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Improved Criticality Search Techniques for Low- and High-Enriched Systems

M. J. Lorek

Prepared for the
Office of Nuclear Regulatory Research
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IMPROVED CRITICALITY SEARCH TECHNIQUES FOR LOW- AND HIGH-ENRICHED SYSTEMS

M. J. Lorek

Sponsor: G. E. Whitesides

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TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

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IMPROVED CRITICALITY SEARCH TECHNIQUES

FOR LOW- AND HIGH-ENRICHED SYSTEMS

M. J. Lorek

ABSTRACT

The purpose of this work is to develop a parameter search capability for use in criticality safety analysis of nuclear fuel shipping containers. This new search capability is being developed for use in the SCALE computer code system. SCALE is being developed for licensing evaluation of various transportation package designs. It can perform criticality safety analysis, shielding analysis, and heat transfer analysis on systems described in multi-dimensional geometry.

The work described in this report is specifically concerned with the criticality safety analysis capability of SCALE, and particularly, with two sequences that will provide SCALE users with the option to perform criticality searches on systems described in either one-dimensional or three-dimensional geometries.

This search package includes a method for an optimization search (maxima or minima) and a method for a fixed value search. The optimization search is a search for the most reactive state of a system. It searches for the value of a parameter, such as fuel assembly lattice pitch or fuel concentration, that corresponds to the maximum K-effective of the system. Similarly, the fixed value search is a search for the value of a parameter that corresponds to a fixed value of K-effective. Both searches rely on least squares curve fitting to obtain the information needed to make an estimate. Specifically, the data points are least squares fitted to a cubic polynomial which is solved analytically for parameter values that correspond to maximum or fixed values of K-effective.

This new search capability has been implemented into a FORTRAN computer routine named OPTMIZ which is used to perform the parameter modifications in SCALE's two criticality search options. Results obtained from OPTMIZ show that fixed value criticality searching is greatly improved with regard to accuracy and computing cost relative to the existing search capability available in KENO-IV. Also, results show that the new optimum search capability available in OPTMIZ is an accurate and reliable search for locating parameter values that correspond to maximum values of K-effective.

CHAPTER I

INTRODUCTION AND PROJECT OVERVIEW

A considerable effort by the Nuclear Regulatory Commission has been under way in recent years to develop a standardized computer analysis methodology to be used for licensing evaluation purposes. The need has arisen for a uniformly accepted method of analysis so that licensees could know in advance how their designs would be evaluated. The result of this effort is a new modular system of computer programs called SCALE[1] which is being developed in the Computer Sciences Division at the Oak Ridge National Laboratory (SCALE is an acronym for Standardized Computer Analysis for Licensing Evaluation). SCALE will benefit the NRC and the industry by simplifying the licensing process. Applicants will have the option of using SCALE to analyze their designs instead of using their own programs and data bases which they must adequately verify.

The SCALE system is a collection of computer programs that perform three basic types of analysis: (1) criticality safety analysis, (2) shielding analysis, and (3) heat transfer analysis. For example, Criticality Safety Analytical Sequence 1 (CSAS1) performs data processing and criticality safety analysis on systems which can be adequately described in one-dimensional geometry. Shielding Analytical Sequence 3 (SAS3) performs data processing and radiation shielding analysis on systems for which the user specifies the radiation source distribution and which must be modeled in three-dimensional geometry. Heat Transfer Analytical Sequence 2 (HTAS2) performs Monte Carlo radiative heat transfer analysis on systems which must be described in three-dimensional geometry.

SCALE consists of a driver module, control modules, functional modules and a data base. It relies heavily on basic neutron transport analysis, data processing, and heat transfer analysis methods that have been developed at the Oak Ridge National Laboratory over the past several years. The neutron transport and heat transfer analyses are performed by well-established analysis codes that have been in use for several years. The data processing is similar to that employed in the AMPX system.[2] SCALE input has been designed to be as simple as possible to help avoid costly input errors. The components of the SCALE system are shown in Figure 1.

This report describes a new search package that is to be used in analytical sequences CSAS3 and CSAS4. These two sequences will allow SCALE users to search for most reactive (maximum K-effective) states of systems that can be described in one-dimensional and three-dimensional geometries, respectively. For example, CSAS4 will have the capability of determining the assembly pitch of an array of fuel assemblies that corresponds to the maximum value of K-effective for the array. CSAS3 and CSAS4 involve iterative processes and will also include the capability to search for fixed states (fixed K-effective) of systems. The end result of this work is a set of FORTRAN subroutines collectively known as OPTMIZ that will be incorporated into CSAS3 and CSAS4. The function of OPTMIZ is to take all previous information and use it to modify the system parameter appropriately, i.e., make an intelligent next guess based on all previous information. It is capable

SCALE

STANDARDIZED COMPUTER ANALYSIS FOR LICENSING EVALUATION

DRIVER

FUNCTIONAL MODULES	DATA BASE	CONTROL MODULES
NITAWL	STANDARD COMPOSITIONS LIBRARY	CSAS1
XSDRNPM	ORIGEN LIBRARIES	CSAS2
COUPLE	HANSEN-ROACH BONDARENKO	CSAS3
ORIGEN-S	123 GROUP AMPX	CSAS4
KENO-IV	22-18 COUPLED	SAS1
BONAMI	218 GROUP ENDF/B-IV	SAS2
ICE	27-18 COUPLED ENDF/B-IV	SAS3
MORSE-SGC/S	27-18 COUPLED ENDF/B-V	SAS4
KENO-V		HTAS1
HEATING-6		HTAS2

Figure 1. The SCALE Computer Code System.

of seeking out parameter values that correspond to maximum values, minimum values, or fixed values of K-effective.

OPTMIZ is a collection of five FORTRAN subroutines: OPTMIZ, MAXMIN, FIXEDK, CUBFIT, and DETERM. MAXMIN is devoted entirely to the optimization search. Similarly, FIXEDK is the fixed value search. Both MAXMIN and FIXEDK rely on least squares fitting to a cubic polynomial, so both routines call CUBFIT (fits input data to a cubic). DETERM is a subroutine that calculates determinants which are needed in the least squares fit, and OPTMIZ is the calling subroutine that sets passing parameters and does preliminary calculations.

During the course of this work, many different methods were considered including interpolation and extrapolation techniques, linear programming, and different optimization techniques. A primary consideration in this work is that during a search, relatively few data points are available, especially at the beginning of the calculation. Most sophisticated techniques, like the ones mentioned above, are useless for this problem because there are so few data points available. Indeed, one of the primary concerns of the SCALE project is to minimize computing cost, which means to generate as few data points as possible. Thus, the primary objective of this thesis project is to develop a method for parameter modification in criticality safety studies that is accurate and reliable and uses a minimum amount of computer time.

Initially, attention was focused on the fixed value search, since there is more information available for this type of search. The object of the first part of the project was to improve the existing fixed v search capability that is available as an option in the KENO-IV[3] Monte Carlo criticality program. This search option is contained in a subroutine known as XXMOD. The parameter modification technique in XXMOD is based on an approximation of the mean value theorem of calculus,[4] which is essentially a truncation of Taylor's series after one term. First, this parameter modification technique was replaced with one based on an approximation of the extended mean value theorem of calculus,[5] which is a truncation of Taylor's series after two terms. Next, the technique of least squares fitting of data points to a curve was added to improve accuracy. The least squares technique has turned out to be the heart of the OPTMIZ method.

One of the initial objectives of this project was to develop a technique that could use all previous information to make a next guess. This information includes standard deviations of data points generated in a Monte Carlo calculation since CSAS4 includes a KENO-V Monte Carlo criticality calculation. Least squares fitting is very appropriate here because each data point can be weighted according to its standard deviation. The existing mean value theorem technique in KENO-IV uses only two data points as previous information — the present and next immediate points. It does not consider the uncertainties in the data that are available. Thus, as shown later in this report, a weighted least squares fitting procedure is quite useful for this problem.

Least squares is also beneficial for the optimization search. Once data points are fitted using least squares, information about critical points (maxima and minima) can be obtained simply by taking derivatives of the fitted curve. Examinations of different curves of parameter values versus K-effective for systems that SCALE would probably encounter show that considerable flexibility and relatively good accuracy can be obtained by least squares fitting to a cubic polynomial. Therefore, OPTMIZ is set up to generate four initial data points by a front-end process, and from four points on, to perform a least squares fit to a cubic polynomial. The roots of the cubic polynomial (or its derivative - a quadratic) are determined analytically to obtain the desired parameter values.

The preceding material is a brief overview of the work. The remainder of this report contains detailed information and explanations about this new search capability. Chapter II describes the actual development of the method. It explains in detail the procedure that has been incorporated into OPTMIZ and describes the mathematical tools that are needed. Chapter III presents the results obtained with this new technique and also results obtained with the KENO-IV mean value theorem technique for comparison. Chapter IV presents conclusions and recommendations for improvements to this method and some suggestions for future work.

CHAPTER II

OPTMIZ METHODOLOGY

This chapter describes the techniques that are incorporated into the OPTMIZ subroutine package. OPTMIZ is essentially divided into two parts: (1) a fixed value search, and (2) an optimization search. Therefore, this chapter is divided into two major sections. The first section describes the development of the fixed value search capability and introduces the concept of least squares fitting as a search tool. The second section describes the development of the optimization search capability and also outlines the role of least squares fitting in seeking out optimum points. OPTMIZ is capable of performing both types of searches while only requiring the user to input an initial guess, a set of boundary constraints which will be described later in this report, and a tolerance for convergence.

2.1 The Fixed Value Search

OPTMIZ development began as an improvement to the fixed value search capability in the KENO-IV criticality code. Even though the primary objective of developing OPTMIZ is to perform searches for most reactive states of systems (i.e., maximum searches), development started with the fixed value search because it is a much easier search to perform. There is more information available to work with initially. Specifically, this means that there is a known fixed value of K-effective available which can be used to decide which direction the search should progress (i.e., whether the parameter should be increased or decreased). This helps to reduce the number of data points that must be generated to reach the desired parameter value relative to the number that must be generated for an optimization search. Knowing the desired value of K-effective also helps to simplify the process that determines when convergence has been reached.

2.1.1 XXMOD and the Mean Value Theorem (MVT) Method

KENO-IV has a built-in fixed value search capability. It is contained in a subroutine called XXMOD. The equation that does the actual modification of the parameter in XXMOD is an approximation of the mean value theorem of calculus. The modifying equation is:

$$R_{new} = R_{old} + \frac{\Delta R}{\Delta K} (K_d - K_{cal}) \tag{1}$$

where:

R_{new} = new parameter guess

R_{old} = R_i = parameter value that is associated with the latest data point that has been generated in the iteration process.

K_d = desired value of K-effective

K_{cal} = K_i = value of K-effective that is associated with the latest data point that has been generated in the iteration process.

$\Delta R = R_i - R_{i-1}$

$\Delta K = K_i - K_{i-1}$

Notice that this equation uses only two data points to make a next guess, and it does not consider the standard deviations that KENO-IV supplies. Equation (1) can be derived from the mean value theorem:[4]

$$f(x) - f(a) = f'(a)(x-a) \tag{2}$$

The first step in the development of OPTMIZ was an improvement to Equation (1).

2.1.2 The Extended Mean Value Theorem (EMVT) Method

Since the mean value theorem is a truncation of Taylor's series, the improvement of Equation (1) is a solution of the mean value theorem plus one more term of Taylor's series, which is known as the extended mean value theorem:[5]

$$f(x) - f(a) = f'(a)(x-a) + f''(a)\,\frac{(x-a)^2}{2} \tag{3}$$

The improved modifying equation, known as the EMVT equation, can be derived from the extended mean value theorem by making some assumptions and solving the equation for x (which is the new parameter value). The modifying equation is:

$$R_{new} = R_{old} - \frac{\Delta R}{\Delta K}\left(1 + |K_{cal} - K_d|\right)^{1/2} \tag{4}$$

where the parameters are defined in Equation (1) of the previous section. This simple improvement has considerably reduced the amount of time needed to run a problem by reducing the number of iterations required to reach convergence on the desired fixed value of K-effective. However, it has done nothing about improving accuracy.

OPTMIZ must be able to accommodate two types of criticality calculations: one-dimensional discrete ordinates and three-dimensional Monte Carlo. All of the work that has been done to test this new fixed value search capability has been done with KENO-IV. Since Monte Carlo is a statistical calculation, the exact value of K-effective can only be determined by running an infinite number of histories. So the answer obtained in a calculation using a finite number of histories is thought of as a range of numbers in which the true answer has some chance of lying in that range. Accuracy then is defined in this work as how close the Monte Carlo estimate is to the true answer. No improvement in accuracy is obtained by the EMVT method because it does not attempt to get closer to the true answer, but merely gets an approximate answer in less computing time. The addition of least squares fitting to OPTMIZ has improved accuracy as well as reduced computing time because the least squares technique uses all previous data points to make a next guess

2.1.3 The Linear Least Squares Fit

Least squares fitting to a polynomial is a powerful mathematical tool for representing experimental data. It happens to be very powerful also in the generation and location of data points for computerized criticality searches. A least squares fit to a polynomial involves fitting data points to a polynomial of some degree by minimizing the sum of the squares of the residuals. This quantity is known as χ^2 and is defined as:

$$\chi^2 = \sum_{i=1}^{n} \left[\frac{\Delta y_i}{\sigma_i}\right]^2 = \sum_{i=1}^{n} \frac{1}{\sigma_i^2} (y_i - a_1 - a_2 x_i - a_3 x_i^2 - \ldots - a_{k+1} x_i^k) \tag{5}$$

where:

- y = dependent variable (= K-effective in this work)
- x = independent variable (= parameter value in this work)
- σ = standard deviation associated with y
- n = number of data points
- k = degree of polynomial

For the particular systems that are described later in this report, the most advantageous polynomial to fit is a cubic. The reasons are: (1) a cubic can fit data with a local maximum (i.e., data with a peak between the boundaries), (2) a cubic can fit data with no local maximums, (3) a cubic can allow for asymmetry (skewness) of data, and (4) a cubic can also fit data with a local minimum. So, for this particular application, Equation (5) becomes:

$$\chi^2 = \sum_{i=1}^{n} \left[\frac{\Delta y_i}{\sigma_i}\right]^2 = \sum_{i=1}^{n} \frac{1}{\sigma_i^2} (y_i - a - bx_i - cx_i^2 - dx_i^3) \tag{6}$$

The object of a least squares fit is to minimize χ^2 with respect to each of the coefficients a, b, c, and d. Therefore, $\frac{\partial\chi^2}{\partial a}$, $\frac{\partial\chi^2}{\partial b}$, $\frac{\partial\chi^2}{\partial c}$, $\frac{\partial\chi^2}{\partial d}$ are determined and set equal to zero. The resulting equations are solved in matrix form for a, b, c, and d, which are the coefficients of the cubic equation that corresponds to the least sum of the squares of the residuals. χ^2 is a measure of the goodness of fit to the data.

After the coefficients of the cubic polynomial have been determined, the next step is to obtain its roots for some desired fixed value of K-effective.

2.1.4 The Analytical Solution of a Cubic Equation

There is another advantage to fitting the data to a third degree polynomial. For cubic equations there exists a fairly simple and easy way to analytically solve for its roots. However, the fact that the solution is analytical rather than numerical is not the only advantage. There is information internal to the analytical solution of a cubic that can be used to determine execution paths. For example, there are two types of cubic equations that can result from a least squares fit. They are: (1) a cubic with no local extrema, and (2) a cubic with two local extrema. These two types of curves are shown in Figures 2 and 3. It will be shown later in the section on optimization searching that information about maximum and minimum points can be obtained by taking the first derivative of the cubic and solving the resulting quadratic for its roots at zero. It is evident from the curves of Figures 2 and 3 that if data points are fit to a cubic with no local extrema, then there is no point in taking the derivative of the cubic to determine maximum or minimum points because the solution will yield the point of inflection, which is of no use in this problem. Thus, information that is internal to the solution of a cubic can be used to determine which type of cubic has been fit and consequently can eliminate calculations that are unnecessary.

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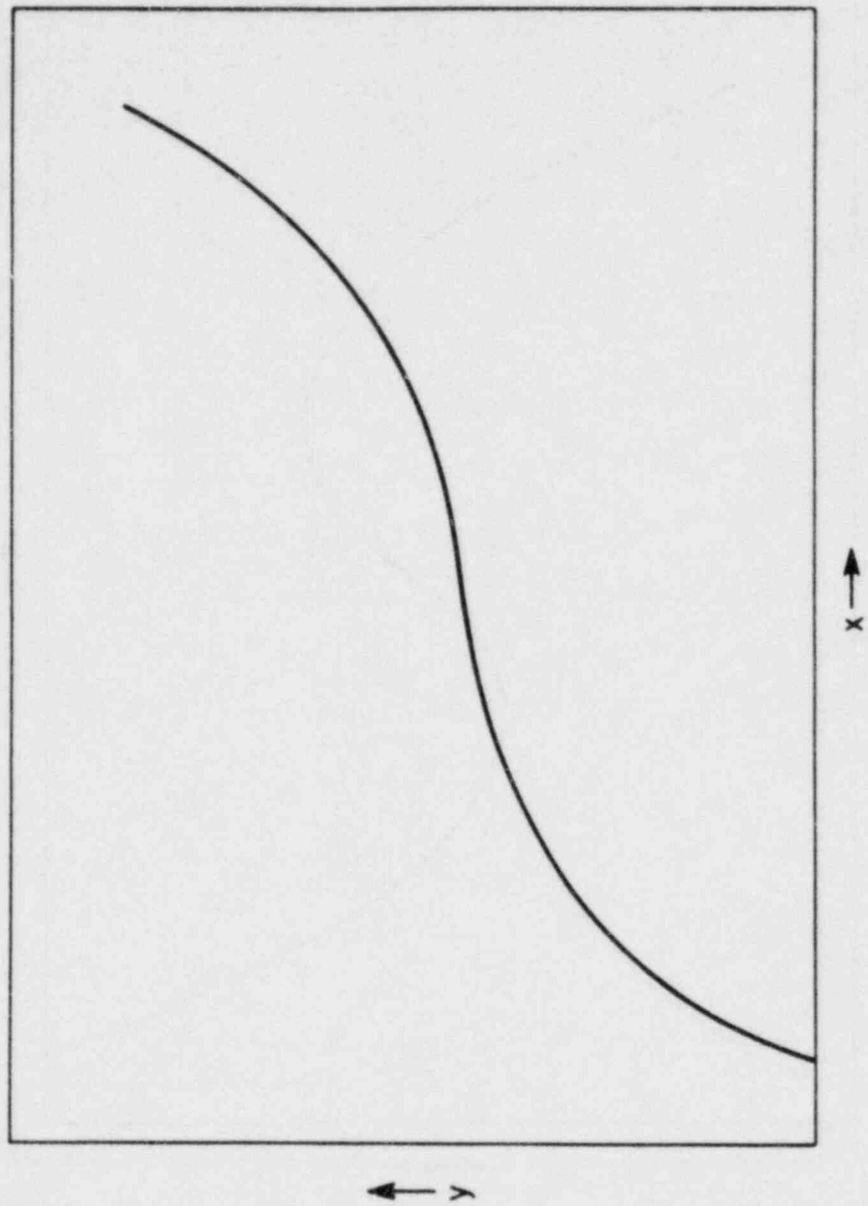

Figure 2. A Cubic with No Local Extrema.

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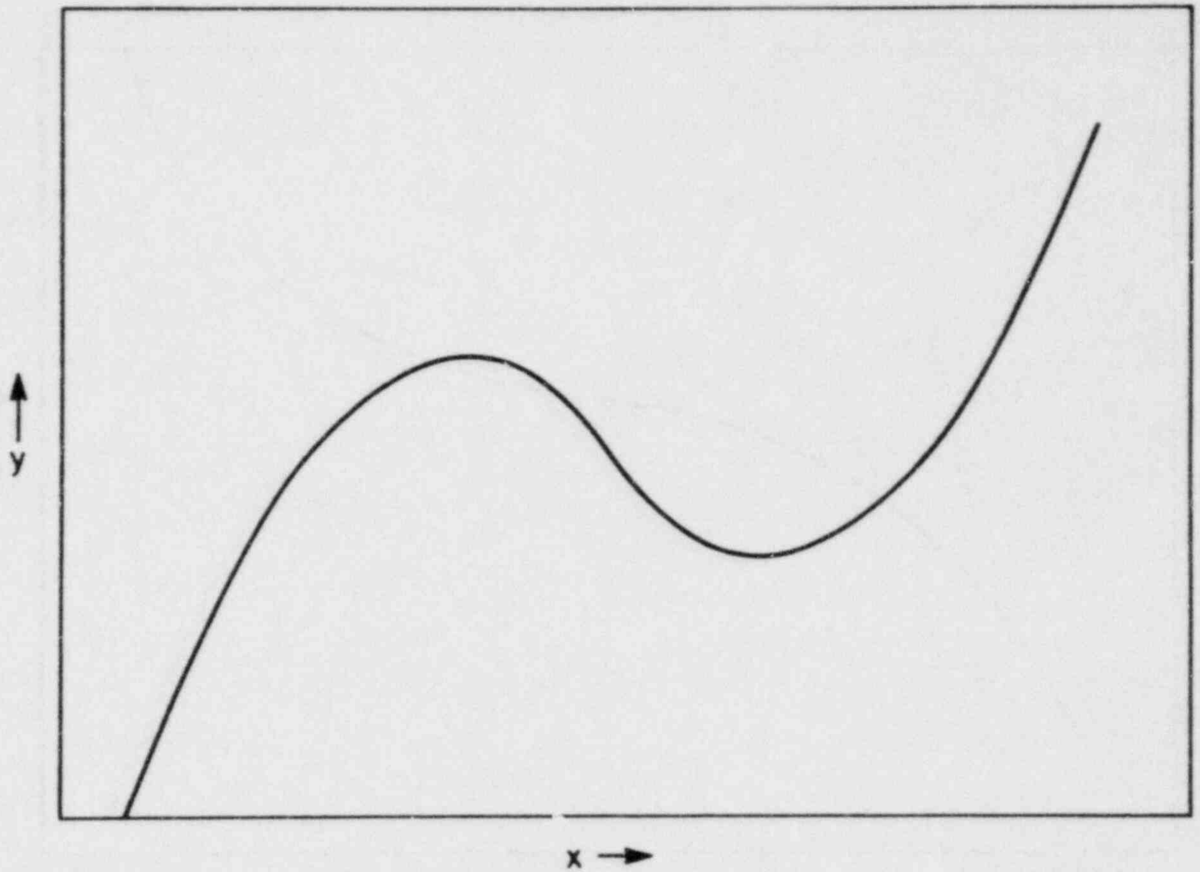

Figure 3. A Cubic with Two Local Extrema.

There are two types of solutions to a cubic equation: (1) a solution that yields one real root and two conjugate imaginary roots, and (2) a solution that yields three real roots. Consider the following cubic equation:

$$x^3 + Px^2 + Qx + R = 0 \tag{7}$$

The solution for one real root is algebraic.[6] Equation (7) reduces to:

$$y^3 + Ay + B = 0 \tag{8}$$

by substituting $x = y - P/3$ into Equation (7). Then, the real root of Equation (7) is:

$$x = z_1 + z_2 - P/3 \tag{9}$$

where:

$$z_1 = \sqrt[3]{-B/2 + \sqrt{B^2/4 + A^3/27}} \tag{10}$$

$$z_2 = \sqrt[3]{-B/2 - \sqrt{B^2/4 + A^3/27}} \tag{11}$$

The solution for three real roots is trigonometric:[7]

$$\begin{aligned} x_1 &= 2\sqrt{-A/3}\ \cos\theta - P/3 \\ x_2 &= 2\sqrt{-A/3}\ \cos(\theta + 2\pi/3) - P/3 \\ x_3 &= 2\sqrt{-A/3}\ \cos(\theta + 4\pi/3) - P/3 \end{aligned} \tag{12}$$

where:

x_1, x_2, and x_3 are the roots, and θ is an angle to be determined.

The analytical solution of the least squares cubic completes the calculations needed for one pass in OPTMIZ.

The next section is a detailed summary of the fixed value search procedure which includes a discussion of the previously mentioned problem of accuracy that the least squares method has helped to alleviate.

2.1.5 The Fixed Value Search Procedure

The procedure for the fixed value search is divided into two parts: (1) a front-end process to generate enough data points for a least squares fit, and (2) the least squares fit itself. The front-end process for the fixed value search is the extended mean value theorem procedure that has been previously discussed. Once enough data points have been generated, the least squares method takes over and is used until the search is terminated. The following is a step-by-step procedure for the fixed value search.

THE OPTMIZ FIXED VALUE SEARCH PROCEDURE

1. Use the extended mean value theorem routine to calculate the first four data points.
2. Perform a least squares fit to a cubic on the data points.
3. Solve the least squares cubic for its root (or roots) at the desired value of K-effective.
4. Use the root (or roots) as the next guess.
5. Go to Step 2; repeat until convergence is reached.

One of the requirements of the OPTMIZ fixed value search is that the user must specify a tolerance for convergence. In the case of a KENO-IV Monte Carlo calculation, this tolerance could be expressed in standard deviations. However, these standard deviations are associated with K-effective and not with the parameter that is being searched for. Therefore, when the calculated K-effective falls within the specified tolerance about the desired value of K-effective, the search is terminated and the parameter that is associated with the final calculated fixed value is assumed to be the right answer. It is at this point that the previously discussed problem of accuracy becomes important.

Consider the coordinate axes illustrated in Figure 4. Since there is a standard deviation associated with K-effective, it is quite valid to assume that there exists a standard deviation associated with the parameter that is being searched for. However, this parameter standard deviation is not known and would be extremely difficult to calculate. It does, however, exist and can be used here to illustrate how improved accuracy can be obtained by using least squares instead of the MVT or EMVT methods.

When an MVT or an EMVT calculation is being performed, the search essentially progresses from the initial guess to the desired value and converges when one of the guesses falls within the user-specified tolerance region. Keep in mind that the only requirement for convergence is that the guess must fall within the tolerance region, meaning that the converged answer could lie very close to the true answer, or it could lie near the outer boundaries of the

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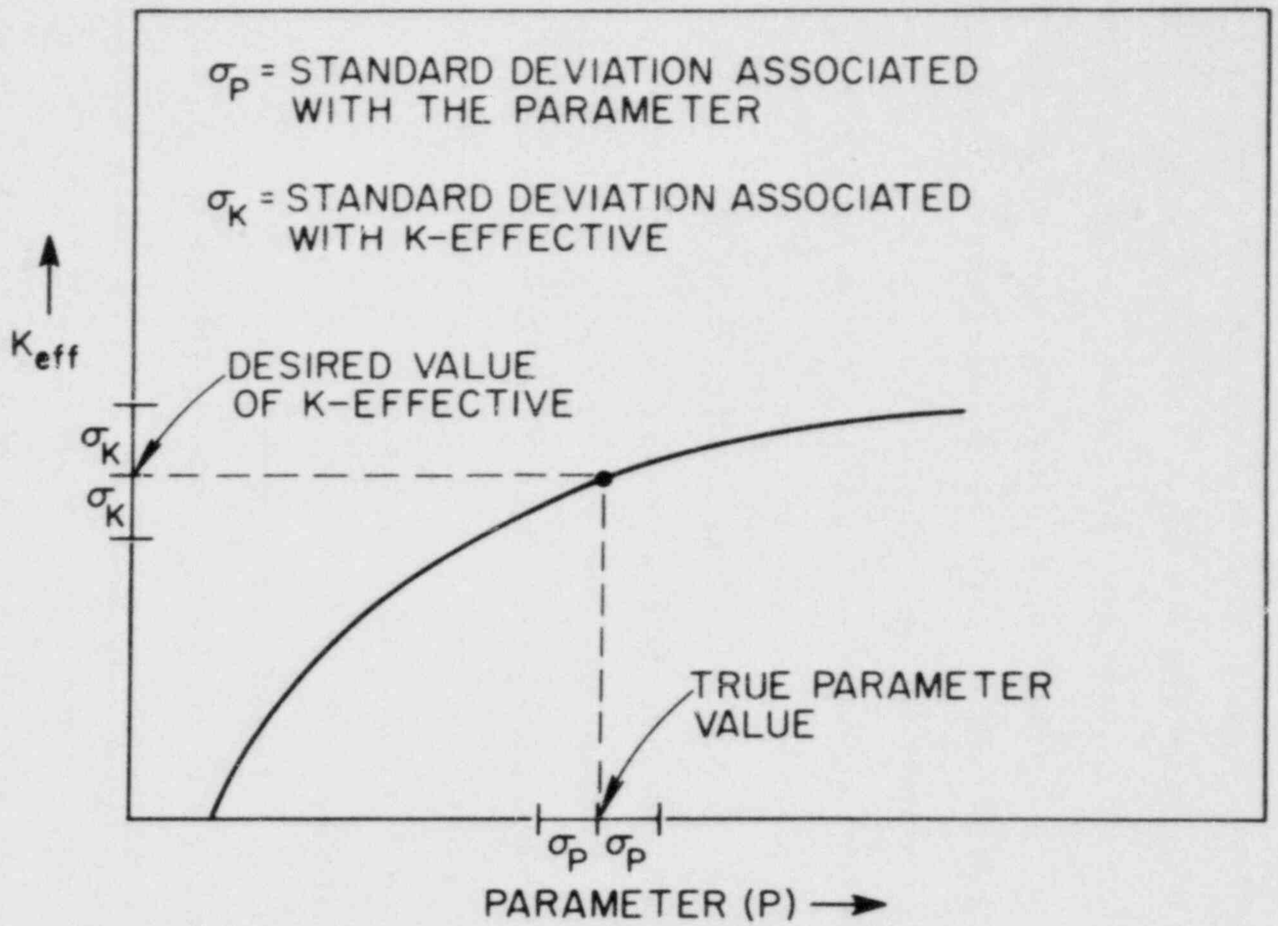

Figure 4. Illustration of Improvement in Accuracy Obtained by Using the Least Squares Method.

region. So essentially, these two methods do not necessarily seek out the true answer, but instead they seek out the tolerance region.

On the other hand the least squares method not only finds the tolerance region, but gets closer to the true answer by using all previous information to make a next guess. The reason is that unlike the MVT and EMVT methods, which are essentially a progression of "jumps" from one data point to the next, the least squares technique is fitting the points to a curve on every iteration. The equation obtained from the least squares fit is then solved for a root. So every iteration provides more information, and when convergence is finally reached, the answer obtained using least squares generally lies closer to the true answer than the answers obtained by the MVT or EMVT methods, as will be shown in Chapter III.

The remainder of this chapter describes the development of the optimization search. Some of the techniques employed in the fixed value search are incorporated into the optimization search, such as the least squares technique.

2.2 The Optimization Search

It is probably very evident that the name OPTMIZ comes directly from the word optimization. The reason for this is that the version of OPTMIZ that will initially be incorporated into modules CSAS3 and CSAS4 will only have optimum searching capabilities. The fixed value search will eventually be available but is considered an extra feature. The CSAS3 and CSAS4 modules are defined as searches for most reactive states of systems (i.e.. optimum states), therefore the package is called OPTMIZ even though it does have the capacity for a fixed value search. The optimization search relies heavily on least squares fitting. Once an equation has been determined, differentiation of the least squares cubic supplies all of the information necessary to locate optimum values.

2.2.1 The Front-End Process

The generation of the first four data points for the optimization search is considerably different than the method used for the fixed value search. The extended mean value theorem method cannot be utilized for an optimum search because a specified desired value of K-effective is needed to perform the EMVT calculation. Since no fixed value is available, a different generation scheme has been developed. This new scheme is relatively simple, yet it is of considerable importance to the least squares fit that follows. It requires the user to input boundary constraints. These constraints essentially define a parameter region in which a maximum can be located.

Given a starting guess and a set of boundary constraints, the idea behind this new generation scheme is quite simple: generate four equally spaced data points within the parameter constraints that will give the least squares method the best chance of approximately locating the maximum after the first curve fit. The generation of equally spaced points across the parameter region is very important assuming there is no prior knowledge about the system available. Equally spaced points provide the least squares method with the best chance of locating the maximum regardless of where in the parameter region it lies. It is not possible to equally space the points exactly because the spacing depends on the initial guess, but an attempt is made to come as close to equal spacing as possible.

The first three points are, respectively, the initial guess, the left parameter constraint, and the right parameter constraint. The fourth point varies according to where in the region the initial guess lies. It is usually generated equidistant between the initial guess and the parameter constraint that is furthest away from the initial guess. In some cases the initial guess may lie so close to one of the constraints that it is not advantageous to use both points. When this happens, the initial guess is assumed to be the constraint. The other constraint becomes the second point and the last two points are generated equidistant from the constraints and from each other. Similar to the fixed value search, after the first four points are generated, the least squares technique takes over and is utilized until the search is terminated.

2.2.2 Locating the Optimum by Differentiation of the Least Squares Cubic

Once again, least squares fitting the data points to a cubic polynomial is the method that is employed. This time, however, the analytical solution of a cubic is not needed. The object of the optimization search is to seek out parameter values that correspond to maximum (or minimum) values of K-effective. These maximum (or minimum) values of K-effective are not known quantities, so it is not clear for what value of K-effective the cubic must be solved. Therefore, some other method of solution must be utilized for this type of search.

Recall from basic calculus that the first and second derivatives of a polynomial provide information about maximum and minimum points. The first derivative of a cubic is a quadratic which can be solved for its roots at zero:

$$f(x) = ax^3 + bx^2 + cx + d \tag{13}$$

$$f'(x) = 3ax^2 + 2bx + c = 0 \tag{14}$$

$$x = \frac{-2b \pm \sqrt{4b^2 - 12ac}}{6a} \tag{15}$$

$$x_1 = \frac{-2b + \sqrt{4b^2 - 12ac}}{6a} \quad , \quad x_2 = \frac{-2b - \sqrt{4b^2 - 12ac}}{6a} \tag{16}$$

The two roots x_1 and x_2 are the maximum and minimum points of Equation (13) as illustrated in Figure 5. The second derivative of Equation (13) tells which root is the maximum and which one is the minimum. The second derivative of a cubic is:

$$f(x) = ax^3 + bx^2 + cx + d \tag{17}$$

$$f'(x) = 3ax^2 + 2bx + c \tag{18}$$

$$f''(x) = 6ax + 2b \tag{19}$$

Substituting x_1 and x_2 into Equation (19) determines which root is the maximum and which one is the minimum. The determination is made by the following procedure:

$$\text{If } f''(x) \begin{cases} > 0 & \text{root is a minimum point} \\ = 0 & \text{root is a point of inflection} \\ < 0 & \text{root is a maximum point} \end{cases}$$

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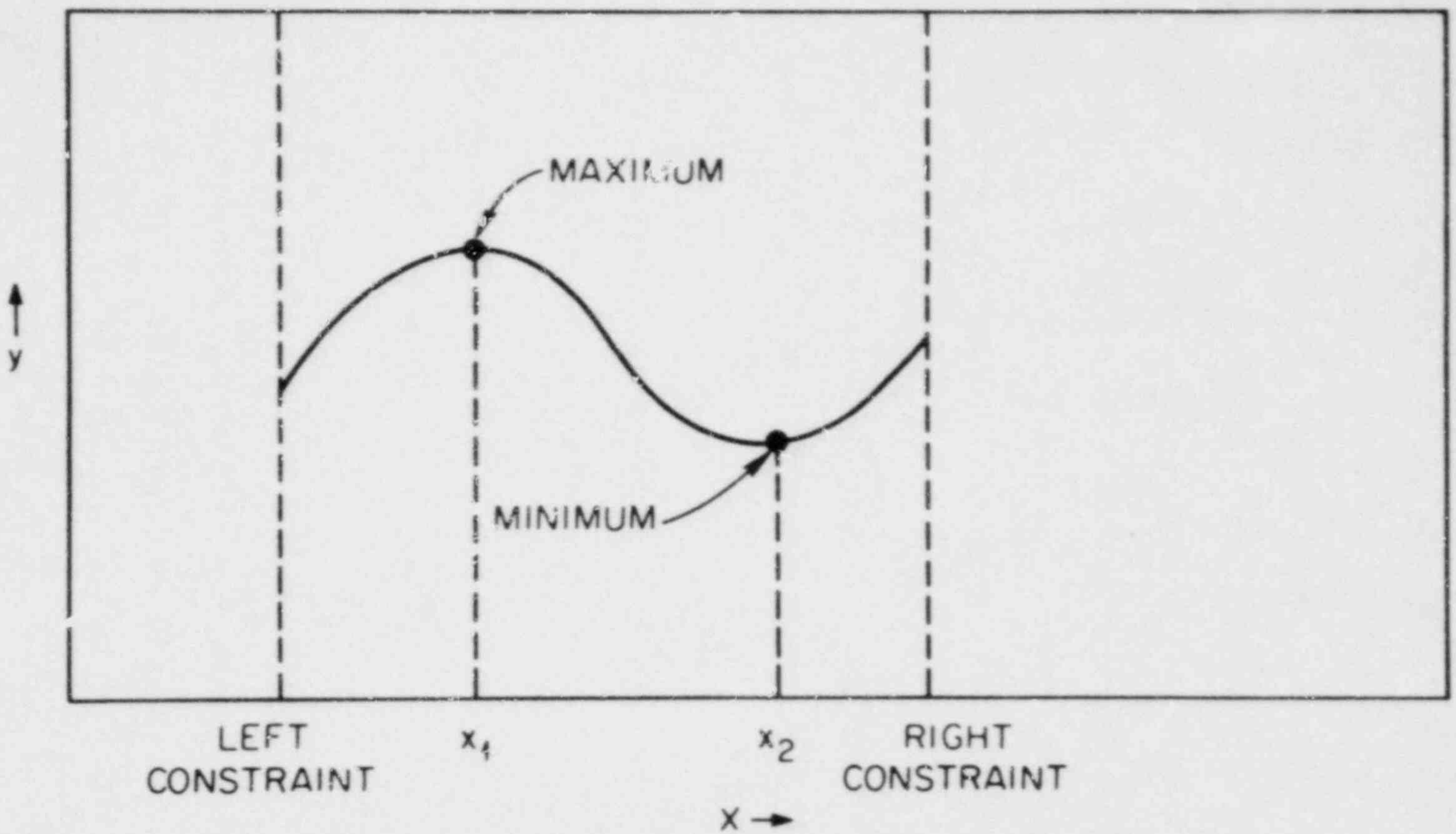

Figure 5. The Maximum and Minimum Points of a Cubic with Two Local Extrema.

Therefore, all of the information necessary to locate and determine the optimum points is contained in the least squares cubic and its derivatives. However, there is one more item to consider.

What if the curve that is fit turns out to be a cubic of the type shown in Figure 2 (page 13)? Then the method involving derivatives that was just discussed is totally useless. All that it will do is locate the point of inflection, as shown in Figure 6. In order to be useful then, OPTMIZ must be able to recognize what type of cubic is being fit, and determine the proper path of execution. This is the advantage that was previously discussed. The analytical solution of a cubic provides information about what type of cubic is being fit. Consider the quantity under the square root in Equations (10) and (11). The type of cubic that has been fit is determined by the following procedure:

If $\frac{b^2}{4} + \frac{a^3}{27} > 0$ There will be one real root and two conjugate imaginary roots;

If $\frac{b^2}{4} + \frac{a^3}{27} = 0$ There will be three real roots of which at least two are equal;

If $\frac{b^2}{4} + \frac{a^3}{27} < 0$ There will be three real and unequal roots.

Of course, the value of this quantity depends on what value of K-effective the cubic equation is set equal to before it is solved for its roots at that value of K-effective. For example, consider the curve of Figure 7. When a cubic with three real roots is set equal to K_1, the analytical solution will yield three real

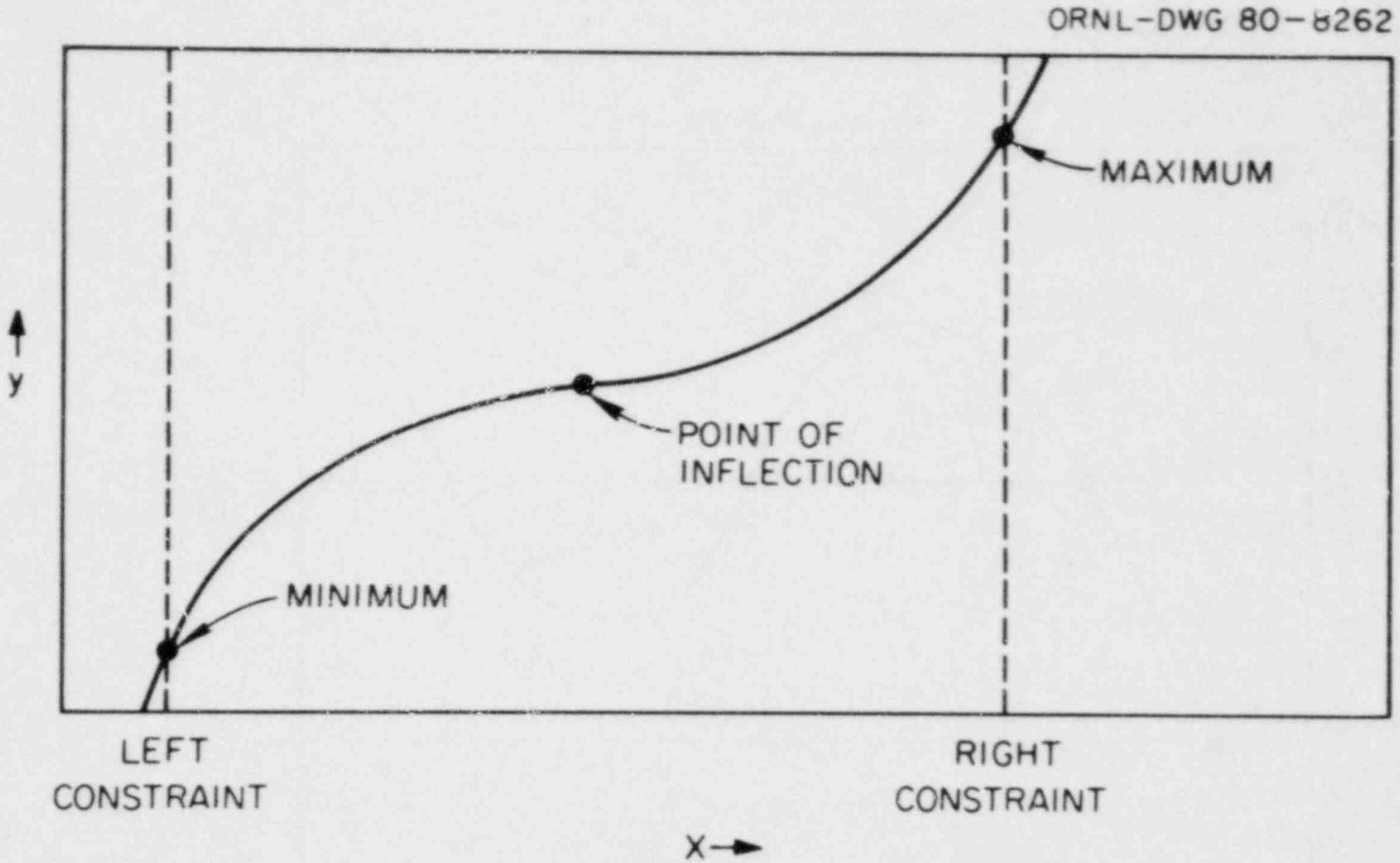

Figure 6. The Maximum and Minimum Points of a Cubic with No Local Extrema.

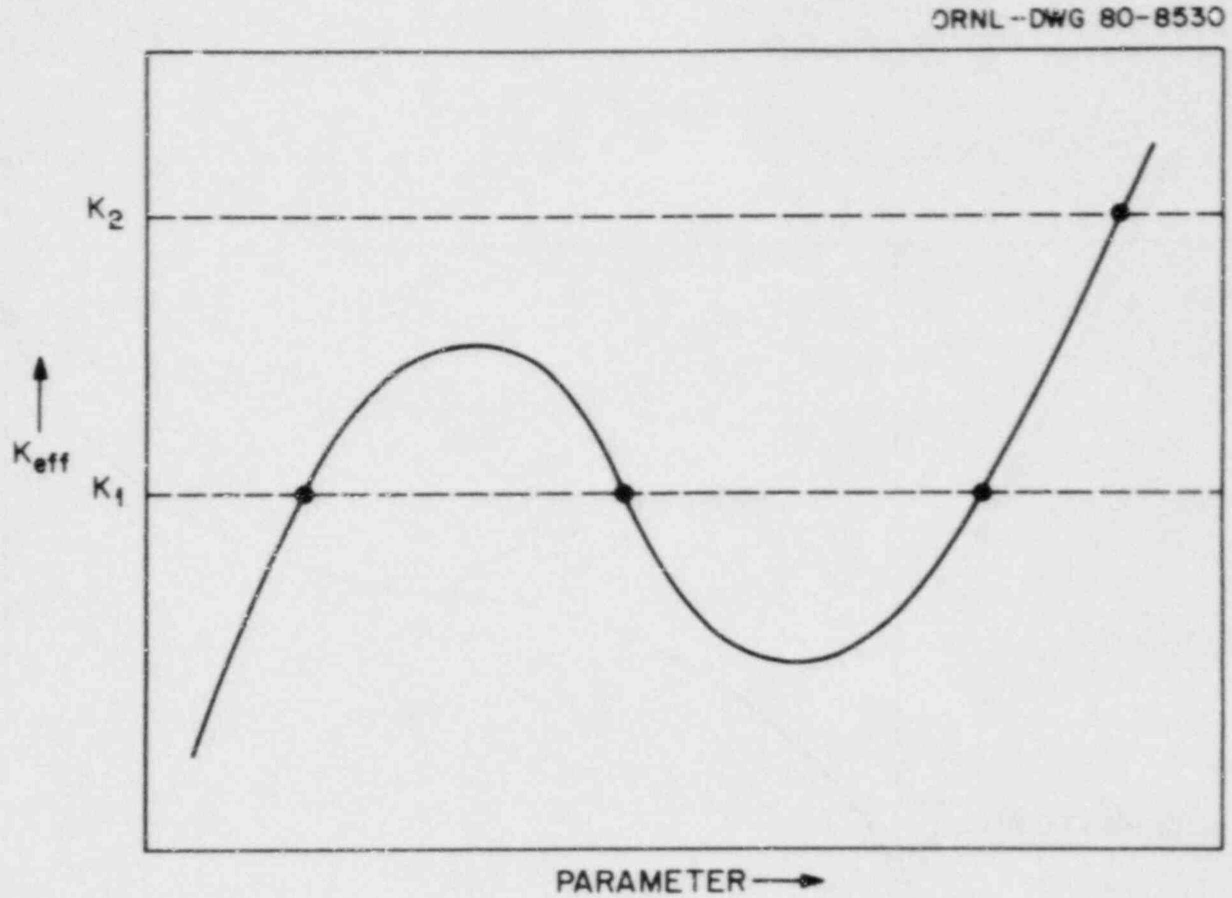

Figure 7. An Illustration of the Effect on the Number of Roots Obtained for the Solution of a Cubic at Different Values of K-effective.

roots. However, if the same cubic is set equal to K_2, the analytical solution will yield only one real root because that is all that is available. Therefore, the procedure for determining whether the least squares method has fit the data to a cubic of the type shown in Figure 2 (page 13) or a cubic of the type shown in Figure 3 (page 14) is to solve the equation for each data point (i.e., set the cubic equation equal to the value of K-effective that corresponds to each data point and solve the equation for its roots at that value of K-effective) and determine if the quantity $\frac{b^2}{4} + \frac{a^3}{27}$ is negative for any of the data points. If this quantity is negative for at least one data point, then the cubic has to be of the type shown in Figure 3 because this situation could not arise for the type shown in Figure 2. If the quantity $\frac{b^2}{4} + \frac{a^3}{27}$ is positive for every data point, then the cubic has to be of the type shown in Figure 2. If $\frac{b^2}{4} + \frac{a^3}{27}$ is zero for any data point, then the cubic must again be of the type shown in Figure 3. However, it is highly unlikely that this latter situation would occur on a computer because of round-off errors associated with floating point arithmetic. The situation of $\frac{b^2}{4} + \frac{a^3}{27} = 0$ is not really important though, because if the fitted curve looks like Figure 3, then there will be at least one data point that causes $\frac{b^2}{4} + \frac{a^3}{27}$ to be negative.

Since an execution path already exists for a cubic of the type shown in Figure 3, then one must be developed for a cubic of the type shown in Figure 2. It turns out to be a relatively simple technique. If CSAS3 and CSAS4 encounter a system with no local extrema (i.e., a system with no maximum or minimum between the boundaries), then most likely it will be similar to the solid portion of the curve of Figure 8. The dashed portion of the curve represents the portion of the least squares cubic that is not a part of the actual system. In other words, the entire curve of Figure 8 (solid and dashed portions) is the cubic that the least squares process has fit to the data, while the actual data points are confined to the portion of the curve that is between the constraints (the solid portion of the curve). For this system the maximum and minimum points lie on the boundaries. Therefore, all OPTMIZ is required to do is to make sure that the system really is similar to Figure 8, and then conclude that the optimum lies on one of the boundaries.

The next section is a summary of the optimization searching method. It also introduces two new concepts that are essential to obtaining accurate results from the optimization search.

2.2.3 The Optimization Search Procedure

The procedure for the optimization search is similar to the procedure for the fixed value search in that it consists of a front-end process, a least squares fit, and an analytical solution for the roots of an equation. However, the front-end process and the analytical solution are considerably different because different information is needed. The least squares fit is essentially the same except for an additional weighting factor. Recall from Equation (6) that the least squares fit for the fixed value search is weighted by $\frac{1}{\sigma_i^2}$ (the inverse of the square of the standard deviation associated with data point i). This weighted least squares process allows for a better fit by weighting each data point according to the uncertainty

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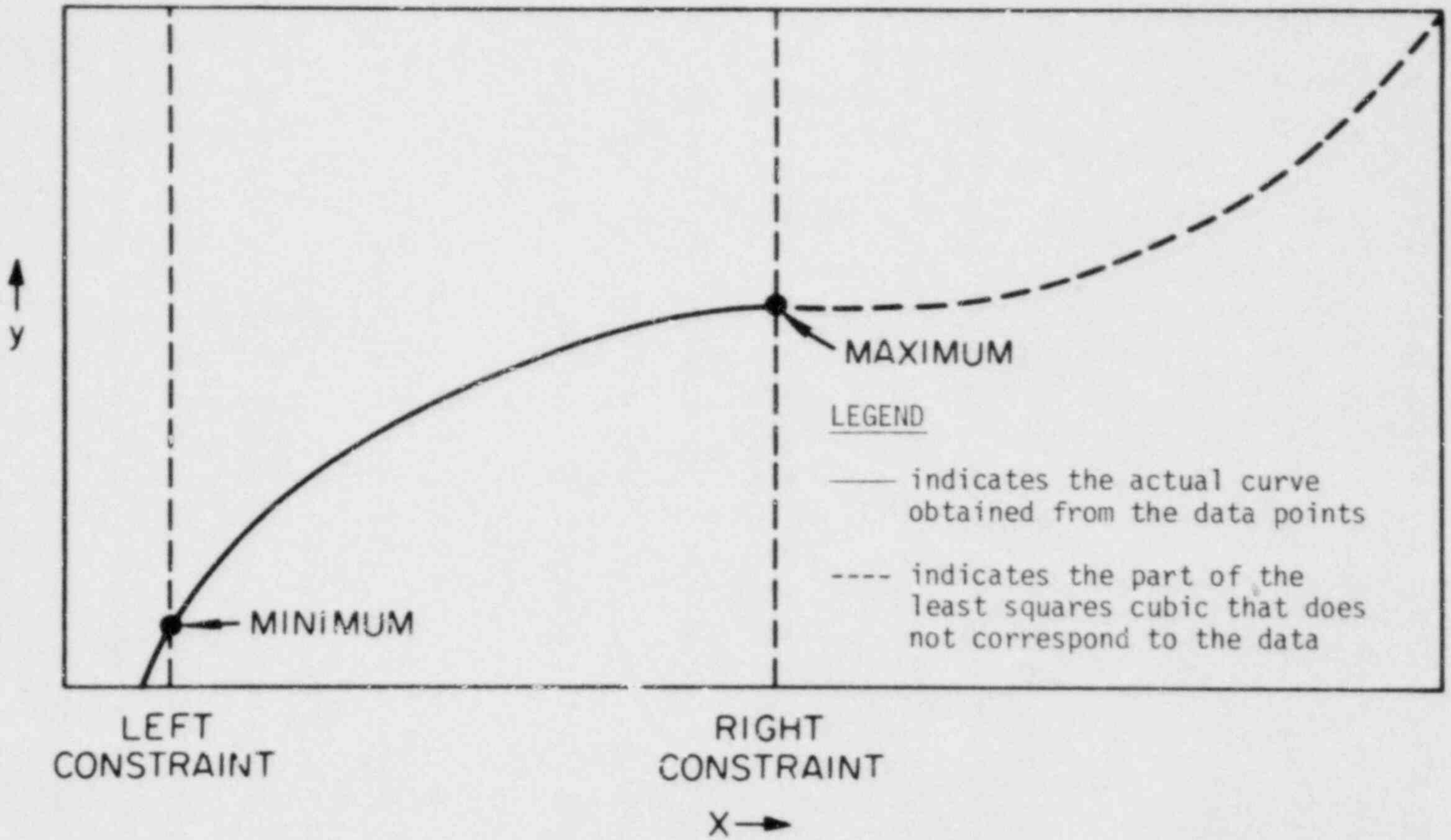

Figure 8. Typical System Curve that Contains No Local Extrema.

associated with it. However, when a least squares fit is performed for the optimization search, the data points are weighted not only according to their standard deviations, but also according to how far away they are from the estimated optimum. The weighting factor for the optimization search is:

$$\text{Weight} = \frac{1}{\sigma_i^2 + D_i^2} \tag{20}$$

where:

σ_i = standard deviation associated with data point i

D_i = parameter distance between data point i and the most recent estimate of the optimum

This new weighting factor has been introduced to help alleviate some convergence problems that will be discussed in the next chapter. Another technique has also been introduced to help with the convergence problems. It is an attempt to locate data points such that the best least squares fit is obtained, as described below.

The object of this "optimum location of data points" is to generate data points on both sides of the optimum. Experience has shown that after the first four data points have been generated, the estimates obtained thereafter from the least squares fit consistently lie on one side or the other of the optimum. The problem that is encountered here is similar to the problem associated with interpolation versus extrapolation of points on a curve. Recall that interpolating a curve is a much more accurate method of obtaining values on that curve than extrapolating it because interpolation implies that there are data points on both sides of the point that is sought. Extrapolation is usually a somewhat dangerous technique because it involves trying to determine a point beyond the realm of data points that are available. The situation is similar for the OPTMIZ least squares process of determining optimum points in that a better fit (and subsequently a better estimate of the optimum) can be obtained if there are data points on both sides of the optimum, and if those points are reasonably close to the optimum. Therefore, this new concept of "optimum location of data points" has been introduced to obtain an even better answer than what could be obtained by using the new weighting scheme described earlier by itself. The following is a step-by-step procedure for the optimization search. It includes procedures for handling both types of cubics (i.e., Figures 2 and 3 on pages 13 and 14, respectively).

THE OPTMIZ OPTIMIZATION SEARCH PROCEDURE

1. Generate four equally spaced points within the parameter boundary constraints.
2. Perform a least squares fit to a cubic polynomial.
3. Determine the type of cubic that has been fit. If it is of the type shown in Figure 2, go to Step 8. If it is of the type shown in Figure 3, go to Step 4.

- -

4. Take the first derivative of the least squares cubic.
5. Solve the resulting quadratic for its roots at zero.
6. Take the second derivative of the least squares cubic to determine which root is the maximum (or minimum). Use root as next guess.

7. Go to Step 2; Repeat until convergence is reached.

- -

8. Generate a few more data points to be sure that a cubic of the type shown in Figure 2 (page 13) is the actual situation that is occurring.
9. If the actual situation is a cubic of the type shown in Figure 2, then conclude that the optimum lies on one of the boundaries. If the fit changes to the type shown in Figure 3 (page 14), then go to Step 4 and continue.

The next chapter presents results that have been obtained from OPTMIZ for both the fixed value search and the optimization search. It also includes some discussion of the improvement of accuracy that has been achieved for the fixed value search and the convergence problems that have been encountered in the optimization search.

CHAPTER III

RESULTS

The results that have been generated to test and validate the OPTMIZ method are divided into two sections. The first section deals with results obtained for the fixed value search. These results include not only OPTMIZ results, but also results for the EMVT method. Both OPTMIZ and EMVT results are compared to results obtained with the existing MVT technique in KENO-IV. The results for the fixed value search were presented at the 1979 American Nuclear Society Winter Meeting in San Francisco, California.[8]

The second section deals with results obtained for the optimization search. Since there is no current automated technique available for optimum searching, there is no standard technique to compare with. Therefore, these results emphasize how accurate and reliable OPTMIZ is in predicting optimum points by testing it on a system for which the maximum is known, as described in the next section, and on a system for which many data points were generated.

3.1 The Fixed Value Search

The OPTMIZ fixed value search procedure was tested on the two systems that are illustrated in Figures 9 and 10. Figure 9 shows how K-effective varies with the radial lattice pitch for a 2 × 2 × 2 array of 93.2% Uranium metal cylinders in air. This particular problem was chosen for the following reasons: (1) critical experiments have been performed and documented for this system,[9] so there is an experimental critical lattice pitch available to compare the various results with, (2) since there is no moderating or reflecting material present, the

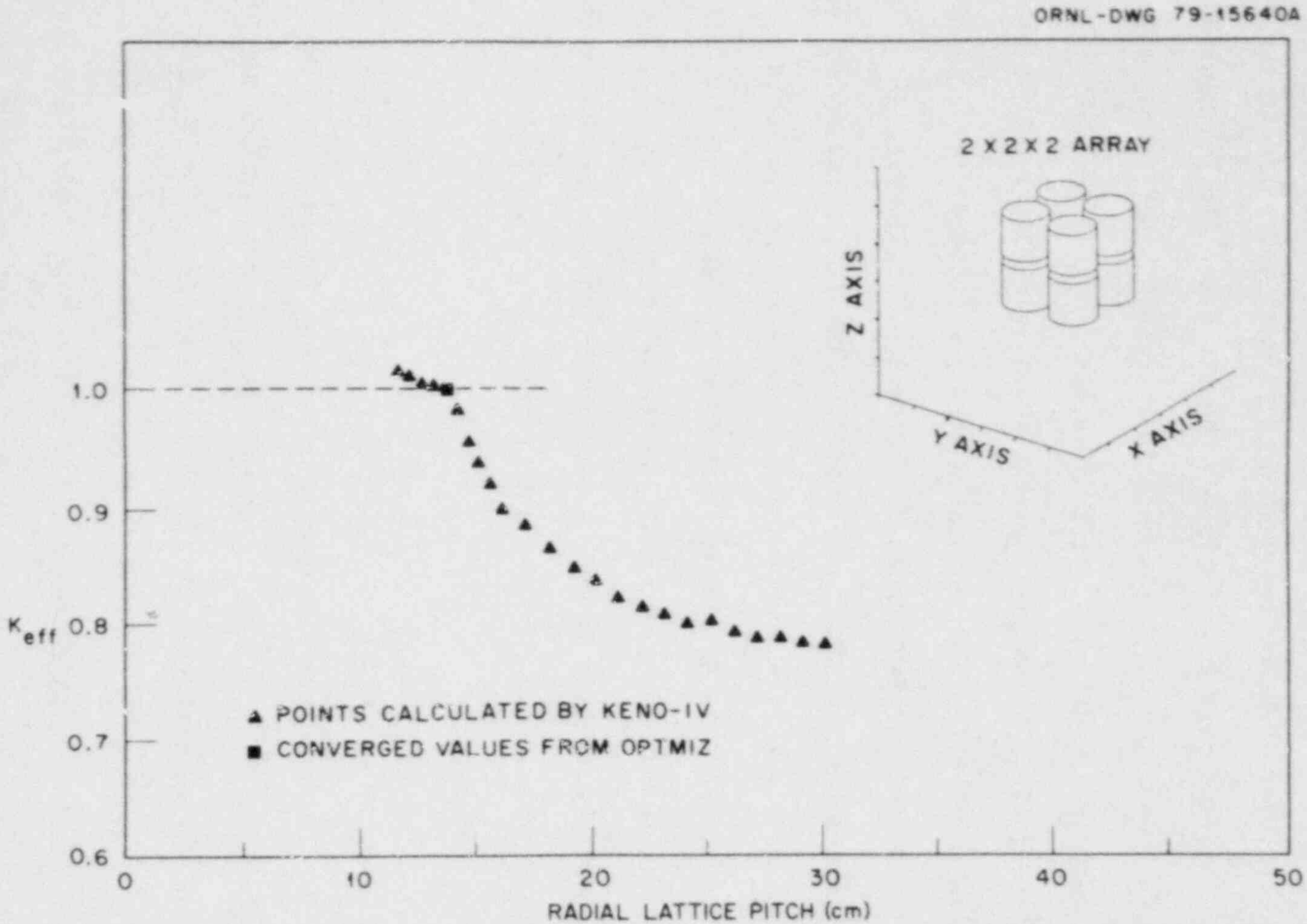

Figure 9. An Illustration of how K-effective Varies with the Radial Lattice Pitch for a 2 x 2 x 2 Array of 93.2% Uranium Metal Cylinders in Air.

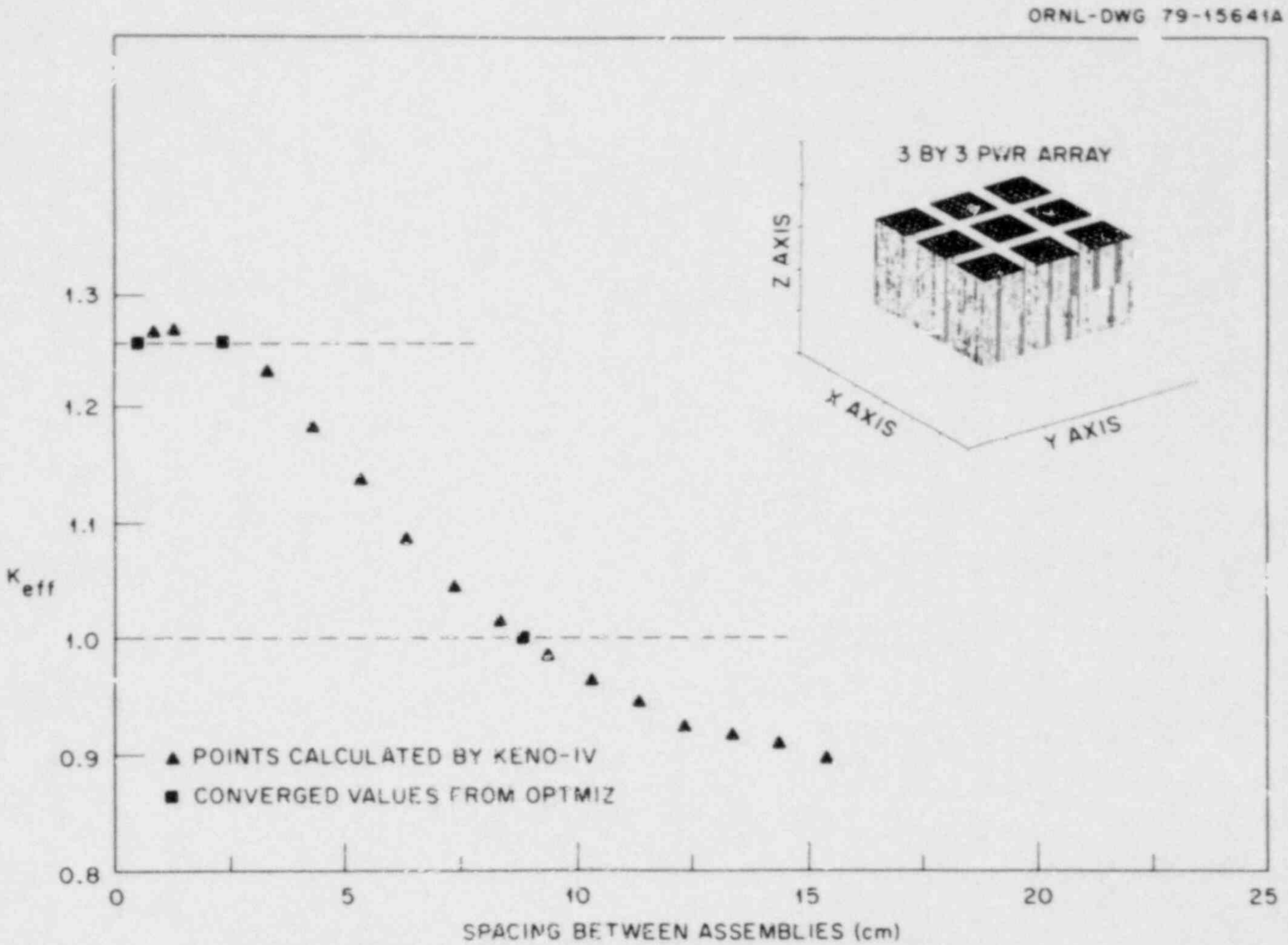

Figure 10. An Illustration of how k effective Varies with the Spacing Between Assemblies for a 3 x 3 Array of PWR Fuel Assemblies in Water.

K-effective calculations for this problem consume relatively modest amounts of computer time, and (3) this problem illustrates how OPTMIZ can handle systems in which the optimum values occur on the boundaries. The results obtained for this high enriched array are presented in Table 1. These results indicate that computational efficiency has been improved. The EMVT method provides a considerable reduction of computer time over the MVT method. Also, OPTMIZ not only reduces computer time but improves accuracy too. Notice that the OPTMIZ converged values of the critical lattice pitch for this system are consistently closer to the value obtained from critical experiments than are the converged values obtained from the EMVT and MVT methods. These results indicate that the concept of least squares curve fitting does indeed improve accuracy relative to the EMVT and MVT methods.

All K-effective calculations for this system were performed by KENO-IV. In Table 1, "method failed" in the MVT column means that the KENO-IV search (XXMOD) was terminated because of a violation of a geometry constraint. For example, for an initial guess of 24 cm, the third guess in the search on radial lattice pitch was less than the diameter of the cylinders. This means that the MVT search was smashing the cylinders together, which is obviously unacceptable. In Table 1, "CPU" is the Central Processor time needed to run each case on an IBM 360 Model 91 computer.

The second system that was used to test the fixed value search is shown in Figure 10. It is an attempt to simulate a problem that CSAS4 is being designed to handle. This problem is criticality safety analysis of fuel assemblies in a shipping cask. Figure 10 shows the

Table 1. A Comparison of MVT, EMVT, and OPTMIZ Results for a 2 x 2 x 2 Array of 93.2% Uranium Metal Cylinders in Air.

K_d = 1.00	MVT		EMVT		OPTMIZ	
Initial Guess	Converged Value	CPU (sec)	Converged Value	CPU (sec)	Converged Value	CPU (sec)
20.00 cm	13.78 cm	360	13.50 cm	195	13.75 cm	200
24.00 cm	Method Failed		Did not Converge in 8 Iterations	350	13.73 cm	240
26.00 cm	Method Failed		13.77 cm	304	13.72 cm	320
30.00 cm	Method Failed		Did not Converge in 8 Iterations	351	13.73 cm	320

Note: Experimental critical lattice pitch = 13.74 cm.

variation of K-effective with the spacing between assemblies for a 3 x 3 array of PWR fuel assemblies surrounded by water. This problem is considerably more expensive than the previous one because a light water moderator and reflector is present. In other words, the Monte Carlo tracking of a neutron requires a lot of computer time scattering in the water thereby driving up the time required to track a specified number of histories. However, this system closely simulates the situation that would arise in the analysis of a spent fuel shipping cask.

Table 2 presents OPTMIZ and MVT results for this low enriched array of PWR assemblies. Results were obtained for searches on two different values of K-effective. The results of the search on K-effective = 1.00 indicate that OPTMIZ is a big help in problems that consume a large amount of computer time. A 10- to 20-minute reduction in computer time was achieved by the OPTMIZ method relative to the KENO-IV MVT method. In Table 2, "CPU" is the Central Processor time needed to run each case on a CDC-7600 computer. The results for K-effective = 1.00 also further illustrate the improved accuracy of the OPTMIZ method over the MVT method. Notice that the converged values from OPTMIZ for 30,000 neutron histories are closer to the values from the MVT method for 100,000 neutron histories than are the values from the MVT method for 30,000 neutron histories. These results indicate that OPTMIZ is a considerable improvement in computational efficiency (i.e., improved accuracy and reduced computing time) over the MVT technique.

Also included in Table 2 are results obtai d for searches on K-effective = 1.26. These results are presented only to show that if

Table 2. A Comparison of MVT and OPTMIZ Results for a 3 x 3 Array of PWR Fuel Assemblies in Water.

K_d = 1.00	MVT		OPTMIZ	
Initial Guess	Converged Value	CPU (min)	Converged Value	CPU (min)
10.00 cm	8.439 cm (30,000 Histories) 8.276 cm (100,000 Histories)	62.9	8.297 cm (30,000 Histories)	43.7
15.00 cm	8.460 cm (30,000 Histories) 8.338 cm (100,000 Histories)	55.7	8.278 cm (30,000 Histories)	44.7

K_d = 1.26	MVT		OPTMIZ	
Initial Guess	Converged Value	CPU	Converged Value	CPU
10.00 cm	1.713 cm (30,000 Histories) 1.834 cm (100,000 Histories)	-	0.172 cm 1.444 cm (30,000 Histories)	-
15.00 cm	0.725 cm (30,000 Histories) 1.506 cm (100,000 Histories)	-	0.109 cm 1.904 cm (30,000 Histories)	-

desired, OPTMIZ can locate two parameter values that correspond to one value of K-effective, if both parameter values exist.

3.2 The Optimization Search

The optimization search procedure was tested on the two systems whose curves of K-effective versus pitch are shown in Figures 11 and 12. The first system shown in Figure 11 does not result from real KENO-IV Monte Carlo K-effective calculations but is rather an attempt to simulate KENO-IV K-effective calculations. The curve of Figure 11 is very similar to the curve of Figure 10. Indeed, the idea here is to simulate a KENO-IV Monte Carlo calculated curve of K-effective versus pitch for a 3 × 3 PWR fuel assembly system with a similar curve that is much cheaper to calculate. The curve of Figure 11 is actually a Gaussian probability distribution curve with a mean value of 0.8100 cm and a standard deviation of 7.00 cm. This simulation has proven to be very efficient in the testing of the new optimization search method. The big advantage of a simulated calculation like this is that the exact maximum value is known. Therefore, it is very easy to see how well OPTMIZ performs in finding the true maximum. OPTMIZ results for this simulated calculation of K-effective are presented in Tables 3 and 4. The results in Table 3 show how the OPTMIZ estimate of the maximum varies with different sets of boundary constraints. Four searches were performed with the same initial guess but with different boundary constraints. These results indicate that the OPTMIZ estimate of the maximum improves as the constraints are tightened. Table 4 presents results that show how well OPTMIZ estimates the maximum for searches

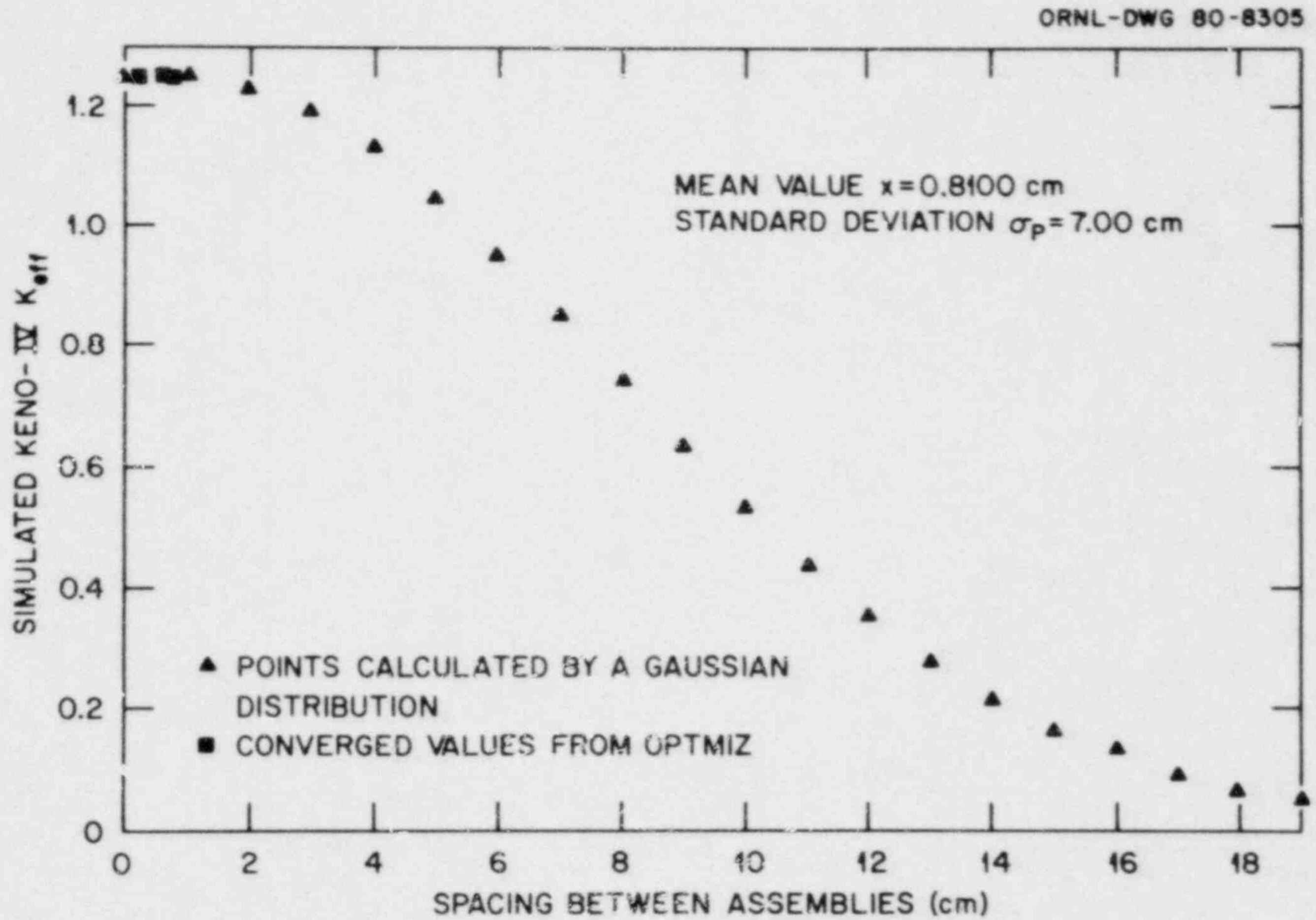

Figure 11. Curve of K-effective Versus Pitch for a Simulated KENO-IV Criticality Calculation of a 3 x 3 Array of PWR Fuel Assemblies in Water by a Gaussian Distribution.

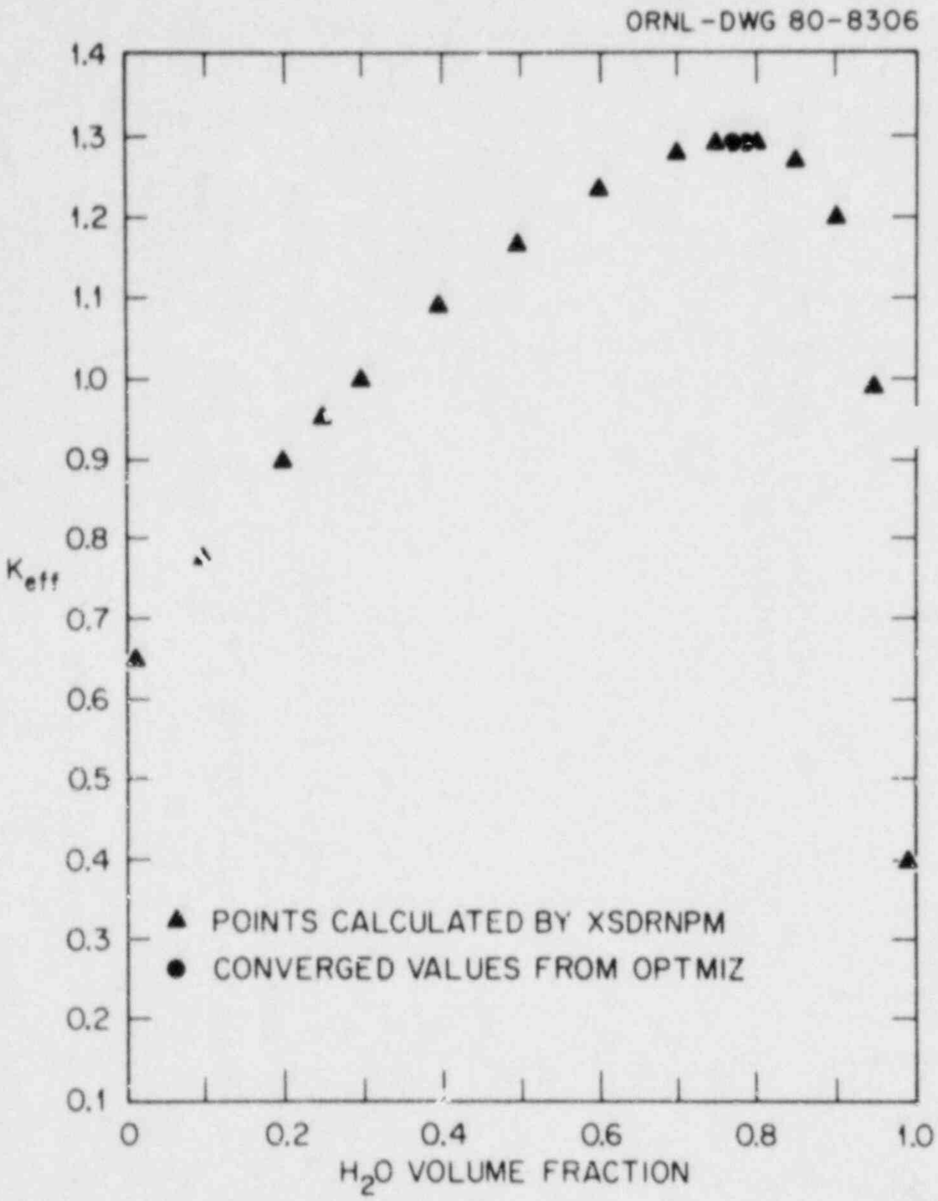

Figure 12. Curve of K-effective Versus Pitch for a Cylindrical Tank of 4% Enriched UO_2 Powder Mixed with Water.

Table 3. Results for the Simulated KENO-IV K-effective Calculation of a 3 x 3 Array of PWR Fuel Assemblies in Water that Show how the OPTMIZ Estimate of the Maximum Varies with the Constraints.

Initial Guess	Left Constraint	Right Constraint	Parameter Value from OPTMIZ that Corresponds to Maximum K-effective	Maximum Value of K-effective
10.00 cm	0.0 cm	25.0 cm	0.211 cm	1.249
10.00 cm	0.0 cm	20.0 cm	0.663 cm	1.253
10.00 cm	0.0 cm	15.0 cm	0.797 cm	1.254
10.00 cm	0.0 cm	10.0 cm	0.797 cm	1.254

Note: Parameter value associated with true maximum value of k-effective = 0.810 cm.

Table 4. Results for the Simulated KENO-IV K-effective Calculation of a 3 x 3 Array of PWR Fuel Assemblies in Water that Show OPTMIZ Estimates of the Maximum for Searches with Different Initial Guesses.

Initial Guess	Parameter Value from OPTMIZ that Corresponds to Maximum K-effective	Maximum Value of K-effective	Number of Iterations
0.0 cm	0.797 cm	1.254	6
5.0 cm	0.797 cm	1.254	6
7.5 cm	0.690 cm	1.254	6
15.0 cm	0.797 cm	1.254	6

Note: Left constraint = 0.0 cm.
Right constraint = 15.0 cm.
Parameter value associated with true maximum value of k-effective = 0.810 cm.

that have the same boundary constraints but different initial guesses. These results indicate that OPTMIZ is very reliable in finding the maximum no matter where the search originates.

The second system used to evaluate the optimization search procedure is shown in Figure 12. This curve illustrates the variation of K-effective with the volume fraction of water in a stainless steel cylindrical tank of 4% enriched UO_2 powder mixed with water. This system is presented to show how OPTMIZ handles one-dimensional CSAS3 problems. When the fuel concentration is being altered, the parameter versus K-effective curves can be very difficult to fit to a cubic and convergence can be a problem. The difficulty is that many times the search will not converge at the true maximum, but rather a little bit to the right or left of the maximum. Convergence in an optimization search is much more difficult to achieve than convergence in a fixed value search because the maximum value of K-effective is not a known quantity. If the data calculated for the system is difficult to fit to a least squares cubic (such as the curve of Figure 12), then locating the maximum value can be very difficult. The concept of weighting the data points according to how far away they are from the estimated maximum, and also the concept of "optimum location of data points" as discussed earlier have been introduced to help obtain a better fit in the region around the maximum.

Table 5 presents results obtained from OPTMIZ for searches that yield the volume fraction of water that corresponds to the maximum value of K-effective in a cylindrical stainless steel tank of 4% enriched UO_2 powder mixed with water. The calculation of K-effective

Table 5. Results from OPTMIZ for the XSDRNPM K-effective Calculation of a Cylindrical Tank of 4% Enriched UO_2 Powder Mixed with Water.

Initial Guess	H_2O Volume Content from OPTMIZ that Corresponds to Maximum K-effective	Maximum Value of K-effective	Number of Iterations
0.01%	0.800%	1.288	10
0.20%	0.780%	1.291	11
0.50%	0.745%	1.288	8
0.60%	0.790%	1.290	11

Note: Left constraint = 0.01%.

Right constraint = 0.99%.

Maximum value of k-effective obtained from generation of numerous data points = 1.291.

H_2O volume content that corresponds to maximum value of k-effective = 0.780%.

Tank inner diameter = 100 cm.

Tank height = 100 cm.

for this system was performed by the SCALE module CSAS1 since CSAS3 is not yet operational. CSAS1 is a one-dimensional criticality safety analysis module that utilizes the discrete ordinates transport code, XSDRNPM,[10] to calculate K-effective. Since the calculation is one-dimensional, a correction must be made for the leakage in the transverse direction of the cylinder so that K-effective will not be over-estimated. The results presented in Table 5 indicate that OPTMIZ is very accurate and reliable even for curves of parameter values versus K-effective that do not fit well to a cubic. The accuracy and reliability of the results in Table 5 are based on the fact that many data points were generated prior to running OPTMIZ searches on this system. So the maximum value has been established by visual observation of the curve of Figure 12 and by the maximum value obtained by the numerous points that were generated in the region around the maximum (all data points calculated are not shown in Figure 12).

The results presented in this section do indicate that the optimization search procedure that has been developed for use in OPTMIZ provides an accurate and dependable method for locating the most reactive states of systems.

The next chapter presents conclusions about the OPTMIZ method for both the fixed value search and the optimization search. It also presents some recommendations for improvements and further work on the OPTMIZ methodology.

CHAPTER IV

CONCLUSIONS AND RECOMMENDATIONS

There are two major conclusions that can be stated regarding the OPTMIZ methodology. First, improved computational efficiency is quite evident for the fixed value search. Having a method (the XXMOD-MVT method) available to compare with makes it very easy to show how OPTMIZ has improved fixed value criticality searches. Based on the results presented in this report, OPTMIZ is consistently more accurate than the KENO-IV MVT method. It also reduces computer time substantially.

Second, the same method used for fixed value searches can be modified and used to perform optimization searches. Since no automated optimization searches are available to compare with, results for this new technique can only show how close OPTMIZ comes to predicting the true maximum of a pre-determined curve. The simulation of the KENO-IV K-effective calculation of a 3×3 array of PWR fuel assemblies in water that is shown in Figure 11 has played a very important part in the development of the optimization search. The advantage of this approach is that the true maximum is a known value, which has helped many times in deciding what kind of intelligence should be incorporated into the search. The cylindrical tank of 4% enriched UO_2 powder mixed with water has also been very important in the development of the optimization search. The concept of "optimum location of data points" was conceived as a result of problems that were encountered with this system. Results indicate that the OPTMIZ optimization search has performed very well even on data that is difficult to least squares fit to a cubic.

Although OPTMIZ has been tested only for fixed value and maximum searches, it should also work for a minimum search, which means that it should just as easily locate a minimum. It can also handle systems that have no local optimum points. In general, OPTMIZ will provide the nuclear criticality safety community with a much improved automated method for performing fixed value searches. More importantly, it will provide an automated capability that heretofore was not available: namely, performing searches for optimum points (i.e., maximums and minimums).

The fixed value search is a fairly straightforward procedure and has been extensively tested. Thus, the bulk of the work that remains is that of improving the optimization searching capability. Optimization searches are inherently more difficult to perform because it is very difficult to decide when the optimum point has been reached. Thus, further research should strive to improve decisions about convergence. The optimization search must also be tested more extensively. Even though the results presented have shown that the optimization search method works, testing on more realistic systems must be performed in order to complete validation of the method.

It should also be pointed out that advanced versions of the searching techniques in CSAS3 and CSAS4 will allow for searches on more than one parameter simultaneously. A preliminary suggestion for this simultaneous search is to use least squares to search on one parameter at a time while holding all other parameters constant. Successive searches on all parameters would hopefully locate the overall optimum of the system (i.e., the determination of the values of all parameters that are being searched on that would yield the most reactive state of the system). There are also more sophisticated techniques that have been developed for locating optimums, such as gradient[11] techniques and acceleration along a ridge.[12] These methods should also be considered for solving the simultaneous parameter search problem.

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