

NOTE

RAPID COMPUTATION OF THE VOIGT PROFILE

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(Received 7 August 1975)

Abstract—A computational procedure is described to evaluate the Voigt function with a maximum relative error of about one part in 10^4 , for use in line-by-line transmittance calculations and other applications. An efficient Fortran IV subprogram is given in the Appendix.

OUTLINE OF COMPUTATIONAL PROCEDURE

ATMOSPHERIC transmittance calculations for regions in which both Doppler and Lorentz line broadening are important require the evaluation of the Voigt profile function, viz.

$$K(x, y) = \frac{y}{\pi} \int_{-\infty}^{\infty} \frac{\exp(-t^2)}{y^2 + (x-t)^2} dt, \quad x, y \geq 0. \quad (1)$$

For an extensive review of the numerical methods employed and references to tabulations, the reader is referred to Armstrong,⁽¹⁾ Young,⁽²⁾ and Armstrong and Nicholls.⁽³⁾ These authors describe computer routines which are suitable for use with arbitrary values of the parameters x and y rather than for the preparation of tables, which was the intent of several earlier authors.

Direct integration or line-by-line methods of computing atmospheric transmittance are now widely employed when high accuracy is required. The computer programs call repeatedly for the evaluation of the Voigt profile, which may account for a considerable fraction of the execution time of the program. For example, computing the Voigt profile with a modified routine from Young⁽²⁾ took about 75% of the total execution time in a test calculation of transmittance using a program developed by Drayson.⁽⁴⁾ Thus, improvement in efficiency of the Voigt routine could considerably reduce the expense of calculating transmittances.

Most routines give an accuracy corresponding to six significant figures or better, although double-precision arithmetic is required to reduce the round-off error on some machines. However, the numerical accuracy of the transmittances in the line-by-line method is usually limited to about four decimal places by the truncation error of the numerical quadrature of the intergral over frequency. The absolute error is further limited by uncertainties in the line parameters, these usually being the dominant source of errors.

An accuracy of 6 decimal figures in the Voigt routines is not normally needed for transmittance calculations. A relative error of 1 part in 10^4 would not contribute to a transmittance error of more than 1 in the fourth decimal place, which is compatible with the other sources of error. In writing the subroutine, speed and accuracy were the primary concern while other factors, such as storage and a small number of statements, were considered only after these criteria has been met. Several techniques described in the literature were programmed and tested for speed and accuracy, with the fastest being incorporated into the function program. Three methods were selected for use in the three regions identified in Fig. 1.

Region I. The method adopted is a variation of the Taylor series expansion [FADDEYERA and TARENTEV⁽⁵⁾]. If $y > 0$, the Voigt function is the real part of the complex probability function

$$w(z) = e^{-z^2} \left(1 + \frac{2i}{\sqrt{\pi}} \int_0^z e^{t^2} dt \right), \quad (2)$$

where $z = x + iy$. Equation (2) may be rewritten as

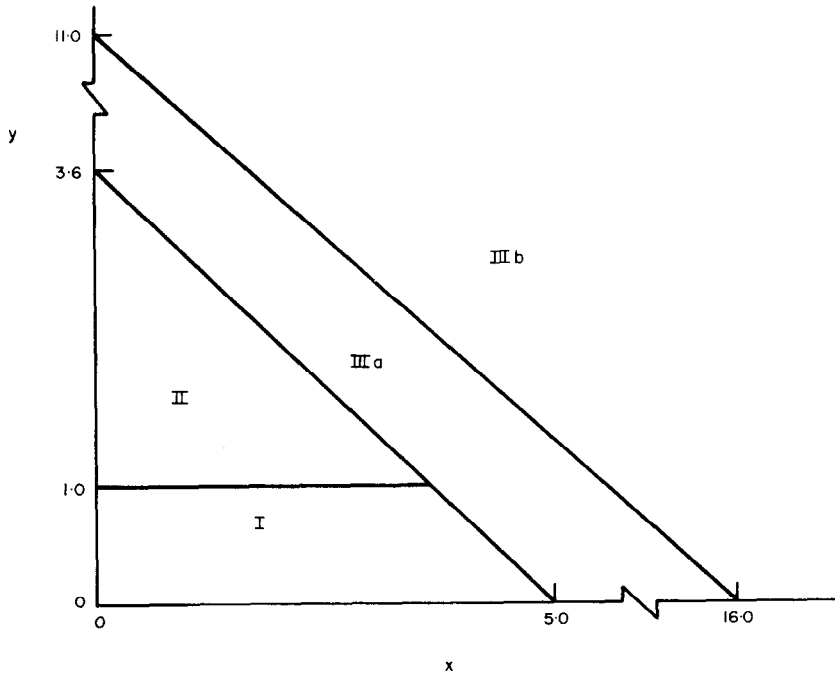


Fig. 1. Computational regions used in this paper.

$$\left. \begin{aligned} w(z) &= e^{-z^2} + \frac{2i}{\sqrt{\pi}} F(z), \\ F(z) &= e^{-z^2} \int_0^z e^{-t^2} dz. \end{aligned} \right\} \quad (3)$$

For real z , the function $F(z)$ is known as Dawson's function. The coefficients d_n of the Taylor series expansion of $F(z)$ about a real point x obey the relationships

$$d_0 = F(x), \quad d_1 = 1 - 2xd_0, \quad d_{n+1} = -\frac{2}{(n+1)}(xd_n + d_{n-1}) \quad \text{for } n = 1, 2, \dots \quad (4)$$

Dawson's function is first evaluated on the x -axis and the Taylor series is used to find the imaginary part of $F(z)$ and hence the real part as $w(z)$.

Dawson's function may be evaluated by series expansion, as asymptotic expansion or a Chebyshev expansion due to HUMMER.⁽⁶⁾ The procedures are time-consuming and add considerably to the execution time of the program if evaluated separately for each entry to the Voigt function. In a faster method developed for the program, Dawson's function is evaluated initially by the Chebyshev expansion at points on the x -axis spaced 0.2 apart at $x = 0.1, 0.3, 0.5, \dots, 4.9$. The coefficients d_1, d_2, d_3, d_4 are also computed at each point using eqn (4) and are then stored for later use. This process is relatively inefficient but has to be done only once for 25 values of x in the interval (0.0, 5.0). Dawson's function is evaluated for arbitrary x by a Taylor series expansion about the nearest point, distance at most 0.1 away, assuring rapid convergence.

The number of terms needed in the Taylor series expansion of $F(z)$ depends on x and y . Testing for convergence slows the program and is not easy since the absolute value of the terms does not always decrease monotonically. The number of terms needed was determined for several values of x and y and an empirical function developed (see program listing).

Region II. The function w has a continued fraction expansion [FRIED and CONTE⁽⁷⁾], viz.

$$\sqrt{(\pi)} w(z) = \frac{1}{z +} \frac{(1/2)}{z +} \frac{1}{z +} \frac{(3/2)}{z +} \dots \frac{(n/2)}{z +} \dots$$

For $y > 1$, the expansion of $w(z)$ converges rapidly so that the continued fraction becomes an

efficient method in Region II. Along the line $y = 1$, which separates Regions I and II, the Taylor series and the continued fraction require about the same computer time but in each region the time decreases with distance from the line.

The number of terms needed in the continued fraction expansion varies from $n = 4$ near the border of Region III to $n = 19$ near the point $x = 0, y = 1$. An empirical function was again developed to avoid the necessity of testing for convergence.

Region III. Numerical integration of the integral (1) by Gauss-Hermite quadrature is simple, fast and accurate for sufficiently large x and y and is employed in Region II. In Region IIIa 4-point quadrature is required to maintain accuracy, while a 2-point quadrature is adequate in Region IIIb. Outside these regions, the required order of the quadrature increases rapidly and other methods must be used.

For very small values of y , the relative error of the method becomes larger than 1 part in 10^4 but, since the numerical value of the integral is small, this is rarely a significant factor.

An efficient FORTRAN IV subroutine was written (see the Appendix for details) and tested for speed and accuracy on an IBM 370/168. This machine was a word length of 32 bits, shorter than that of other machines commonly used in scientific calculations, so that problem due to round-off error on different machines should not arise. Table 1 gives the CPU time in each computational region. Also shown is the CPU time for a method due to Rybicki [see ARMSTRONG and NICHOLLS⁽³⁾] in which the function $w(z)$ is expanded in a series. Limiting the sum from $n = -8$ to $+8$ gives about the same accuracy as the routine described here, but is slower except in a small region of comparable speed. A routine given by GAUTSCHI⁽⁶⁾ is more than five times slower than the routine described in this paper, so no attempt was made to increase speed at the expense of accuracy. The technique employed by KIELKOPF⁽⁹⁾ is not suitable for transmittance calculations since it sometimes gives only an accuracy of one significant figure.

In a test of transmittance calculations described earlier, the new routine evaluation the Voigt profiles almost five times faster and the execution time of the entire program was less than half. The transmittances, averaged over 0.1 cm^{-1} intervals, differed at most by 2×10^{-6} , which is considerably more accurate than the original aim, partly because the function accuracy was usually better than 1 part in 10^4 and partly because the integrations in the transmittance program tended to average the alternating signs of the errors.

Table 1. CPU time of routines for calculating Voigt profiles, in microseconds (IBM 370/168).

Region		This paper	Rybicki
I	Maximum	185	250
	Minimum	125	
II	Maximum	250	
	Minimum	45	
IIIa		40	
IIIb		30	

Summary of computational methods

(a) *Region I.* $y \leq 1.0, x < 5.0 - 0.8y$. In the initial entry, only Dawson's function is evaluated at 25 points on the x -axis using a Chebyshev expansion [HUMMER⁽⁶⁾]. Dawson's function $F(x)$ is obtained from a Taylor-series expansion about the nearest of the 25 points. A second Taylor series with $x = \text{constant}$ is used to obtain $F(z)$ [FADDEYEVA and TERENCEV⁽⁵⁾].

(b) *Region II.* $y > 1.0$ and $x < 1.85(3.6 - y)$. We used a continued fraction [FRIED and CONTE⁽⁷⁾].

(c) *Region III.* All x, y not in I and II. For $y \geq 11.0 - 0.6875x$, we used a 2-point Gauss-Hermite quadrature; for $y < 11.0 - 0.6875x$, we used a 4-point Gauss-Hermite quadrature.

Acknowledgements—The work described in this paper was supported by the National Environmental Satellite Service, NOAA, and by the NASA Langley Research Center.

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APPENDIX: A

FORTRAN program for the Voigt function

The Fortran IV computer program for the evaluation of the Voigt function uses the efficient numerical methods described in the text and the following FORTRAN code.

```

C *** FUNCTION VOIGT (X,Y)
C *** ROUTINE COMPUTES THE VOIGT FUNCTION: Y/PI*INTEGRAL FROM -
C *** - TO + INFINITY OF EXP(-T*T)/(Y*Y+(X-T)*(X-T)) DT
REAL B(22)/0.,.7093602E-7/,RI(15),XN(15)/10.,9.,.2*8.,.7.,.6.,.5.,.4.,.7
1*3./,YN(15)/3*.,6.,.5.,.2*.,4.,.4*.,3.,.1.,.9.,.8.,.2*.,7/,D0(25),D1(25),D2(25),
2D3(25),D4(25),HN(25),H/.,201/,XX(3)/.,5246476.,1.,65066.,.7071066/,HN(3
3)/.,2562121.,.2588268E-1.,.2820946/,NBY2(19)/9.,5.,9.,.8.,.5.,.8.,.7.,.5.,.7.,.6.,5
4/.,5.,.5.,.4.,.5.,.4.,.3.,.5.,.3.,.2.,.5.,.2.,.1.,.5.,.1.,.5/,C(21)/.,7093602E-7.,.251
58434E-6.,.8566874E-6.,.2787638E-5.,.866074E-5.,.2565551E-4.,.728775E
6.,.4.,.1933631E-3.,.4899580E-3.,.1173267E-2.,.2648762E-2.,.5623190E-2.,
7.,.119601E-1.,.2084976E-1.,.3621573E-1.,.5851412E-1.,.8770816E-1.,.12
81664.,.15584.,.184.,.2/
LOGICAL TRU/.FALSE./
IF (TRU) GO TO 104
C *** REGION I. COMPUTE DAWSON'S FUNCTION AT MESH POINTS ***
TRU=.TRUE.
DO 101 I=1,15
  RI(I)=-I/2.
DO 103 I=1,25
  HN(I)=H*(I-.5)
  CO=4.*HN(I)*HN(I)/25.-2.
DO 102 J=2,21
  B(J+1)=CO*B(J)-B(J-1)+C(J)
  DO(I)=HN(I)*(B(22)-B(21))/5.
  D1(I)=1.-2.*HN(I)*DO(I)
  D2(I)=(HN(I)*D1(I)+DO(I))/RI(2)
  D3(I)=(HN(I)*D2(I)+D1(I))/RI(3)
  D4(I)=(HN(I)*D3(I)+D2(I))/RI(4)
DO 104 IF (X-.5.) 105,112,112
DO 105 IF (Y-.1.) 110,110,106
DO 106 IF (X.GT.1.85*(3.6-Y)) GO TO 112
C *** REGION II: CONTINUED FRACTION. COMPUTE NUMBER OF TERMS NEEDED. ***
IF (Y.LT.1.45) GO TO 107
I=Y+Y
GO TO 108
DO 107 I=11.*Y
  J=X+X+1.85
  MAX=XN(J)*YN(I)+.46
  MIN=MINO(16,21-2*MAX)
C *** EVALUATE CONTINUED FRACTION ***
UU=Y
VV=X
DO 109 J=MIN,19
  U=NBY2(J)/(UU*UU+VV*VV)
  UU=Y+U*UU
  VV=X-U*VV
DO 109 VOIGT=UU/(UU*UU+VV*VV)/1.772454
RETURN
Y2=Y*Y
IF (X+Y.GE.5.) GO TO 113
C *** REGION I. COMPUTE DAWSON'S FUNCTION AT X FROM TAYLOR SERIES. ***
N=X/H
DX=X-HN(N+1)
U=C((D4(N+1)*DX+D3(N+1))*DX+D2(N+1))*DX+D1(N+1))*DX+D0(N+1)
U=1.-2.*X*U
C *** TAYLOR SERIES EXPANSION ABOUT Y=0.0 ***
UU=EXP(Y2-X*X)*COS(2.*X*Y)/1.128379-Y*Y
UU=-Y
MAX=5.+(12.5-X)*.8*Y
DO 111 I=2,MAX,2
  U=(X*U+U)/RI(I)
  V=(X*U+U)/RI(I+1)
  UU=-UU*Y2
DO 111 VV=VV+V*UU
  VOIGT=1.128379*VV
RETURN
Y2=Y*Y
IF (Y.LT.11.-.6875*X) GO TO 113
C *** REGION IIIB: 2-POINT GAUSS-HERMITE QUADRATURE. ***
U=X-XX(3)
V=X+XX(3)
VOIGT=Y*(HH(3)/(Y2+U*U)+HH(3)/(Y2+V*V))
RETURN
C *** REGION IIIC: 4-POINT GAUSS-HERMITE QUADRATURE. ***
U=X-XX(1)
V=X+XX(1)
UU=X-XX(2)
VV=X+XX(2)
VOIGT=Y*(HH(1)/(Y2+U*U)+HH(1)/(Y2+V*V)+HH(2)/(Y2+UU*UU)+HH(2)/(Y2+
1VV*VV))
RETURN
END

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