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A COMPARISON OF METHODS FOR THE CALCULATION OF VOIGT PROFILES

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Abstract—Six algorithms and approximations for the calculation of Voigt profiles are compared for accuracy and time required for calculation. For high-precision calculations, a GAUTSCHI program is recommended; for calculations with a few per cent of error, the Matvejev and the Kielkopf approximations are recommended.

INTRODUCTION

For precise calculations of the transmittance function of the atmosphere, application of the Voigt profile is indispensable. Here a comparison is shown of different computing programs and approximation formulas. We follow the definition of Armstrong[1] and distinguish between the Voigt profile P_V and the Voigt function K. The Voigt function K contains only two parameters. It is preferably used in tables. For numerical calculation of the transmittance on computers, the Voigt profile P_V is more convenient. It contains three parameters: the distance from the line centre $(\nu - \nu_0)$, the Lorentz half-width (α_L), and the Doppler half-width (α_D). For the comparison, only those methods of calculation have been chosen that were available as programs ready for use (Armstrong,[1] Poljakov,[2] Gautschi,[3] Drayson[4]) or as approximation formulas (Kielkopf,[5] Matvejev,[6] Whiting[7]). These have been written as real-function Fortran subroutines.

COMPARISON OF ACCURACY

The accuracy of the various computing methods has been assessed by comparison of methods and numerical values from the tables of Posener,[8] Finn and Muggelstone,[9] and Hummer.[10] However, these tables are not sufficient for a detailed accuracy test. The accuracy of the Posener table is insufficient. The table by Hummer, Finn, and Mugglestone cover only a minor portion of the needed range of values. Hence, an intercomparison of the programs is required. For this purpose, the Voigt profile P_V was calculated by each of the algorithms that were to be tested for $(\nu - \nu_0)$ values between 0.0 and 135.0, on an approximately logarithmic scale and for α_L/α_D equal to 1×10^{-4}, 5×10^{-4}, etc. up to 100.0, 200.0, and 500.0. The absolute values of α_L and α_D do not affect the accuracy of the results. We are here concerned with comparisons of the computing programs. From a comparison of results derived from the Armstrong[1] and Gautschi[3] programs, we have found that these differ on the average by 10^{-8}; only a few points show differences in excess of 10^{-6}. We shall use Armstrong's program as the reference. Results using the approximations of Kielkopf,[5] Matvejev,[6] Poljakov,[2] and Whiting[7] are presented in Figs. 1(a–e) in the form of curves of relative error $= P_V^{(I)}/P_V^{(A)} - 1$, with $I =$ Kielopf, Matvejev, Poljakov, Whiting, and A = Armstrong. As expected, the relative error reaches a maximum when the Voigt profile contains equal contributions from the Doppler and Lorentz profiles (Fig. 1d). Kielkopf[5] claims a relative error of 10^{-4} for the zero point. This requirement is met, excluding a narrow region around $\alpha_L/\alpha_V = 0.83$ (ratio of the Lorentz and Voigt half-widths, see Fig. 2), where the relative error of the zero point value becomes 10^{-3}. This disadvantage may be avoided by using a different approximation formula for the zero point value, e.g. the Oldham[11] formula which has an error smaller than 1.5×10^{-4} for all values α_L/α_V. At the half-width, the Voigt profile is exactly reproduced by the Kielkopf formula. When the Doppler profile prevails (Figs. 1a–d), the relative error is negative at small x. In the line-wings, it becomes positive and reaches values of 10%, 20%, and more. In this case, the Kielkopf approximation does not describe the curvature of the Voigt profile very well. When the Lorentz profile prevails (Fig. 1e), the relative error tends to zero in the line-wings. The Matvejev[6]

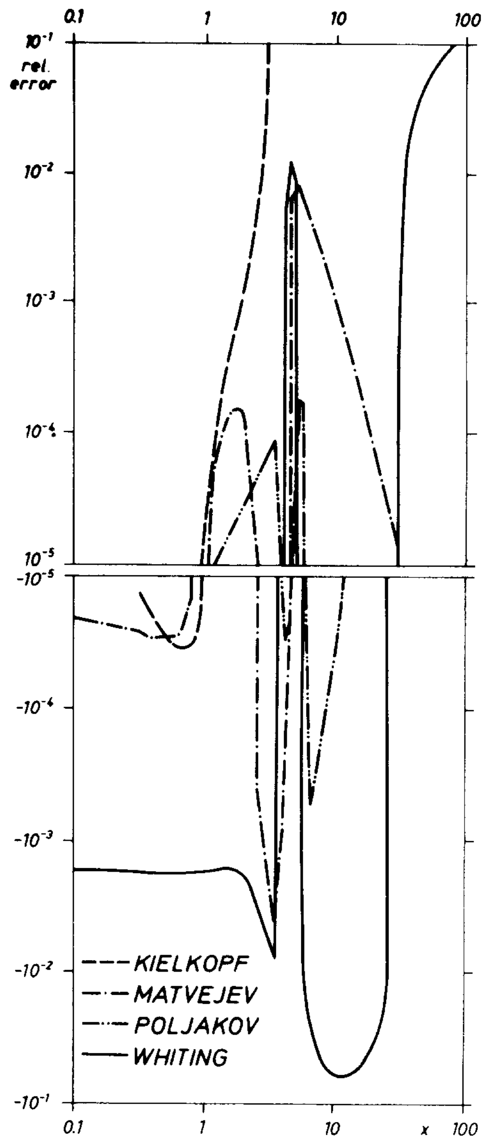

Fig. 1(a–e). Relative errors in the results of different computing programs for the Voigt profiles as a function of x; x and y are the two parameters of the Voigt function: x is defined as $(\nu - \nu_0)\sqrt{\ln 2}/\alpha_D$ and $y = \alpha_L \sqrt{\ln 2}/\alpha_D$. In Figs. 1(a–e), the y values are: Fig. 1(a), $y = 10^{-3}$; Fig. 1(b), $y = 10^{-2}$; Fig. 1(c), $y = 10^{-1}$; Fig. 1(d), $y = 1$; Fig. 1(e), $y = 10$. For values y greater than 10, the relative errors in all of the computing programs are smaller than 10^{-4}.

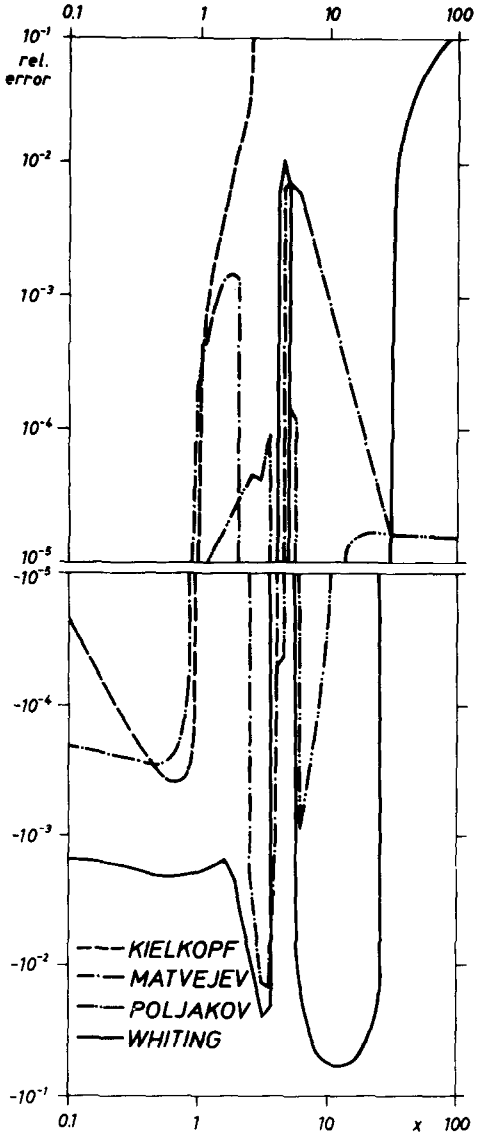
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Fig. 1(b).

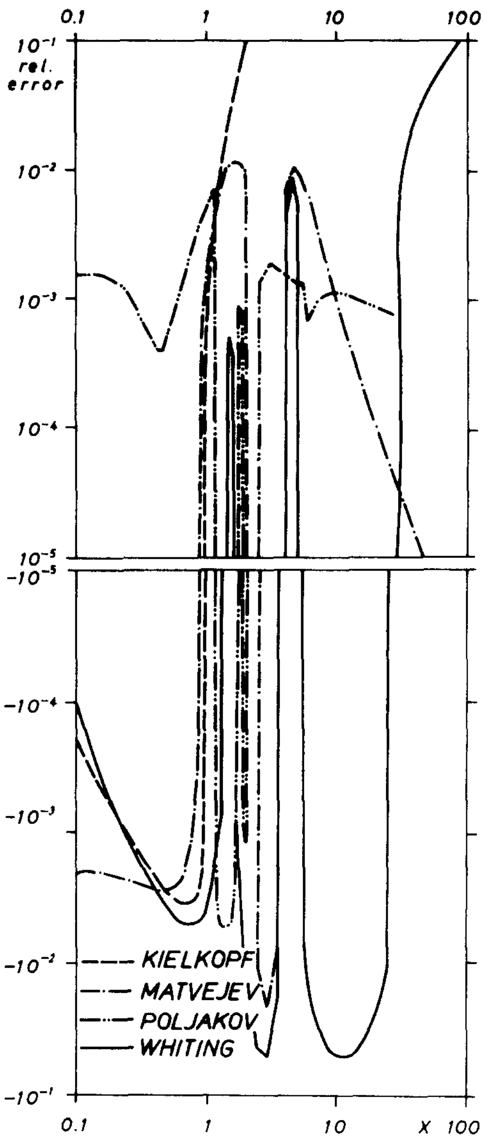
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Fig. 1(c).

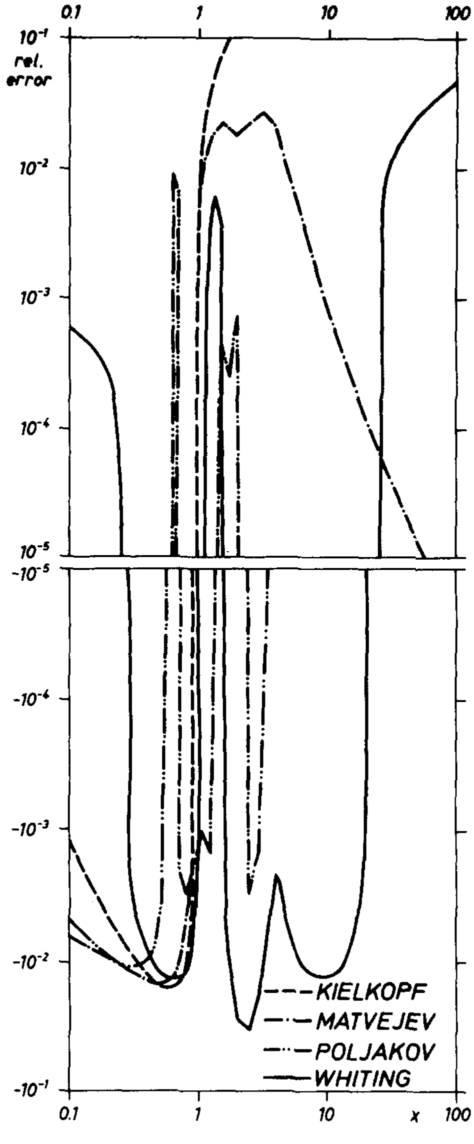
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Fig. 1(d).

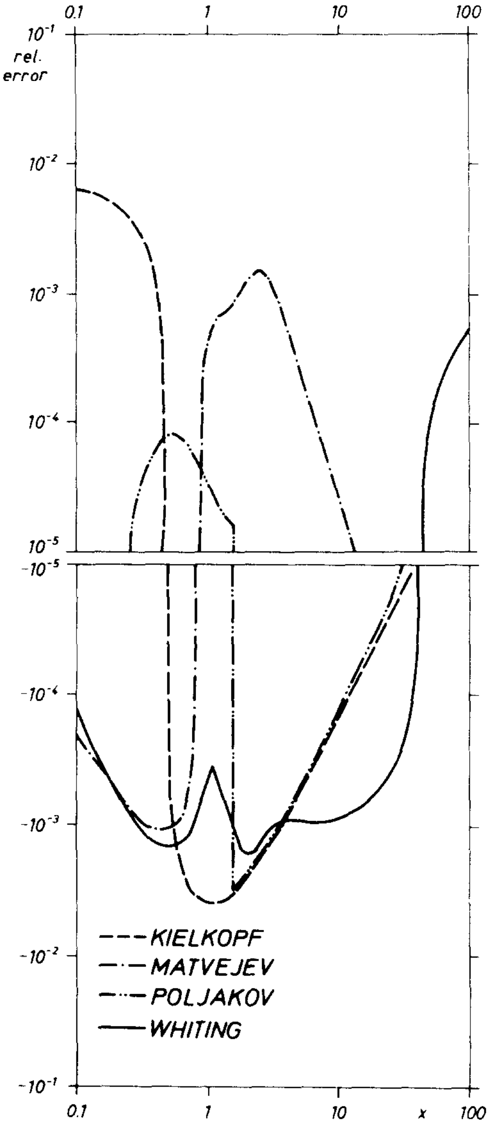
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Fig. 1(e).

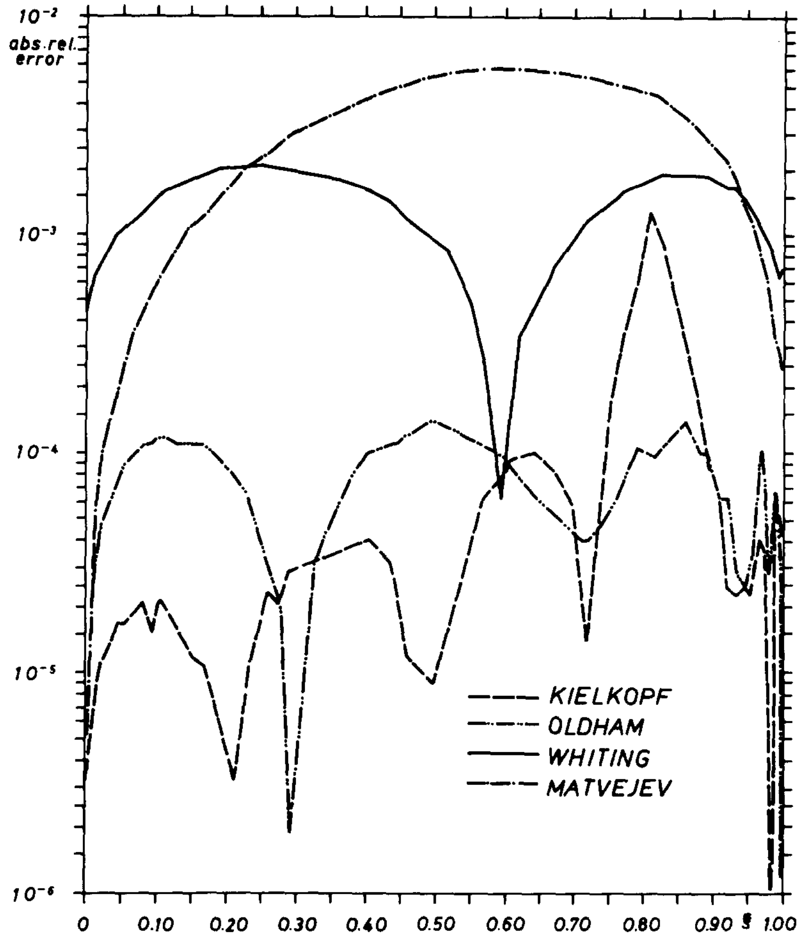

Fig. 2. Absolute values of the relative errors of the Zero-point values for different approximations to the Voigt profiles as a function of ξ($\xi = \alpha_L/\alpha_V$ = ratio of Lorentz to Voigt half-widths). The transformation of variables from $y = \alpha_L/\alpha_D\sqrt{\ln 2}$ to ξ simplifies the plotting. The y range from 0 to ∞ while the ξ range from 0 to 1; $\xi = 0$ corresponds to the pure Doppler profile, $\xi = 1$ to the pure Lorentz profile. Approximations for calculation of the Voight half-width α_V from the Lorentz and Doppler half-widths are presented by Matvejev[6] and Olivero and Longbothum[12].

approximation describes the curvature of the Voigt profile better. All relative errors are less than 3%. For all y (Figs. 1a–e), the curve of relative error begins with negative values, runs through an extremum, crosses to positive values, runs through an extremum, and tends to zero in the line-wings. When the Doppler contribution prevails in the Voigt profile, one finds a sharp and deep dip near the positive extremum. When the Lorentz profile rises, the dip becomes shallower and finally disappears. The Matvejev formula is a much poorer approximation for the zero point than either the Kielkopf or the Whiting formulas (see Fig. 2). The Whiting[7] formula is the simplest, but does not yield a reasonable description for the curvature. The relative error of 10% in the line-wings is not surprising. The Poljakov[2] program furnishes results with relative errors, for narrow regions of the input values, of less than 2% (Fig. 1d). For most of the input values, the relative error does not exceed 10^{-3}. The precision of the Poljakov program is the result of many of approximations used for all values. Many peaks and jumps in the curve reflect this fact very clearly. In Fig. 3, we show regions of validity of the different formulas for the programs of Armstrong[1] and Poljakov.[2] Drayson[4] claims for his program a relative error smaller than 10^{-4}. This requirement is met. With the exception of a few points in the input value domain, the error is smaller than 10^{-5}.

COMPARISON OF THE TIME REQUIRED FOR CALCULATIONS

For comparison, each of the computing programs was used to calculate the Voigt profile P_V for the same input values. The time needed by each program for different $\nu - \nu_0$ and constant

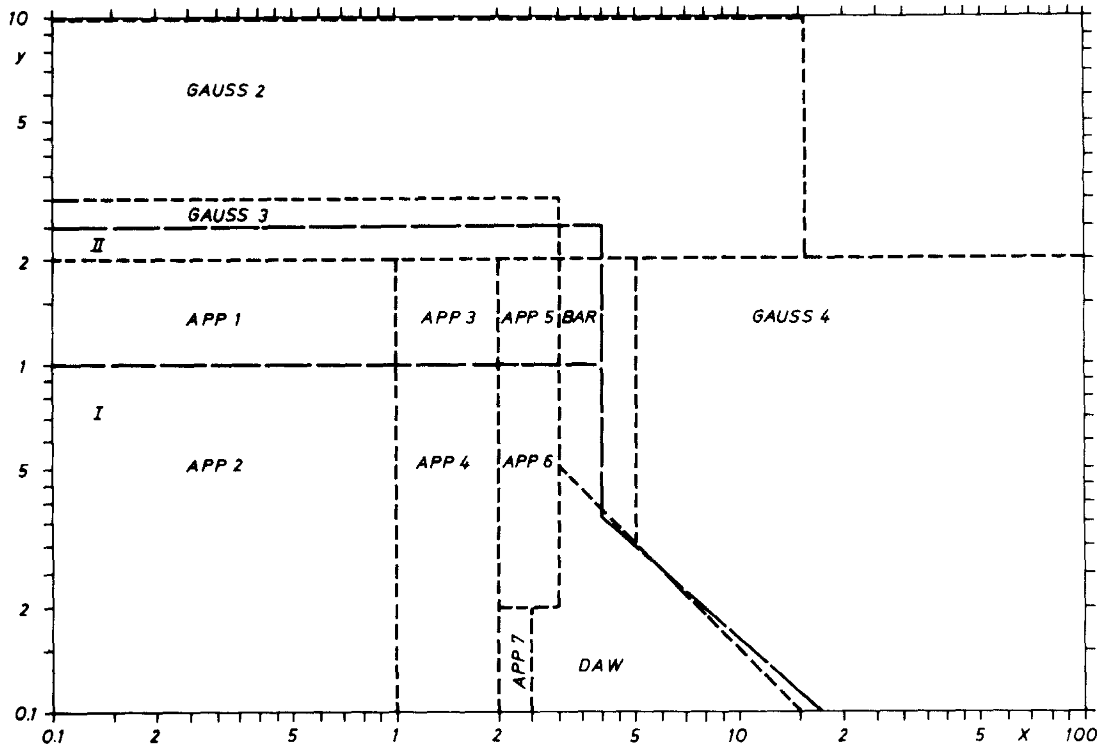

Fig. 3. Partition of the x-y-domain into regions in which different formulas are used. The lines with long dashes indicate the region in which we used the formulas I and II of the Armstrong[1] program. In the remainder of the x-y-domain, the formula III is used. The lines with short dashes show regions for different formulas in the Poljakov[2] program. In the remainder of the x-y-domain, Gauss 1 is used.

α_L/α_D, was estimated. We used 50–150 $\nu - \nu_0$ values distributed in different ways over the $\nu - \nu_0$ interval. The influence of α_L/α_D on the computing time could be determined exactly, whereas the influence of $\nu - \nu_0$ on the computing time could only be estimated. The absolute values of the computer time are, of course, typical for the machine used and for the calculated values selected. The ratios of computer times are believed to be of importance. The results are shown in Fig. 4.

For $\alpha_L/\alpha_D > 3$ (the Lorentz profile prevails in the Voigt profile), the computer times are rather short. The Armstrong[1] program needs about half the time of the Gautschi[3] program. The computer times do not depend on x.

For $\alpha_L/\alpha_D < 1$ (the Doppler profile prevails in the Voigt profile), the calculation times are longer. In this domain, the needed times increase with decreasing $\nu - \nu_0$. The Armstrong program requires about 3–6 times more computer time than the Gautschi program. The running times of the programs using approximation formulas are not influenced by $\nu - \nu_0$ and α_L/α_D. The computing speed of the Drayson program lies between the speed of the Poljakov program and the speed of the Kielkopf, Matvejev, and Whiting programs.

The results of our comparisons of calculation times between the Armstrong and Gautschi programs do not agree with those of Ref. 13, presumably because an improved program was used.

CONCLUDING REMARKS

After completion of our calculations, new methods[13-16] were published. These were not included in the comparisons. The relative error gives only rough information about the practical usefulness of the programs. In calculating transmittance, we must integrate over the entire line profile, for which absolute rather than relative errors are important. Since Voigt profiles with different α_L/α_D contribute to the transmittance, and since the sign in the errors may change, the errors will, possibly, compensate for each other. The following recommendations relate to these qualifications. Because of its good accuracy, the Gautschi[3] program should be used for

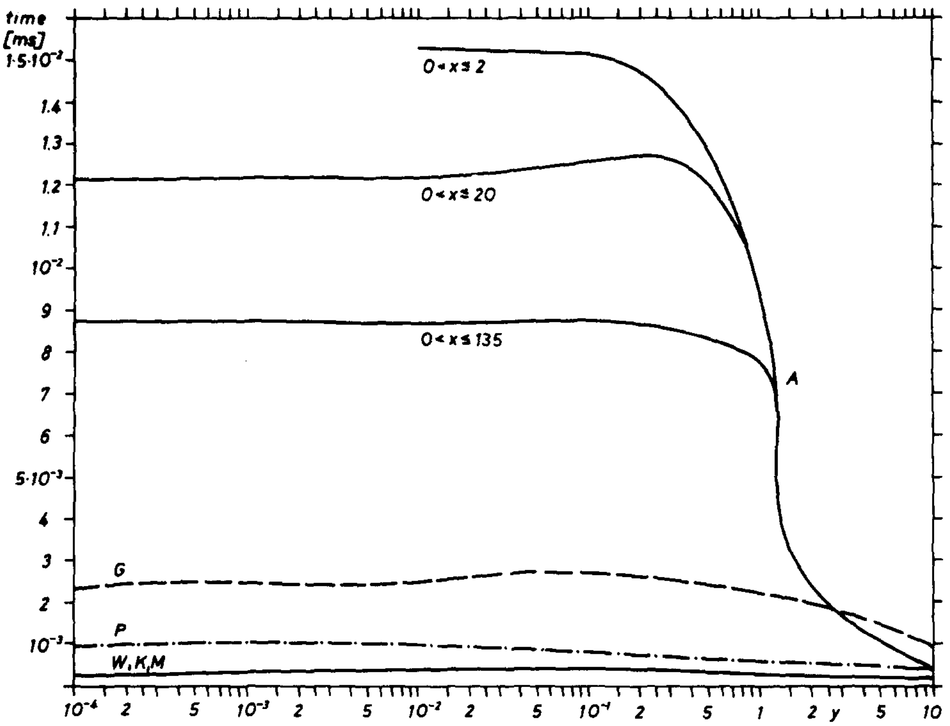

Fig. 4. Computing times for the programs under test as a function of y. The capital letters denote the following programs: A, Armstrong;[1] G, Gautschi;[3] K, Kielkopf;[5] M,Matvejev;[6] P, Poljakov;[2] Whiting.[7]

high-precision calculations. If we can accept a few percent of error in the Voigt profile and need to save time, both the Kielkopf[5] (for $0 \leq x \leq 1$ and $y < 1$) and the Matvejev[6] approximations may be used jointly to yield reasonable accuracy and high-speed calculations. In all other cases, the Drayson[4] program is useful.

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