was minimized by solving the standard infinite time linear quadratic state feedback problem (Athans and Falb 1966). Second, optimal settings were chosen for single input, single output loops using a non-linear optimization package. Table 2 shows the resulting optimal performance indices for each case, corresponding to an initial perturbation in all the states of 5% of their steady-state values.

It can be seen that the ranking implied by Table 1 also shows up in the ranking of closed loop performance. Also, small differences in performance index are reflected in small differences in condition number. To gauge the significance of the differences, responses of the methanol stream composition are plotted in Fig. 2 for each configuration under multi-loop control.

It can be seen that there is a significant difference between {A, A′} and {B, C}: the times to recover from the disturbance being about 30 minutes and 5 minutes respectively. Although there are differences between A and A′ and between B and C these are much less marked. These results, combined with those of other case studies described by Wong (1985), suggest that differences in condition number of about a factor of two do correspond to significantly different closed loop performance, under multi-loop control. Perhaps this sensitivity is explained by the fact that assuming a diagonal transfer function matrix is a gross modeling error for most process systems (i.e. $\|\delta G\|$ is large).

The conclusion of this study, which has been confirmed by several others performed by the authors (Wong (1985)), is that indicators of controllability suggested by a linear theory do indeed give useful information on the performance of non-linear processes in the neighbourhood of a steady-state. These indications are easy to compute from a non-linear model, and are easier to produce and interpret than a set of non-linear simulation results.

5. Switchability of chemical plants

The operability of chemical plants in the neighbourhood of a particular steady-state has been discussed in the last two sections. Case studies exemplified by that

	Optimal indices	
Configuration	Using state feedback	Multiloop
A	33	42
A′	27	29
B	11	12
C	14	16

Table 2. Optimal performance indices

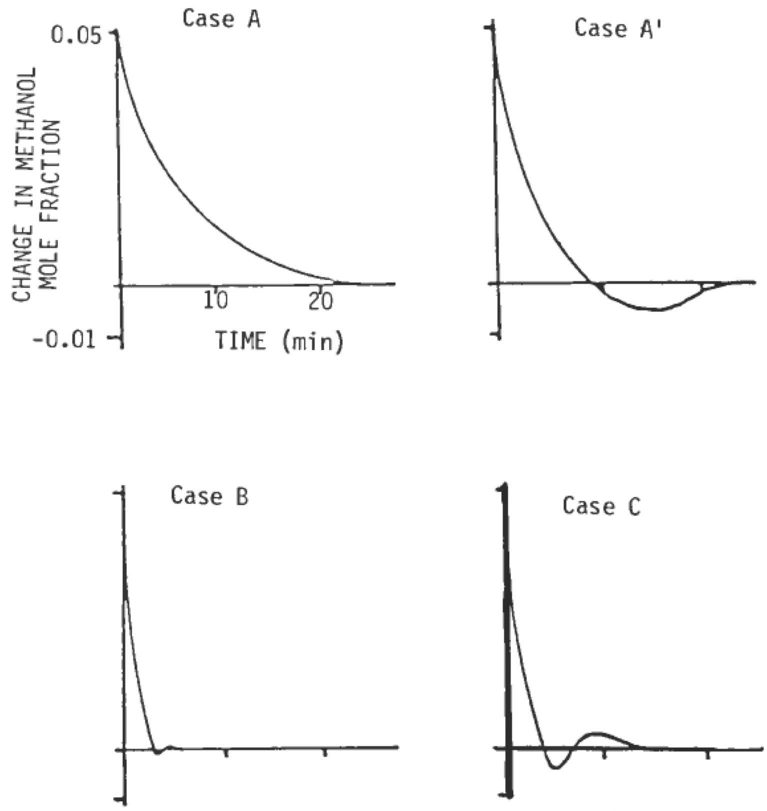


Figure 2. Change in Methanol Mole Fraction v. Time (minutes) for each Configuration (same scales in each case)

described in § 4 have demonstrated the utility of a theory based on linearized models for that situation. However, there are cases where the non-linear dynamics of the plant will be excited. One example is where the steady-state operating point is being deliberately changed in response to a large external disturbance (e.g. a change in feedstock). During process design, we may be interested in the ability of the plant to cope with such large changes. We shall call this ability: *switchability*.

The first question to be answered is whether a desired switch is feasible. The problem has been studied by Howell (1984). It turns out that if both steady states are feasible operating points for the plant, and they are stable in some sense, the switch will indeed be feasible. Thus, feasibility of switches will not be an issue for carefully designed plants, although Howell (1984) does present examples of what can happen if the design is not carefully done.

The next question is one of optimality. Are there features of plant that make switching more expensive, and which therefore should be avoided if possible? One feature which may be relevant is energy integration. The effect of different levels of energy integration on the switchability of a particular plant will be assessed in the remainder of this section.

The plant consists of a multi-component complex distillation column and the associated heat recovery network for the separation of crude oil. The column structure is shown in Fig. 3. The feedstock is split into four fractions, the exact ratio being determined by the feed composition. Liquid is drawn off at intermediate

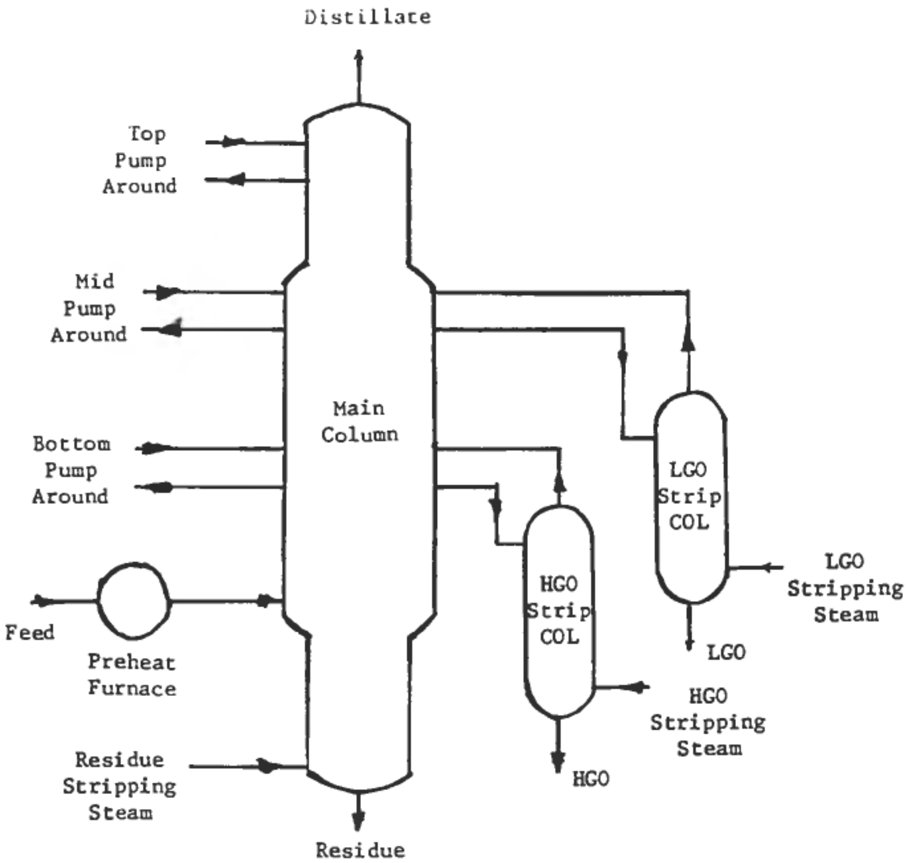


Figure 3. Main column schematic. Dist, distillate; LGO, light gas oil; HGO, heavy gas oil; RES, residue; TPA, top pump around; MPA, mid pump around; BPA, bottom pump around.

stages and cooled, then returned to the column to provide inter-section cooling. These 'pump-around' streams, as they are called, regulate the reflux ratio in each section. The main vapour flow comes from partial vapourization of the feed, but direct steam injection is used to strip valuable light products out of the residue and side streams.

Crude oil separation consumes a substantial amount of energy, and the recovery of waste energy is a very important aspect of the operation. The feed is heated to a temperature equivalent to around 700 K in the unvapourized liquid before injection into the main column. Most of this heat is in practice recovered from the product streams, and the oil fired heater only accounts for about one third of the final heat content of the feed. There are many different heat exchanger networks which will accomplish this task. The purpose of this case study is to investigate how the choice of heat exchange network affects the switchability of the combined column and heat exchange system.

Three networks have been selected for study (Fig. 4). The first is a simplified version of the original network currently in use at the refinery. The temperatures and flowrates within this network were used to define the heat recovery problem. The second network is a solution to this problem reported by Hanson (1984),

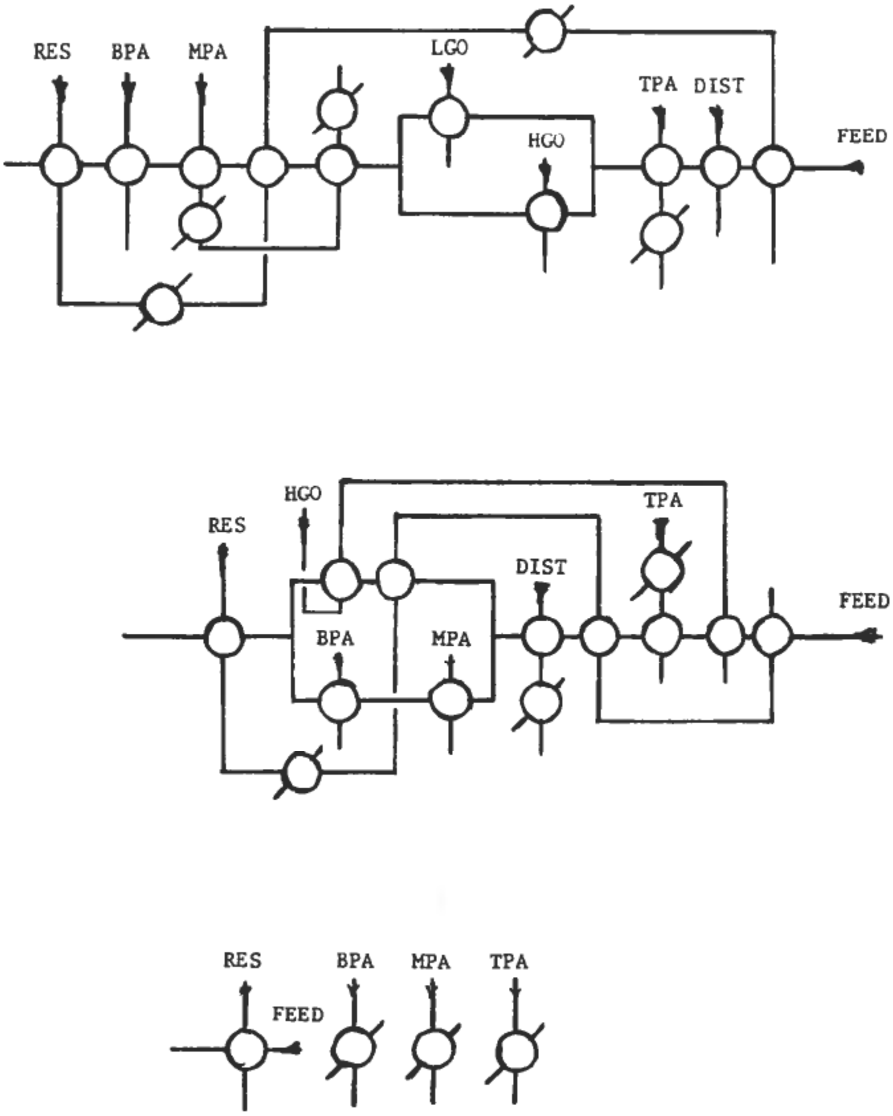


Figure 4. Heat exchanger networks for the crude distillation column.

subject to a minimum approach temperature of 50 K. The third network is a 'minimum equipment' solution developed to represent a scheme with virtually no interaction between column and network. Even so, this network recovers over two thirds of the heat which either of the complex networks recover.

We will use the least costs associated with switches as measures of the switch-abilities of different designs. The models used to represent the column and heat exchangers are of the kind described in the previous section, i.e. lumped section models for the column, and simplified models for the heat exchangers. Care was taken to match the steady-state behaviour of the plant closely; the dynamics were matched to dominant eigenvalues of more rigorous models. To simplify the model as much as possible without losing the essential features of the problem. the crude oil was represented by a small number of chemical components (four). Even with these simplifications, the determination of the optimal switching policies using an optimal control package is a substantial computational problem. Full details of the models used are presented in Howell (1984).

The objective function used for this study was:

$$J = \int_0^t F(0{\cdot}0174 \sum_i (T_i - T_{i,ss})^2 + \sum_j c_j(u_j - u_{j,ss}) - \sum_i c_i(F_i - F_{i,ss}))\,.\,dt \qquad (6)$$

where c is the stream cost
T is the stream temperature
F is the stream flowrate
u is the utility flowrate
i is the product stream identification
j is the utility stream identification
ss indicates the final steady state value.

The first term represents a penalty on off-specification product, where product quality is measured by the proximity of the stream bubble point to its desired value. The second term represents the cost of utilities associated with control action, and the third term gives the contribution of product values.

The controls chosen for the optimal control study are as follows:

Top pumparound flow
Middle pumparound flow
LGO product flow
HGO product flow
LGO offtake
HGO offtake
Feed preheater furnace duty.

Switches associated with changes between heavy and light crudes were studied, the optimal switching policies being determined by an optimal control package interfaced to our SPEEDUP simulation package. Details of these packages may be found in Howell (1984).

Table 3 shows costs associated with a particular pair of switches from heavy to light crude and back. The 'steady state switch cost' corresponds roughly to normal practice; the controls are set to their new values at the initial time, and the system is left to settle to the new steady-state. We see that network 1 is the cheapest network using this policy, with network 2 a poor third. Network 1 also performs best under the optimal switching policy, although the differences in performance between the three cases are much smaller. Since these differences correspond to the profit associated with only roughly 5 minutes of steady state operation, they are not a significant factor in choosing between the alternative heat exchanger networks for this plant.

Two other significant facts emerge from study of Table 3. First, the profits associated with switching are significantly larger than those associated with steady-state operation! Thus it appears that this is another example of a distillation process that would benefit from transient operation (cf. Pollard and Sargent (1970)).

The second point of interest is the difference in cost between normal and optimal switching policies. This difference is significant, corresponding to roughly 8 hours steady-state profit for network 1, and confirms the earlier work of Sargent and

Network	1	2	3
Steady state switch cost			
A–B tons	10·7	9·2	16·2
B–A tons	21·8	47·0	18·3
A–B–A tons	32·5	56·2	35·5
Optimal switch cost			
A–B tons	−7·4	−7·9	−7·0
B–A tons	−1·7	−0·7	−1·1
A–B–A tons	−9·1	−8·6	−8·1

Key: state A—processing heavy crude; state B—processing light crude

Table 3. Switching costs for the three networks

Sullivan (1979). It seems that efforts made to optimize the way in which changes of steady-state operating point are made will be amply rewarded.

6. Conclusion

The paper has attempted to demonstrate the significance of process dynamics in plant design by two means. Several examples of industrial cases where dynamics turned out to be crucial have been discussed. These examples range from cases where plants were designed and built which turned out to be unstable to a case where an explosive transient between two safe steady states was discovered by dynamic simulation.

Some effects of process dynamics on plant operability have been discussed. Indications of closed-loop control performance based on plant characteristics have been described, and demonstrated to highlight significant differences in plant performance under control. It has also been shown that consideration of non-linear dynamic effects may have economic benefits in some circumstances.

Acknowledgements

The financial support of British Petroleum PLC through an Extra Mural Research Award is gratefully acknowledged.

References

Anderson, J. S. (1966). A practical problem in dynamic heat transfer. *Chem. Engr.* (Lond.) p. CE97.

Athans, M., and Falb, P. L. (1966). Optical control, McGraw-Hill: New York.

Brockett, R. W., and Mesarovic, M. D. (1965). The reproducibility of multivariable systems, *J. Math Anal. Appl.*, **11,** 548.

Grossman, I. E., and Morari, M. (1983). Operability, resiliency and flexibility—process design objectives for a changing world. Presented at *FOCAPD–83*, Snowmass, Colorado, USA, June 19–24, (CACHE Corporation).

Hanson, K. W. (1984). The synthesis of heat exchanger network subject to variable sets of constraints. PhD Thesis, University of London.

Holt, and Morari, (1984). Design of resilient processing plants VI, *Chem. Eng. Sci.* (in press).

Howell, J. M. (1984). The effect of energy integration on the switchability of chemical processes. PhD Thesis, University of London.

PERKINS, J. D. (1985). Survey of existing systems for the dynamic simulation of industrial processes. *Modeling, Identification and Control*, **7,** 2.

PERKINS, J. D., SARGENT, R. W. H., and THOMAS, S, (1982). SPEEDUP: A computer program for steady-state and dynamic simulation of chemical processes. Presented at Inst. Chem. Engrs. Annual Research Meeting *Computers in Chemical Engineering* London, April.

PERKINS, J. D., and WONG, M. P. F. (1985). On the controllability of chemical plants. Presented at *PSE 85*, Cambridge, Mar. 31–Apr. 3, EFCE Publication Series No. 40. pp. 481–92.

PERRIS, F. A., and GROGAN, J. C. (1981). Computer aids for process plant operability studies. Presented at *CHEMCONTROL81*, Vienna, Austria, Sept.

POLLARD, G. P., and SARGENT, R. W. H. (1970). Offline computation of optimal controls for a plate distillation column. *Automatica*, **6,** 59.

ROSENBROCK, H. H. (1970). *State-space and Multivariable Theory* (Nelson).

SARGENT, R. W. H., and SULLIVAN, G. R. (1979). Development of feed changeover policies for refinery distillation units *Ind. Eng. Chem. PD & D*, **18,** 113–24.

TSITSOURAS, K. (1984). Dynamic simulation with an equation oriented flowsheeting system. MSc Thesis, University of London.

TYREUS, and LUYBEN, (1975). Controlling heat integrated distillation columns, *CEP 72* (6), 59.

VAN DEN BUELK, (1984). Operability, reliability and maintenance differences onshore and offshore. Presented at *Offshore/Onshore Engineering Practices Symposium*, Glasgow, Scotland, Nov. 21–22.

WONG, M. P. F. (1985). The assessment of controllability of chemical processes. PhD Thesis, University of London.