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Part IV

EVALUATION OF MOLECULAR WEIGHT FROM EQUILIBRIUM SEDIMENTATION

PART IV: APPLICATION OF TIKHONOV'S REGULARIZING FUNCTIONS

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AIR FORCE MATERIALS LABORATORY
AIR FORCE SYSTEMS COMMAND
WRIGHT-PATTERSON AIR FORCE BASE, OHIO

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Part IV

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The following corrections are applicable to AFML-TR-67-121, Part IV, (UNCLASSIFIED Title) Evaluation of Molecular Weight From Equilibrium Sedimentation. Part IV: Application of Tikhonov's Regularizing Functions, UNCLASSIFIED Report, August 1970:

Page 6

Change equation (8) to read

$$L_n^{\alpha}[f] = \alpha\left\{\sum_{i=0}^{n+1}(-1)^{i+1}\frac{d^i}{dm^i}\left[K_i(m)\frac{d^i f}{dm^i}\right]\right\} - \left\{\int_0^{M_{max}} \bar{K}(m,\xi)f(\xi)\,d\xi - \bar{b}(m)\right\} = 0 \quad (8)$$

Air Force Materials Laboratory
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FOREWORD

This report was prepared by the Polymer Branch of the Nonmetallic Materials Division. The work was initiated under Project No. 7342, "Fundamental Research on Macromolecular Materials and Lubrication Phenomena," Task No. 734203, "Fundamental Principles Determining the Behavior of Macromolecules," with Dr. M. T. Gehatia acting as task scientist. The work was administered under the direction of the Air Force Materials Laboratory, Directorate of Laboratories, Air Force System Command, Wright-Patterson Air Force Base, Ohio 45433.

The report covers research conducted from January 1969 to February 1970. The manuscript was released by the authors in April 1970 for publication as a technical report.

This technical report has been reviewed and is approved.

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SECTION I

INTRODUCTION

The determination of molecular weight distribution (MWD) from equilibrium sedimentation was investigated in 1928 by Rinde (Reference 1). Fujita (Reference 2) expressed the relationship between the frequency function, f(m), of MWD and an experimental curve $u(\xi)$, obtained from ultracentrifugal sedimentation in the form of the two following equations:

$$u(\xi) = \frac{C(\xi)}{C_0} = \int_0^{m_{max}} \frac{\lambda m e^{-\lambda m \xi}}{1 - e^{-\lambda m}} f(m)\, dm \qquad (1)$$

$$u(\xi) = -\frac{1}{C_0}\frac{dC(\xi)}{d\xi} = \int_0^{m_{max}} \frac{\lambda^2 m^2 e^{-\lambda m \xi}}{1 - e^{-\lambda m}} f(m)\, dm \qquad (2)$$

where C is concentration; Co, initial concentration; m, molecular weight, r, distance from the center of rotation; r_a, r_b-r to the meniscus and bottom respectively; ρ, density of solution; V, partial specific volume of polymer; ω, angular viscosity; R, universal gas constant; and T, temperature in °K; and

$$\lambda = \frac{(1 - V\rho)\omega^2 (r_b^2 - r_a^2)}{2RT} \; ; \; \xi = \frac{r_b^2 - r^2}{r_b^2 - r_a^2}$$

The determination of MWD can now be defined as a solution of Equation 1 or 2.

In recent years the need to know the MWD of polymers has significantly increased and spurred many new attempts to develop a good computational technique for this purpose (References 3 through 17). The determination of MWD was also an objective of this laboratory (References 18 through 21). Unfortunately, the efforts to develop a good method for MWD determination were, in general, not very successful and the results proved to be disappointing. In some cases such results lacked precision and reproducibility and they did not seem to provide a routine which would work in all circumstances. Elucidation of this enigmatic behavior of Fujita's equations, and the difficulties arising during their solution is a subject of investigation in this laboratory.

Lee (Reference 21) first recognized that Equations 1 and 2 constitute an Improperly Posed Problem (IPP) in the Hadamard sense (Reference 22) and, therefore, a conventional mathematical approach cannot provide satisfactory solutions. There is, however, the possibility of finding an approximate solution to IPP in general and to Fujita's equations in particular by applying Tikhonov's regularizing functions. Application of this method and solution of Fujita's equations is the objective of this Technical Report.

SECTION II

IMPROPERLY POSED PROBLEM

The notion of a mathematical IPP (Improperly Posed Problem, also known as an Ill Posed Problem or Incorrectly Formulated Problem) goes back to Hadamard (Reference 22) in conjunction with the Cauchy problem for the Laplace equation. At that time Hadamard believed an IPP is evidence that the expression under consideration does not have any real physical meaning, and therefore, it cannot express any physical rule or situation. This belief proved to be wrong, and the existence of IPP was established in many other "physical" expressions such as the heat equation for negative time and Cauchy data on the boundary, the non-hyperbolic Cauchy problem for the wave equation, the inverse problem of potential, and a number of inverse problems for differential and integral equations.

In the recent decade IPP was intensively investigated. The following considerations are based upon the works of C. Pucci (References 23 through 28); F. John (References 29 through 32); M. M. Lavrentiev (References 33 through 43); A.N. Tikhonov (References 44 through 61); V.K. Ivanov (References 62 through 66); V.A. Morozov (References 67 through 70); and others (References 71 through 83).

Consider the equation:

$$u(\xi) = Af(m) = Q\left[\xi, f(m)\right]$$

where A is an operator, $u \in U$, $f \in F$, U, and F are some complete metric spaces, and Af is a function with the domain of definition F and the range of values U.

The solution of Equation 2 is a properly posed problem if the following conditions are satisfied:

(2a.) The solution of (2) exists for any $u(\xi) \in U$.

(2b.) The solution of (2) is unique in F(m).

(2c.) The solution of (2) depends continuously on $u(\xi)$ in the metrics of F and U.

In such a case there exists a function $Bu(\xi)$, defined and continuous over all U, and B is an inverse operator of A, where:

$$A^{-1}u(\xi) = f(m) = R\left[m, u(\xi)\right] \tag{3}$$

If even one of the conditions 2a, 2b, or 2c is not satisfied [$u(\xi) = Af(m)$] is an IPP. In such a case due to the unboundedness of the operator A^{-1} the solution does not exist for all $u(\xi)$ and is unstable. To arbitrarily small variations of $u(\xi)$ may correspond arbitrarily large changes in f(m).

As an example consider a Fredholm Integral Equation of the First Kind.

$$u(\xi) = A\left[\xi, f(m)\right] = \int_a^b K(\xi, m) f(m) dm; \quad c \leq \xi \leq d \tag{4}$$

It can be shown that the inverse problem of Equation 4, e.g., computation of $f(m)$ on the basis of a given function $u(\xi)$, is improper. Indeed, to the functions $f_1(m)$ and $f_2(m) = f_1(m) + p \cos \omega m$, $f_1(m)$, $f_2(m) \in \bar{F}$, where p is an arbitrarily large given number, there will correspond functions $u_1(\xi)$ and $u_2(\xi)$ for which the norm $\| u_1(\xi) - u_2(\xi) \|$ is arbitrarily small if ω is sufficiently large. However, if the class of admissible solutions is the compact class $\tilde{F}$, the inverse mapping $U \rightarrow \tilde{F}$ will be stable (Reference 48). In other words, for every $\epsilon > 0$, there will exist a $\delta(\epsilon, \tilde{F})$ such that the inequality $\| u_1 - u_2 \| < \delta(\epsilon, \tilde{F})$ implies $\| f_1 - f_2 \| < \epsilon$ if u_1 and $u_2 \in U = \{ u(\xi) = A[\xi, f(m)],\ f \in \tilde{F} \}$, where $\tilde{F}$ is a compact class of functions.

An IPP will be called a Regularizable Problem in Tikhonov's sense if it has at least one regularizing algorithm defined in the following. Such regularizing algorithms are practical aids for solving an IPP.

Let an IPP, $f = R[m, u]$ be given, where, to a special function $\bar{u}(\xi)$, there corresponds a solution $\bar{f}(m) = R[m, \bar{u}(\xi)]$. Let also an approximating function $\tilde{u}(\xi)$ for $\bar{u}(\xi)$ be given, such that $\| \tilde{u} - \bar{u} \| < \delta$, where δ is known. It is required to find $\tilde{f}(m)$, an approximation to $\bar{f}(m)$, with an assigned precision $\| \tilde{f} - \bar{f} \| \leq \epsilon$ if δ is sufficiently small.

$R[m, u(\xi)]$ will be called a regularizing operator if the following conditions are fulfilled:

(1.) $R_\delta[m, u(\xi)]$ is defined for every $\tilde{u} \in U$ and $\delta > 0$.

(2.) If for $\bar{u}(\xi)$ there exists a $\bar{f}(m) = R[m, u(\xi)]$, then for every positive ϵ, there exists a $\delta(\epsilon, f)$ such that if $\| \tilde{u} - \bar{u} \|_U < \delta$, then $\| \tilde{f} - \bar{f} \|_F \leq \epsilon$ where $\tilde{f}_\delta = R[m, \tilde{u}]$.

Consider a Fredholm Integral Equation of the First Kind as expressed by Equation 4, with the boundaries a = 0, b = m_{max}, c = 0, and d = 1. If the kernel $K(\xi, m)$ is continuous, and if for $\bar{u}(\xi) = 0$ there exists just one solution $\bar{f}(m) = 0$, the Integral Equation can be solved in the following way by applying variational calculus and Tikhonov's regularizing algorithm.

Instead of dealing with the conventional functional:

$$N\left[f(m); \bar{u}(\xi)\right] = \int_0^1 \left[A\left[\xi, f(m)\right] - \bar{u}(\xi)\right]^2 d\xi \qquad (5)$$

Tikhonov suggests applying another smoothing functional:

$$M_n^{\alpha}\left[f(m); \bar{u}(\xi)\right] = N\left[f(m); \bar{u}(\xi)\right] + \alpha\Omega^{(n)}\left[f(m)\right] \qquad (6)$$

where $\Omega^{(n)}$ is the regularizing functional. Then,

$$\Omega^{(n)}(f) = \int_0^{M_{max}} \left\{\sum_{i=0}^{n+1} K_i(m)\left[f^{(i)}(m)\right]^2\right\} dm, \qquad (7)$$

where the $K_i(m)$'s are positive continuous functions, and α is an arbitrary parameter, which minimizes the functional M_n^{α}.

The application of the variational Euler Equation and boundary conditions transform Equation 6 into a new expression:

$$L_n^{\alpha}\left[f\right] = \alpha\left\{\sum_{i=0}^{n+1}(-1)^{i+1} K_i(m)\frac{d^i f}{dm^i}\right\} - \left\{\int_0^{M_{max}} \bar{K}(m,\xi)f(\xi)\,d\xi - \bar{b}(m)\right\} = 0 \qquad (8)$$

with the boundary conditions

$$\pi^{\ell}(m) = \left\{ \sum_{i=\ell+1}^{n+1} (-1)^{i-\ell-1} \left[K_i(m) f^i(m) \right]^{(i-\ell-1)} \right\} \Bigg|_{0, m_{max}} = 0; \; (\ell = 1, 2, \cdots n+1) \quad (9)$$

where

$$\bar{K}(m,\xi) = \int_0^1 K(\xi, m) K(\xi, \xi) d\xi \quad (10\text{-a})$$

and

$$\bar{b}(m) = \int_0^1 K(\xi, m) \bar{u}(\xi) d\xi \quad (10\text{-b})$$

Equation 8 will lead to an approximate computation of the function f(m).

SECTION III

COMPUTATION

Consider a Fredholm Integral Equation of the First Kind:

$$u(\xi) = \int_a^b K(\xi,m)\, f(m)\, dm \qquad (11)$$

where $K(\xi,m)$ is a continuous kernel within a range $a \leq \xi \leq b$ and $c \leq m \leq d$. The distribution function, $f(m)$, fulfills the following boundary conditions:

$$f(c) = f(d) = 0 \qquad (12\text{-}a)$$

and

$$\left(\frac{df}{dm}\right)_{m=c} = \left(\frac{df}{dm}\right)_{m=d} = 0 \qquad (12\text{-}b)$$

The function $\bar{f}(m)$ can be mapped to generate the function $\bar{u}(\xi)$. If an inverse operation will be applied on $\bar{u}(\xi)$, a function $\tilde{f}(m)$ can be calculated. Finally, $\tilde{f}(m)$ can be mapped again to generate a function $\tilde{u}(\xi)$. The norms $\| \bar{u}(\xi) - \tilde{u}(\xi) \|$ and $\| \bar{f}(m) - \tilde{f}(m) \|$ will show the quality of the transformation. Such a quality is influenced by the following factors:

(a.) The nature of $f(m)$ function;

(b.) The nature of the kernel;

(c.) The way of obtaining $u(\xi)$;

(d.) The type of regularizing function applied;

(e.) The type of matrix used for approximate calculations.

To examine these factors, various distributions, kernels, methods of integration, regularizing functions, and approximate matrices have been considered.

The following f(m) distributions have been examined:

(a-1.) A mono-modal distribution:

$$\bar{f}(s) = 8s^2(1-s)^2; \quad 0 \le s \le 1 \tag{13}$$

(a-2.) A bi-modal distribution:

$$\bar{f}(s) = f_1(s) + f_2(s); \quad 0 \le s \le 1 \tag{14}$$

where

$$f_1(s) = 78.125\, s^2(s-0.6)^2; \quad 0 \le s \le 0.6 \tag{14-a}$$
$$f_1(s) = 0; \; 0.6 \le s \le 1 \tag{14-b}$$
$$f_2(s) = 0; \quad 0 \le s \le 0.5 \tag{14-c}$$
$$f_2(s) = 162(s-0.5)^2(1-s)^2; \; 0.5 \le s \le 1 \tag{14-d}$$

The following kernels have been applied:

(b-1.) The kernel appearing in Fujita's Equation for concentration gradient, (Equation 2) is

$$K_2(\xi, m) = \frac{\lambda^2 m^2 e^{-\lambda m \xi}}{1 - e^{-\lambda m}}; \; 0 \le m \le m_{max}; \; 0 \le \xi \le 1 \tag{15}$$

Letting $m = m_{max} s$; $\lambda = \beta / m_{max}$; $\bar{u}(\xi) = u(\xi)/m_{max}$, and $\bar{f}(s) = f(s m_{max})$, Equation 15 can be transformed:

$$K_2(\xi, s) = \frac{\beta^2 s^2 e^{-\beta s \xi}}{1 - e^{-\beta s}}; \; 0 \le s \le 1; \; 0 \le \xi \le 1 \tag{15-a}$$

and Equation 2 will be replaced by Equation 16:

$$\bar{u}(\xi) = - \frac{1}{m_{max} C_0} \frac{dC(\xi)}{d\xi} = \int_0^1 K_2(\xi, s)\, \bar{f}(s)\, ds \tag{16}$$

(b-2.) The kernel appearing in the Fujita's Equation for concentration (Equation 1) is

$$K_3(\xi,m) = \frac{\lambda m e^{-\lambda m \xi}}{1-e^{-\lambda m}}; \quad 0 \le m \le m_{max}; \; 0 \le \xi \le 1 \tag{17}$$

Using a previous setting, we will obtain:

$$K_3(\xi,s) = \frac{\beta s e^{-\beta s \xi}}{1-e^{-\beta s}} \tag{17-a}$$

and

$$\bar{u}(\xi) = \frac{C(\xi)}{m_{max} C_0} = \int_0^1 K_3(\xi,s)\, \bar{f}(s)\, ds \tag{18}$$

Two methods of numerical integration have been applied:

(c-1.) The integration was achieved by applying the trapezoidal rule.

(c-2.) The Simpson formula was applied in integration.

Various types of regularizing functions Ω have been used:

(d-1.) $\Omega = \| f^{(1)} \|^2$

and

(d-2.) $\alpha\,\Omega = \alpha(\| f^{(1)} \|^2 + \gamma_1 \| f^{(2)} \|^2)$

To examine weighting of elements of a matrix used in an approximation the variable of the function u was defined in the two different ways:

$$(e-1)\; \xi_1 = \frac{r_b^2 - r^2}{r_b^2 - r_a^2}; \qquad \text{and} \qquad e-2 \cdot \xi_2 = \frac{r^2 - r_a^2}{r_b^2 - r_a^2}$$

SECTION IV

RESULTS OF COMPUTATION

To emphasize the importance of regularization: 1) a mono-modal distribution (Equation 13) was assumed, 2) $\bar{u}(\xi)$ was computed by Equation 19 with the aid of Simpson's formula for integration, and 3) variational calculus (see Equation 5) without Tikhonov's regularizing function was applied so as to obtain a "best fit" computed distribution. The result of this computation is shown by Figure 1. Note that although the results are very erratic the error analysis $\| \bar{u}(\xi) - \tilde{u}(\xi) \|$ was a minimum. The behavior is typical for an IPP.

Upon including a regularizing function Ω (see Equation 7) and applying Euler's equation from variational calculus to the functional $M_1^{\alpha}[f;\bar{u}]$ (see Equation 6) a distribution $\tilde{f}^{\alpha}(s)$ was obtained for each value of the parameter α . The objective of the search is to find the value of α which will produce a minimum error analysis. Using $\inf |M^{\alpha}|$ as the error criterion, Figure 2 shows a typical example of how the appropriate value of α is determined. This tells the experimenter that for the error he has in the experimental values $\bar{u}(\xi)$, this is the best initial approximate distribution. From this starting approximation the experimenter can then apply some algorithm to infer a distribution which will produce a still smaller error analysis. He is now in a position to do this because he has an admissible solution to his originally improperly posed problem.

Using the concentration kernel (Equation 17-a) and the gradient kernel (Equation 15-a) with the mono-modal distribution (Equation 13) and the regularizing function $\Omega^{(1)}(f)$, the results obtained are shown in Figures 3 and 4 respectively. For both cases the integration involved in obtaining $\tilde{u}(\xi)$ was performed by the trapezoidal rule. Since the concentration kernel provided a better solution to the problem, especially for low molecular weights, this kernel was used for all further investigations. It can easily be shown that the gradient kernel (Equation 15) degenerates for very low molecular weights, thus

$$\lim_{m \to 0} \left[\frac{\lambda^2 m^2 e^{-\lambda m \xi}}{1 - e^{-\lambda m}} \right] = 0$$

and the concentration kernel (Equation 17) does not degenerate under identical circumstances:

$$\lim_{m \to 0} \left[\frac{\lambda m e^{-\lambda m \xi}}{1 - e^{-\lambda m}} \right] = 1$$

Therefore, computationally the concentration kernel is preferred when considering low molecular weights. For Figures 3 and 4 the error criterion minimized was $\| \tilde{u}(\xi) - u^*(\xi) \|$. Here $u^*(\xi)$ was computed by using the calculated function $\tilde{f}^{\alpha}(s)$. To demonstrate the numerical agreement between $\tilde{u}(\xi)$ and $u^*(\xi)$ Figure 5 presents the curves for $\tilde{u}(\xi)$ and $[\tilde{u}(\xi) - u^*(\xi)] \times 10^3$ associated with Figure 3. If $\tilde{u}(\xi)$ and $u^*(\xi)$ had been plotted on the same graph, for the ordinate scale used the two curves would have coalesced. The numerical values of $\tilde{u}(\xi)$ and $u^*(\xi)$ agreed to three significant figures.

The computation of a bi-modal distribution proved to be more complex. At first Equation 18 was applied using the trapezoidal rule for integration.

The resulting $\tilde{f}^{\alpha}(s)$ obtained by minimizing $\| \tilde{u}(\xi)-u^*(\xi) \|$ was the three-peaked curve shown in Figure 6. Upon using Simpson's formula for integration and varying α so as to minimize $\| \tilde{u}(\xi)-u^*(\xi) \|$ a good "fit" to the initial distribution (Equation 14) was obtained (see Figure 6).

To study the effect of the error analysis on choosing the appropriate value for α, three criteria were applied:

$$(1).\ \inf \left| M^{\alpha}\left[\bar{f}(s), \tilde{u}(\xi)\right] \right|$$

$$(2).\ \inf \left\{ \max \left| \bar{f}(s) - \tilde{f}^{\alpha}(s) \right| \right\}$$

$$(3).\ \| \tilde{u}(\xi) - u^*(\xi) \|$$

The results are shown in Figure 7. In a true experimental situation the error analysis $\inf \left\{ \max \left| \bar{f}(s)-\tilde{f}^{\alpha}(s) \right| \right\}$ would not be available. Choosing between the other two criteria it would qualitatively appear from Figure 7 that $\| \tilde{u}(\xi)-u^*(\xi) \|$ is better than one could expect to derive deductively from Tikhonov's theory.

For all computations mentioned above $\beta = 4.25$. Recall that $\beta = \lambda m_{max}$, where β is proportional to the square of the rotor speed (see Equation 1). If $\lambda = 1.02 \times 10^{-10}\omega^2$, and $\omega^2 = 4.1693 \times 10^5$ sec^{-2} (6,166 RPM), then $\lambda = 4.25 \times 10^{-5}$ $(\text{mol wt})^{-1}$. Assuming $m_{max} = 10^5$, the value of β $(=\lambda m_{max})$ is $\beta = 4.25$. The following values for m_{max} were chosen: 4.706×10^4; 4.706×10^5; 7.059×10^5; and 1.8824×10^6. The corresponding values for β are respectively 2.00, 20.00, 30.00, and 80.00. The results obtained by varying α so as to minimize the error criterion $\| \tilde{u}(\xi)-u^*(\xi) \|$ are shown in Figure 8. No attempt was made to determine the exact optimum value for β.

To express the integral operation (Equations 17-a and 18) of the concentration kernel in matrix form, the matrix is weighted by large numerical values in the upper right-hand corner. Since use of the regularizing functions tends to enhance the diagonal and near-diagonal elements, modification of the concentration kernel so as to have the large numerical values of the matrix near the diagonal should greatly improve the computations. This was easily performed by redefining ξ to be

$$\xi = \frac{r^2 - r_a^2}{r_b^2 - r_a^2}$$

Previously ξ was defined as

$$\xi = \frac{r_b^2 - r^2}{r_b^2 - r_a^2}$$

In using the same bi-modal distribution applied previously and the modified concentration kernel it was found that the computed distribution $\tilde{f}^{\alpha}(s)$ was in poorer agreement with the assumed $\bar{f}(s)$ than when the unmodified concentration kernel was applied (see Figure 9).

SECTION V

CONCLUSIONS

Tikhonov's regularizing functions have proved excellent as a tool to solve the inverse problem associated with the Fredholm Integral Equation of the First Kind which correlates the ultracentrifugal data obtained by sedimentation-diffusion equilibrium and the desired molecular weight distribution (MWD). This technique is especially desirable since a MWD can be obtained from data at only one rotor speed. Computationally this technique has provided excellent results when the MWD is a mono-modal distribution and good results for a bi-modal distribution. However, for a multi-modal distribution (fine structure) an additional algorithm has to be applied.

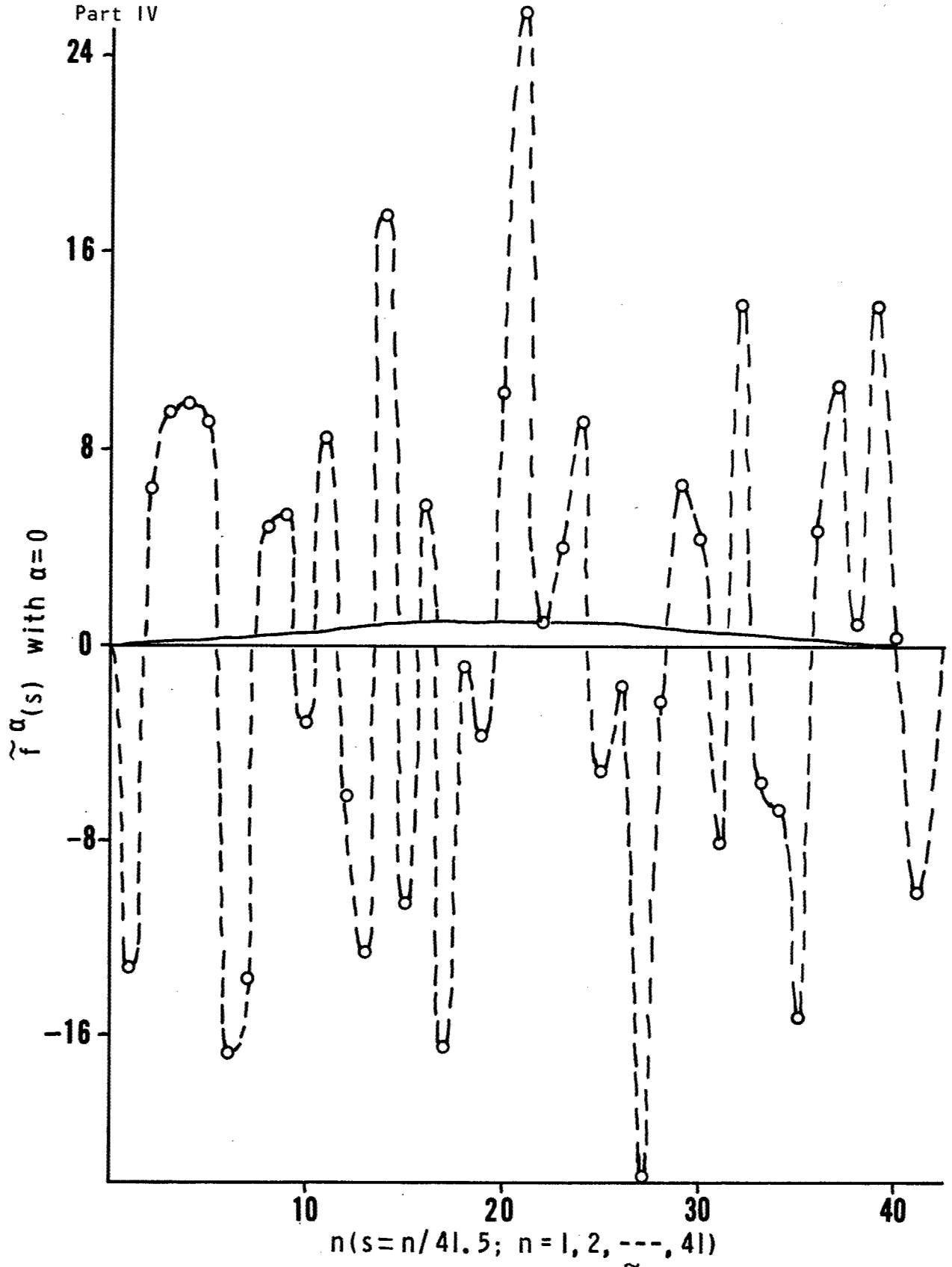

Figure 1. Calculation of the inverse problem, $\tilde{f}(S)$ distribution without regularization. The solid curve is the original distribution $\bar{f}(S)$, the dashed curve is the resulting distribution $\tilde{f}^{\alpha}(S)$.

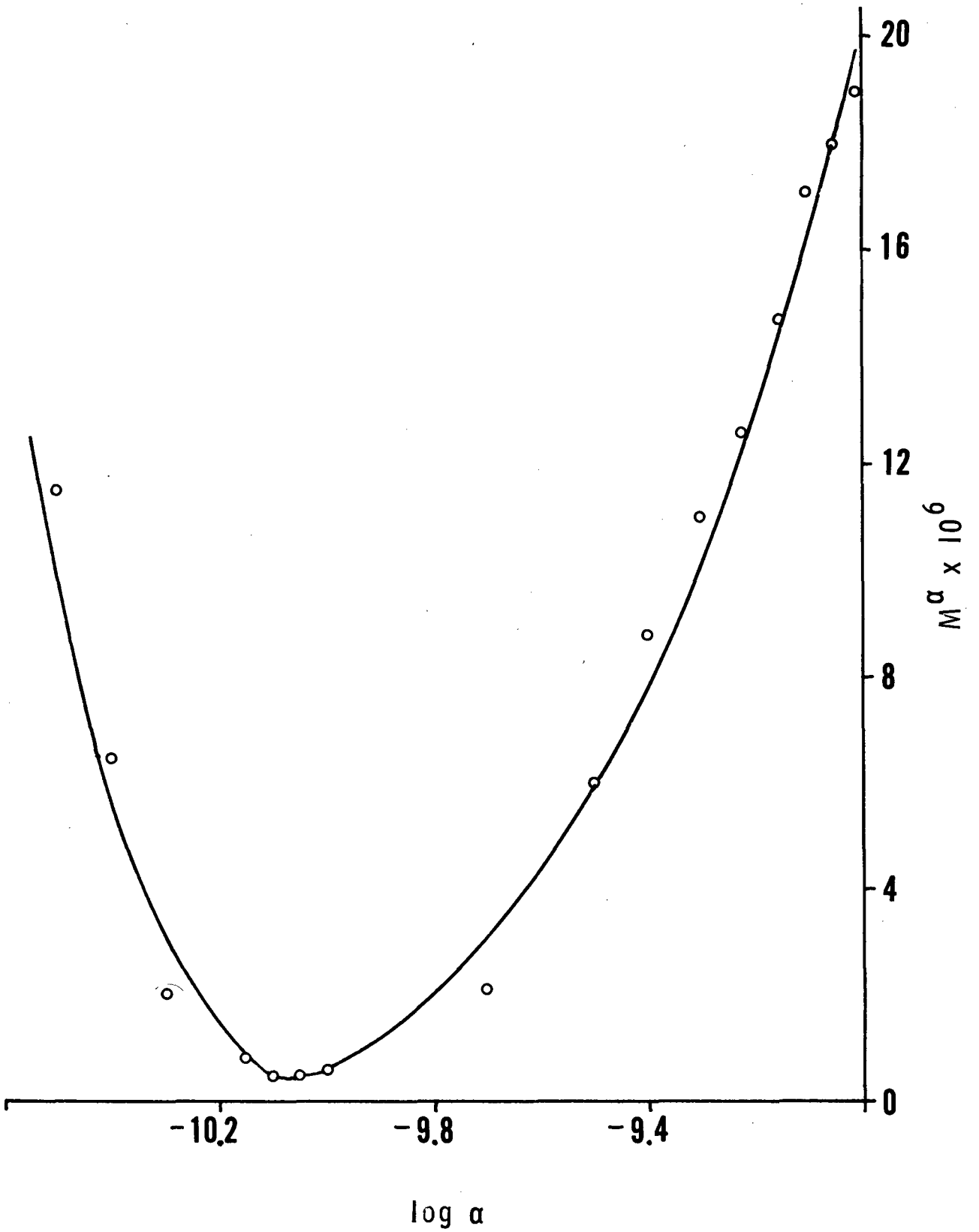

Figure 2. Minimizing the smoothing functional $M^{\alpha}[\bar{f}(s),\tilde{u}(\xi)]$. A plot of log α versus M^{α}.

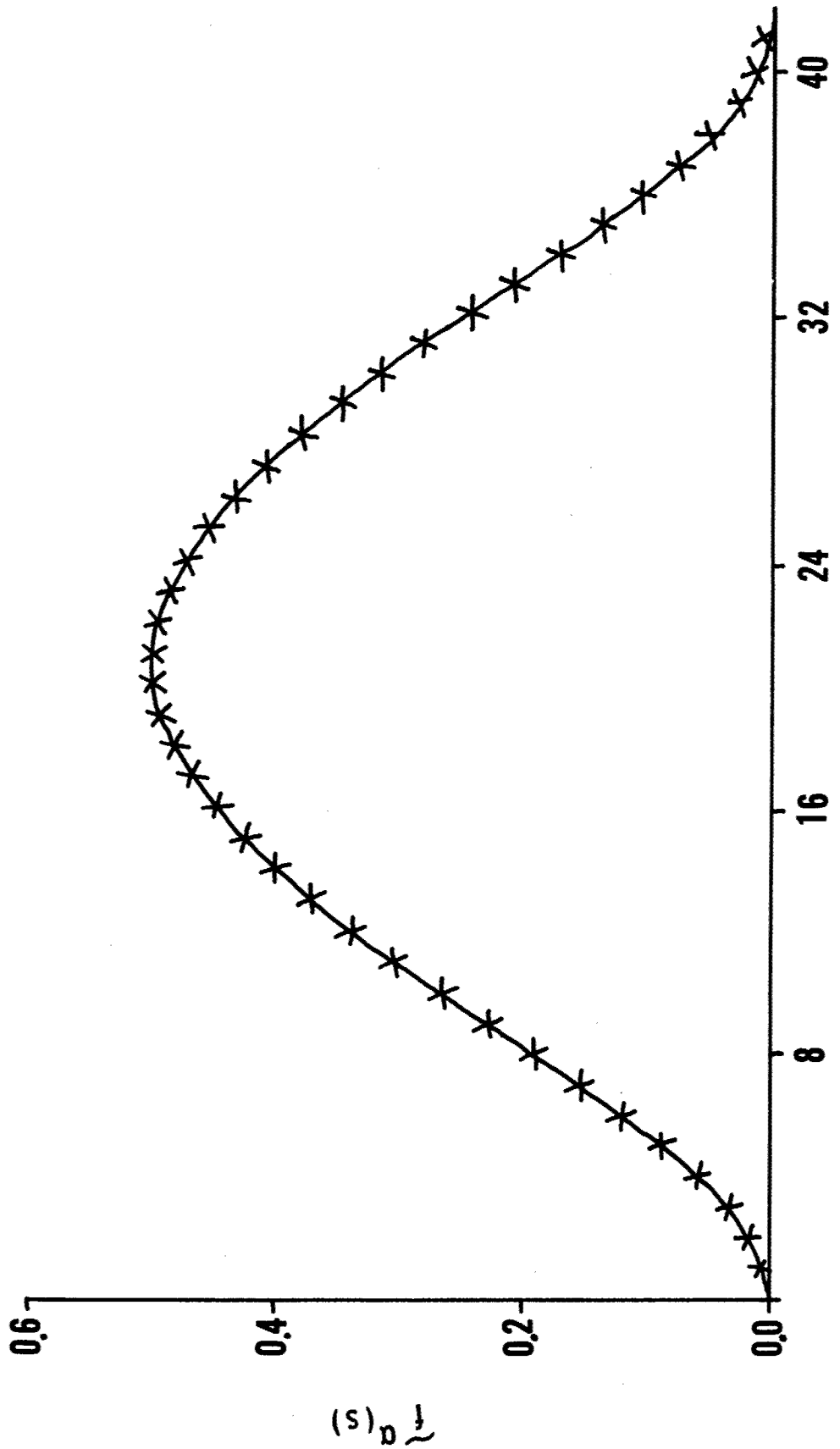

Figure 3. Determination of MWD for a mono-modal distribution by applying Tikhonov's regularizing function and the concentration kernal. The solid curve represents the original $\bar{f}(s)$ and the crosses represent the computed distribution $\tilde{f}^{\alpha}(s)$.

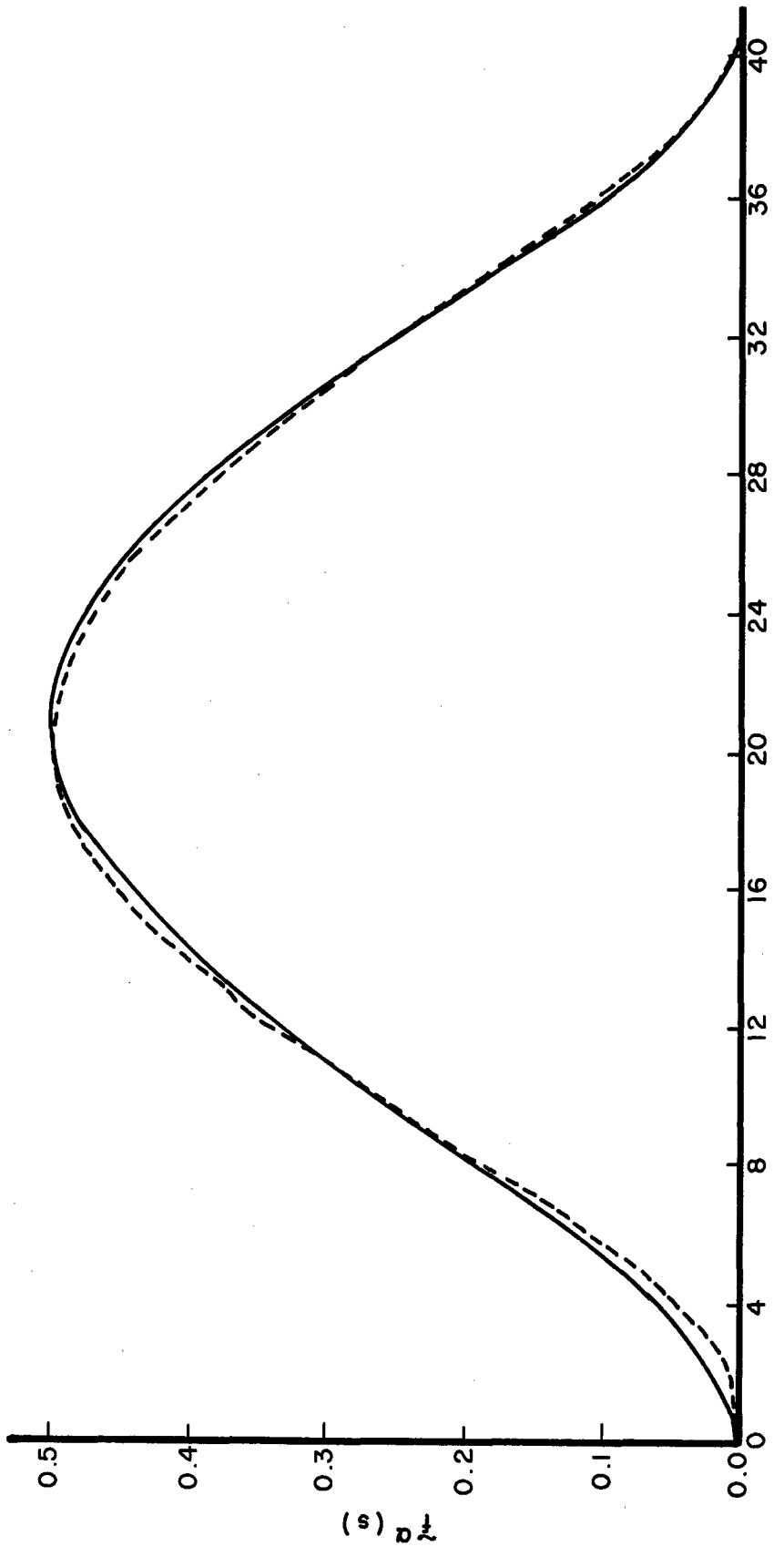

Figure 4. Determination of MWD for a mono-modal distribution by applying Tikhonov's regularizing function and the concentration kernel. The solid gradient curve represents the original $\bar{f}(s)$ and the crosses represent the computed distribution $\tilde{f}^{\alpha}(s)$.

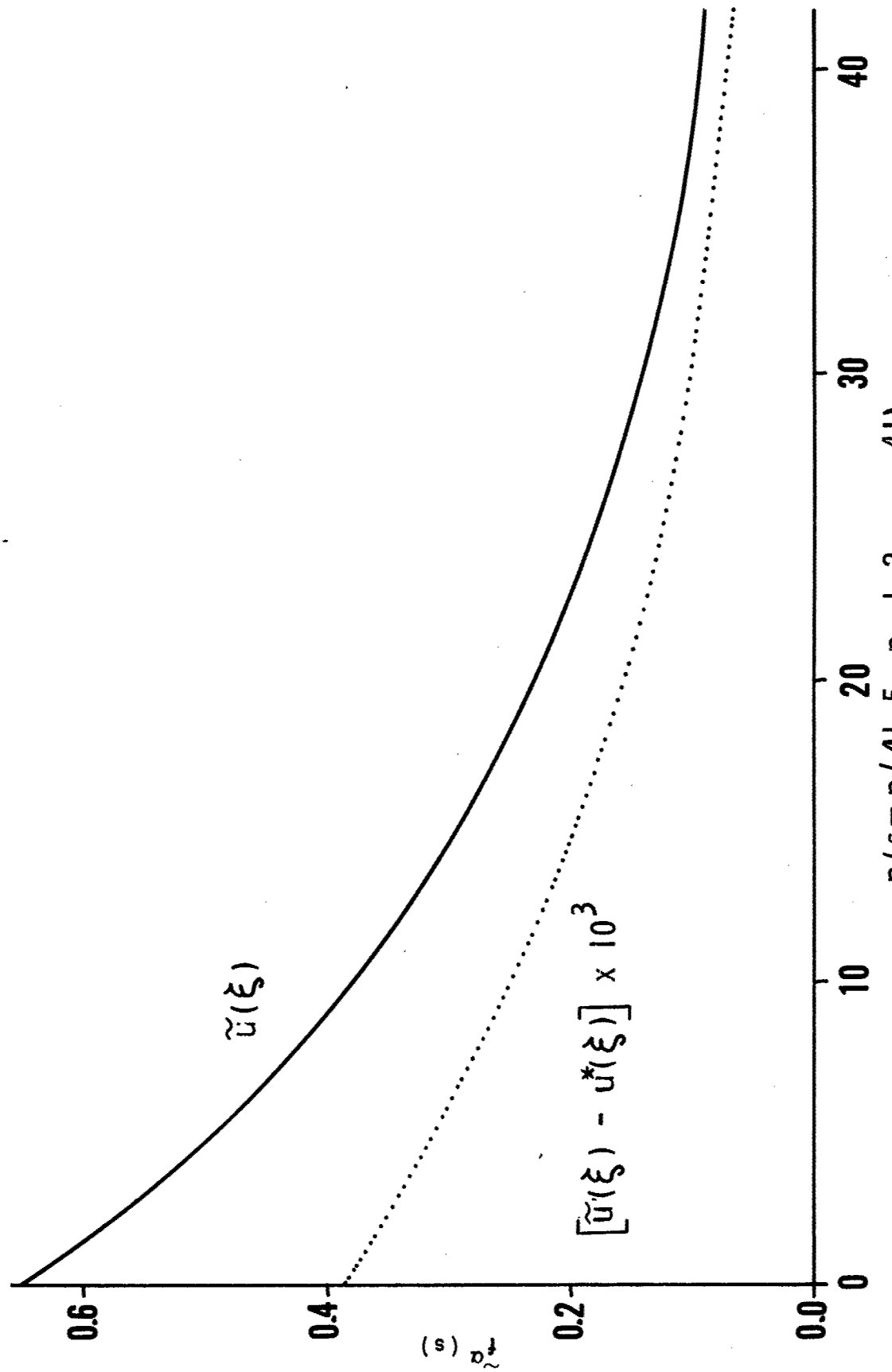

Figure 5. The ultracentrifugal $u(\xi)$ functions computed from the original distribution and the calculated distribution. The solid curve represents the original $\tilde{u}(\xi)$. The dotted line is $[\tilde{u}(\xi)-u^{*}(\xi)] \times 10^{3}$.

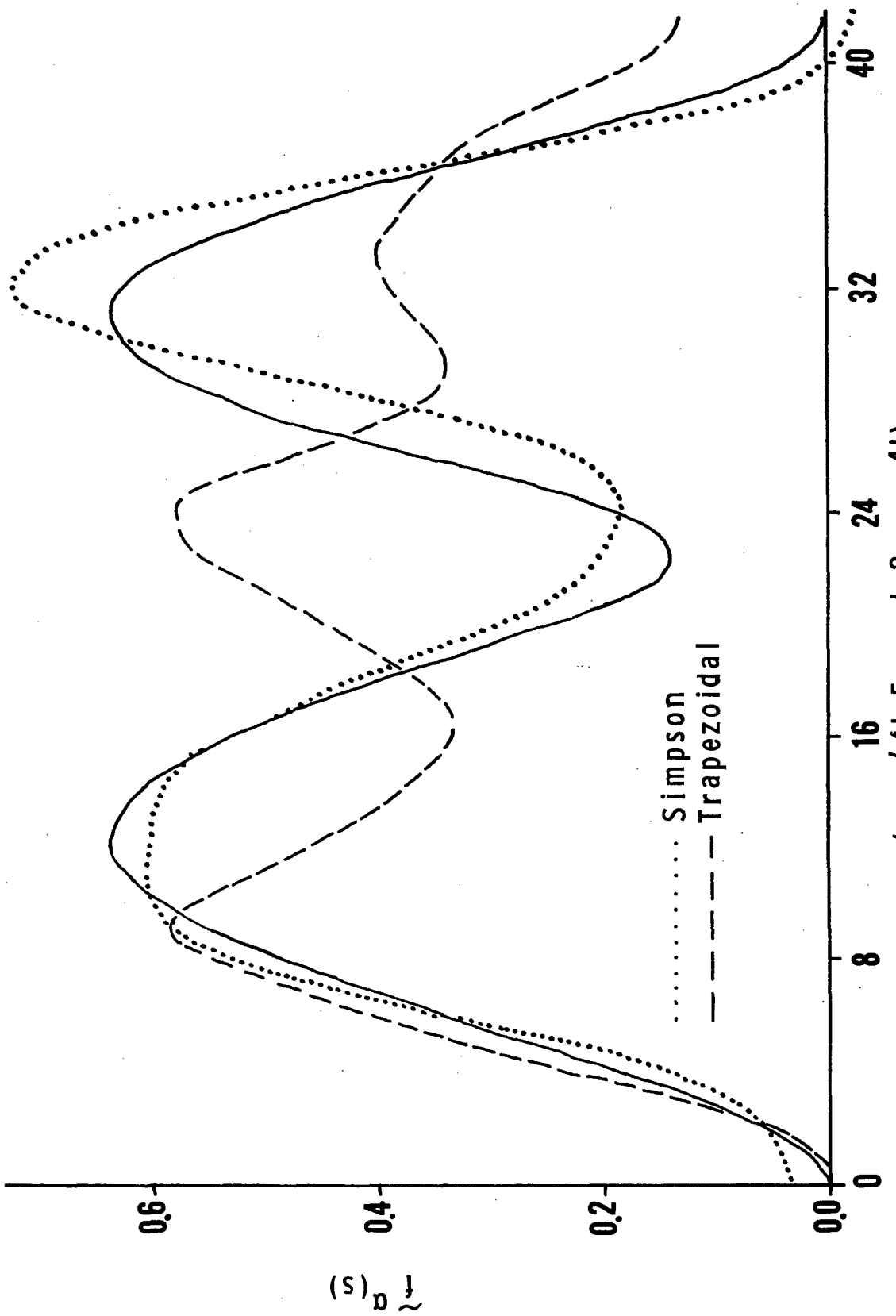

Figure 6. Evaluation of the bi-modal distribution. The solid line represents the original distribution. The dotted line was the resulting distribution using Simpson's formula for integration. The dashed curve resulted from application of trapezoidal integration.

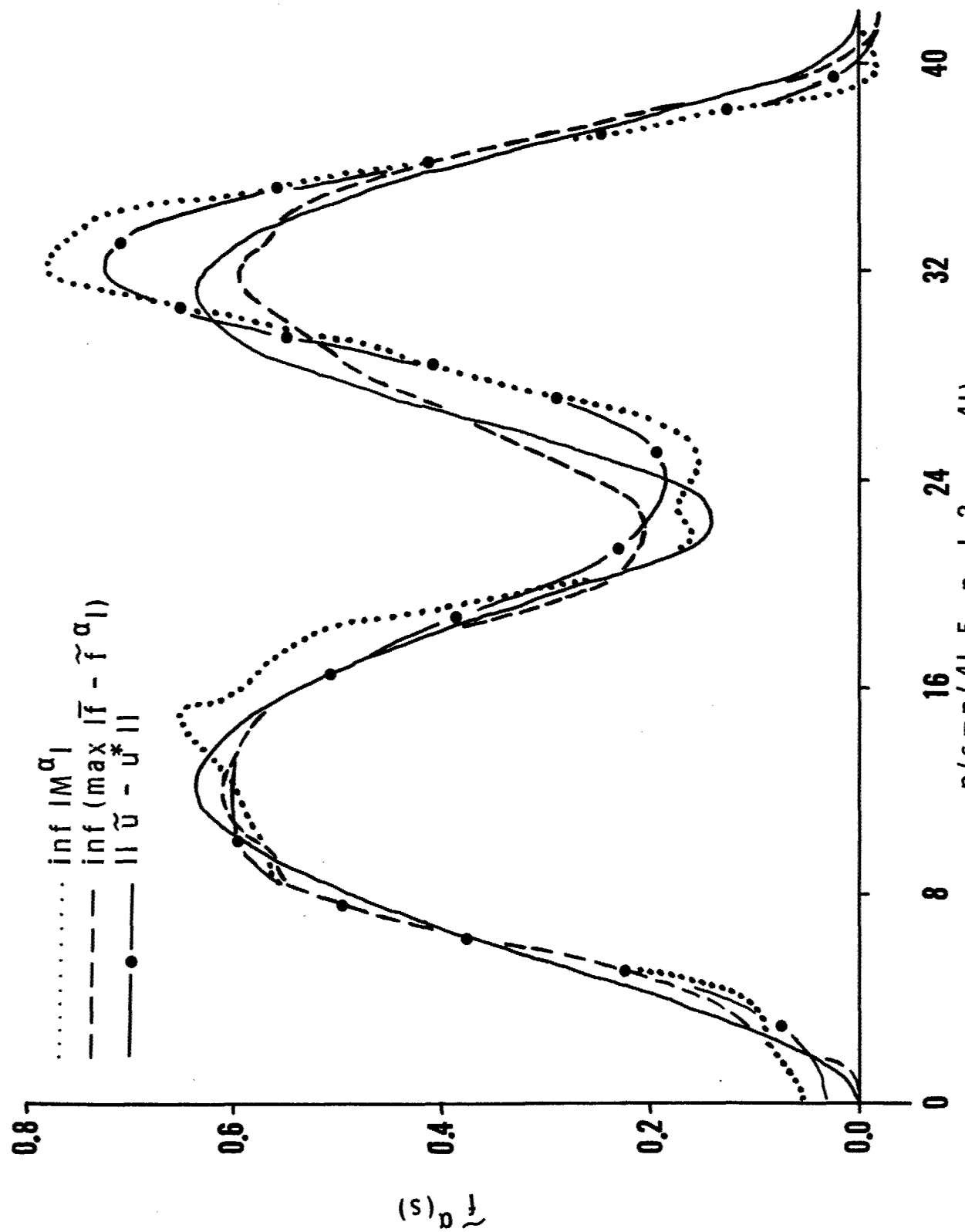

Figure 7. Resulting distributions evaluated according to different error criterion. The solid curve is the original distribution.

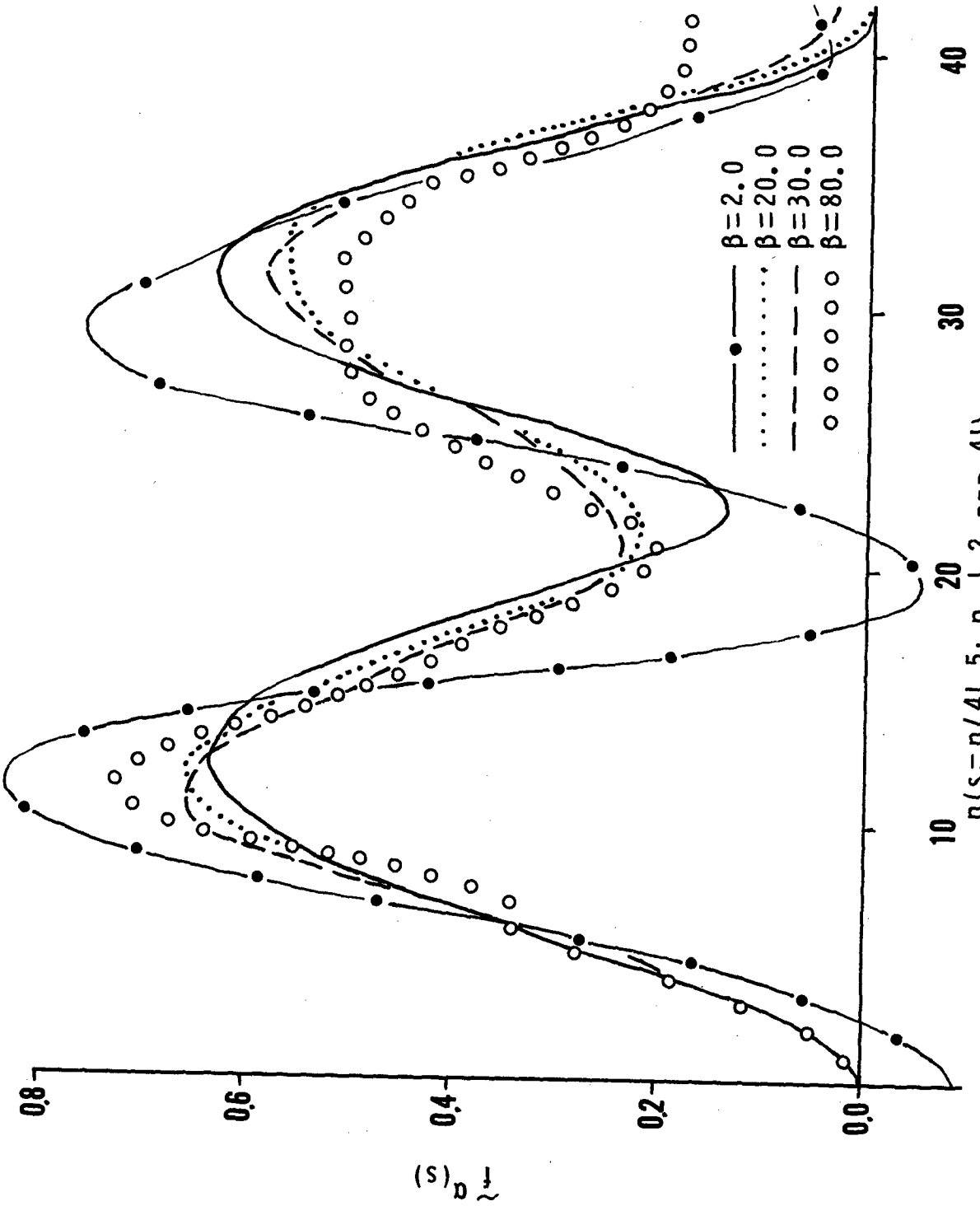

Figure 8. Evaluation of a bi-modal distribution for various values of β ($= \lambda m_{max}$). The original distribution is indicated by the solid curve.

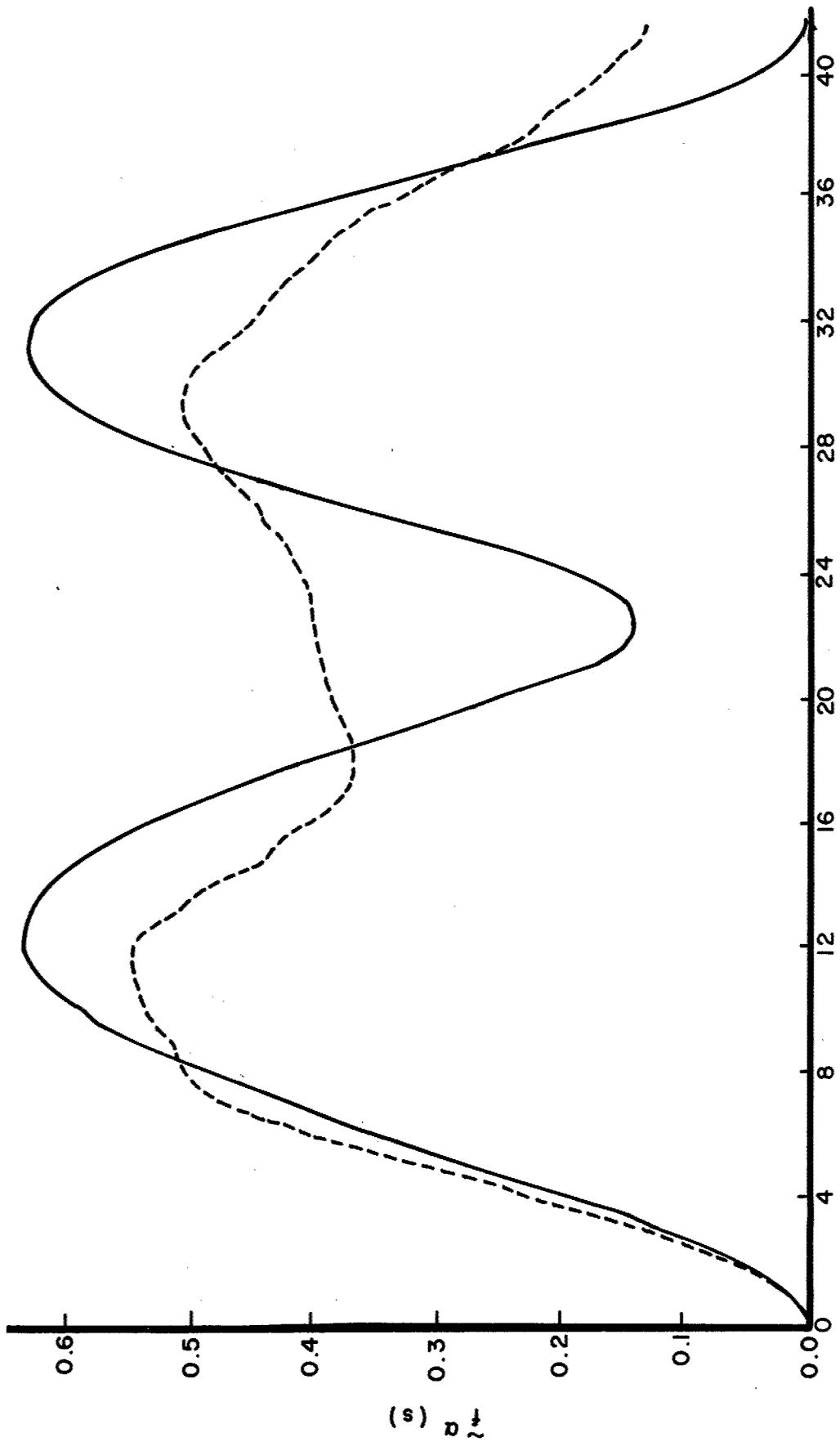

Figure 9. Evaluation of a bi-modal distribution using a modified concentration kernal. Here $\xi = (r^2-r_a^2)/(r_b^2-r_a^2)$. The solid curve represents the original distribution.

APPENDIX

COMPUTER PROGRAM LISTING

```
$IBJOB          MAP
$IBFTC REGLAR
      COMMON/ZYT/X1,X2,U,A
C           DIMENSION FOR COMMON
      DIMENSION U(60),A(60,60)
C
      DIMENSION XK(60,60),S(60),X(60),Z(60),BK(60,60),B(60),ZP(60),ALPHA
     1(10),UP(60)
C
C
C        CODED NOVEMBER 1969 BY D.R. WIFF  AND M.T. GEHATIA
C        TO CHANGE INITIAL DISTRIBUTION, THE SECTION SO LABELED
C        MUST BE MODIFIED.
C        THIS PROGRAM IS CODED TO RUN ON A 41 POINT MESH.  IF ANOTHER
C        MESH (EVEN A VARIABLE) IS DESIRED THE APPROPRIATE CHANGES
C        MUST BE MADE.   PROGRAM SEARCHES FOR ALPHA WHICH MINUMIZES THE
C        GIVEN ERROR CRITERION (SO INDICATED).   IT BEGINS WITH
C        1.0E-ALPHA1 AND SEARCHES TO 1.0E-ALPHA2 . THEN THE
C        MINIMUM REGION IS AGAIN SUBDIVIDED.
C
C
      READ(5,200)
      WRITE(6,1000)
      WRITE(6,200)
      WRITE(6,1001)
      DLX = 41.5
      DLS = 41.5
      XC1 = 0.78125000E 02
      XC2 = 0.16200000E 03
      AXX = 1.
C
C        EVALUATE INITIAL DISTRIBUTION
      DO 1 I = 1,41
      A1 = I
      S(I) = A1/DLS
    1 X(I) = A1/DLX
      DO 2 I = 1,41
      A1 = S(I)**2
      A2 = (S(I)-1.)**2
    2 Z(I) = 8.*A1*A2
C
C        XSIG = LAMBDA*MAXIMUM MOLECULAR WEIGHT
      READ(5,103) XSIG
      DO 4 I = 1,41
      COEF = 0.
      DO 3 J = 1,41
      A1 = XSIG*S(J)
      A2 = A1
      A3 = EXP(-A1*X(I))
      A4 = EXP(-A1)
      A5 = 1. - A4
      A6 = A2*A3/A5
      XK(I,J) = A6
      IF(J.EQ.1.OR.J.EQ.41) GO TO 41
      IF(J.EQ.2.OR.J.EQ.40) GO TO 42
      KNUM = J/2
      JNUM = (J+1)/2
      IF(JNUM.EQ.KNUM) GO TO 42
      SIG = 2.
      GO TO 43
   41 SIG = 1.
      GO TO 43
   42 SIG = 4.
```

```
   43 CCEF = CCEF + SIG*XK(I,J)*Z(J)/(3.*DLS)
    3 CONTINUE
C        CALCULATION OF U(ZI) BY SIMPSON'S FORMULA
    4 U(I) = CCEF
      CALL REG2(XK,B,BK,DLX)
C
C
C        PROGRAM READS ALPHA(NLAST) AS DATA FROM NFIRST THROUGH
C        NCODE.   THEN PROGRAM CONTINUES FROM NCODE+1  THROUGH
C        NUPP SEARCHING FOR MINIMUM FOR EACH DERIVATIVE RETAINING
C        PREVIOUS VALUES.   IF NCODE = 0 , SEARCH BEGINS WITH NFIRST.
C        IF NFLAG.GT.0  PROGRAM READS ONE VALUE OF ALPHA AND
C        COMPUTES FOR ONLY THIS ONE VALUE
C
C
      READ(5,101) NCODE,NFIRST,NUPP,NFLAG
      DO 30 NLAST = NFIRST,NUPP
      IF(NFLAG.GT.0) GO TO 40
      IF(NLAST.LE.NCODE) GO TO 31
      READ(5,100) LPHA1,LPHA2
      LXP = IABS(LPHA2 - LPHA1) + 1
      NUM = 0
      DO 20 II = 1,LXP
      IXP = LPHA1 + II - 1
      DO 21 KL = 1,9
      ALPHA(NLAST) = FLOAT(KL)*10.**IXP
C        OBTAIN MODIFIED MATRIX
      CALL REG3(NFIRST,NLAST,ALPHA,BK,B,DLX,DLS)
C        OBTAIN INVERSE SOLUTION
      CALL EQS(41)
C        EVALUATE ERROR
      CALL REG4(Z,ZP,XK,DLS,UP,UAVG,NFIRST,NLAST,ALPHA,DLX)
      IF(KL.EQ.1.AND.II.EQ.1) GO TO 22
      IF(UAVG.GT.AVG1) GO TO 28
      AVG1 = UAVG
C        STORE MINIMUM ERROR AND CORRESPONDING ALPHA
      XM = ALPHA(NLAST)
      NX = IXP
      NUM = 0
      GO TO 21
   22 AVG1 = UAVG
C        STORE FIRST ALPHA USED AND ASSOCIATED ERROR
      XM = ALPHA(NLAST)
      NX = IXP
      GO TO 21
   28 CONTINUE
   21 CONTINUE
   20 CONTINUE
   23 CONTINUE
      XMM = XM - 10.**NX
      NUM = 0
      DO 25 I = 1,20
      ALPHA(NLAST) = XMM + FLOAT(I-1)*10.**(NX-1)
C        OBTAIN MODIFIED MATRIX
      CALL REG3(NFIRST,NLAST,ALPHA,BK,B,DLX,DLS)
C        OBTAIN INVERSE SOLUTION
      CALL EQS(41)
C        EVALUATE ERROR
      CALL REG4(Z,ZP,XK,DLS,UP,UAVG,NFIRST,NLAST,ALPHA,DLX)
      IF(I.EQ.1) GO TO 26
      IF(UAVG.GT.AVG1) GO TO 29
      AVG1 = UAVG
```

```
C         STORE MINIMUM ERROR AND CORRESPONDING ALPHA
        YM = ALPHA(NLAST)
        GO TO 25
   26 AVG1 = UAVG
C         STORE FIRST ALPHA USED AND ASSOCIATED ERROR
        YM = ALPHA(NLAST)
        GO TO 25
   29 NUM = NUM + 1
        IF(NUM.EQ.4) GO TO 27
   25 CONTINUE
C         START EVALUATION FOR ALPHA WITH MINIMUM ERROR
   27 ALPHA(NLAST) = YM
        GO TO 51
   40 READ(5,102) ALPHA(NLAST)
C         IF COMPUTATION PROCEEDS FOR ONLY ONE ALPHA BEGIN HERE
   51 CONTINUE
C         OBTAIN MODIFIED MATRIX
        CALL REG3(NFIRST,NLAST,ALPHA,EK,B,DLX,DLS)
C         OBTAIN INVERSE SOLUTION
C         EVALUATE ERROR
        CALL EQS(41)
        CALL REG4(Z,ZP,XK,DLS,UP,UAVG,NFIRST,NLAST,ALPHA,DLX)
        DO 24 I = 1,41
C         Z(I) = ORIGINAL DISTRIBUTION
C         ZP(I) = BACK SOLUTION
C         U(I) = CORRESPONDS TO INPUT DATA, COMPUTED USING Z(I)
C         UP(I) = BACK SOLUTION COMPUTATION
C         S(I) = VARIABLE FOR Z(I), CORRESPONDING TO
C         MOLECULAR WEIGHT
        WRITE(6,2001) I,ZP(I),I,Z(I),I,UP(I),I,U(I),I,S(I)
   24 CONTINUE
        WRITE(6,2000) (I,ALPHA(I),I = NFIRST,NLAST)
        WRITE(6,2002) UAVG
        WRITE(6,104) XSIG
  104 FORMAT(1H ,7HXSIG = ,1PE10.3)
        WRITE(6,1000)
        GO TO 30
   31 READ(5,102) ALPHA(NLAST)
   30 CONTINUE
        WRITE(6,1001)
        WRITE(6,7000)
        STOP
  100 FORMAT(2I3)
  101 FORMAT(4I2)
  102 FORMAT(1PE9.2)
  103 FORMAT(E10.3)
  200 FORMAT(72H
     1                    )
 1000 FORMAT(1H1/1HA)
 1001 FORMAT(1HA/1HA)
 2000 FORMAT(1H ,6HALPHA(,I2,4H) = ,1PE9.2)
 2001 FORMAT(1H ,7HZ-CALC(,I2,4H) = ,E12.5,2X,7HZ-TRUE(,I2,4H) = ,E12.5,
     12X,7HCALC U(,I2,4H) = ,E12.5,2X,2HU(,I2,4H) = ,E12.5,2X,2HS(,I2,4H
     2) = ,E12.5)
 2002 FORMAT(1H ,11HM(ALPHA) = ,E12.5)
 7000 FORMAT(1H ,20X,6(5X,10HEND OF RUN)/1H1)
        END
$IBFTC RRR4     DECK
        SUBROUTINE REG4(Z,ZP,XK,DLS,UP,UAVG,NFIRST,NLAST,ALPHA,DLX)
C         THIS SUBROUTINE PROCESSES THE COMPUTED ZP(I)
C         CALCULATES UP(I) AND THE ERROR
C         ERROR CRITERION
```

```
      COMMON/ZYT/X1,X2,U,A
C     DIMENSIONS FOR COMMON
      DIMENSION U(60),A(60,60)
      DIMENSION ZP(60),XK(60,60),UP(60)
      DIMENSION Z(60),ALPHA(10)
      DO 14 I = 1,41
      ZP(I) = A(I,42)
   14 CONTINUE
      UAVG = 0.
      DO 40 I = 1,41
      COEF = 0.
      COEF1 = 0.
      DO 41 J = 1,41
      IF(J.EQ.1.OR.J.EQ.41) GO TO 42
      IF(J.EQ.2.OR.J.EQ.40) GO TO 43
      KNUM = J/2
      JNUM = (J+1)/2
      IF(JNUM.EQ.KNUM) GO TO 43
      SIG = 2.
      GO TO 44
   42 SIG = 1.
      GO TO 44
   43 SIG = 4.
   44 COEF = COEF + SIG*XK(I,J)*ZP(J)/(3.*DLS)
      IF(I.LT.41) GO TO 41
      IF(J.EQ.1) GO TO 1
      KL = J-1
      GO TO 2
    1 KL = 1
    2 IF(J.EQ.41) GO TO 3
      KJ = J+1
      GO TO 4
    3 KJ = 41
    4 COEF1 = COEF1 + SIG*((ZP(KJ)-ZP(KL))**2)*DLS/3.
   41 CONTINUE
      UP(I) = COEF
      IF(I.EQ.1.OR.I.EQ.41) GO TO 30
      IF(I.EQ.2.OR.I.EQ.40) GO TO 31
      KNUM = I/2
      JNUM = (I+1)/2
      IF(JNUM.EQ.KNUM) GO TO 31
      SIG = 2.
      GO TO 33
   30 SIG = 1.
      GO TO 33
   31 SIG = 4.
   33 UAVG = UAVG + SIG*((UP(I)-U(I))**2)/(3.*DLX)
   40 CONTINUE
      UAVG = UAVG + ALPHA(1)*COEF1
      RETURN
      END
$IBFTC RRR2    DECK
      SUBROUTINE REG2(XK,B,BK,DLX)
C        THIS SUBROUTINE INTEGRATES XK(I,J)*XK(I,J) OVER ZI-VALUES
C        TO OBTAIN NEW MATRIX  BK(I,J)
      COMMON/ZYT/X1,X2,U,A
C     DIMENSIONS FOR COMMON
      DIMENSION U(60),A(60,60)
      DIMENSION XK(60,60),BK(60,60),B(60)
C
C          SIMPSON RULE
C
```

```
      DO 5 I = 1,41
      DO 5 J = 1,41
      CCEF1 = 0.
      CCEF = 0.
      DO 20 K = 1,41
      IF(K.EQ.1.OR.K.EQ.41) GO TO 21
      IF(K.EQ.2.OR.K.EQ.40) GO TO 23
      KNUM = K/2
      JNUM = (K+1)/2
      IF(JNUM.EQ.KNUM) GO TO 23
   22 SIG = 2.
      GO TO 24
   21 SIG = 1.
      GO TO 24
   23 SIG = 4.
   24 A1 = SIG*XK(K,I)*XK(K,J)/(3.*DLX)
      IF(I.GT.1) GO TO 7
      A2 = SIG*XK(K,J)*U(K)/(3.*DLX)
      CCEF1 = CCEF1 + A2
    7 CCEF = CCEF + A1
   20 CONTINUE
      IF(I.GT.1) GO TO 8
      B(J) = CCEF1
    8 BK(I,J) = CCEF
    5 CONTINUE
      RETURN
      END
$IBFTC RRR3     DECK
      SUBROUTINE REG3(NFIRST,NLAST,ALPHA,BK,B,DLX,DLS)
C        THIS SUBROUTINE INTRODUCES THE REGULARIZATION TERMS
C        IN THE MATRIX BK(I,J).    THE FINAL REGULARIZED MATRIX
C        IS A(I,J)
      COMMON/ZYT/X1,X2,U,A
C     DIMENSIONS FOR COMMON
      DIMENSION U(60),A(60,60)
      DIMENSION BK(60,60),B(60),ALPHA(10)
      DO 9 I = 1,41
      DO 9 J = 1,41
      A(I,J) = BK(I,J)/DLS
    9 CONTINUE
      DO 63 N = NFIRST,NLAST
      DO 60 I = 1,41
      NUM = 2*N + 1
      DO 60 K = 1,NUM
      A2 = CALC(N,K,DLS)
      A1 = ALPHA(N)*A2
      LABEL = I + N - K + 1
   64 CONTINUE
      IF(LABEL.LE.0) GO TO 61
      IF(LABEL.GT.41) GO TO 62
      A(I,LABEL) = A(I,LABEL) + A1
      GO TO 60
   61 LABEL = IABS(LABEL) + 1
      GO TO 64
   62 LABEL = 82 - LABEL + 1
      GO TO 64
   60 CONTINUE
   63 CONTINUE
      DO 50 I = 1,41
   50 A(I,42) = B(I)
      RETURN
      END
```

```
$*
$IBFTC EEXX    DECK
      SUBROUTINE EQS(N)
C        STANDARD SUBROUTINE TO OBTAIN THE INVERSION SOLUTION.   THE
C        SOLUTION IS IN COLUMN J+1  IN A(I,J) MATRIX.
      COMMON/ZYT/X1,X2,U,A
C          DIMENSION FOR COMMON
      DIMENSION U(60),A(60,60)
      DIMENSION B(60)
53    N1=N+1
    5 M=N1
   13 DO 23 K=1,N
      K1=K+1
      IF(A(K,K))20,14,20
   14 IF(K-N)15,19,15
   15 DO 18 L=K1,N
      IF(A(L,K))16,18,16
   16 DO 17 J=K,M
      B(J)=A(K,J)
      A(K,J)=A(L,J)
   17 A(L,J)=-B(J)
      GO TO 20
   18 CONTINUE
   19 WRITE(6,101)
      GO TO 30
   20 DO 23 I=1,N
      IF(I-K)21,23,21
   21 C=A(I,K)/A(K,K)
      DO 22 J=1,M
   22 A(I,J)=A(I,J) - C*A(K,J)
   23 CONTINUE
   46 DO 29 J=N1,M
      DO 25 I=1,N
  25  A(I,J)=A(I,J)/A(I,I)
29    CONTINUE
  101 FORMAT(19H MATRIX IS SINGULAR)
   30 RETURN
      END
$IBFTC CALF    DECK
      FUNCTION CALC(N,K,DLS)
C        THIS FUNCTION SUBROUTINE EVALUATES THE
C        COEFFICIENTS (BINOMIAL), ETC.
C        CALLED BY REG3
C
      L = 2*N
      M = L - K + 1
      J = K - 1
      IF(K.EQ.1.OR.K.EQ.L+1) GO TO 10
      I1 = 1
      I2 = 1
      I3 = 1
      DO 1 I = 1,L
    1 I1 = I1*I
      DO 2 I = 1,M
    2 I2 = I2*I
      DO 3 I = 1,J
    3 I3 = I3*I
      I4 = I1/(I2*I3)
      I5 = (-1)**(N+K+1)
      X = FLOAT(I4*I5)
      CALC = X*DLS**L
      GO TO 99
```

```
      10 IA = (-1)**N
         A1 = FLOAT(IA)
         CALC = A1*CLS**L
      99 RETURN
         END
$DATA
  CONCENTRATION KERNEL,41PTS.,8*(V*(V-1))**2
 0.425E 01
 0 1 1 1
 1.00E-07
$EOF
```

REFERENCES

1. H. Rinde, thesis, University of Uppsala, Sweden, 1928 (unpublished).

2. H. Fujita, Mathematical Theory of Sedimentation Analysis, Academic Press Inc., New York 1962.

3. G. V. Shulz, Z. Physik Chem. (Leipzig) Vol. B43, 25 (1939).

4. E. O. Kramer in The Ultracentrifuge, T. Svedberg and K. O. Pedersen, Oxford University Press, p. 350, New York (1940).

5. M. Wales, thesis, University of Wisconsin, 1947 (unpublished).

6. M. Wales, J. Phys. Colloid Chem., Vol. 52, 235 (1948).

7. M. Wales, J. W. Williams, J. O. Thompson, and R. H. Ewart, J. Phys. Chem., Vol. 52, 983 (1948).

8. H. Wesslan, Macromol. Chem., Vol. 20, 111 (1956).

9. D. G. Gardner, J. C. Gardner, G. Laush, and W. W. Meinke, J. Chem. Phys., Vol. 31, 978 (1959).

10. T. H. Donnelly, J. Phys. Chem., Vol. 64, 1830 (1960).

11. J. E. Blair, J. Polymer Sci., Vol. 68, 253 (1965).

12. L. O. Sundelöf, Arkiv Kemi, Vol. 25, 1 (1965).

13. T. H. Donnelly, J. Phys. Chem., Vol. 70, 1862 (1966).

14. S. W. Prowencher, J. Chem. Phys., Vol. 46, 3229 (1967).

15. L. O. Sundelöf, Arkiv Kemi, Vol. 29, 279 (1967).

16. Th. G. Scholte, J. Polymer Sci., Part A-2, Vol. 6, 91 (1968).

17. Th. G. Scholte, J. Polymer Sci., Part A-2, Vol. 6, 111 (1968).

18. M. Gehatia, AFML-TR-67-121, Part 1.

19. M. Gehatia, and D. R. Wiff, AFML-TR-67-121, Part 2.

20. R. R. Jurick, D. R. Wiff, and M. Gehatia, AFML-TR-67-121, Part 3.

21. D. A. Lee, J. Polymer Sci., (1970).

22. J. S. Hadamard, Lectures on Cauchy Problem, Dover Publication, New York, p. 4, (1952).

REFERENCES (CONTD)

23. C. Pucci, Ann. Sci. Pisa, Vol. 3, 7 (1953).

24. C. Pucci, Rend. Accad. Naz. Lincei, Vol. 8, No. 18, 473 (1955).

25. C. Pucci, Ann. mat. pura et appl., Vol. 46, 131 (1958).

26. C. Pucci, Ann. mat. pura et appl., Vol. 48, 131 (1959).

27. C. Pucci, Ann. mat. pura et appl., Vol. 49, 131 (1959).

28. C. Pucci, Symposium Numeric Treatment Partial Diff. Equations with Real Characteristics, Rome, pp. 140-144, (1959).

29. F. John, Ann. mat. pura et appl., (4), Vol. 40, 129 (1955).

30. F. John, Comm. Pure Appl. Math., Vol. 8, 591 (1955).

31. F. John, Differential Equations with Approximate and Improper Data, Lectures, New York (1955).

32. M. M. Lavrentiev, Dokl. Akad. Nauk SSSR, Vol. 92, (1952), (Russ).

33. M. M. Lavrentiev, Math. Sbor., Vol. 34, 76 (1954), (Russ).

34. M. M. Lavrentiev, Dokl. Akad. Nauk SSSR, Vol. 102, 205 (1955), (Russ).

35. M. M. Lavrentiev, ISvest. Akad. Nauk SSR, Ser. Math., Vol. 20, (1956), (Russ).

36. M. M. Lavrentiev, Proceeding of the Third All Union Mathem. Congress, Vol. 2, (1956), (Russ).

37. M. M. Lavrentiev, Dokl. Akad. Nauk SSSR, Vol. 110, (1956), (Russ).

38. M. M. Lavrentiev, Dokl. Akad. Nauk SSR, Vol. 106, 389 (1956), (Russ).

39. M. M. Lavrentiev, Dokl. Akad. Nauk SSSR, Vol. 112, 195 (1957), (Russ).

40. M. M. Lavrentiev, Uniqueness and Stability of Analytic Functions Helsinki Suomalainan Tiedekademia (1958).

41. M. M. Lavrentiev, Doklady Akad. Nauk SSSR, Vol. 127, (1959), (Russ).

REFERENCES (CONTD)

42. M. M. Lavrentiev, Some Improperly Posed Problems of Math. Physics, Springer Verlag, New York Inc., (1967), (English).

43. M. M. Lavrentiev, Siberian Math. Z., Vol. 4, 4 (1963), (Russ).

44. A. N. Tikhonov, Dokl. Akad. Nauk SSSR, Vol. 39, No. 5, 195 (1943), (Russ).

45. A. N. Tikhonov, Dokl. Akad. Nauk SSSR, Vol. 151, No. 3, 501 (1963), (Russ).

46. A. N. Tikhonov, Dokl. Akad. Nauk SSSR, Vol. 153, No. 1, 49 (1963), (Russ).

47. A. N. Tikhonov, Dokl. Akad. Nauk SSSR, Vol. 156, No. 2, 268 (1964), (Russ).

48. A. N. Tikhonov, Dokl. Akad. Nauk SSSR, Vol. 156, No. 6, (1964), (Russ).

49. A. N. Tikhonov, Dokl. Akad. Nauk SSSR, Vol. 161, No. 5, (1965), (Russ).

50. A. N. Tikhonov, Dokl. Akad. Nauk SSSR, Vol. 162, No. 4, 763 (1965), (Russ).

51. A. N. Tikhonov, Dokl. Akad. Nauk SSSR, Vol. 163, No. 3, 591 (1965), (Russ).

52. A. N. Tikhonov, Dokl. Akad. Nauk SSSR, Vol. 164, No. 3, 507 (1965), (Russ).

53. A. N. Tikhonov, Z. Vycisl. Math. i Math. Fiz., Vol. 5, No. 4, 718 (1965), (Russ).

54. A. N. Tikhonov, Z. Vycisl. Math. i Math. Fiz., Vol. 6, No. 1, 81 (1966), (Russ).

55. A. N. Tikhonov, Computational Methods and Programming Collective Works of Computational Center of Moscow University., Vol. VIII, Moscow University Press (1967), (Russ).

56. A. N. Tikhonov, and A. A. Samarskii, Z. Vycisl. Mat. i Mat. Fiz., Vol. 1, 5 (1961), (Russ).

57. A. N. Tikhonov, and B. V. Glasko, Z. Vycisl. Math. i Mat. Fiz., Vol. 4, No. 3, 564 (1964), (Russ).

REFERENCES (CONTD)

58. A. N. Tikhonov, and B. V. Glasko, Z. Vycisl. Math. i Math. Fiz., Vol. 5, No. 3, 463 (1965), (Russ).

59. A. N. Tikhonov, and V. Ya. Arsenic, L. A. Vladinirov, G. G. Droshenko, and L. A. Lumor, IZV Akad. Nauk SSSR Ser. Fiz., Vol. 24, No. 5, 815 (1965), (Russ).

60. A. N. Tikhonov, and V. Ya. Galkin, Z. Vycisl. Mat. i Mat. Fiz., Vol. 7, No. 2, (1967), (Russ).

61. A. N. Tikhonov, V. Ya. Galkin, and P. N. Zapkin, Z. Vycisl. Mat. i Mat. Fiz., Vol. 7, No. 2 (1967), (Russ).

62. V. K. Ivanov, IZV. Dokl. Akad. Nauk SSSR, Vol. 20, 793 (1956), (Russ).

63. V. K. Ivanov, Dokl. Akad. Nauk SSSR. Vol. 142, No. 5, 997 (1962), (Russ).

64. V. K. Ivanov, Dokl. Akad. Nauk SSSR, Vol. 145, No. 2, 270 (1962), (Russ).

65. V. K. Ivanov, Mat. Sbornik, Vol. 61, No. 2, 212 (1962), (Russ).

66. V. K. Ivanov, and L. E. Kazakov, Sibir. Mat. Z., Vol. 4, No. 6 (1963), (Russ).

67. V. A. Morozov, Z. Vycisl. Mat. i Mat. Fiz., Vol. 7, No. 4, (1964), (Russ).

68. V. A. Morozov, Vesti Mosc. un-ta, No. 4 (1965), (Russ).

69. V. A. Morozov, Z. Vycisl. Mat. i Mat. Fiz., Vol. 6, No. 1 (1966), (Russ).

70. V. A. Morozov, Dokl. Akad. Nauk SSSR, Vol. 167, No. 3 (1966), (Russ).

71. D. J. Newman, J. Math. and Phys., Vol. 39, No. 1, 72 (1960).

72. L. E. Pane, Arch. Rational. Anal., Vol. 5, No. 1,35 (1960).

73. G. Fichera, Rend. Mat. e. appl., Vol. 19, No. 1-2, 95 (1960).

74. C. N. Megrelian, Uspehy Mat. Nauk, Vol. 11, No. 5, 3 (1956), (Russ).

75. E. M. Landis, Dokl. Akad. Nauk SSSR, Vol. 107, No. 5, 640 (1956), (Russ).

REFERENCES (CONTD)

76. Lin Tsia Tiao, Mechanica, Vol. 52, 37 (1958), (Russ).

77. C. G. Kreyn, and I. Prozovskaya, Dokl. Akad. Nauk SSSR, Vol. 133, No. 2, 277 (1960), (Russ).

78. PP. Rederenk, Z. Vycisl. Mat. i Mat. Fiz., Vol. 4, No. 6 (1964), (Russ).

79. A. B. Bakushinskiy, Z. Vycisl. Mat. i Mat. Fiz., Vol. 5, No. 4 (1965), (Russ).

80. L. V. Mayoror, Z. Vycisl. Mat. i Mat. Fiz., Vol. 5, No. 2 (1965), (Russ).

81. V. Ya. Arcenin, Z. Vycisl. Mat. i Mat. Fiz., Vol. 5, No. 5 (1968), (Russ).

82. V. P. Maslov, Dokl. Akad. Nauk SSSR, Vol. 176, No. 5, (1967), (Russ).

83. D. L. Phillips, J. Assoc. Comput. Machinery, Vol. 9, No. 1 (1962).

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13. ABSTRACT

Determination of a molecular weight distribution (MWD) from equilibrium sedimentation has been investigated. Such a determination requires a solution of the Fujita equations, which proved to be a mathematically Improperly Posed Problem in Hadamard sense. To avoid these difficulties an approximate computational technique has been applied which is based on variational calculus widened to include Tikhonov's regularizing functions.

It has been shown that this is an excellent method for determining a monomodal distribution. Also, the determination of a bi-modal distribution provided satisfactory results. However, a multi-modal distribution (fine structure in a MWD) requires the application of an additional algorithm.

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