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Computer Program Descriptions

Computation of Dielectric Properties from Short-Circuited Waveguide Measurements on High- or Low-Loss Materials

- PURPOSE:** Computation of the relative complex permittivity components ϵ_r' and ϵ_r'' , loss tangent, and conductivity from measurements data on materials in coaxial, rectangular, or cylindrical waveguides.
- LANGUAGE:** Fortran IV; 393 cards, including comments.
- AUTHORS:** S. O. Nelson, C. W. Schlaphoff, and L. E. Stetson, U.S. Department of Agriculture, ARS, and University of Nebraska, Lincoln, Nebr.
- AVAILABILITY:** ASIS/NAPS Document No. 02272. Listing, typical I/O data and description in U.S. Department of Agriculture Publication No. ARS-NC-4, November 1972.
- DESCRIPTION:** The program was developed for calculation of dielectric properties from data obtained using the short-circuited waveguide technique originally reported by Roberts and von Hippel [1] and employing relationships for wall-loss corrections described by Westphal [2]. In preliminary calculation stages, the program employs simplified relationships developed by Dakin and Works [3] that are valid for low-loss materials. Final calculations, however, are based on the general equations that are valid for high-loss materials as well.

Required information for determining the dielectric properties of a sample include the voltage or current standing-wave node locations with respect to the short-circuit termination, both with and without the sample in the waveguide, and the respective standing-wave ratios for these two situations. Also required are the frequency, the length of the sample, and the dimensions of the waveguide unless it is a coaxial line.

The program accommodates input data from measurements on coaxial lines, or cylindrical or rectangular waveguides. It properly performs all necessary calculations for either low-loss or high-loss dielectric samples and provides values for ϵ_r' , ϵ_r'' , the loss tangent ($\tan \delta$), and the conductivity (σ).

Input data include sample description and other sample identifying information, waveguide dimensions, width of the slot in the slotted waveguide section, a reference dimension corresponding to the approximate distance (within $\pm \lambda_g/4$) between the short-circuit termination and the slotted-section probe when the probe is positioned at zero on its scale, frequency (either directly or in terms of adjacent standing-wave node data), slotted-section scale readings taken at 3-dB points (or any other decibel level) on both sides of the air node (empty line or waveguide) and sample node (sample in place at short-circuited end of line or waveguide), the decibel level employed for each node-width measurement, the length of the

sample, and an estimate of the value of the dielectric constant (ϵ_r'). The program accepts any air node or any sample node without regard to relative positional relationships.

The program corrects all slotted-waveguide-section data for the influence of the slot. An iterative method is employed to solve the necessary cubic equations for the true guide wavelength in rectangular and cylindrical waveguides. Standing-wave ratios are calculated from node-width measurements using an exact relationship. The fact that measurements are taken in air rather than vacuum is taken into account.

Detailed explanations of the computations and subroutines employed have been described [4]. The input estimate for ϵ_r' provides, through simplified relationships of Dakin and Works [3], an estimate for $\beta_2 d$, the product of the phase constant in the sample (β_2), and the sample length (d). A special subroutine is then employed to find the three values of $\beta_2 d$ closest to the initial estimate of $\beta_2 d$, that satisfy the equation of Dakin and Works, $(\tan \beta_2 d)/\beta_2 d = C$, where C is a real number obtained from measurements data. Estimates for $\alpha_2 d$ are then obtained using another equation of Dakin and Works [3], and the three corresponding values of $\gamma_2 d = \alpha_2 d + j\beta_2 d$ are provided by another subroutine that alternately adjusts values of $\alpha_2 d$ and $\beta_2 d$ until the complex transcendental equation $(\tanh \gamma_2 d)/\gamma_2 d = Ce^{j\delta}$ is satisfied to within the desired limit. $Ce^{j\delta}$ is a complex number obtained from measurements data.

The values of $\gamma_2 d$, the product of sample length, and the complex propagation constant in the sample material, thus provide three sets of values for ϵ_r' and ϵ_r'' that have ϵ_r' values closest to the estimated dielectric constant of the sample. Three sets of values for ϵ_r' , ϵ_r'' , $\tan \delta$, and σ are printed out along with the input data and a few diagnostics. When calculations are performed by the program for a number of different sample measurements (up to 50), a summary table is provided in the printout which includes only that set of dielectric properties for each sample that matches most closely the input estimate for the dielectric constant. The detailed printout of input data and three sets of values for the dielectric properties of each sample measurement can be suppressed if desired.

Calculations were programmed for computation on an IBM 360 model 65 computer. When compiled under IBM OS/MVT, the program executes in 40K of core. Typical central-processing-unit time required for processing 50 sample measurements is less than 20 s. There are no files other than the input (reader) and the output (printer) files.

On rare occasions when the sample length is an odd-multiple quarter-wavelength, values for some of the functions become infinite. The program includes tests to circumvent this problem and prints out a statement identifying the problem, approximate values for the dielectric constant, and zeros for the other properties.

This computer program has been used successfully for several different systems for dielectric-properties measurement, including a rectangular waveguide X-band system, a cylindrical waveguide system operating at 8.5 GHz, and three coaxial systems operating in the range from 1 to 6.3 GHz. It incorporates a number of convenience features for an already convenient measurement method whose principal disadvantage is in the tedium of calculation. The computer program eliminates this disadvantage and improves the precision of calculation, making the method more attractive, especially for the determination of dielectric properties of high-loss materials.

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The Complex Program for Constrained Minimization

PURPOSE: The complex program is a package of sub-routines that minimizes a nonlinear objective function subject to nonlinear inequality constraints.

LANGUAGE: Fortran IV G Level 21 for the IBM 360/65 computer; 270 cards including comments but not including the user-supplied subprograms.

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AVAILABILITY: ASIS/NAPS Document No. 02272.

DESCRIPTION: The COMPLEX method [1]-[3] is a direct search procedure for the minimization of a nonlinear objective function subject to nonlinear inequality constraints. The problem under consideration can be mathematically described as follows:

minimize the objective function $f(x_1, x_2, \dots, x_n)$
 subject to the implicit constraints $g_j(x_1, x_2, \dots, x_n) \leq 0, \quad j = 1, 2, \dots, m$
 and the explicit constraints $x_i^l \leq x_i \leq x_i^h, \quad i = 1, 2, \dots, n$.

The method is based on the construction of a flexible figure of $v \geq (n + 1)$ vertices. This figure, or complex, can expand or contract in any direction and, at the same time, is made to satisfy all the constraints. A set of explicit constraints is required for each variable. These explicit constraints define a rectangular region within which the initial complex is generated about an initial feasible point. The additional $(v - 1)$ vertices are generated by the formula

$$x_i = x_i^l + r_i(x_i^h - x_i^l), \quad i = 1, 2, \dots, n$$

in which the r_i are pseudorandom numbers over the interval 0 to 1.

The initial complex will be within the rectangular region of search, and the variables will be, therefore, automatically scaled. The implicit constraints may, however, not all be satisfied. If this is the case, those vertices which are outside the feasible region are moved halfway towards the centroid of the remaining vertices. This procedure is repeated for each vertex until all the implicit constraints are satisfied. The centroid is calculated from the expression

$$x_i^c = \frac{1}{v-1} \sum_{k=1, k \neq w}^v x_{i,k}, \quad i = 1, 2, \dots, n \quad (1)$$

in which $k = w$ corresponds to the worst vertex (largest function value).

After the initial complex is generated, the algorithm consists of the following steps.

Step 1: The objective function is calculated at each vertex and

the one with the largest function value is rejected and replaced by another located a distance $\alpha (\alpha > 1)$ times as far from the weighted centroid of the remaining vertices. If this new vertex is feasible the process is repeated.

Step 2: If the new vertex generated in step 1 has the largest function value, then it is moved a distance $\beta (\beta < 1)$ times closer to the weighted centroid of the previous complex.

Step 3: If the new vertex generated in step 2 is also the worst, then a contraction of the whole complex is initiated about the best vertex so far obtained.

Step 4: If a vertex generated at any of the previous steps does not satisfy an implicit constraint, then that vertex is moved a distance $\beta (\beta < 1)$ times closer to the centroid of the previous complex. The process is repeated until the vertex enters the feasible region.

Step 5: If a vertex generated at any of the previous steps contains a variable which does not satisfy an explicit constraint, that variable is reset at a suitable distance (10^{-6}) inside the appropriate boundary.

The weighted centroid is calculated from the expression

$$x_i^c = \frac{\sum_{k=1, k \neq w}^v (f_k)^\gamma x_{i,k}}{\sum_{k=1, k \neq w}^v (f_k)^\gamma}, \quad i = 1, 2, \dots, n \quad (2)$$

in which f_k is the value of the objective function which corresponds to the vertex x_k . The weighting factor γ may be chosen in the range $0 \leq \gamma \leq 2$. For $\gamma = 0$ (2) reduces to (1).

The iterative procedure is terminated when

$$\sigma = \left[\frac{1}{v} \sum_{k=1}^v (f_k - f_m)^2 \right]^{1/2} \leq \varepsilon \quad (3)$$

in which σ is the standard deviation, f_m the mean of the function values at all the vertices, and ε a predetermined tolerance. For double precision arithmetic (12 significant digits for the IBM 360/65) ε may be chosen as low as 10^{-5} ; otherwise a value of 10^{-2} is recommended.

The computer program may be called as follows:

CALL COMPLEX(N,X,F,M,V,XL,XH,ALFA,BETA,GAMMA,SIGMA,EPS)

where N,X,F,M,V,XL,XH,ALFA,BETA,GAMMA,SIGMA,EPS correspond to $n, x_i, f(x_1, \dots, x_n), m, v, x_i^l, x_i^h, \alpha, \beta, \gamma, \sigma, \varepsilon$, respectively, and $i = 1, 2, \dots, n$.

It was convenient to place the following user-specified variables in COMMON/COMPLX/COUNT,EVAL,T,IT,LOOP,NLOOP,UNIT,IPRINT,IDATA in which

COUNT	integer variable specifying the number of iterations; initially set to zero;
EVAL	integer variable specifying the number of function evaluations; initially set to zero;
T,IT	integer variables (if $\tau = 1$ printing occurs every τ iterations; otherwise every τ function evaluations);
LOOP,NLOOP	integer variables for convergence criterion (the iterative procedure is tested every NLOOP iterations by the counter LOOP which is initially set to zero);
UNIT	integer variable specifying the output device;
IDATA	logical variable (if IDATA = .TRUE. the input data is printed out, otherwise not);
IPRINT	logical variable (if IPRINT = .TRUE. intermediate printing will occur, otherwise not).

All the parameters, except F, must be supplied in the main program by the user. The user must supply the tolerance ε and he has some control over the printout. The random numbers are generated internally. This is described in ASIS/NAPS Document No. 02272.

REQUIRED SUBPROGRAMS

SUBROUTINE FUNCT (N,X,F): This user-supplied program provides the value of the objective function F at point x.

SUBROUTINE MONIT (N,X,F,COUNT,EVAL,M,SIGMA,UNIT): This user-supplied program provides the variables in the argument list for printing. This program is used for the intermediate printing as well as for the final printing.

FUNCTION G(L,X,N): This user-supplied program provides the implicit constraints. Considering the case of two implicit constraints

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