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# Small-Angle-Scattering-Data Treatment by the Regularization Method

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## Abstract

The application of Tikhonov's regularization method [Tikhonov & Arsenin (1977). *Solution of Ill-Posed Problems*. New York: Wiley] for the solution of ill-posed problems in small-angle-scattering-data treatment is considered. Simple regularization algorithms are proposed for solving convolution equations in data desmearing (slit-width and polychromaticity problems) as well as for polydispersity problems. A general indirect approach of data processing based on the regularization method is described. Comparison with other data-treatment methods is made.

## Introduction

Small-angle scattering (SAS) is widely used for structure investigations of substances of different natures. SAS studies are of much importance for disordered disperse systems with colloidal inhomogeneities since their inner structures are difficult to study by other methods (Glatter & Kratky, 1982; Feigin & Svergun, 1987).

Experimental data processing (the reduction of instrumental distortions) is the necessary step in the structural analysis of SAS data. Smearing effects in SAS owe their origin to finite dimensions and polychromaticity of the radiation beam. The main equations connecting the experimental data set $u_e(s_i)$ [$s = 4\pi(\sin\theta)/\bar{\lambda}$, $2\theta$ is the scattering angle, $\bar{\lambda}$ is the average wavelength] with ideal curve $I(s)$ can for isotropic scattering be written as

$$u_e(s_i) = u(s_i) + \varepsilon_i$$

($\varepsilon_i$ is the statistical error in the point $s_i$),

$$u(s) = \int_{-\infty}^{\infty} W_w(x) F(s-x)\,\mathrm{d}x \qquad (1)$$

(smearing caused by the slit-width effect),

$$F(s) = \int_{-\infty}^{\infty} W_l(t) J[(s^2+t^2)^{1/2}]\,\mathrm{d}t \qquad (2)$$

(slit-height effect),

$$J(s) = \int_{0}^{\infty} W_\lambda(\lambda) I(s/\lambda)\,\mathrm{d}\lambda \qquad (3)$$

(smearing caused by the beam polychromaticity). Here the normalized weighting functions $W_w(x)$, $W_l(t)$ and $W_\lambda(\lambda)$ depend on the experimental conditions.

A number of methods was developed to solve these equations separately (step-by-step). The slit-height-correction problem, which is of much importance in X-ray SAS investigations, has been treated by many authors and several reliable algorithms have been developed (Heine & Roppert, 1962; Schedrin & Feigin, 1966; Vonk, 1971; Deutsch & Luban, 1978). Fewer papers have been devoted to slit-width (Taylor & Schmidt, 1967; Rolbin, Feigin & Schedrin, 1977) and polychromaticity (Zipper, 1969) problems, which can now be of value in synchrotron and neutron SAS studies. When solving (1)–(3), one faces the problem that they are unstable with respect to experimental data errors. Therefore, preliminary data smoothing is frequently necessary to reduce the random noise. Moreover, the termination effects arise because the experimental data are known only in a finite angle region $[s_{\min}, s_{\max}]$.

Several methods have been suggested for simultaneous reduction of the experimental distortions, *i.e.* for solving the general equation

$$u(s) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{0}^{\infty} W_w(u) W_l(t) W_\lambda(\lambda) \times I\{[(s-u)^2+t^2]^{1/2}/\lambda\}\,\mathrm{d}\lambda\,\mathrm{d}t\,\mathrm{d}u. \qquad (4)$$

The iteration procedure of Lake (1967) was probably the first attempt to do this. Another type of general procedure, the so-called indirect approach, where the solution is represented by some parametrization, has recently been developed. Here the methods making use of the sampling theorem (Moore, 1980; Taupin & Luzzati, 1982) should be mentioned which allow one to describe the solution with minimal number of parameters. Spline functions are also used for the parametrization (see Schelten & Hossfeld, 1971; Glatter 1977, 1980*a*,*b*).

Among the indirect methods, Glatter's (1977, 1980*a*,*b*) approach found widest practical application. Here a characteristic function describing the system in real space is represented as a sum of *B*-spline functions and the coefficients of the expansion are to be found. For monodisperse systems the

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parametrization of the distance distribution function

$$p(r)=\frac{1}{2\pi^2}\int_0^\infty s^2 I(s)\frac{\sin(sr)}{sr}\,ds \qquad (5)$$

is used; for polydisperse systems, the size distribution function $D(R)$ is searched for (see below). Indirect methods are stable to random errors and to termination effects, being, however, more complicated in use than the step-by-step algorithms and requiring more *a priori* information about the object.

Equations of data treatment represent the so-called ill-posed problems. Such problems can be effectively solved with the Tikhonov regularization method (Tikhonov & Arsenin, 1977). Here the possibilities of application of the regularization method to SAS data treatment are examined in comparison to other desmearing procedures.

### *Tikhonov's regularization method*

First of all we shall briefly describe Tikhonov's method for solving incorrect problems. The conditions of correctness (Hadamard, 1932) are as follows: let us consider the operator equation

$$\mathbf{A}[z]=u, \qquad (6)$$

$z\in Z$, $u\in U$; $Z$ and $U$ are some metric spaces. The problem is called correct if (i) a unique solution exists for any $u\in U$; (ii) the solution is stable with respect to errors in $u$ and $\mathbf{A}$ (*i.e.* operator $\mathbf{A}^{-1}$ determined over all $U$ is continuous). Otherwise the problem is called ill posed or incorrect.

The regularization method for ill-posed problems was proposed and substantiated by Tikhonov (1943, 1963) and is now of wide application (Tikhonov & Arsenin, 1977; Hofmann, 1986). The main idea of the method is to use the *a priori* information about the solution. It can be done as follows. Instead of solving with respect to function $z$ an ill-posed problem (6), where the inverse operator $\mathbf{A}^{-1}$ exists, but is not necessarily continuous, function $u$ and operator $\mathbf{A}$ are known with error bounds $\delta$ and $h$ respectively:

$$\|u-u^0\|_U\le\delta;\quad \sup_{z\in Z,z\neq 0}\frac{\|\mathbf{A}^0[z]-\mathbf{A}[z]\|_U}{\|z\|_Z}\le h$$

($u^0$ and $\mathbf{A}^0$ are exact right-hand part and operator, respectively), a correct problem of minimization of Tikhonov's functional

$$\mathbf{T}_\alpha[z]=\|\mathbf{A}[z]-u\|_U^2+\alpha\Omega[z] \qquad (7)$$

is to be solved. Here $\|u\|_U$ and $\|z\|_Z$ denote the norms in $U$ and $Z$ spaces, $\Omega$ is a non-negative stabilizing functional, $\alpha>0$ is a regularization parameter. It was shown by Tikhonov that if the parameter $\alpha$ is specifically correlated with $\delta$ and $h$, then $z_\alpha$, minimizing functional (7), is tending to the exact solution of (6) being stable to random errors under $\delta$ and $h$ tending to zero. The regularization parameter $\alpha$ may be chosen, for example, using the generalized discrepancy method (Tikhonov & Arsenin, 1977) as a solution of the equation

$$\|\mathbf{A}[z_\alpha]-u\|_U^2=(\delta+h\|z_\alpha\|_Z)^2+\mu^2(u,\mathbf{A}),$$

where

$$\mu(u,\mathbf{A})=\inf_{z\in Z}\|\mathbf{A}[z]-u\|_U.$$

If the operator $\mathbf{A}$ is given exactly, the discrepancy method can be used:

$$\|\mathbf{A}[z_\alpha]-u\|_U^2=\delta^2.$$

Other ways of choosing the regularization parameter are considered below.

The stabilizer $\Omega[z]$ is taken so as to fulfil *a priori* information about the solution (boundness, smoothness *etc.*). The squared norm of solution $\|z\|_Z^2$ is frequently used. Then the functional $\mathbf{T}_\alpha$ is strictly convex, being minimized by a unique function $z_\alpha$. So the problem of minimization (7) can easily be solved by standard routines (see Tikhonov, Goncharsky, Stepanov & Yagola, 1983).

For further considerations of the ill-posed problems dealt with, the norms in $U$ and $Z$ spaces are to be defined. With experimental data accuracy and discretization taken into account, it is natural to take

$$\|u\|_U^2=(1/N)\sum_{i=1}^N u^2(s_i)/\sigma_i^2, \qquad (8)$$

where $N$ is the number of data points, $\sigma_i$ is the mean square deviation in the $i$th experimental point. Then $\delta=\|u^0-u\|_U\simeq 1$, being in fact a sum of normalized random numbers (Brandt, 1970). The $Z$ space can be defined with the norm

$$\|z\|_Z^2=\{z^2(x)+\rho[z'(x)]^2\}\,dx, \qquad (9)$$

which demands the function $z$ and its first derivative to be integrable ($\rho$ is a constant chosen from the metric considerations).

## Solution of convolution equations

### *Slit-width correction*

Integral equation (1) for the slit-width correction is a convolution equation. From the convolution properties of the Fourier transformation (denoted as $\mathbf{F}$) its solution

$$F(s)=\mathbf{F}^{-1}\{\mathbf{F}[u(s)]/\mathbf{F}[W_w(s)]\}$$
$$=\mathbf{F}^{-1}\{\bar{u}(\omega)/\bar{W}_w(\omega)\} \qquad (10)$$

can be readily derived (Sneddon, 1951). This 'exact' solution is, however, rather sensitive to random errors in $u(s)$. The regularization method enables one to write down a stable solution. For the stabilizer of

type (9) with $\rho = 1$ the function minimizing the functional (7) is (Goncharsky, Cherepaschuk & Yagola, 1978)

$$F_\alpha(s) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{\bar{W}_w(-\omega)\bar{u}(\omega)\exp(-i\omega s)\,d\omega}{\bar{W}_w(-\omega)\bar{W}_w(\omega) + \alpha(1+\omega^2)}. \quad (11)$$

To verify the stability of the solution several model calculations were made. Model scattering curves were smeared according to (1) and statistical noise was imposed on the smeared curves. After this the curves were restored from the obtained data sets taken in intervals $[s_{\min}, s_{\max}]$; the $\alpha$ value was determined by the discrepancy method. Fig. 1 presents the results of application of the regularization method and of Taylor & Schmidt's (1967) algorithm to a model curve. One can see that the solution (11) is much more stable.

*Correction for polychromaticity*

The same idea can be applied to the equation of polychromaticity. On taking the Mellin transform from both parts of (3) and using the convolution theorem for this transform (Sneddon, 1951), one obtains

$$\tilde{J}(\xi) = \tilde{I}(\xi)/\tilde{K}(\xi),$$

where $K(\lambda) = \lambda W_\lambda(\lambda)$, and

$$\tilde{f}(\xi) = \int_0^\infty f(s)s^{\xi-1}\,ds$$

is a Mellin image of the function $f(s)$. Svergun & Semenyuk (1986) showed that for the stabilizer (9) the regularized solution can be written as

$$I_\alpha(s) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} \frac{\tilde{K}^*(\xi)\tilde{J}(\xi)s^{-\xi}\,d\xi}{\tilde{K}^*(\xi)\tilde{K}(\xi) + \alpha(1+|\xi|^2)^2}. \quad (12)$$

Here $c$ is a constant which can be chosen so as to facilitate the computations.

The solution was tested on model examples and compared with several other methods for solving (3). The restoration of a homogeneous-sphere scattering curve by Glatter's (1977) method, Lake's (1967) iteration procedure and the regularization method is presented in Fig. 2. The iteration procedure is unstable, Glatter's method, although stable, consumes more computer time and memory (it also needs more parameters adjusted). It should be noted here that Glatter's indirect approach offers much wider possibilities than polychromaticity corrections (see *Introduction*). However, comparison with the approach was done since up to now it has in fact been the only reliable method for polychromaticity correction.

*Polydispersity equation*

The regularization approach using the convolution properties can also be applied to solve the equation of polydispersity. If the investigated system is represented by an ensemble of randomly oriented similar particles described by a distribution function $D(R) = m^2(R)D_N(R)$ [$m(R)$ is the scattering length, $D_N(R)$ the number of particles of size $R$], then the SAS intensity is given by

$$I(s) = \int_{R_{\min}}^{R_{\max}} D(R)I_0(sR)\,dR, \quad (13)$$

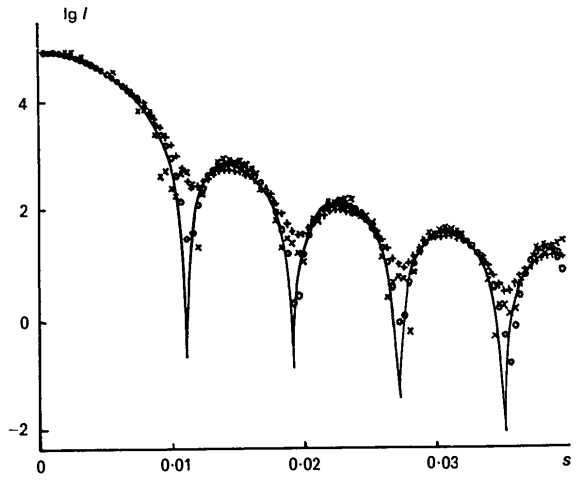



Fig. 1. Restoration of model scattering intensity of homogeneo sphere smeared by slit-width effect: — exact curve; +++ smear curve with statistical noise of 3%; ××× and ○○○ are desmeared curves according to Taylor & Schmidt (1967) and as obtained by the regularization technique, respectively.

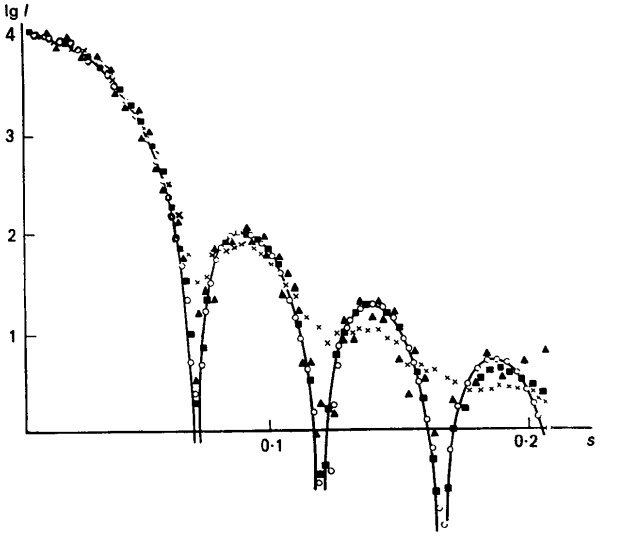



Fig. 2. Corrections for polychromaticity: — exact curve; ××× smeared curve with 3% noise; restoration by ▲▲▲ Lake (1967), ■■■ Glatter (1977), ○○○ regularization technique.

where $I_0(sR)$ is the form factor of particles, $R_{min}$ and $R_{max}$ are the minimal and maximal sizes of particles in the ensemble. The problem of finding $D(R)$ under the given $I(s)$ and $I_0(sR)$ is of great practical value.

Several methods have been proposed for solving (13). Among them the analytical approach (Fedorova & Schmidt, 1978) is of wide practical application, where the exact solution is written for some types of form factor [the solid-sphere form factor is used most frequently, see Letscher & Schmidt (1966), Walter, Gerber & Kranold (1983)]. The solution is, unfortunately, rather sensitive with respect to termination effects, therefore strong artificial oscillations may deteriorate the resulting $D(R)$ function. Another simple method proposed by Plavnik, Troshkin, Kozhevnikov, Ruzinov & Khrustaleva (1985) allows one to estimate both the $D(R)$ function and the anisometry of the particles (however, only rough estimation can be achieved). The indirect method (Glatter, 1980*a*) enables reliable solutions to be obtained but requires *a priori* information about the range of definition of the $D(R)$ function.

This proves that the polydispersity equation can be easily solved using the Mellin transform, as for the polychromaticity problem. In fact, substituting $x = 1/R$ in (13) and denoting $W(x) = RD(R)$, one gets

$$I(s) = \int_0^\infty W(x) I_0(s/x)\, dx/x \qquad (14)$$

and similar to (12) the regularized solution can be written as

$$D_\alpha(R) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} \frac{\tilde{I}_0^*(\xi)\tilde{I}(\xi)R^{\xi-1}\, d\xi}{\tilde{I}_0^*(\xi)\tilde{I}_0(\xi) + \alpha(1+|\xi|^2)^2}. \qquad (15)$$

The regularization approach was compared to the methods of Letscher & Schmidt (1966) and Glatter (1980*a*). Fig. 3 illustrates the results obtained with the bimodal volume distribution function $D_V(R) = m(R)D_N(R)$. One can see that all the methods enable one to restore the model distribution fairly well; however, it should be noted that a special extrapolation procedure was applied to avoid termination effects in Schmidt's approach whereas the regularization method is stable with respect to these effects. As to Glatter's method, the same reasoning as for the polychromaticity problem can be repeated.

A Fortran-77 program package based on the considered regularization procedures has been written [the slit-height-correction routine of Schedrin & Feigin (1966) was also used]. Selection of the regularization parameters was done by the discrepancy method; with no information about the input errors available, reasonable $\alpha$ estimation could be obtained from the condition $\|A[z_\alpha] - u\|_U^2 = \min$ (Svergun & Semenyuk, 1986). The package was applied to neutron SAS data processing for the 'Membrane-2' diffractometer (Institute of Nuclear Physics, Gatchina, USSR). Here the collimation and especially polychromaticity smearing effects were rather strong (see Agamalyan, Drabkin, Deriglazow & Krivshich, 1984; Agamalyan, Krivshich, Svergun & Semenyuk, 1985). Model calculations with spectral and collimation functions of the diffractometer have proved the high reliability of the package. Fig. 4 illustrates the

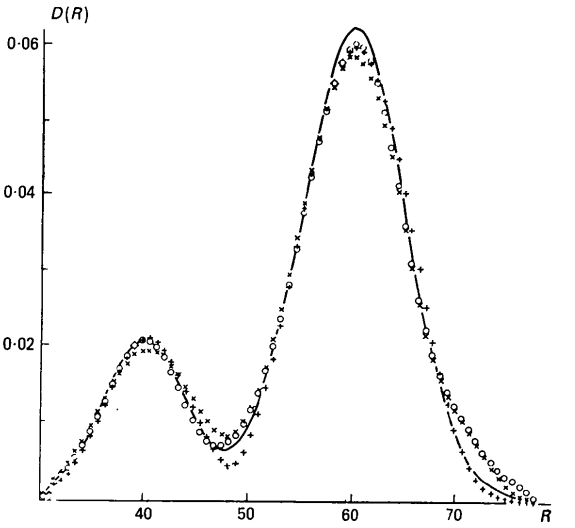



Fig. 3. Restoration of model volume distribution function for a polydisperse system of homogeneous spheres: — exact curve; ○○○ Letscher & Schmidt's (1966) method; ××× Glatter's (1977) method, +++ regularization technique.

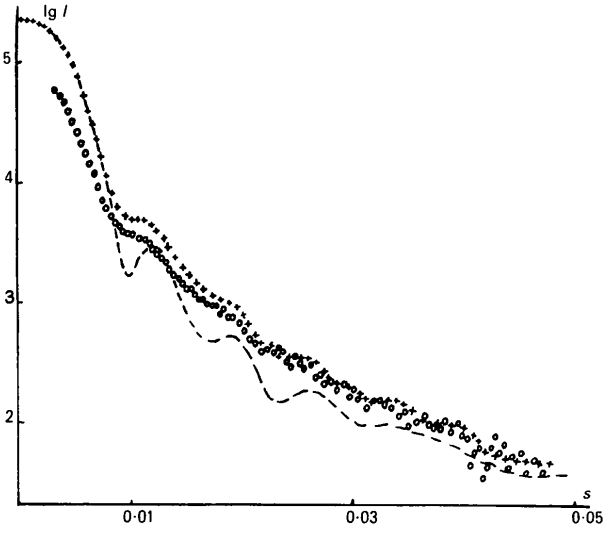



Fig. 4. Application of the regularization procedures for neutron-scattering-data treatment of polystyrene latex sample: ○○○ experimental data; +++ after collimation corrections; --- completely desmeared curve.

application of the package for the desmearing of the experimental scattering intensity of polystyrene latex samples; the restored size distribution function is shown in Fig. 5 together with the histogram obtained by electron microscopy. This example illustrates the reliability of the regularization procedures described and their usefulness in the data treatment problems.

### General method of SAS data treatment

This is a substantial shortcoming in the application of the step-by-step algorithms of data processing. Although ill-posed problems (1)–(3) can be solved successfully, only a rough estimation can be obtained about the error bounds in each solution. Therefore, a full account of experimental data accuracy cannot be expected. A general approach of SAS data treatment using the regularization technique is described below.

Let us consider scattering by monodisperse and polydisperse systems. For the monodisperse system, ideal scattering intensity is connected to the function $p(r)$ by

$$I(s)=4\pi\int_0^{l_{max}} p(r)\sin(sr)/sr\,dr, \qquad (16)$$

$l_{max}$ is a maximal chord in the particle. For the polydisperse system of similar particles, scattering intensity is connected to the size distribution function according to (13). In these important cases the problem of data treatment can be solved indirectly by finding a finite distribution function (see *Introduction*).

The indirect approach can be realized in a simple way without parametrization of the solution to be found. Let us substitute integral expressions (16) and (13) in (4) and change the order of integration. Thus, for monodisperse systems one can write

$$u(s)=\int_0^{l_{max}} K_1(s,r)p(r)\,dr, \qquad (17)$$

where

$$K_1(s,r)=4\pi r^2\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_0^{\infty} W_w(x)W_l(t)W_\lambda(\lambda)\times(\sin\{[(s-x)^2+t^2]^{1/2}r/\lambda\})\times\{[(s-x)^2+t^2]^{1/2}r/\lambda\}^{-1}\,d\lambda\,dt\,dx. \qquad (18)$$

For polydisperse systems we obtain

$$u(s)=\int_{R_{min}}^{R_{max}} K_2(s,R)D(R)\,dR, \qquad (19)$$

where

$$K_2(s,R)=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_0^{\infty} W_w(x)W_l(t)W_\lambda(\lambda)\times I_0\{[(s-x)^2+t^2]R/\lambda\}\,d\lambda\,dt\,dx. \qquad (20)$$

The kernels $K_1$ and $K_2$ are fixed under given experimental conditions and can be evaluated with any quadratures.

Therefore, the problem of data treatment for monodisperse and polydisperse systems is reduced to the solution of (17) and (19) respectively, which are in fact Fredholm integral equations of the first kind. The Tikhonov functional for (17) can be written as

$$\mathbf{T}_\alpha[p]=\sum_{i=1}^{N}(\Delta s_i/\sigma_i^2)\left[\Delta r\sum_{j=1}^{M}K_1(s_i,r_j)p(r_j)-u(s_i)\right]^2+\alpha\left[\Delta r\sum_{j=1}^{M}p^2(r_j)+\rho(\Delta r)^{-1}\times\sum_{j=2}^{M}[p(r_j)-p(r_{j-1})]\right]^2=\min.$$

Here $\Delta s_i=s_i-s_{i-1}$, and the function $p(r)$ is searched for at $M$ equidistant points, $\Delta r=l_{max}/(M-1)$. Differentiating $\mathbf{T}_\alpha[p]$ over $p(r_j)$ and putting the result to zero for $j=1,\ldots,M$, we obtain an $M\times M$ system of linear equations [$p(r_j)$ are unknowns] with a symmetric positive-definite matrix, which can easily be solved by standard routines.

A similar equation can be written for the $D(R)$ function. Special cases of monodisperse systems [lamellar particles, long rods, see Glatter (1980*b*)] can also be treated in this way.

Fast and reliable choice of the regularization parameter is probably the most important problem. It is known that when solving equations of type (17) the best $\alpha$ value proves to be somewhat smaller than the value provided by the discrepancy method (see *e.g.*

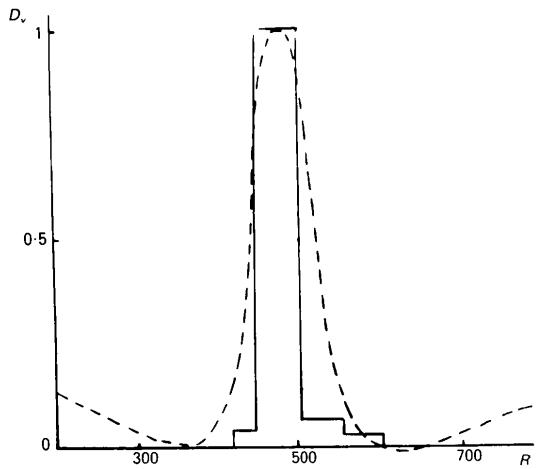
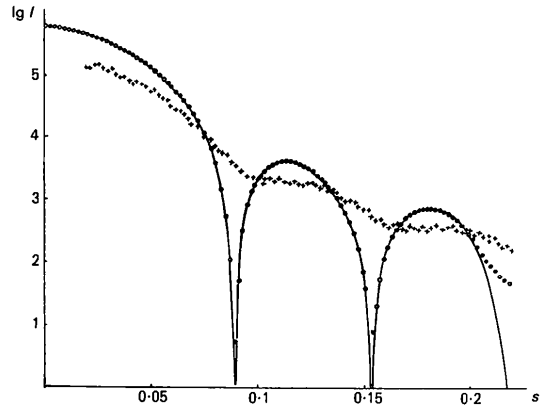



Fig. 5. Volume distribution function of polystyrene latex as calculated by regularization technique (---) and electron microscopy (—).

Hofmann, 1986). To avoid oversmoothing of the solution, several methods were tested for refining the regularization parameter, in particular, the so-called quasioptimality criterion [$\|\alpha\, \partial p_\alpha/\partial\alpha\| = \min$, $\alpha > 0$; (Tikhonov & Arsenin, 1977)], point-of-inflection criterion [$-\partial\|p_\alpha\|/\partial\alpha = \min$, $\alpha > 0$, see Glatter (1977)]. It proved that rough estimation of $\alpha$ by the generalized discrepancy method followed by its refinement with the quasioptimality criterion ensures reliable determination of the $\alpha$ value.

A Fortran 77 program using the approach described has been written which allows data treatment *via* both $p(r)$ and $D(R)$ functions. Economic computing algorithms (Tikhonov *et al.*, 1983) are used for fast solving the Euler equation for different $\alpha$ values; the selection of $\alpha$ is performed as a straightforward routine. Fig. 6 presents an example of application of the method to a model curve smeared with both collimation and polychromaticity effects.

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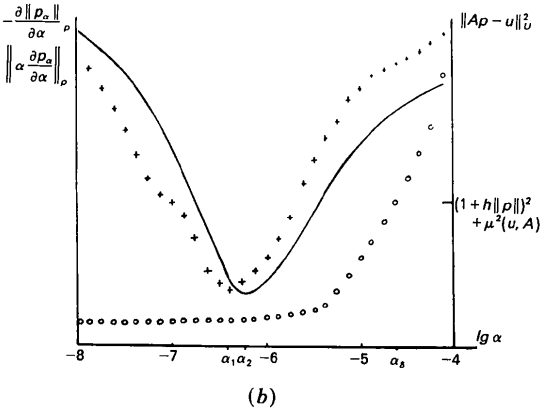
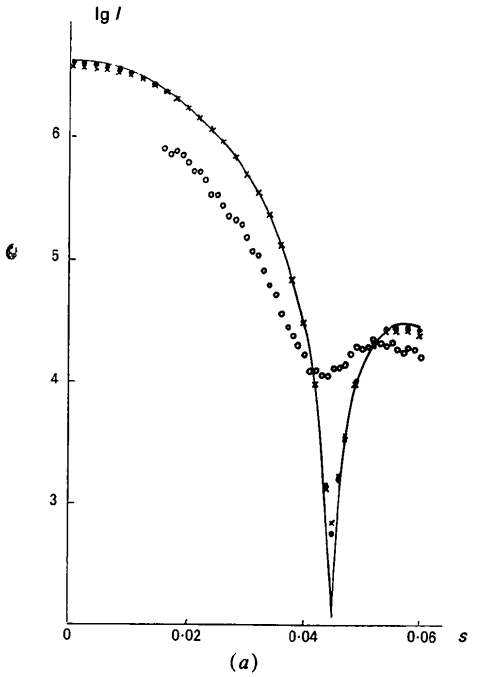



(*b*)

Fig. 6. Restoration of the model curve smeared with collimation and polychromaticity effects using the regularization approach. (*a*) The scattering curves: — exact curve; +++ smeared curve with 5% noise; OOO restored curve. (*b*) Selection of regularization parameter: OOO general discrepancy method gives $\alpha_\delta$ value; +++ point of inflection method: $\alpha_1$ value; — quazioptimal method: $\alpha_2$ value.

The approach described is similar to the indirect transform techniques (in particular to Glatter's). In Fig. 7 a model example is presented where the two methods are compared. They give nearly the same results being rather stable with respect to statistical errors and termination effects. Both of them require information about the range of definition of the $p(r)$ [or $D(R)$] function. At the same time, the fact that no parametrization is used makes the regularization approach more general; automatic choice of the regularization parameter facilitates its application (a

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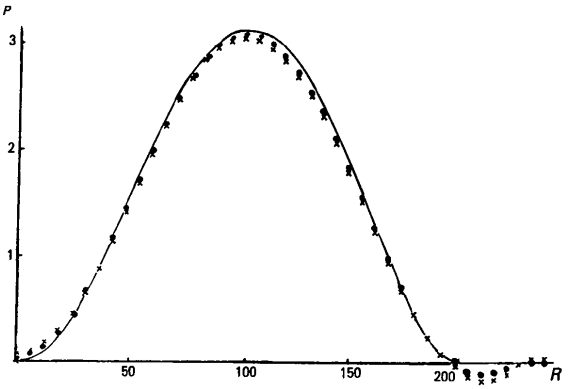


(*b*)

Fig. 7. Comparison of Glatter's method with the regularization technique. (*a*) The scattering curves: — exact scattering curve from the sphere of radius $R = 100$; OOO smeared curve with 5% noise, $s_{min} = 0{\cdot}016$, $s_{max} = 0{\cdot}06$ Å$^{-1}$; ××× and ●●● restoration with the two methods, respectively, $l_{max} = 240$. (*b*) The distance distribution functions: notations are the same as in (*a*).

similar parameter in Glatter's approach needs to be selected by the user).

The regularization method has been also applied by Provencher (1982) for inverting noisy linear operator equations. A general Fortran IV program described in the paper allows a constrained solution to be found by means of quadratic programming algorithms; the discrepancy method is used to select the $\alpha$ value. One may expect that Provencher's package as applied to SAS problems would lead to similar results. At the same time our algorithm differs from Provencher's in computing procedures (type of stabilizer, solving the least-squares problems, choice of regularization parameters). Moreover, the presented algorithm is designed especially for SAS problems being much more compact in program realization.

## Concluding remarks

Two possibilities of application of the regularization method in SAS data treatment have been considered. The use of the method for solving the convolution equations shows a number of advantages in comparison with other methods. Simple and stable regularized solutions can be written for the problems of slit-width and polychromaticity desmearing as well as for the polydispersity equation. Therefore the application of the regularization technique combines reliability of the indirect transform methods with the simplicity of standard routines.

The general approach based on regularization is similar to several indirect algorithms (*e.g.* those of Moore, Glatter and Provencher). However, some features (such as the ways of using *a priori* information, stabilization of the solution, computing algorithms) are different in these methods. A forthcoming paper is planned where the problems of constraints, choice of stabilizers and error propagation will be discussed.

The question may arise whether it is better to use stepwise procedures or an indirect approach. One cannot answer this definitely. In fact, with appropriate information in hand one can obtain excellent results by indirect methods even if the quality of the experimental data is not very good (poor accuracy, small angular range measured). On the other hand, when the experimental data set is representative it would be better to use stepwise algorithms which do not require *a priori* information about the object.

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