The rapidly increasing activity coefficients of NMe_4OH with concentration (Abdel-Salam et al., 1976) suggest that the reaction rate constant depends, in some way, on the OH^- concentration. Further support of that view comes from the early work on the alkaline decomposition of diacetone alcohol in presence of NMe_4OH and KOH, successively (Halberstadt and Prue, 1952). The reaction rate in that case increased with increasing NMe_4OH concentration but decreased slightly in the case of KOH. This behavior is consistent with the activity coefficients of the two electrolytes.

The dependence of the gas-catholyte interface area on the current density and the electrode configuration is less clearly understood. It is known that the equilibrium of the electrolyte meniscus inside the electrode pores depends on several factors, such as the capillary forces, gas pressure, etc. It may be that the electroosmotic forces, which depend on the current density distribution in the electrode, affect the air-electrolyte equilibrium and hence their interface area.

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Methodology for Simultaneous Optimization with Reliability: Nuclear PWR Example

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SCOPE

The determination of optimal process reliability can be described as a mixed integer optimization problem. Although not usually included in the optimization study, reliability is an important aspect of process design, affecting both the safety and economics of the installation.

Process reliability can be improved by redundancy (spares), by use of more expensive components (or controls), and by subdividing large units into smaller units that will accomplish the same task. Differing reliability requirements involve new, and sometimes quite different, process arrangements. Improving reliability of a process usually adds to the cost, and this added cost must be offset by better operation.

Reliability can be incorporated in the process study as a constraint that must be met by the process arrangement, or reliability might be built into the cost function as a penalty imposed for less reliable systems. Both of these methods require manipulation of the process arrangement to determine the best configuration. At the same time, however, it is necessary to consider other independent

variables in the process in order to arrive at an optimum. This type of optimization study is mixed integer, with different process configurations represented as discrete variables.

Previous approaches to combining optimization and reliability usually treat the two as separate problems, determining the reliability by integer programming. The purpose of this paper is to describe a method for including reliability in the usual process optimization problem. The algorithm applied to this mixed integer problem is the adaptive random search, which can search both discrete and continuous variables simultaneously. This method is applied to optimization of the primary cooling system of a nuclear PWR, which has twelve independent variables, three of which are integers directly affecting system reliability. Reliability data were obtained from USAEC-WASH 1400 report. Optimization results are presented for various levels of reliability.

CONCLUSIONS AND SIGNIFICANCE

The adaptive random search was found to be an appropriate method for solving mixed integer optimization problems. Only slight modifications to the basic search procedure are required to accommodate discrete variables.

The optimal design for the PWR was found to consist of two coolant loops, each with one pump and one exchanger. The reliability of this minimum cost arrangement was only 0.93. Improvements in reliability of the PWR are obtained by adding loops and pumps, with an attendant increase in cost. In this study, reliability was incorporated as a constraint to be satisfied by the process. The adaptive random search was successful in locating new optima as the reliability constraint was varied and for different methods of computing reliability.

This method of design permits improvement in reliability, not only by adding safety features but also by modifying the system design. The algorithm is easy to program, and computational times are reasonable. The method should find wide application in reliability studies, as well as other types of synthesis problems.

Optimization of chemical processes involves manipulation of certain independent variables in the process to achieve a minimum cost or a maximum profit. These independent variables are usually continuous, although discrete variables, such as number of stages, are frequently encountered. The search of continuous and discrete independent variables simultaneously poses severe obstacles for most optimization techniques (Weisman and Holzman, 1969). The method usually employed to handle this difficulty is to treat all variables as continuous, rounding the discrete variables at the termination of the search. This procedure produces erroneous results unless the objective function is well behaved (Beveridge and Schechter, 1970). Another method, somewhat tedious, is to apply an optimization algorithm to the continuous variables and to enumerate the discrete variables externally by brand and bound procedures (Weisman, 1968; Dakin, 1965).

Process reliability is a function of the type and arrangement of equipment in the process. Reliability has a very definite influence on process economics although reliability is rarely considered in the optimization problems. Inclusion of process reliability in the process optimization study would involve manipulation of the process arrangement to adjust reliability and maximize profitability. Such a study is analogous to the synthesis of the optimal process (Hendry et al., 1973; Umeda et al., 1972). The variables in these studies will include discrete quantities, number of spares, type of equipment, etc. Therefore, optimization procedures for reliability and synthesis analyses usually involve integer or discrete programming methods (Henley and Gandhi, 1975; Menzies and Johnson, 1972).

The usual statement of the optimal reliability problem is to maximize the reliability subject to a maximum cost constraint. These problems treat equipment type or redundancy as integers and do not include continuous variables. Therefore, solutions can be obtained by integer programming (Tillman and Luttschwager, 1967; Proschan and Bray, 1965) or integer gradient methods (Henley and Gandhi, 1975).

A more general optimization problem for the chemical process would be to include the reliability as a cost item in the profit function to be optimized (Gandhi and Henley, 1975; Allen and Pearson, 1975). A similar approach is to treat the reliability as a minimum constraint that must be satisfied. Both of these procedures introduce integer variables associated with manipulating the reliability, thereby complicating the optimization procedure.

The purpose of this paper is to describe a method for solving the mixed integer, process reliability-synthesis optimization problem. The method utilizes the adaptive random search procedure which can be modified to allow search of continuous and discrete independent variables simultaneously. The example chosen for demonstration of this method is the optimization of the primary cooling system of a nuclear reactor. This process was chosen because of the importance of the reliability of these systems and because it offers an interesting optimization problem with twelve discrete and continuous variables.

THE ADAPTIVE RANDOM SEARCH

The adaptive random search technique, proposed by Gall (1966) and examined in detail by Heuckroth and Gaddy (1976), searches each variable randomly by simulation of values of the variables from a probability density function given by Equation (1):

$$x_i = x_i^* + \frac{R}{k}(2\theta - 1)^k \tag{1}$$

The search is centered about values of the independent variables which have given the best objective function; thus, the search converges in a systematic manner to the optimum. The efficiency of the search is controlled by increasing the distribution coefficient k and by reducing the range R as the optimum is approached. This procedure has been found to be quite effective in solving a variety of problems and exhibits certain advantages for process optimization problems (Gaines and Gaddy, 1976; Heuckroth and Gaddy, 1976).

The adaptive random search procedure can be applied to discrete variables by sampling from the distribution given by Equation (2):

$$\theta \leq \sum_{j=1}^{M} k'p(x_{ij}) \quad \begin{matrix} (j = 1, N) \\ k' = 1, \quad x_{ij} \neq x_i^* \\ k' > 1, \quad x_{ij} = x_i^* \end{matrix} \tag{2}$$

The new value of the independent variable is x_{iM}. The probabilities $p(x_{ij})$ are found from Equation (3):

$$\sum^{N} k'p(x_{ij}) = 1 \quad (3)$$

Initially, the probabilities are all the same $[p(x_{ij}) = 1/N]$, and an exhaustive random search is performed. As the search converges toward the optimum, k' is increased to raise the probability of obtaining a value which is near optimal.

When the number of possible values of a discrete variable becomes large ($N > 50$), the sampling can be performed in two steps to reduce the computational effort. First, the range of possible values is divided into a number of equal regions, and each region is treated as a discrete variable. Once the proper region is chosen, by means of Equations (2) and (3), the value of the discrete variable within that region is calculated by Equation (4)

$$\max(x_{ij}) \leq x_{iL} + \frac{\theta - p(x_{iL})}{p(x_{iU}) - p(x_{iL})} [x_{iU} - x_{iL}] \quad (4)$$

Rounding the variable x_i, as in Equation (4), is necessary, since the fraction $[\theta - p(x_{iL})]/[p(x_{iU}) - p(x_{iL})]$ is not always an integer. The above sampling procedure corresponds to a uniform search within the selected region. An alternative procedure would be to apply Equations (2) and (3) to the selected region.

Since the search procedure does not associate the independent variables, except through the objective function, it can be applied to mixed integer optimization problems. Separate random numbers are generated for each variable, and convergence is controlled by the distribution coefficients.

NUCLEAR POWER PLANT PRIMARY COOLING SYSTEMS

Figure 1 shows the flow diagram of a pressurized water nuclear reactor system. The nuclear fuel is cooled by water circulated through the core. The coolant then exchanges heat to produce steam that drives a turbine generator. Water pressure, generally in excess of 2000 lb/in.^{2} to suppress bulk boiling, is maintained by an electrically heated pressurizer. Only one coolant loop is shown in Figure 1, although several identical parallel loops are generally used.

The plant size studied is 384 MW, net electrical output, and is identical to the unit constructed at San Clemente, California, in 1963. The objective of the optimization study is to minimize the investment for this facility. Long experience with turbine-generator design has led to standard units, and it is assumed that the cost of generating equipment for 384 MW is constant. Also, it is assumed that the cost of reactor fuel, auxiliary systems, and safety features is fixed. With these assumptions, the design which minimizes the cost is only concerned with the primary coolant loop. This study is similar to one performed for the same facility by Weisman and Holzman (1972).

The cost equations include the following parameters: reactor core and vessel size, size and number of reactor coolant loops, number and power requirements of coolant pumps, number and size of steam generators, and coolant and steam pressure. A number of design constraints are imposed: size and weight of steam generators, size of reactor vessel, linear flow in main coolant piping, and the departure from nucleate boiling ratio. The equations describing this system (objective function and constraints) have been presented earlier (Weisman, 1968; Weisman and Holzman, 1972) and are not repeated.

The twelve independent variables are listed in Figure 1. As noted, the number of loops, number of pumps per loop, number of heat exchangers per loop, and number of fuel rods are integer variables. Tubing diameter and lengths

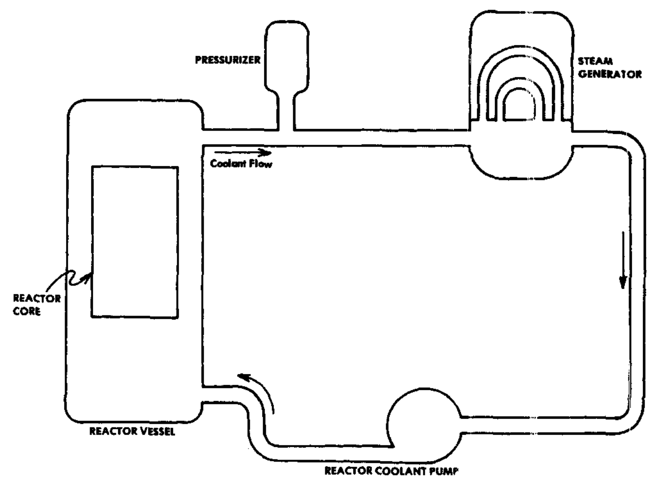

Fig. 1. Pressurized water reactor (PWR) primary cooling system.

Independent design variables

1. Total coolant flow
2. Coolant temperature at reactor inlet
3. Delta T between steam and coolant at outlet
4. Steam generator tube diameter
5. Steam generator tube length
6. Operating pressure
7. Number of fuel rods in the core
8. Thermal shield flow passage width
9. Coolant piping diameter
10. Number of coolant loops
11. Number of pumps per loop
12. Number of steam generators per loop

TABLE 1. RANGE OF DESIGN VARIABLES FOP PWR

Variables	Minimum	Maximum
Number of coolant loops (N)	2	10
Number of pumps per loop (NPN)	1	2
Number of stm. gen. per loop (NHN)	1	2
Total coolant flow (W), lb/hr	2.5×10^7	2.5×10^8
Coolant temp. to reactor (TIN), °F	490	660
ΔT @ stm. gen. outlet ($DELT2$), °F	50	170
Stm. gen. tube diameter (D), in.	0.5	1.0
Stm. gen. tube length (ZL), ft	10	80
Max. operating pressure($ZPMAX$), lb/in.^{2}	1 000	2 500
Thermal shield flow passage width (B), ft	0.1	3.0
Coolant piping diameter ($CAPD$), ft	1.0	3.5
Fuel rods in code (NN)	15 000	40 000

TABLE 2. PWR DESIGN OPTIMIZATION WITHOUT RELIABILITY

Variables	Optimal value
Number of coolant loops	2
Number of pumps per loop	1
Number of stm. gen. per loop	1
Total coolant flow	6.26×10^7
Coolant temp. to reactor	549
ΔT @ stm. gen. outlet	50.1
Stm. gen. tube diameter	0.994
Stm. gen. tube length	26.33
Max. operating pressure	1 411
Thermal shield flow passage width	2.46
Coolant piping diameter	2.56
Fuel rods in core (NN)	36 598
Minimum total cost, MM$	18.89

may also be considered discrete variables. Table 1 lists the upper and lower limits of the design variables. The variable names given are used in subsequent tables. Since the range of the number of fuel rods is quite large, this variable was sampled by the method given in Equation (4).

TABLE 3. COOLING SYSTEM COMPONENT FAILURE PROBABILITIES

Component	Component failure rates	
	Failures per hour	Failures per year
Pumps (failure to run)	3×10^{-5}/hr	2.628×10^{-1}/yr
Pipe, ≤ 3 in. diam (per section-rupture/plug)	1×10^{-9}/hr	8.76×10^{-6}/yr
Pipe, > 3 in. diam (per section-rupture)	1×10^{-10}/hr	8.76×10^{-7}/yr

TABLE 4. COMPONENT RELIABILITY CALCULATIONS

I. Reliability of pump(s) in a loop (parallel)
$R_{pumps} = 1.-(0.2628)^{NPN}$

II. Reliability of steam generator(s) in a loop (parallel)
$R_{sgs} = 1.-(1.-(1.-8.76 \times 10^{-6})^{NTH})^{NHN}$

III. Reliability of coolant piping in a loop (series)
$R_{pipe} = (1.-8.76 \times 10^{-7})^{6}$

IV. Coolant loop reliability (series)
$R_{loop} = R_{pumps} \times R_{sgs} \times R_{pipe}$

TABLE 5. OPTIMIZATION RESULTS WITH RELIABILITY CONSTANTS

Reliability constraint	System reliability	Number of loops	Pumps per loop	Stm. gen. per loop	Min. cost, $MM
0.80	0.9309	2	1	1	18.89
0.90	0.9309	2	1	1	18.89
0.95	0.9817	3	1	1	18.94
0.98	0.9817	3	1	1	18.94
0.99	0.9952	2	2	1	20 04
0.995	0.9952	2	2	1	20.04
0.996	0.9997	3	2	1	22.34
0.999	0.9997	3	2	1	22.34
0.9999	0.99998	4	2	1	23.76

OPTIMIZATION OF THE PWR

The adaptive random search procedure was used to search the twelve independent variables of the PWR system shown in Figure 1. The results of this optimization study are presented in Table 2. Two coolant loops, each with one pump and one heat exchanger, were found to be optimal. The minimum cost of the system is about $19 million. This figure represents the cost of equipment in 1968 and does not include installation. If appropriate installation and time correction factors are applied, this cost compares favorably with other cost data for this size facility (US-AEC Report, WASH-1150, 1970; Bowers and Meyers, 1971).

It should be noted that the optimal solution shown in Table 2 is somewhat different from the optimal solution of $23 million presented by Weisman (1968). Weisman followed a direct search procedure to locate the optimum region, treating all variables as continuous. A branch and bound procedure was then used to locate the true optimum. Rather than introduce discrete variables, a penalty function was added to the objective function when the value of a variable was not discrete. Weisman also imposed a substantial design margin on his solution by requiring a low probability of a constraint violation. Therefore, a different solution with a lower cost would be expected with the adaptive random search.

OPTIMIZATION WITH RELIABILITY

The reliability of the PWR is dependent upon the ability of the system to maintain an adequate coolant flow (Reactor Safety Study, 1974). This is in turn dependent upon the configuration of the design, number of loops, pumps, etc. Therefore, as certain independent variables are manipulated in the optimization procedure, the reliability of the system changes. If the reliability must be maintained above some minimal level, a further constraint is imposed upon the optimization procedure. This constraint can only be checked by determing the reliability of each process configuration synthesized. As described earlier, the reliability could be built into the cost equations; however, the constraint approach seems to be appropriate for nuclear systems design.

The reliability of the primary cooling system is the product of the series-parallel arrangement of the components. Loops are, of course, in parallel, as are multiple pumps and steam generators within a loop. The reliability of an individual loop is the product of the reliabilities of the coolant piping, steam generator(s), and pump(s), since these items are arranged in series.

Failure rate data for the system components were taken from USAEC WASH-1400 Report (1974) and are shown in Table 3. Previous PWR designs (Ark. Power & Light, 1974; Duke Power Co. 1972) indicate that six series piping sections are required per loop and confirm the parallel arrangement of loops, pumps and steam generators. The pressurizer and reactor vessel were assigned reliabilities of unity (USAEC WASH-1400 Report, 1974).

Table 4 summarizes the reliability calculations. Reliability is calculated on an annual basis. The reliability of a single generator is calculated with the tubes (pipe ≤ 3 in. diam) in series, since failure of one tube causes failure of the unit. The number of exchanger tubes is a computed (dependent) variable.

The usual calculation of system reliability would be to treat the loops as a parallel arrangement, in which all would have to fail to cause a system failure. This approach is not strictly applicable to the nuclear reactor, since a system failure can be effected by loss of a single loop, if the heat transfer capability of the remaining coolant flowing through the reactor core is not adequate to suppress film boiling at the fuel rod surface. However, when loss of coolant results, because of a loop failure, the thermal output of the reactor is reduced by moderation of the reaction. With this method of operation, system failure would result only when all loops fail, and the primary cooling system reliability R_s is calculated by the redundancy equation

$$R_s = 1 - (1 - R_{loop})^N \tag{5}$$

The above treatment is, of course, an oversimplification of the reliability computations for a very complex system. For example, redundancy does not protect against common failure, such as electric power loss. The intent here is to demonstrate a method of analysis, and the method will permit more elaborate treatment of reliability, as illustrated later.

Optimization with the adaptive random search was repeated as before, except with a minimum reliability imposed as a constraint. The results of these runs with several values of reliability are presented in Table 5. The basic design of two loops, each with one pump and exchanger, has a system reliability of 0.93. Therefore, the reliability constraint has no effect on the solution until the required reliability exceeds 0.93. The system which most economically satisfies this higher reliability constraint has three loops, each with one pump and exchanger. This design has a reliability of 0.98 and costs very little more than the optimal design. Interestingly, the San Clemente design consists of three loops, each with one pump and one exchanger. Therefore, this near optimal, but more reliable system, was chosen by the actual designers.

When reliability must exceed 0.99, the most economical design consists of two loops, each with two pumps and one exchanger, and produces a reliability of 0.995. This 2-2-1 system costs about 6% more than the optimal design. To find the optimum design for each of these reliability situations, all twelve of the independent variables were optimized. Only the optimal process configuration is shown in Table 5.

As noted from Table 3, the failure rate of exchanger tubes is quite low; therefore, significant improvements in reliability are achieved only by increasing loops and pumps. To obtain a reliability exceeding 0.995, an additional loop is required, increasing the cost approximately 11%. The reliability of the 3-2-1 system is 0.9997. Further improvements in the reliability can be obtained only by adding loops, since only two pumps per loop are permitted. To exceed a reliability of 0.9997, a 4-2-1 system is required. The last increment of reliability improvement is quite costly, 0.03% improvement in reliability for $1.4 million. Each of these optimization runs with the adaptive random search required about 1.5 min of CPU time on the IBM 370/165.

ALTERNATIVE RELIABILITY COMPUTATION

The previous treatment of redundant loops in the reliability calculation probably represents the maximum reliability case. There are cases where failure of one loop would necessitate system shut down: failure in capability to moderate reaction, failure of the loop with the pressurizer, coolant leak that cannot be valved off, etc. An alternative reliability computation, which probably represents the minimum reliability case, would be to assume that the reactor thermal output is always constant; that is, the reaction moderation efforts fail. With this failure, the heat transfer conditions in the reactor core necessitate shut down upon violation of a nucleate boiling criterion. This procedure is described as follows:

1. One of the coolant loops is assumed to fail. This failure is assumed to reduce the total coolant flow by the ratio of number of coolant loops not operating to the design number of coolant loops.
2. The thermal conditions for the system are calculated, with no reduction in the reactor thermal output.
3. If the departure from nucleate boiling ratio (Weisman, 1968) does not exceed unity, the system is operable.
4. Another loop is assumed to fail, and steps 2 and 3 are repeated. When the system fails in step 3 or the number of operable loops goes to zero, the system reliability is calculated by

$$R_s = 1 - (1 - R_{\text{loop}})^{N_f} \tag{6}$$

The optimization results with reliability computed by Equation (6) are presented in Table 6. The design (2-1-1) to achieve 0.9 reliability does not change with the new reliability computation, since a design was located in which adequate cooling could be achieved with half the coolant flow. However, different designs are required to meet each of the other reliability constraints. The result of a constant reactor thermal output is a requirement for more redundancy (loops, pumps, etc.) to achieve a given reliability. As expected, the optimal cost of the designs to meet the reliability constraints in Table 6 are higher than those in Table 5. A reliability of near unity can be achieved with ten loops, but at a cost of almost double the optimum.

The above data are presented to illustrate how the system reliability can be affected by process conditions. These additional constraints can readily be incorporated in the process model used for optimization.

CATASTROPHIC RELIABILITY

An interesting extension of this study is to consider the calculation of the probability of a catastrophic reactor failure. In order to have a catastrophic failure (melt down), both the coolant system and the engineered safety features (control rods, water spray, etc.) must fail. The combined reliability of the safety features is given as 0.94158 (US-AEC WASH-1400, 1974). A combination of this reliability with the reliability of a 4-2-1 system from Table 5 gives a reliability against catastrophic failure of 0.9999998. Therefore, about one catastrophic failure in one million reactor years could be expected for the 4-2-1 reactor configuration.

This analysis emphasizes the ability to increase the reliability against catastrophe, not only by adding safety features but also by modifying the system design. The latter procedure may prove more economical in many cases.

TABLE 6. OPTIMIZATION RESULTS WITH ALTERNATIVE RELIABILITY COMPUTATION

Reliability constraint	System reliability	Number of loops	Pumps per loop	Steam gen per loop	Min. cost, $MM
.9	.9309	2	1	1	18.89
.99	.9952	4	2	1	23.76
.999	.9997	5	2	1	26.03
.9999	.99998	7	2	2	31.71
.99999	.999998	9	2	1	33.71
.999999	.9999999	10	2	1	35.43

CONCLUSIONS

In summary, it has been shown that the adaptive random search procedure can be used to solve mixed integer optimization problems. The solution obtained for the nuclear reactor coolant system was in reasonable agreement with another study of this same process.

The adaptive random search was also used to synthesize the optimal coolant system design to achieve a certain level of reliability. This was accomplished by adding the reliability computation as a constraint to the optimization problem. This method proved satisfactory in finding the optimal design with various methods of computing reliability and for various levels of reliability. Computational times for this method are reasonable. The adaptive random search is also applicable to other types of synthesis problems.

NOTATION

k = distribution coefficient (odd integer 1, 3, 5 . . .)
k' = weighting coefficient for x_{ij}
M = smallest value of j that satisfies Equation (3) for a given random number, θ
N = number of possible discrete values of the i^{th} variable
N_f = number of loops that have to fail to cause system failure
NHN = number of steam generators per loop
NPH = number of pumps per loop
NTH = number of tubes per steam generator
$p(x_{ij})$ = probability of obtaining x_{ij}
x_i = new value of the i^{th} continuous independent variable
x_i^* = value of variable x_i which has produced highest (lowest) objective function
x_{ij} = j^{th} discrete value of i^{th} independent variable
x_{ij}^* = value of the i^{th} independent variable producing the previous best value of the objective function
x_{iL} = lower bound of chosen region
x_{iU} = upper bound of chosen region
R = allowable search region (range) about x_i^*

R_{loop} = reliability of a coolant loop
R_{pipe} = reliability of the coolant piping
R_{pumps} = reliability of the pump(s) in a loop
R_{sgs} = reliability of the steam generator(s) in a loop
θ = uniform random number between zero and one

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Equilibrium Staged Parametric Pumping

I. Single Transfer Step per Half-cycle and Total Reflux—the Analogy with Distillation

Equilibrium staged batch parametric pumps are studied with nonlinear isotherms. The half cycle is composed of one single equilibration step and one discrete transfer. The limiting regime (for infinite number of cycles) is shown to correspond to a staircase construction between the two isotherms, the number of steps being equal to the number of stages. The reservoir concentrations are then connected by Fenske's equation. Several analogies with binary total reflux distillation are suggested.

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SCOPE

Parametric pumping is a separation technique based on the periodic movement of a fluid phase over a solid adsorbent bed and a coupled energy input into the system to effect the separation. The most common form of parametric pumping is one in which a packed bed of adsorbent, undergoing a cyclic temperature change, is subjected to a synchronous, alternating, axial flow. The variation of adsorptivity with temperature and the synchronized relative motion of the fluid over the fixed phase makes possible the enrichment of a given component at one end of the column and its depletion at the other end. In this form, parametric pumping was first described by Wilhelm et al. (1966). Since this paper, several similar processes have been described and studied, including continuous, semicontinuous, and nonthermal processes.

The scope of the present paper may be explained by the following key words, in addition to parametric pumping:

1. Finite staging. The continuous column of Wilhelm's scheme is here replaced by a cascade of discrete stages; the number of these stages is finite and in some examples small.

2. Discrete transfer. The continuous flow of Wilhelm's