CONCLUSIONS

Based on the results of this experimental study, the following conclusions can be drawn:

1. The convective heat transfer from a packed bed to a flowing gas-solid suspension was measured using microwave heating.
2. Analysis of the data led to a correlation which may be used to estimate the convective Nusselt number.
3. The important correlating parameters were found to be the particle Reynolds number, the Archimedes number, and the loading ratio.

NOTATION

A = surface area of arbitrarily shaped particle
$A_{p\text{-}e}$ = surface area of the particles in the bed, m^2
A_s = surface area of spherical particle
A_t = cross-sectional area of test section, m^2
Ar_m = Archimedes number, $D_p{}^3 g\rho_f(\rho_p - \rho_f)\ (1 - \epsilon)^2/\mu_f{}^2$, dimensionless
c_{pf} = specific heat of fluid, J/kg·°K
c_{ps} = specific heat of fines, J/kg·°K
D_p = diameter of particles in bed, m
G_f = fluid mass velocity, kg/m²·s
G_s = fines mass velocity, kg/m²·s
h_{fp} = convective heat transfer coefficient, J/m²·s·°K
jh_{fp} = Colburn-J factor for convective heat transfer, $(h_{fp}/c_{pf}G_f)Pr^{2/3}$, dimensionless
k_f = fluid thermal conductivity, J/m·s·°K
$\dot{m}_f$ = fluid mass flow rate, kg/s
$\dot{m}_s$ = solid (fines) flow rate, kg/s
Nu_{fp} = convective Nusselt number, $h_{fp}\cdot D_p/k_f$, (dimensionless)
Nu_t = total Nusselt number, Nu_{ts}, increase in Nusselt number due to fines
Pr_f = Prandtl number, $c_{pf}\cdot\mu_f/k_f$, dimensionless
Re_p = Reynolds number, $D_p\cdot u_f\cdot\rho_f/\mu_f$, dimensionless
t = temperature, °K, t_p of packing, t_f of fluid
u_f = fluid velocity, m/s

Greek Letters

ϵ = bed porosity, dimensionless
η = loading ratio $(\dot{m}_s/\dot{m}_f)$ dimensionless
μ_f = fluid viscosity, N·s/m²
ρ_p = bed particle density, kg/m³
ρ_f = fluid density, kg/m³
ϕ_s = shape factor, dimensionless

LITERATURE CITED

Baden Fuller, A. J., *Microwaves*, Pergamon Press, Oxford, England (1969).

Balakrishnan, A. R., "Thermal Transport in Gas-Solid Suspension Flow through Packed Beds," Ph.D. thesis, Univ. Waterloo, Ontario, Canada (1976).

———, and D. C. T. Pei, "Heat Transfer in Fixed Beds," *Ind. Eng. Chem. Process Design Develop.*, **13**, 441 (1974).

———, "Heat Transfer in Packed Bed Gas-Solid Systems: Part 1—A critical Review," (in press).

Barker, J. J., "Heat Transfer in Packed Beds," *Ind. Eng. Chem.*, **47**, No. 4, 43 (1965).

Barlow, H., and A. Cullen, *Microwave Measurements*, Constable and Co., London, England (1950).

Bhattacharyya, D., and D. C. T. Pei, "Application of Microwave Power in Heat Transfer Studies," *J. Microwave Power*, **8**, 287 (1973).

———, "Heat Transfer in Fixed Bed Gas-Solid Systems," *Chem. Eng. Sci.*, **30**, 293 (1975).

Davidson, J. F., and D. Harrison, ed., *Fluidization*, Academic Press, London, England (1971).

Depew, C. A., and T. J. Kramer, "Heat Transfer to Flowing Gas-Solid Mixtures," *Advan. Heat Transfer*, **9**, 113 (1973).

Ford, J. D., and D. C. T. Pei, "High Temperature Chemical Processing via Microwave Absorption," *J. Microwave Power*, **2**, 61 (1967).

Gutfinger, C., and N. Abauf, "Heat Transfer in Fluidized Beds," *Advan. Heat Transfer*, **10**, 167 (1974).

Hewlett-Packard Company, *Microwave Theory and Measurements*, Prentice Hall, London, England (1963).

Kelligian, R., and C. L. Jones, *Microwave Measurements Manual*, McGraw Hill, New York (1965).

Leva, M., *Fluidization*, McGraw Hill, New York (1959).

Royston, D., "Heat Transfer in the Flow of Solids in Gas Suspensions through a Packed Bed," *Ind. Eng. Chem. Process Design Develop.*, **10**, 145 (1971).

Saad, T. S., *Microwave Engineers' Handbook*, Vol. 1, Artech. House, Dedham, U.K. (1971).

Zabrodsky, S. S., *Hydrodynamics and Heat Transfer in Fluidized Beds*, Mass. Inst. Technol. Press, Cambridge, Mass. (1966).

Manuscript received March 21, 1977; revision received January 23, and accepted February 23, 1978.

Reliability of Optimization Procedures for Obtaining Global Optimum

The importance of the starting point, the size of initial search region, and the search region reduction rate is examined with respect to the reliability of different direct search optimization procedures in being able to furnish the global optimum for nonunimodal systems. Although, in general, the reliability of an optimization procedure is problem dependent, it is nevertheless clear that reliability cannot be increased simply by selecting larger search regions or by reducing the rate of contraction of the search region. A more efficient means of increasing reliability is to embody a pseudo one-dimensional search in the optimization procedure to enable the search to leave a local optimum and proceed to a better optimum.

BI-CHONG WANG

and

REIN LUUS

Department of Chemical Engineering and Applied Chemistry
University of Toronto
Toronto, Ontario, M5S 1A4, Canada

SCOPE

The ease of programming and the ease with which inequality constraints can be handled make direct search optimization procedures attractive from user's point of view. Luus and Jaakola (1973) presented a direct search method (LJ method) based on random sampling and search region contraction. The method is easy to program and is also computationally efficient for solving general nonlinear programming problems.

Recently, Gaines and Gaddy (1976) introduced a method (GG method) where the random points are chosen from a nonuniform distribution where the distribution is made more peaked about the best point during the course of the search. In essence, the effect is the same as obtained by the systematic search region contraction in the LJ method, but the convergence rate is different as pointed out by Heuckroth et al. (1976) in the optimization of six nonlinear programming problems. Heuckroth et al. (1976) improved the rate of convergence of the GG method by incorporating a systematic search region reduction (HGG method). A skewing technique was also embodied when the search was near the boundary to change the distribution of search points and thus to increase the number of testing points inside the feasible region.

When multiple optima exist, however, the optimization procedures may converge to a local optimum instead of the global optimum. The reliability of obtaining the global optimum is not only problem dependent but is also influenced by the choice of the starting point, the size of initial search region, and the rate of reduction of the size of search region. To handle problems with numerous local optima, Wang and Luus (1977) modified the LJ method by incorporating into the LJ method a pseudo one-dimensional search (WL method). Heuckroth et al. (1976) suggested periodically expanding the search region for multimodal problems to enable the search to move away from a local optimum. No comprehensive evaluation, however, exists among the various direct search methods as to their suitability for nonunimodal optimization problems.

By means of optimization of four nonunimodal problems, the reliability and convergence of these direct search methods are examined in detail, and a modification to the WL method is suggested to make it more effective. The effect of periodic search region expansion was not studied, so that for comparison only the basic GG and HGG methods were examined.

CONCLUSIONS AND SIGNIFICANCE

Since in the optimization of nonlinear systems there may exist more than one local optimum, the knowledge of reliability of an optimization procedure in obtaining the global optimum is important. The present investigation was undertaken to provide such information with respect to direct search optimization procedures. Four widely different problems were used for the study.

Of the direct search methods considered in this paper, the LJ method is the simplest to use. The search is uniformly distributed in the entire search space, and the rate of reduction of the search region is uniform. Although the GG method may converge faster than the LJ method to the vicinity of the global optimum (for example, within 1%), the LJ method eventually converges to much tighter tolerances (for example, 0.001%) without requiring too much extra computational effort. The appropriate reduction rate of search region is about 5% ($\epsilon = 0.05$). It is important to note that too small a reduction rate not only increases the number of iterations required to reach the same level of accuracy but also tends to reduce the reliability. Too rapid a reduction rate also reduces reliability by restricting the search to the vicinity of a local optimum.

The GG method using nonuniform random scanning in the search space and adopting the best point immediately as the center point for the next search was found to yield about the same reliability as the LJ method. Because of the immediate replacement of the center point once improvement has been obtained, it usually converges faster than the LJ method to the vicinity of the global optimum. However, since the region contraction is accomplished by using higher peaked distributions during the course of iterations, it is slow in converging to close tolerances (0.01%) and is not as effective as the 5% reduction rate of the LJ method as the search progresses. The convergence rate of the GG method can be increased by incorporating a very small amount of search region contraction after each iteration, for example, $\epsilon = 0.01$. The HGG method without periodic search region expansion yielded considerably lower reliability as compared to the LJ and GG methods.

The WL method exhibited better reliability than the LJ and the basic GG methods. Its convergence rate is comparable to the LJ method, but because of the pseudo one-dimensional search, the computation time may be doubled. Although the optimal choices of k_{ii} and k_{jj} are problem dependent, $k_{ii} = 2$, and $k_{jj} = 0.05$ to 0.1 are suitable. The WL method's reliability is not very sensitive to the reduction rate of the search region and is also less sensitive to the size of the initial search region than the LJ and GG methods. The modified WL method (MWL) eliminates the choice of k_{ii} and k_{jj} but retains the reliability and convergence property of the WL method.

The detailed comparison among the direct search optimization procedures presented here provides a good understanding of the effects of the initial search region and the search region reduction rate. Although perfect reliability cannot be obtained by any method for all nonlinear problems, the global optimum can usually be obtained without difficulty if a few starting points chosen at random are used.

In recent years, several direct search optimization procedures have been applied to various chemical processes (Luus and Jaakola, 1973; Gaines and Gaddy, 1976; Heuckroth et al., 1976; Chen and Fan, 1976) since they are easy to use and are computationally efficient. For complex systems, multiple optima may exist. Therefore, the suitability of the existing direct search methods for problems possessing multiple optima is of special interest.

The main purpose of this paper is to examine the existing direct search optimization procedures using random scanning (Luus and Jaakola, 1973; Gaines and Gaddy, 1976; Heuckroth et al., 1976; Wang and Luus, 1977) in order to test their usefulness in the optimization of problems where more than one local optimum exists. Of direct interest are the reliability of the method in locating the vicinity of the global optimum and the rate of convergence to the global optimum. In order to carry out the investigation, we have chosen four examples, of which two are chemical engineering problems. Thus, a detailed evaluation of different methods should provide a valuable guide to those involved in process optimization.

During the course of this investigation we also develop and evaluate an alternative to the pseudo one-dimensional search procedure presented by Wang and Luus (1977).

The problem frequently encountered by chemical engineers is to maximize the function

$$P = f(x_1, x_2, \ldots, x_n) \tag{1}$$

subject to the constraints

$$g_j(x_1, x_2, \ldots, x_n) \geq 0 \qquad j = 1, 2, \ldots, s \tag{2}$$

and

$$\alpha_i \leq x_i \leq \beta_i \qquad i = 1, 2, \ldots, n \tag{3}$$

through the appropriate choice of $x_1, x_2, \ldots, x_n$. We consider the general case where P given by Equation (1) is nonunimodal, and the feasible region given by Equations (2) and (3) is not necessarily convex. If the upper and lower bounds on each of the variables as given by Equation (3) are not expressed explicitly in some problems, then the bounds simply indicate the region of interest and may be easily added to the problem without affecting the results. Since the reliability of many optimization methods depends on the region allowed for the variables, we use Equation (3) to standardize the search region for the evaluation of different optimization procedures.

The direct search optimization method suggested by Luus and Jaakola (1973) involves really two steps:

1. Choose a number of testing points (for example, 100), each established by the equation

$$\mathbf{x} = \mathbf{x}^* + \mathbf{Z}\,\mathbf{r} \tag{4}$$

For each testing point $\mathbf{Z}$ is different.

2. At the end of each iteration, $\mathbf{x}^*$ is replaced by the best feasible value of $\mathbf{x}$ obtained in step 1, and the region $\mathbf{r}$ is contracted by a small amount ϵ; that is

$$\mathbf{r}^{(j+1)} = (1 - \epsilon)\,\mathbf{r}^{(j)} \tag{5}$$

Recently, Gaines and Gaddy (1976) suggested that instead of using a number of testing points before a best feasible value of $\mathbf{x}$ is determined, only a single testing point is chosen at a time. Whenever a feasible testing point is better than the previous one, $\mathbf{x}^*$ is immediately replaced by this new point. Furthermore, instead of region contraction, they suggested the use of peaked distribution for the testing points in the form

$$\mathbf{x} = \mathbf{x}^* + \mathbf{Z}^k\,\mathbf{r} \tag{6}$$

where k is a positive odd integer. When k is 1, then Equation (6) becomes simply Equation (4), and the distribution from which the random numbers are taken becomes uniform. When k is greater than 1, the distribution becomes peaked.

Heuckroth et al. (1976) modified the GG method by introducing a systematic search region reduction, namely, $\mathbf{r}$ used in Equation (6) is replaced by $\mathbf{r}/k$. When the search was near the boundary, they also used a skewing technique which changes the random distribution to increase the number of feasible testing points.

For consistency, we specify the initial search region by means of bounds on the variables given by Equation (3):

$$\mathbf{r}^{(1)} = \lambda\,(\boldsymbol{\beta} - \boldsymbol{\alpha}) \tag{7}$$

For the method of Gaines and Gaddy (GG), Equation (7) is used to specify the search region at each iteration, since no region contraction is used. The search region parameter λ is introduced to allow the search region to be changed systematically from run to run.

To handle problems of numerous local optima, Wang and Luus (1977) modified the LJ optimization procedure by incorporating a pseudo one-dimensional search over all the variables to locate the vicinity of the global optimum and then switching back to the standard LJ method to obtain the refined optimum. The method consists of choosing a number of testing points (for example, 100) by

TABLE 1. DIFFERENT STARTING POINTS USED FOR EXAMPLE 1

x_1	x_2	x_3	x_4	x_5	x_6
4.395	3.305	1.436	4.128	1.700	8.790
1.815	3.500	1.780	5.160	2.908	1.310
4.455	2.145	2.864	2.634	2.252	9.750
4.850	4.130	1.100	1.878	1.580	9.010
2.250	4.005	3.720	2.178	1.524	1.210
0.995	4.875	1.716	4.056	1.296	6.770
4.530	2.285	3.580	0.948	1.864	5.670
0.165	0.415	1.056	0.330	3.444	9.750
4.575	3.420	3.692	3.378	1.556	3.980
4.445	1.385	2.568	3.348	1.960	4.420
2.500	2.500	3.000	3.000	3.000	5.000
0.000	0.000	1.000	0.000	1.000	0.000
5.000	5.000	5.000	6.000	5.000	10.000

$$\mathbf{x} = \mathbf{x}^* + \mathbf{K}\,\mathbf{Z}\,\mathbf{r} \tag{8}$$

where $\mathbf{K}$ is an $n \times n$ diagonal matrix with diagonal elements $k_{ii} = 2$ and $k_{jj} = 0.05$ for $j = 1, 2, \ldots, i-1, i+1, \ldots, n$. This allows a search to be performed on the i^{th} variable while restricting the range for the other variables. The search region is contracted as in Equation (5), and only a small number of iterations (for example, 10) are performed. The original search region then is restored, and the search proceeds to the next variable. This is continued until the pseudo one-dimensional search has been used on each of the variables. Thereafter, the LJ method with a small search region (for example, 30% of the original search region) is used to refine the solution.

It is not at all clear how the reliability of the GG method and its modifications (HGG method) compare to the LJ method and WL method (modified LJ method) when numerous local optima are encountered. The aim here is to carry out detailed comparisons with nonunimodal problems and to find the appropriate conditions for using these methods. The GG and HGG methods were not tried by periodically expanding the search region. This modification may increase the reliability of these methods but at too great an increase in computation time.

EXAMPLES

As the first example, consider the problem presented by Hesse (1973), where it is required to maximize

$$P = 25(x_1 - 2)^2 + (x_2 - 2)^2 + (x_3 - 1)^2 + (x_4 - 4)^2 + (x_5 - 1)^2 + (x_6 - 4)^2 \tag{9}$$

subject to

$$2 \leq x_1 + x_2 \leq 6 \tag{10}$$

$$-x_1 + x_2 \leq 2 \tag{11}$$

$$x_1 - 3x_2 \leq 2 \tag{12}$$

$$(x_3 - 3)^2 + x_4 \geq 4 \tag{13}$$

$$(x_5 - 3)^2 + x_6 \geq 4 \tag{14}$$

$$0 \leq x_1 \tag{15}$$

$$0 \leq x_2 \tag{16}$$

$$1 \leq x_3 \leq 5 \tag{17}$$

$$0 \leq x_4 \leq 6 \tag{18}$$

$$1 \leq x_5 \leq 5 \tag{19}$$

$$0 \leq x_6 \leq 10 \tag{20}$$

There exist eighteen local maxima, of which the global

Table 2. Comparison of Different Methods for Solving Example 1

Method	λ	Reliability success ratio	Average number of function evaluations required to reach the global maximum within 0.1%	0.01%	0.001%	Average computation time, s/run
LJ	1	5/13	1 959 (1 458)*	2 468 (2 025)	3 292 (2 877)	2.13
	2	11/13	1 674 (1 194)	2 334 (1 664)	2 532 (2 153)	2.08
GG†	1	9/13	1 339 (767)	>5 156 (1 404)	NC**	4.90
	2	12/13	1 201 (505)	>4 591 (1 384)	NC	4.90
WL	1	13/13	1 950 (1 457)	2 560 (1 995)	2 858 (2 450)	4.29
	2	13/13	1 787 (1 487)	2 378 (1 898)	2 977 (2 601)	4.29

* Minimum number of function evaluations are shown in parenthesis.
** Nonconvergence to this level in any of the runs.
† Start with $k = 3$; after twenty improvements of P, $k = 5$. For another twenty improvements, $k = 7$. This policy is used unless otherwise specified.

maximum is at $\mathbf{x} = (5, 1, 5, 0, 5, 10)^T$ with $P = 310$.

To examine the reliability of the methods, we choose thirteen different starting points given in Table 1. The first ten points were chosen at random in the allowable range. The last three correspond to the bounds on the variables and the midpoint. Reliability is expressed as the ratio of the number of successful runs reaching the vicinity of global optimum to the total number of runs. With these thirteen starting points and for two different values of initial search region parameter λ, the results are given in Table 2. The GG method gave a higher success ratio than the LJ method for each value of λ. Also, it is noted that the larger initial search region yielded substantially higher reliability for both of these methods. The WL method, however, gave a success ratio of 13/13 for both values of λ.

The convergence rate of the GG method, however, is rather slow to close tolerances of the optimum. To reach to within 0.01% of the global optimum requires more than twice as many function evaluations as the LJ method. In none of the cases could we reach 0.001% as shown in Table 2. Here, the average number of function evaluations is the arithmetic mean of the successful runs. A greater sign indicates an estimated average value, because not all successful runs could reach this specified level. The ratio of the average number of function evaluations to reach 0.001% level as compared to 0.1% level is about 1.7 for the LJ method. This illustrates the fact that the LJ method can reach within 0.001% of the global optimum without too much extra effort.

Further investigation showed that if seventeen local maxima were used as the starting points with initial search region parameter $\lambda = 2$, the number of successful runs were 8, 9, 16 for the LJ, GG, and WL methods, respectively. This illustrates the different capabilities of each of these methods in proceeding to the region containing the global maximum when the search starts with the most adverse starting points, namely, at other local optima.

The second example to be considered is the geometrical problem presented by Luus (1974). This problem is to find the maximum of the function

$$P = x_1^2 + x_2^2 + x_3^2 \qquad (21)$$

Table 3. Starting Points for Example 2

x_1	x_2	x_3	P
1.04400	2.48909	1.78541	10.47319
1.37172	−2.13008	1.77488	9.56906
2.22288	−0.17259	1.98899	8.92706
1.57411	−1.79381	−1.75688	8.78221
2.04195	−0.95967	−1.90526	8.72054
−1.41862	−0.16050	1.01260	3.06360
−1.40498	−0.24513	−1.00200	3.03807

subject to

$$4(x_1 - 0.5)^2 + 2(x_2 - 0.2)^2 + x_3^2 + 0.1\,x_1x_2 + 0.2\,x_2x_3 \leq 16 \qquad (22)$$

$$2\,x_1^2 + x_2^2 - 2\,x_3^2 \geq 2 \qquad (23)$$

$$-2.3 \leq x_i \leq 2.7 \quad i = 1, 2 \qquad (24)$$

This problem corresponds to the one considered by Luus (1974) to illustrate the two-pass method for solving optimization problems containing difficult equality constraints. There are four local maxima, of which the global maximum is at $\mathbf{x} = (0.988, 2.674, -1.884)^T$ with $P = 11.67664$.

Seven starting points given in Table 3 were used for the investigation. The initial search region parameter λ was taken to be 2. For this example, the reliability of the LJ method was the same as the WL method, both higher than for the GG method, as shown in Table 4. The rate of convergence of the GG method to close tolerances was again poor. It could not converge to even 0.01% level and had difficulty in converging to the 0.1% level. The LJ and WL methods, however, exhibited no such difficulty in convergence.

The minimum cost of a reactor-heater system with an auxiliary cooler (Chen and Fan, 1976) is considered next. The optimum obtained by Chen and Fan (1976) was obtained by all of the existing direct search optimization procedures considered in this paper. None of the procedures failed to identify the global minimum cost from

Table 4. Comparison of Different Methods for Solving Example 2

Method	Reliability success ratio	Average number of function evaluations required to reach the global maximum within 0.1%	0.01%	Average computation time, s/run
LJ	6/7	2 175 (1 683)	>3 723 (2 869)	1.46
GG	4/7	>3 571 (1 274)	NC	3.43
WL	6/7	1 942 (1 441)	>4 186 (3 029)	2.57

every starting condition which was considered. Less than 250 average function evaluations and 0.1 s were required to reach within 0.001% of the global minimum for the LJ method.

MODIFIED PSEUDO ONE-DIMENSIONAL SEARCH

In the last section, the pseudo one-dimensional search procedure presented by Wang and Luus (1977) has been shown to be more reliable than the other two procedures. However, it did fail to locate the global maximum twice out of fifty runs performed on the first two examples. An alternative way of random scanning which enlarges the pseudo one-dimensional search region while retaining the original distinct characteristic is to replace Equation (8) by the expression

$$\mathbf{x} = \mathbf{x}^* + \mathbf{M}\,\mathbf{Z}\,\mathbf{r} \tag{25}$$

where $\mathbf{M}$ is an $n \times n$ diagonal matrix with diagonal elements $m_{ii} = 1$ and $m_{jj} = z_{jj}^4$ for $j = 1, 2, \ldots, i-1, i+1, \ldots, n$. The rest of the procedure is the same as the WL method outlined earlier in this paper. The results of applying this procedure to examples 1 and 2 yield considerably better reliability as is shown in Table 5. The rate of convergence is rapid and corresponds to the LJ rate.

APPLICATION TO AIR POLLUTION CONTROL

In monitoring air pollution, it is useful to know the maximum ground level concentration of pollutants resulting from the emission from multiple sources.

For the purpose of testing the usefulness of the direct search optimization procedures in air pollution control, the simple Holland's plume rise equation and Gifford's dispersion equation are used (Turner, 1973) for estimating the ground level sulfur dioxide concentration. Let us consider an environment with ten stacks. Under adiabatic conditions, the ground level concentration of sulfur dioxide is given by

$$C = \frac{0.8}{\pi u} \sum_{i=1}^{10} \frac{Q_i}{\sigma_{yi}\sigma_{zi}} \exp\left[-\frac{1}{2}\left(\frac{Y_i}{\sigma_{yi}}\right)^2 - \frac{1}{2}\left(\frac{H_i}{\sigma_{zi}}\right)^2\right] \tag{26}$$

where

$$Y_i = \sin\theta\,(x - a_i) + \cos\theta\,(y - b_i) \quad i = 1, 2, \ldots, 10 \tag{27}$$

By curve fitting Figures 3-2 and 4-1 of Turner (1973), the standard deviations σ_{yi} and σ_{zi} are given by

$$\sigma_{yi} = \begin{cases} 0.9591 & X_i \le 10 \\ 0.1136\,X_i^{0.9265} & 10 < X_i \le 2 \times 10^3 \\ 0.1385\,X_i^{0.9015} & 2 \times 10^3 < X_i \le 10^4 \\ 0.2030\,X_i^{0.8600} & 10^4 < X_i \le 10^5 \end{cases} \tag{28}$$

$$\sigma_{yi}\sigma_{zi} = \begin{cases} 0.07925 & X_i \le 10 \\ 4.828 \times 10^{-5}\,(\ln X_i)^{8.8766} & 10 < X_i \le 200 \\ 3.108 \times 10^{-6}\,(\ln X_i)^{10.5295} & 200 < X_i \le 10^3 \\ 1.808 \times 10^{-7}\,(\ln X_i)^{11.9998} & 10^3 < X_i \le 5 \times 10^3 \\ 1.892 \times 10^{-9}\,(\ln X_i)^{14.1284} & 5 \times 10^3 < X_i \le 10^5 \end{cases} \tag{29}$$

where the downwind distance from the i^{th} stack is given by

$$X_i = \cos\theta\,(x - a_i) - \sin\theta\,(y - b_i) \quad i = 1, 2, \ldots, 10 \tag{30}$$

The effective stack height H_i in Equation (26) is the sum of the stack height H_{si} and the plume rise ΔH_i which (Turner, 1973) is given by

$$\Delta H_i = \frac{V_{si}\,d_i}{u}\left[1.5 + 2.68\,\frac{T_{si} - T_a}{T_{si}}\,d_i\right] \quad i = 1, 2, \ldots, 10 \tag{31}$$

The problem is to find the coordinates on the ground x, y, the wind velocity u, and the wind direction θ for which C given by Equation (26) is maximum. From physical considerations, we impose the following constraints:

$$-20\,000 \le x \le 20\,000 \tag{32}$$

$$-20\,000 \le y \le 20\,000 \tag{33}$$

$$0 < u \le 12.5 \tag{34}$$

$$0 \le \theta \le 2\pi \tag{35}$$

The stack and emission data are given in Table 6. This problem has numerous local maxima, of which the global maximum is at $x = -8\,039.6$, $y = 9\,369.2$, $u = 5.6371$, $\theta = 3.996$, with $C = 7.7114 \times 10^{-4}$ g/m^3 (or 28.4 pphm). What makes the problem challenging is the existence of a large local maximum $C = 7.5316 \times 10^{-4}$ g/m^3 at $x = 18\,103.2$, $y = -1\,579.6$, $u = 6.0238$, $\theta = -0.00447$. This local maximum is only 2.3% less than the global maximum.

In order to ensure that we are seeking the maximum in a downwind direction, we seek θ by the equation

$$\theta = \begin{cases} 2\pi - \tan^{-1}(y/x) + \theta' & x > 0,\ y > 0 \\ \pi - \tan^{-1}(y/x) + \theta' & x < 0 \\ -\tan^{-1}(y/x) + \theta' & x > 0,\ y < 0 \end{cases} \tag{36}$$

where θ' is a small value. Therefore, the new four independent variables are x, y, u, and θ'.

In this approach, nine ground locations (10 000, 10 000), (10 000, 0), (10 000, −10 000), (0, 10 000), (0, 0), (0, −10 000), (−10 000, 10 000), (−10 000, 0), (−10 000, −10 000) with $u = 6.0$, $\theta' = 0.0$ were used as nine starting points. The initial search region for θ' was 0.1λ. The results are shown in Table 7. The reliability of all methods is not as high as that for solving examples 1 and 2 owing to the fact that, as stated before, there is a local maximum which differs only 2.3% from the global maximum and is far away (in the fourth quadrant) from the global maximum.

To improve the reliability, however, we may transform the problem into polar coordinates. Thus

$$x = \rho\cos\phi, \quad y = -\rho\sin\phi \tag{37}$$

$$\theta = \phi + \theta' \tag{38}$$

$$0 \le \rho \le 20\,000 \tag{39}$$

$$0 \le \phi \le 2\pi \tag{40}$$

$$0 < u \le 12.5 \tag{41}$$

When the search center is near the vicinity of the local maximum located in the fourth quadrant, in polar coordinates a proper change of only ϕ can bring the search into the vicinity of the global maximum located in the second quadrant, whereas changes in both x and y are required for Cartesian coordinates. Therefore, by requiring a change

Table 5. Reliablility and Convergence Properties of the Modified Pseudo One-Dimensional Search Procedure (MWL)

Example	Starting condition	Reliability success ratio	Average number of function evaluations required to reach the global maximum within 0.1%	0.01%	0.001%	Average computation time, s/run
1	Table 1 $\lambda = 2$	13/13	1 634 (816)	2 372 (2 048)	2 900 (2 504)	4.43
1	Local maxima $\lambda = 2$	17/17	1 667 (618)	2 211 (1 712)	2 827 (2 525)	4.41
2	Table 4 $\lambda = 2$	7/7	1 815 (1 769)	>3 461 (2 720)	>4 029 (4 029)	2.57

Table 6. Stack and Emission Data

a_i	b_i	H_{si}	d_i	T_{si}	Q_i	V_{Si}
−3 000	−2 500	183.0	8.0	413	2 882.6	19.245
−2 600	−300	183.0	8.0	413	2 882.6	19.245
−1 100	−1 700	160.0	7.6	413	2 391.3	17.690
1 000	−2 500	160.0	7.6	413	2 391.3	17.690
1 000	2 200	152.4	6.3	413	2 173.9	23.404
2 700	1 000	152.4	6.3	413	2 173.9	23.404
3 000	−1 600	121.9	4.3	413	1 173.9	27.128
−2 000	2 500	121.9	4.3	413	1 173.9	27.128
0	0	91.4	5.0	413	1 304.3	22.293
1 500	−1 600	91.4	5.0	413	1 304.3	22.293

Table 8. Starting Points for Air Pollution Problem in Polar Coordinates

ρ	ϕ	u	θ'
0	0	5	0
0	2.2	10	0
6 000	0	20	0
2 000	0.9	5	0
15 000	1.6	2	0
8 000	4.4	12	0
18 000	0.7	7	0
6 000	2.6	17	0
10 000	1.3	1	0
5 000	3.5	15	0

of only one variable to leave the local optimum, the polar coordinate system is expected to provide a higher reliability.

By using ten random starting conditions given in Table 8, the reliability success ratios obtained are 7/10, 8/10, 8/10, and 8/10 for the LJ, WL, GG, and MWL methods, respectively. The dependence of the reliability on the choice of λ is discussed in the following section.

DISCUSSION

Three principal factors affecting the reliability of direct search optimization procedures are the starting point, the size of the initial search region, and the rate of search region reduction. If the starting point is close to a local optimum, large initial search region with slow rate of search region reduction provides a good chance for the search to leave the vicinity of such a local optimum to proceed to a global optimum. The effects of the choices of λ, ϵ, k_{ii}, and k_{jj} on the reliability of the direct search methods are now analyzed in greater detail.

The Effect of Initial Search Region on the Reliability

The initial search region should cover the entire feasible region during the first few iterations in order to have access to any feasible point. By using ten random starting

Table 7. Comparison of Different Methods for Solving Air Pollution Problem

Method	Reliability success ratio $\lambda = 1$	$\lambda = 2$
LJ	6/9	3/9
GG	5/9	2/9
WL	5/9	6/9
MWL	4/9	8/9

Table 9. The Effect of λ on the Reliability of Direct Search Methods for Example 1

λ	Reliability success ratio LJ ($\epsilon = 0.05$)	WL ($\epsilon = 0.05$)	MWL ($\epsilon = 0.05$)	GG*	HGG*
1	3/10	10/10	7/10	7/10	2/10
2	8/10	10/10	10/10	9/10	5/10
3	7/10	9/10	8/10	4/10	4/10
4	6/10	6/10	6/10	4/10	3/10

* Start with $k = 1$. After five improvements of P, $k = 3$. After another fifteen improvements of P, $k = 5$. For another twenty improvements, $k = 7$. This policy was used for all runs in the section of discussion.

Table 10. Random Starting Points for Example 2

x_1	x_2	x_3
−1.430	1.090	1.400
−1.180	−0.632	−1.400
−1.405	0.880	−0.100
0.747	0.908	−0.200
1.332	−0.273	−0.900
1.082	−1.422	1.000
−0.974	0.704	0.600
−0.327	−0.577	1.100
0.006	0.051	−0.300
1.260	0.315	0.800

Table 11. The Effect of λ on the Reliability of Direct Search Methods for Example 2

λ	Reliability success ratio LJ ($\epsilon = 0.05$)	WL ($\epsilon = 0.05$)	MWL ($\epsilon = 0.05$)	GG	HGG
1	8/10	10/10	7/10	9/10	4/10
2	6/10	9/10	10/10	7/10	6/10
3	5/10	8/10	10/10	6/10	4/10
4	6/10	9/10	10/10	7/10	5/10

Table 12. The Effect of λ on the Reliability of Direct Search Methods for Air Pollution Problem in Polar Coordinates

λ	Reliability success ratio LJ ($\epsilon = 0.05$)	WL ($\epsilon = 0.05$)	MWL ($\epsilon = 0.05$)	GG
1	7/10	4/10	8/10	8/10
2	4/10	8/10	8/10	4/10
3	3/10	3/10	5/10	5/10
4	5/10	4/10	4/10	6/10

Table 14. The Effect of Region Reduction Rate ϵ on the Reliability of Direct Search Methods for Example 2

Region reduction rate ϵ	Reliability success ratio LJ λ = 1	LJ λ = 2	WL λ = 1	WL λ = 2	MWL λ = 1	MWL λ = 2
0.01	8/10	3/10	10/10	9/10	10/10	10/10
0.03	7/10	7/10	10/10	9/10	9/10	10/10
0.05	8/10	6/10	10/10	9/10	7/10	10/10
0.07	7/10	7/10	10/10	9/10	8/10	10/10
0.10	8/10	7/10	10/10	9/10	8/10	10/10

points (from Table 1) to solve example 1, the reliabilities of the five direct search methods for four different values of λ are reported in Table 9. It is observed that the WL and MWL methods achieved reliability of 6/10 or greater for the entire range of λ, but as λ increases beyond the value 2, the reliability of all methods decreases. Thus the reliability cannot be increased simply by increasing the size of the search region. Also, it is noted that the search region reduction suggested by Heuckroth et al. (1976) does not improve the reliability. Similar results were obtained for example 2 by using the random starting points given in Table 10 to give the results in Table 11. For solving the air pollution problem, the starting points from Table 8 yielded the reliabilities shown in Table 12. Here, the MWL method yielded the best reliability and was least sensitive to the choice of λ. Unlike examples 1 and 2, for this example none of the methods can yield perfect reliability for any value of λ. However, the reliability success ratio of 8/10 is very good for this problem.

The Effect of Search Region Reduction Rate on the Reliability

Table 13 shows the effect of ϵ on the performance of the LJ, the WL, and the MWL methods for example 1. It is noted that decreasing ϵ does not necessarily increase the reliability. Table 14 shows similar results for example 2. From these examples we conclude that the reduction rate should be intermediate, such as $\epsilon = 0.05$, for good reliability. The WL and MWL methods are least sensitive to the choice of ϵ.

The Effects of k_{ii} to k_{jj} on the Performance of the WL Method

Different ratios of k_{ii} to k_{jj} were used to examine their effects on the WL method. Table 15 shows that when $k_{ii}/k_{jj} < 40$, the reliability was decreased. Table 16 shows similar results in reliability for example 2. The reliability of the WL method ($k_{ii} = 2$) for solving the air pollution problem in the Cartesian coordinates was 6/9, 8/9, and 7/9 for $k_{jj} = 0.05$, 0.10, and 0.15, respectively. Therefore, for example 4, the choice of $k_{ii}/k_{jj} = 20$ is better than the other two choices.

Although only four examples were fully examined in this paper, it is clear that direct search methods are very useful in the optimization of systems possessing numerous

Table 13. The Effect of Region Reduction Rate ϵ on the Reliability of Direct Search Methods for Example 1

Region reduction rate ϵ	Reliability success ratio LJ λ = 1	LJ λ = 2	WL λ = 1	WL λ = 2	MWL λ = 1	MWL λ = 2
0.01	5/10	3/10	10/10	8/10	7/10	10/10
0.03	6/10	8/10	10/10	9/10	7/10	9/10
0.05	3/10	8/10	10/10	10/10	7/10	10/10
0.07	1/10	7/10	10/10	9/10	8/10	10/10
0.10	1/10	6/10	10/10	9/10	5/10	10/10

Table 15. The Dependence of the WL Method on the Choice of K for Example 1

k_{ii}	k_{jj}	k_{ii}/k_{jj}	Reliability success ratio λ = 1	λ = 2
2	0.01	200	10/10	10/10
2	0.05	40	10/10	10/10
2	0.10	20	9/10	8/10
2	0.20	10	6/10	7/10

Table 16. The Dependence of the WL Method on the Choice of K for Example 2

k_{ii}	k_{jj}	k_{ii}/k_{jj}	Reliability success ratio λ = 1	λ = 2
2	0.01	200	10/10	9/10
2	0.05	40	10/10	9/10
2	0.10	20	10/10	8/10
2	0.20	10	10/10	8/10

local optima. When proper choice of the parameters such as λ and ϵ is used, only a few different starting points are required to locate the global optimum. For the LJ and the GG methods, if the global optimum is not expected on the bounds of independent variables (for example, examples 2 and 4), λ = 1 tends to be better than λ = 2. If, however, the global optimum is on the bounds (for example, example 1), then the larger search region with λ = 2 is better. For the WL and MWL methods, λ = 2 tends to be better. The search region reduction is an important feature, and the rate should be neither too large nor too small. Although the optimum reduction rate is problem dependent, for numerous systems it was found that $\epsilon = 0.05$ is a very good choice. The convergence rate of the GG method is slow when the search is close to the global optimum because no search region contraction is used. On the other hand, the reduction rate in the HGG method appears to be too rapid for any improvement in the reliability over the GG method. Unless periodic expansion of the search region is used, therefore, the basic HGG method is not well adapted for multimodal systems.

In all of the direct search optimization procedures there are some parameters which one may change to suit a particular problem. Since the WL and MWL methods are least sensitive to the changes of λ and ϵ, their usefulness should be greater in solving unfamiliar problems. Even for very complex problems possessing numerous local optima, the direct search optimization procedures provide sufficiently high reliability in obtaining the global optimum, so that only a few random starting points are necessary to locate the global optimum.

ACKNOWLEDGMENT

This work was performed with the assistance of a grant from the Canadian National Research Council, A-3515. Computations were carried out with the facilities of the University of Toronto Computer Center.

NOTATION

a_i = x coordinate of stack i, m
b_i = y coordinate of stack i, m
C = average ground level sulfur dioxide concentration based on 30 min sampling time, g/m^3
d_i = exit diameter of stack i, m
H_i = effective height of stack i, m
H_{si} = height of stack i, m
k = weighting parameter defined by Equation (6)
$\mathbf{K}$ = $n \times n$ diagonal matrix defined by Equation (8)
$\mathbf{M}$ = $n \times n$ diagonal matrix defined by Equation (25)
Q_i = emission rate of stack i, g/s
$\mathbf{r}$ = search region defined by Equation (7)
T_a = air temperature, taken as 283°K
T_{si} = exit gas temperature at top of stack i, °K
u = wind velocity, m/s
V_{si} = exit gas velocity of stack i, m/s
$\mathbf{x}$ = independent variable
$\mathbf{x}^*$ = best value of $\mathbf{x}$
X_i = downwind distance from stack i, m
Y_i = crosswind distance from the plume center line of stack i, m
$\mathbf{Z}$ = $n \times n$ diagonal matrix consisting of random numbers between −1.0 and 1.0

Greek Letters

α = lower bound of $\mathbf{x}$
β = upper bound of $\mathbf{x}$
ΔH_i = plume rise from stack i, m
ϵ = amount of size reduction defined by Equation (5)
θ = wind direction measured clockwise from x axis, radian
λ = search region parameter defined by Equation (7)
ρ = radius defined by Equation (37), m
σ_{yi} = standard deviation defined by Equation (28), m
σ_{zi} = standard deviation defined by Equation (29), m
ϕ = angle defined by Equation (37), measured clockwise from x axis, radian

Superscripts

j = iteration number

LITERATURE CITED

Chen, H.T., and L. T. Fan, "Multiple Minima in a Fluidized Reactor-Heater System," *AIChE J.*, **22**, 680(1976).

Gaines, L. D., and J. L. Gaddy, "Process Optimization by Flow Sheet Optimization," *Ind. Eng. Chem. Process Design Develop.*, **15**, 206 (1976).

Hesse, R., "A Heuristic Search Procedure for Estimating a Global Solution of Nonconvex Programming Problems," *Opns. Res.*, **21**, 1267 (1973).

Heuckroth, M. W., J. L. Gaddy, and L. D. Gaines, "An Examination of the Adaptive Random Search Technique," *AIChE J.*, **22**, 744 (1976).

Luus, R., "Two-pass Method for Handling Difficult Equality Constraints in Optimization," *ibid.*, **20**, 608 (1974).

———, and T. H. I. Jaakola, "Optimization by Direct Search and Systematic Reduction of the Size of Search Region," *ibid.*, **19**, 760 (1973).

Turner, D. B., *Workbook of Atmospheric Dispersion Estimates*, Environmental Protection Agency, Office of Air Programs, Research Triangle Park, N. C. (1973).

Wang, B-C., and R. Luus, "Optimization of Nonunimodal Systems," *Intern. J. Num. Meth. Eng.*, **11**, 1235 (1977).

Manuscript received February 4, 1977; revision received January 13, and accepted February 22, 1978.

Internal Boiling and Superheating in Vaporizing Multicomponent Droplets

The vaporization and combustion of a miscible multicomponent droplet in a quiescent atmosphere is analyzed by assuming transient-diffusive transport within the droplet, quasi steady diffusive-convective transport in the gas phase, and ideal solution behavior for the mixture. Results on the vaporization of a binary droplet show that owing to the significant liquid phase diffusional resistance, the vaporization process approximately consists of an initial transient regime, an intermediate, diffusion limited, almost quasi steady regime, and a final volatility limited regime. It is further demonstrated that the entrapment of the volatile components within the rapidly heated droplet interior may lead to the initiation of either homogeneous or heterogeneous nucleation, which can result in the fragmentation of the parent droplet with the internal pressure buildup.

C. K. LAW

Department of Mechanical Engineering and Astronautical Sciences Northwestern University Evanston, Illinois 60201

SCOPE

For vaporizing multicomponent droplets without much internal circulation, the extremely slow process of liquid phase mass diffusion is rate limiting such that vaporization ceases to resemble the batch distillation process as governed by volatility differentials. The entrapment of the volatile components within the rapidly heated droplet interior may subsequently lead to homogeneous or heterogeneous nucleation and hence further atomization of the liquid droplet due to the internal pressure buildup. It is also suggested that the heterogeneously induced fragmentation is a possible mechanism in preventing the formation of large coal particle agglomerates in vaporizing coal slurry droplets. The present study aims to explore and quantify the vaporization and nucleation characteristics of a multicomponent droplet in typical combustor environments.