DEPARTMENT OF GEOPHYSICAL SCIENCES
SCHOOL OF SCIENCES AND HEALTH PROFESSIONS
OLD DOMINION UNIVERSITY
NORFOLK, VIRGINIA

Technical Report GSTR-79-9

THE DETERMINATION OF ATMOSPHERIC TRACE GASES USING THE CORRELATION INTERFEROMETER TECHNIQUE

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By

Jerold T. Twitty

and

Earl C. Kindle
Principal Investigator

Final Report
For the period ending January 31, 1979

Prepared for the
National Aeronautics and Space Administration
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Hampton, Virginia

Under
Research Grant NSG 1131
J.A. Dodgen, Technical Monitor
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By

Jerold T. Twitty[1] and Earl C. Kindle[2]

INTRODUCTION

This report describes the total research efforts and results obtained under NASA grant NSG 1131. The discussion is presented under four major headings:

(1) Summary of results of the cumulative research efforts conducted during the entire grant period,

(2) Summary of results of research efforts during 1975,

(3) Summary of results of research efforts during 1976, and

(4) Summary of results of research efforts for 1977.

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SUMMARY OF RESULTS OF THE CUMULATIVE RESEARCH EFFORTS CONDUCTED DURING THE ENTIRE GRANT PERIOD

The work presented in this report and in previous annual reports has demonstrated the theoretical feasibility inherent in the correlation interferometry technique. High signal-to-noise and increased information content in a given partial interferogram are attractive features of the technique. The main difficulty is in the separation of interfering gas species, particularly methane. This can be overcome by a precise measurement program for methane and other species spectral line parameters. The work of Toth (private communication) is a step in that direction.

In reality, the most important consideration to be dealt with in the demonstration of correlation interferometry has been the hardware design problem. This hardware, COPE, has elecontric, optical, and mechanical difficulties that are simply impossible to fix at this late date. After a one-year refurbishment of the electronics, the digital interface fails intermittently and the analog AGC network has a strange nonlinear response.

Flight data from Cessna 402 over southeastern Virginia during April 1978 yielded amplitude fluctuations that were not explainable except as internal nonlinearities. Misalignment of the AGC/interferometer optical axis also contributed to a large error source in the flight data. The conclusion is that no useful data on gas burdens was obtained from these flights.

It is hoped that the second generation correlation interferometer, CIMATS, will solve all of these problems and that it will be able to fulfill the expectations for the technique.

SUMMARY OF RESULTS OF RESEARCH EFFORTS DURING 1975

Several months at the beginning of this grant were spent in gaining familiarity with the correlation interferometer technique and with existing CO Pollution Experiment (COPE) instrumentation. A computer program to simulate the COPE instrument was developed during this time by extending an existing program which was written by General Electric, the COPE contractor. A substantial effort has been expended toward understanding the COPE signal. This has included laboratory testing of stability, sensitivity, and theoretical analyses. In addition, COPE data obtained during a flight field test in Washington, DC, in July 1974, were reanalyzed to determine the source of observed methane variations in that data. The results of these various tasks are presented in the technical report mentioned on page 4.

Work was also performed on theoretical aspects of Correlation Interferometric Measurements of Atmospheric Trace Species (CIMATS), which is a multigas version of COPE. Computer programs exist for the analysis of the CIMATS experiment, and some preliminary work has been done.

Two papers were published during 1975 and two papers presented at the AMS Radiation Conference in Arlington, Virginia. Another paper was submitted for publication in April 1976. These publications are listed below:

DeLuisi, J.; Charlson, R.; Fegley, R.; Furukawa, P.; Gillette, D.; Herman, B.; Schuster, B.; Twitty, J.T.; and Weinman, J.: Results of a Comprehensive Aerosol-Radiation Field Experiment in the Southwestern United States. Presented at the Second Annual Radiation Conference of AMS (Arlington, VA), October 29, 1975.

Twitty, Jerold T.: The Inversion of Aureole Measurements to Derive Aerosol Size Distributions. J. Atmos. Sci., Vol. 32, 1975, pp. 584-591.

Twitty, Jerold T.: Airborne Measurements of the Solar Aureole and the Remote Determination of Atmospheric Aerosol Size Distributions. Presented at the Second Annual Radiation Conference of AMS (Arlington, VA), October 29, 1975.

Twitty, J.T.; Parent, R.J.; Weinman, J.A.; and Eloranta, E.W.: Aerosol Size Distributions: Remote Determination from Airborne Measurements of the Solar Aureole. To be published in April 1976 in Appl. Opt.

Weinman, J.A.; Twitty, J.T.; Browning, S.R.; and Herman, B.: Derivation of Phase Functions from Multiple Scattered Sunlight Transmitted through a Hazy Atmosphere. J. Atmos. Sci., Vol. 32, 1975, pp. 577-583.

In addition, the technical report contained in the following section was published and forwarded through channels to the Technical Monitor in 1976.

SUMMARY OF RESULTS OF RESEARCH EFFORTS DURING 1976

Work performed under grant NSG 1131 during 1976 contributed to the objectives of the grant in two ways. First, a theoretical error analysis for the CO/CH_4 measurement for the solar reflected channel for both the CIMATS and the COPE instruments was completed. Second, an empirical/theoretical analysis of COPE field data obtained at NASA/Langley Research Center (LaRC) was undertaken. The aim of these analyses was to assess the general outlook of the correlation technique and to assess the capability of COPE to performs to its specifications.

The theoretical error analysis was undertaken for the CO/CH_4 CIMATS reflected solar channel. These calculations included errors induced by noise and by the algorithm application necessary to separate out the individual gas burdens. A line-by-line atmospheric radiative transfer model was developed. This model includes temperature, humidity, CO, and CH_4 vertical profiles with approximately 2-km resolution. This model was used to calculate a high-resolution absorption spectrum as a function of various atmospheric parameters. Estimated optical and electronic filters were applied to this spectrum, and CIMATS interferometer visibility curves were applied to the Fourier transformed spectrum to yield interferograms as a function of delay. This represents simulated CIMATS output. This signal was calculated for various gas burdens, including water vapor and for different temperature profiles. A set of base interferograms was used to obtain derivatives of these interferograms with respect to CO, CH_4, and H_2O gas burdens. These derivatives were used to calculate least square solutions for individual gas burdens by determination of weights applicable to a linear variation in gas burden change. These weights, when applied to a measured (or simulated) interferogram, yield an estimate of total gas burdens. Noise was added to these simulated derivatives to estimate errors in the instrument transfer function, i.e., errors in the parameters characterizing the instrument response.

The results of this analysis are presented in table 1. The model was used to calculate interferograms with random gas burdens (within stated limits) for CO, CH_4, and H_2O. Noise representative of instrument NEP was added to these interferograms and the gas burdens estimated by application of the algorithm. As shown in table 1, the average error for CO was 0.002 atm-cm. This corresponds to a change of 2 ppb throughout the atmosphere or a change of 0.2 ppm in a 100-m layer. These errors are well within the stated objectives for CIMATS.

The second analysis used real data from the COPE correlation interferometer. During the period reported a number of instrument difficulties with COPE prevented an assessment of the capabilities of the instrumentation. Beginning in October 1976, atmospheric data was gathered routinely. In the absence of an accurate instrument transfer function to enable the theoretical calculation of gas burden derivatives, this data has been analyzed using empirically determined derivatives and calibrations. Some of this data is presented in figure 1a. The measurement represents the total burden of CH_4 between the Sun and the Earth's surface and, therefore, varies with Sun elevation angle. The solid line represents the variation due to the change in solar elevation angle for a constant amount of methane in the atmosphere. Figure 1b represents similar results for CO. At this time, these results are preliminary and the variations away from the nominal line cannot be considered to be real. These fluctuations correspond to variations of 0.02 atm-cm for CO and 0.075 atm-cm for CH_4: this is only a factor of 2 worse than the estimated error limit for COPE obtained by extrapolation of the simulated CIMATS results presented in table 1.

In conclusion, the CIMATS and COPE instrumentation appear to have the theoretical capability to make excellent remote measurement of CO, CH_4, and H_2O gas burdens. To reach this theoretical limit, the proper handling of water vapor effects must be included. This can be done only by interfacing the theory with the instrument through the instrument transfer function (ITF). Work is underway by GE to obtain this function for CIMATS. The ITF is needed for COPE also, but as yet a satisfactory measurement has not been made.

TABLE 1

Gas	Average Error (atm-cm)	Maximum Error (atm-cm)	Range of Gas Burden (atm-cm)
CO	0.002	0.005	0.07-0.13
CH_4	0.01	0.02	1.2 - 1.6
H_2O	14.	28	350 - 3800 (dry) (moist)

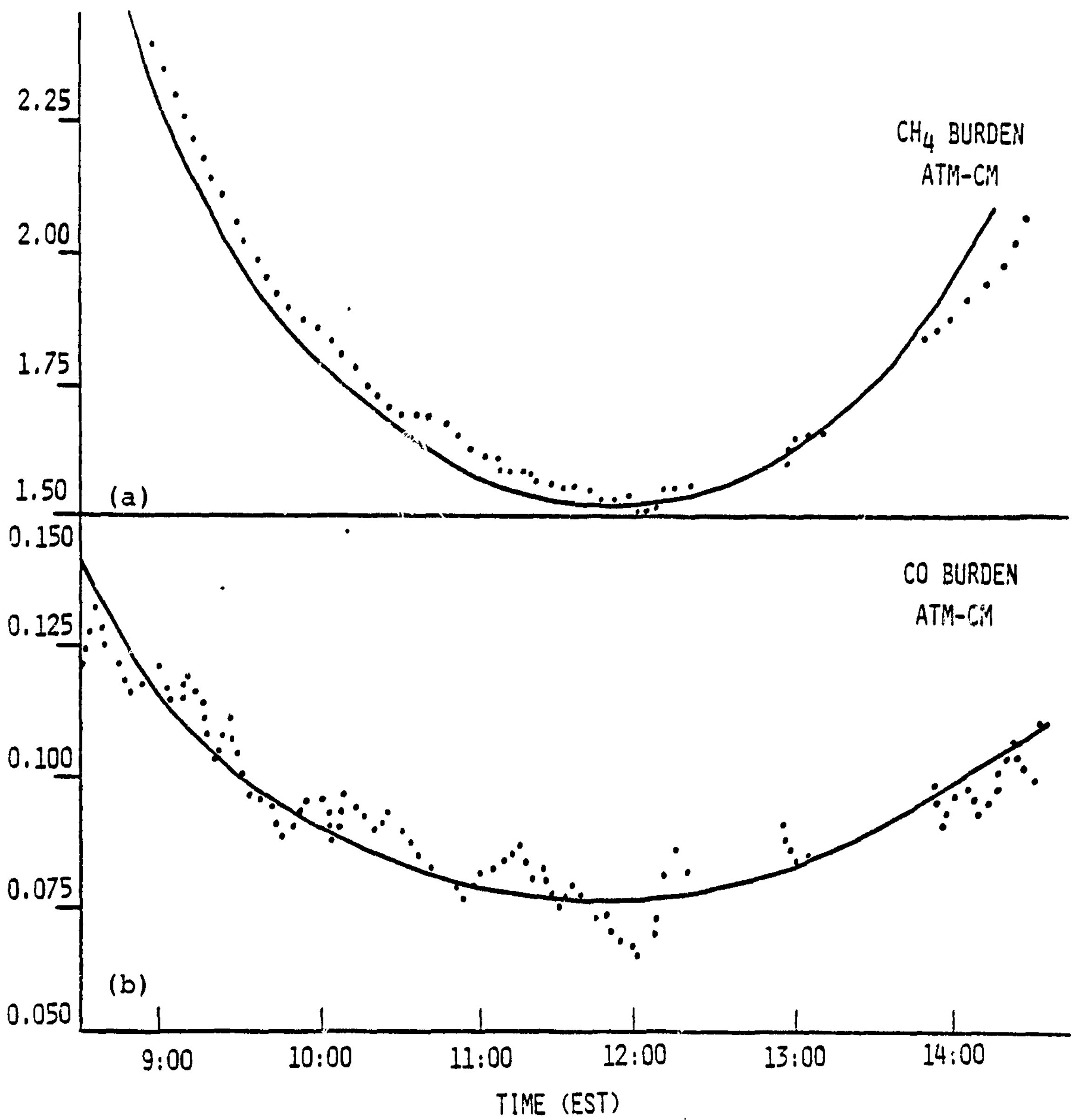

Figure 1. Estimation of CO + CH_4 atmospheric gas burdens, November 5, 1976 at Langley Research Center.

SUMMARY OF RESULTS OF RESEARCH EFFORTS FOR 1977

Efforts for the first half of this year were reported in the semiannual report of July 1977. The problems reported therein with the optical components of CIMATS have been solved, and an acceptable beamsplitter was delivered to General Electric in February 1978. An assessment of the improvement in signal-to-noise ratio has begun. A second problem which was slowing analysis at that time was the lack of good CH_4 line parameter data. Improved line parameter positions and strengths have been measured by Dr. Toth at JPL and recently delivered to NASA/LaRC. However, some discrepancies between this data and the previous preliminary data have been discovered. These discrepancies are being investigated.

A major new effort begun during the second half of this year was to iniciate the writing of a modular atmospheric line-by-line radiative transfer program for the STAR computer. Such a program would be faster than current CDC-6600 software and would aid in further analyses. As a part of this effort, new Voigt profile software has been written for both NOS-6600 and STAR computers for several new fast algorithms reported recently in the literature. This study is reported in Appendix A.[3]

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3 In the preparation of this report an error was discovered in the derivation of the Kielkopf approximation to the Voigt profile. Hence the errors of approximation described herein are not valid and the graphical representation in Appendix A should be recalculated.

APPENDIX A

This appendix represents a part of a paper on a new atmospheric radiative transfer development effort currently underway, and is intended to be part of a future publication documenting that effort.

COMPARISON OF VARIOUS COMPUTATIONAL METHODS FOR THE CALCULATION OF THE VOIGT PROFILE FUNCTION

In line-by-line radiative transfer calculations, the line shape of individual lines is, in general, described by the Voigt profile function, an integral expression requiring substantial computational time. Several proposed procedures for the calculation of this function have been investigated as to their accuracies and computational speed on the NASA/LaRC NOS-6600 and STAR computer systems. This is intended as part of a development of a radiative transfer program in a structured modular approach for general atmospheric application. Limits where the Lorentz or Doppler approximations are appropriate are given in terms of the parameterized profile, and considerations on the calculational termination of typical atmospheric conditions are discussed.

Atmospheric radiative transfer calculations, in general, require the evaluation of the Voigt profile function:

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

where

$$x = 2.326 \times 10^6 (\Delta\nu/\nu_o)(M/T_o)^{1/2}$$

$$y = 2.326 \times 10^6 \alpha_o (P/P_o)(M/T_o)^{1/2}/\nu_o$$

ν_o = center frequency of line

α_o = line width at reference pressure P_o and temperature T_o

M = molecular weight of gas

$\Delta\nu = \nu - \nu_o$

for atmospheric pressure and temperature conditions where both Lorentz and Doppler line broadening are important. Several recent authors (refs. 1 to 3) have reported computational procedures for the rapid evaluation of this function.

As part of an effort to improve the accuracy and speed of existing radiative transfer codes in use at NASA/LaRC for the COPE/CIMATS program, the relative accuracy and speed of these methods have been reviewed for typical values of the parameters x and y needed in tropospheric calculations. In addition, for comparison, two existing codes (refs. 4, 5) which are used currently in NASA/LaRC radiative transfer codes were included.

The actual codes tested on the NOS system were written in FTN FORTRAN and represent either syntactical conversions of the codes presented in the references or codes based on the described algorithm. These codes are given in Appendix B (methods A through H). In order to test the relative computational times of these codes for realistic conditions, a range of x and y parameters was used and the total CPU time was determined for each code. The values of y used were y = 0.1(0.1)1.0(1.0)11.0 and the values of x used were x = 0.0(0.25)25.0. It will be shown later that these are a typical range of parameters needed for tropospheric calculations.

The results of this timing test are given in table A1. These results confirm that the computational schemes D and E of references 2 and 3 are indeed faster, but that method C of reference 1 is neither faster nor as accurate. Comparison of the Kielkopf method (ref. 1) with the actual Voigt profile is shown in figure 1A. All of the remaining algorithms are accurate to five decimal places for the calculated parameters. Since the codes D and E were comparable in speed and accuracy, the latter was chosen to be used in the improved radiative transfer code because of its simplicity and easier vectorizability for the STAR computer. It should be noted that the Drayson code (method D) as given in that reference is not exactly the same as that described in the text of that paper, but in fact has some odd subregions. These do not appear to affect the results, however.

The method E has been coded for the STAR using the NASA/LaRC language SL/1, a vector language structured like PL1. This language allows for the use of the halfword capability of STAR and easy vector manipulation. This code is also given in Appendix B. The timing result for the same sample space is given as case H in table A1. A disappointing result is that the STAR vectorized function is no faster than the fast NOS-6600 CPU times, at least for vectors of length 101. Since times improve as vector length increases on STAR, it may yet be possible to gain by using STAR. Further investigations are underway.

The requirements on sampling of the profile, on cutoff limits for the profile, and the applicability of the Lorentz or Doppler approximation have been investigated. Figures A2, A3, and A4 show three Voigt profiles for values of the parameter y of 0.1, 1.0, and 10.0. This represents the typical range for y in the atmosphere. This would correspond roughly to pressues of 10, 100, and 1000 mbar. Note that the Doppler limit is not reached even at the lowest pressure. Note also that the Lorentz profile is an excellent approximation for the highest pressure (lowest altitude) as would be expected. However, even at $y = 1.0$ the Lorentz profile is good in the wings of the line. This would seem to allow for a generalized Voigt/Lorentz routine with regions where the Lorentz profile could be used. Since the profile is only a function of x and y and does not depend on the specific molecule or line except through these parameters, such a function would be uniquely defined. The computational speed of such a hybrid function has not been investigated as yet, but since the simple Lorentz form is faster, one would expect an improvement.

A final consideration is the necessary sampling and the limit of a line. Since a line extends to infinity in principle, a cutoff must be defined for the practical calculation. Typically this cutoff has been given in wave number space with values of 3 to 5 cm^{-1} commonly used. For values of Doppler half width this would be a cutoff limit of $x = 500$ to 1000. From figures A2 to A4, it can be seen that this is an extreme limit. It would appear that a limit of $x = 100$ is sufficient for all atmospheric conditions. This would be typically one wave number either side of the line center. Since this limit is very important from the computational viewpoint, this conclusion will be incorporated into the new radiative transfer program. The typical sampling used in radiative transfer programs is 0.01 cm^{-1}. This corresponds to a sampling of steps of 2 in x space. This is seen to be adequate except for the highest altitudes (fig. A2). The new program will be written with this as the nominal sampling, but with provisions for increasing the sampling if necessary.

ACKNOWLEDGMENTS

The work of P.L. Rarig of Systems and Applied Sciences Corp. is acknowledged in the coding of the various algorithms and in the design and coding of the SL/1 code for the STAR. L. Vian is thanked for his assistance in the plotting of the data used in this paper. This research was supported by NASA grant NSG 1131.

APPENDIX A REFERENCES

1. Kielkopf, J.F.: New Approximation to the Voigt Function with Applications to Spectral-Line Profile Analysis. JOSA, 63, pp. 987-994, 1973.

2. Drayson, S.R.: Rapid Computation of the Voigt Profile. JQSRT, 16, pp. 611-614, 1976.

3. Pierlussi, J.H.; Vanderwood, P.C.; and Gomez, R.B.: Fast Calculational Algorithm for the Voigt Profile. JQSRT, 18, pp. 555-556, 1977.

4. Bortner, M.H.; Alyea, F.N.; Grenda, R.N.; Liebling, G.R.; and Levy, G.M: Analysis of the Feasibility of an Experiment to Measure Carbon Monoxide in the Atmosphere. NASA Contractor Report, NASA CR-2303, 1973.

5. Kyle, T.: Unpublished data, 1976.

Table A1

Method	Case	CPU Time (sec)
Bortner et al.	A	0.147
Kyle	B	0.411
Kielkopf	C	0.132
Drayson	D	0.050
Pierlussi et al.	E	0.050
Lorentz approximation	F	0.026
Doppler approximation	G	0.037
Method E on STAR	H	0.057

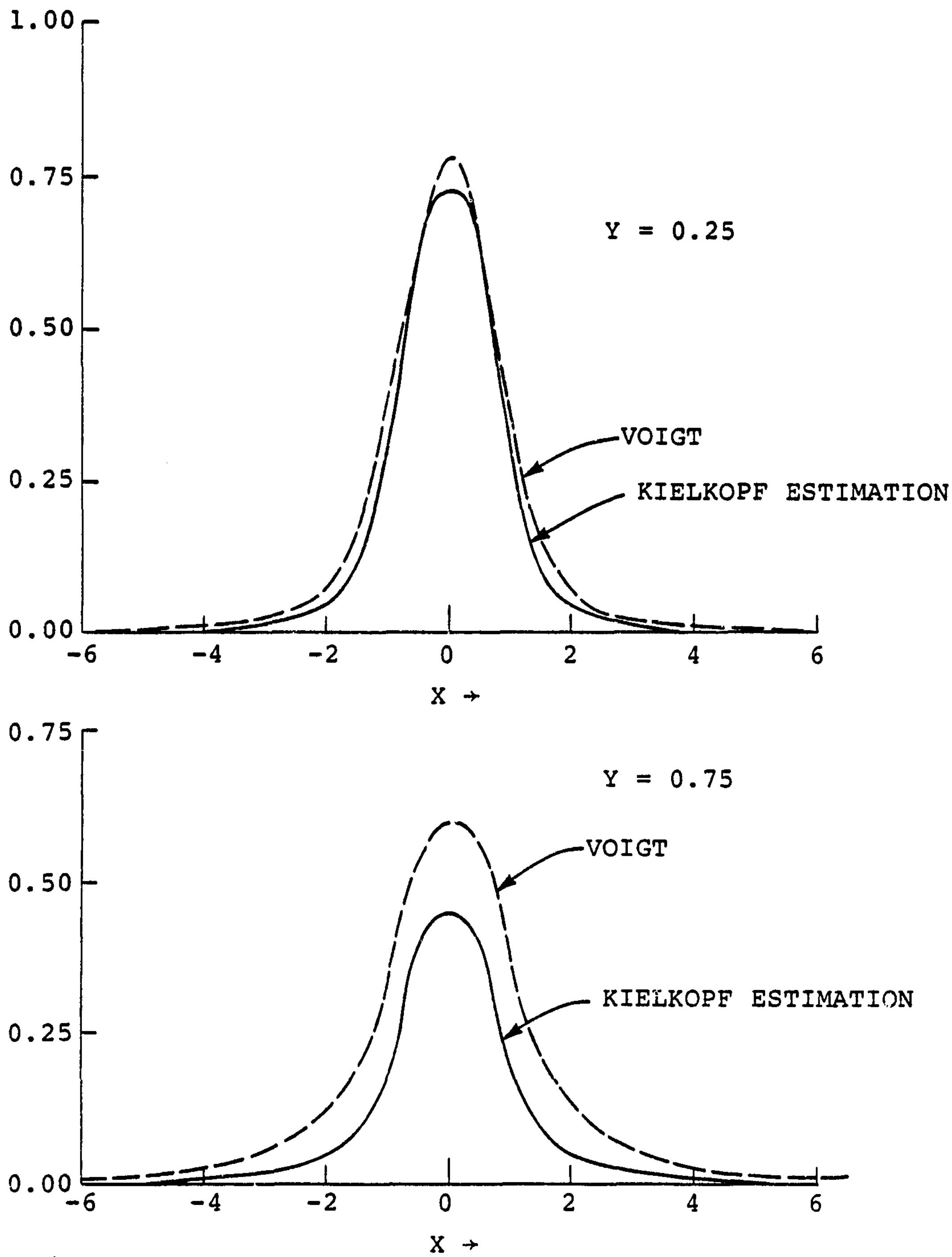

Figure A1. Comparison of the Kielkopf approximation to the actual Voigt profile for two values of the parameter y.

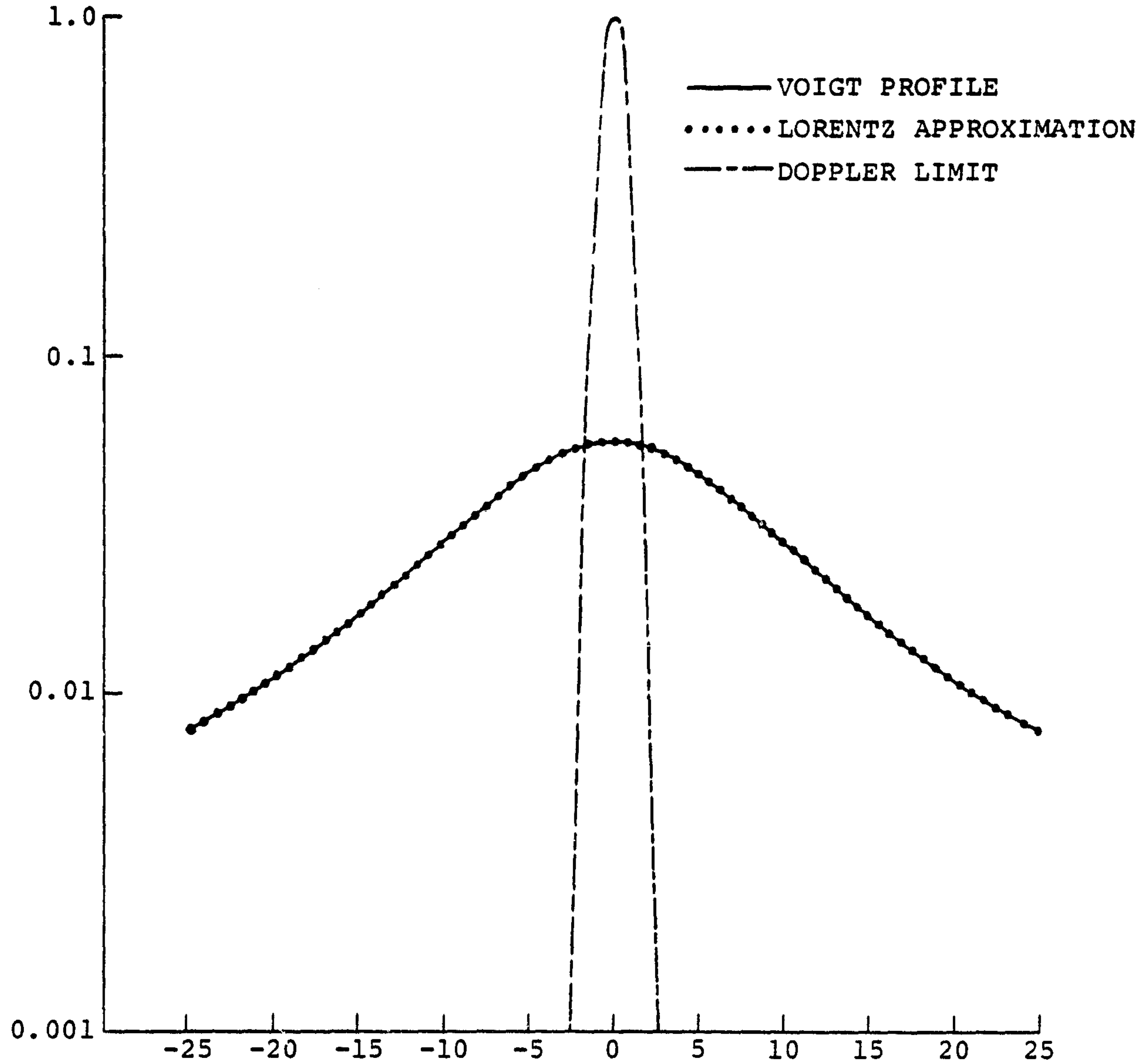

Figure A2. Comparison of the Voigt profile to the Lorentz approximation and the Doppler limit for the parameter y = 10.

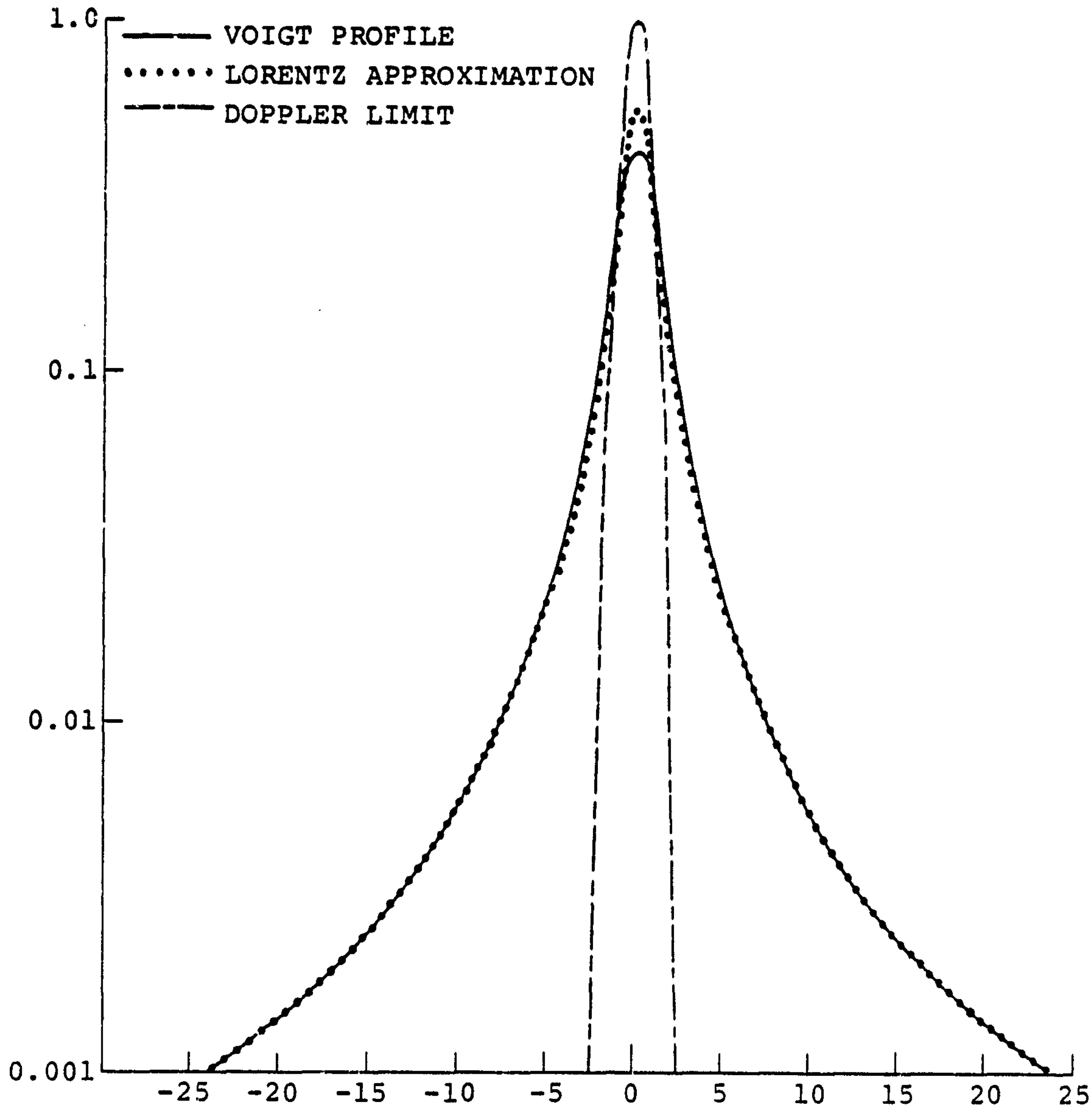

Figure A3. Comparison of the Voigt profile to the Lorentz approximation and the Doppler limit for the parameter y = 1.0.

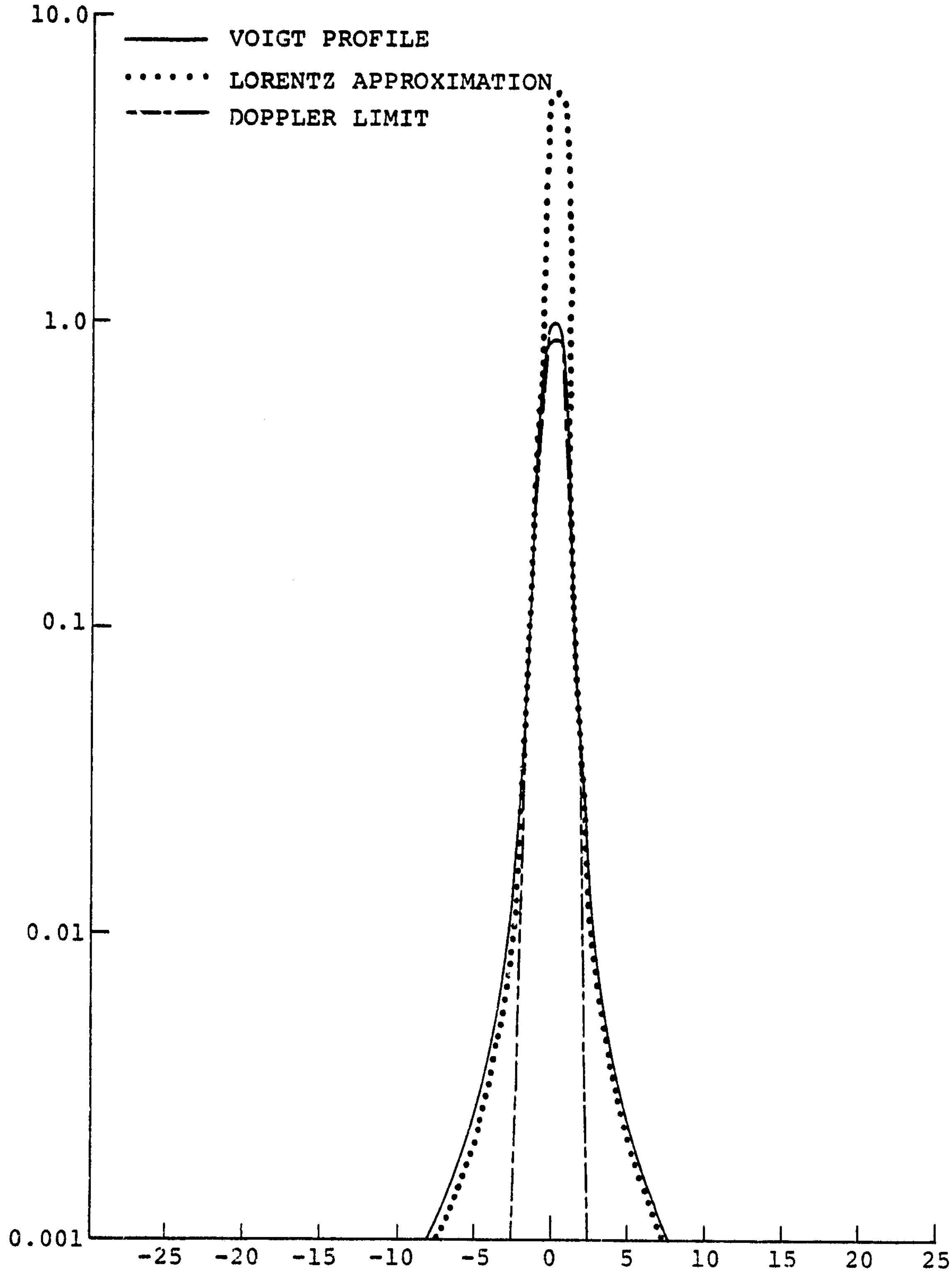

Figure A4. Comparison of the Voigt profile to the Lorentz approximation and the Doppler limit for the parameter y = 0.1

APPENDIX B

This appendix contains computer programs for methods A through H.

METHOD A

```
      FUNCTION K(X,Y)
C           THIS FUNCTION IS THE REAL PART OF THE COMPLEX PROBABILITY
C           FUNCTION OR THE VOIGHT SPECTRUM LINE PROFILE
      REAL K,K1,K2,K3
      IF (Y.LT.1.0.AND.X.LT.4.0.OR.Y.LT.1.8/(X+1.0)) GO TO 300
      IF (Y.LT.2.5.AND.X.LT.4.0) GO TO 200
  100 K = K3(X,Y)
      RETURN
  200 K = K2(X,Y)
      RETURN
  300 K = K1(X,Y)
      RETURN
      END
      FUNCTION K1(X,Y)
      REAL K1
      DOUBLE PRECISION C(34),COEF,BN01,BN02,BN,X1,F
C     ENTER HUMMERS CHEBYSHEV COEFFICIENTS C(I)
      DATA C/  0.19999999999972224D+00,  -0.18400000000029998D+00,
     1         0.15583999999965025D+20,  -0.12166400000043988D+00,
     2         0.03770815059940391D+20,  -0.05851412480086007D+00,
     3         0.03621573016239140D+00,  -0.02084972543980360D+00,
     4         0.01115601163462700D+20,  -0.56231896167109000D-02,
     5         0.25487634172265000D-02,  -0.11732670757784000D-02,
     6         0.48995199783888000D-03,  -0.19336300015280000D-03,
     7         0.72287744678800000D-04,  -0.25655512497900000D-04,
     8         0.86620736841000000D-05,  -0.27876379719000000D-05,
     9         0.85668736270000000D-06,  -0.25184337840000000D-06,
     1         0.70935022100000000D-07,  -0.19173225700000000D-07,
     2         0.49801256000000000D-08,  -0.12447734200000000D-08,
     3         0.29977770000000000D-09,  -0.69645033060000000D-10,
     4         0.15626200000000000D-10,  -0.33897000000000000D-11,
     5         0.71160000000000000D-12,  -0.14470000000000000D-12,
     6         0.285D-13,  -0.550D-14,    0.100D-14   -0.200D-15/
      Y2 = Y**2
      IF ((X**2-Y2).GT.70.0) GO TO 2
      U1 = EXP(-X**2+Y2)*COS(2.*X*Y)
      GO TO 5
    2 U1 = 0.0
    5 IF (X.GT.5.0) GO TO 1000
C     FROM HERE TO STATEMENT 30 WE CALCULATE DAWSONS FUNCTION
C     CLENSHAUS ALGORITHM AS GIVEN BY HUMMER
      BN01 = 0.0D0
      BN02 = 0.0D0
      X1 = X/5.0D0
      COEF = 4.0D0*X1**2-2.0D0
      DO 20 I = 1,34
      II = 35-I
      BN = COEF*BN01-BN02+C(II)
      BN02 = BN01
   20 BN01 = BN
   30 F = X1*(BN-BN02)
   40 DN01 = 1.0-2.*X*SNGL(F)
 1100 DN02 = SNGL(F)
      GO TO 1200
 1000 AX = 0.0
      BX = 0.0
      CX = 0.0
      IF (X .GE. 1000.0)  GO TO 1005
      AX = 29.53125 / X**10
      BX = 162.4218 / X**12
      CX = 1055.7421 / X**14
 1005 DN01 = -(.5/X**2+.75/X**4+1.875/X**6+6.5625/X**8
??
     1      +AX + BX + CX )
      DN02 = (1.-DN01)/(2.*X)
 1200 FUNCT = Y*DN01
      IF (Y.LE.1.0E-08) GO TO 2500
      Q = 1.0
      YN = Y
      DO 2000 I = 2,50
      DN = (X*DN01+DN02)*(-2.)/FLOAT(I)
      DN02 = DN01
      DN01 = DN
      IF (MOD(I,2)) 2000,2000,1500
 1500 Q = -Q
      YN = YN*Y2
      G = DN*YN
      FUNCT = FUNCT+Q*G
      IF (ABS(G/FUNCT).LE.1.0E-08) GO TO 2500
 2000 CONTINUE
 2500 K1 = U1-1.12837917*FUNCT
      RETURN
      END
      FUNCTION K2(X,Y)
      REAL K2
      DIMENSION U(10), T(10)
      DATA U/4.62243670E-1,2.86675505E-1,1.09817206E-1,2.48105209E-2,
     1       3.24377334E-3,2.28338636E-4,7.80255648E-6,1.08606937E-7,
     2       4.39934099E-10,2.22939365E-13/
      DATA T/0.245340708,0.737473729,1.23407622,1.73853771,2.25497400,
     1       2.78880606,3.34785457,3.94476404,4.60368245,5.38748089/
      Y2 = Y * Y
      G = 0.0
      DO 100 I = 1,10
      R = T(I)-X
      S = T(I)+X
  100 G = G+(4.*T(I)**2-2.)*(R*ATAN(R/Y)+S*ATAN(S/Y)-.5*Y*(ALOG(Y2+R**2)
     1+ALOG(Y2+S**2)))*U(I)
      K2 = 0.31830988*G
      RETURN
      END
      FUNCTION K3(X,Y)
      REAL K3
      DIMENSION U(10), T(10)
      DATA U/4.62243670E-1,2.86675505E-1,1.09817206E-1,2.48105209E-2,
     1       3.24377334E-3,2.28338636E-4,7.80255648E-6,1.08606937E-7,
     2       4.39934299E-10,2.22939365E-13/
      DATA T/0.245340708,0.737473729,1.23407622,1.73853771,2.25497400,
     1       2.78880606,3.34785457,3.94476404,4.60368245,5.38748089/
      Y2 = Y * Y
      G = 0.0
      DO 100 I = 1,10
  100 G = G+(1.0E0/((X-T(I))**2+Y2)+1.0E0/((X+T(I))**2+Y2))*U(I)
      K3 = 0.31830988*Y*G
      RETURN
      END
```

METHOD B

```
$VOIGTK
      FUNCTION VOIGTK(XIN,YIN)
C  THUS SUBROUTINE IS YOUNG,S METHOD FOR CALCULATING THE VOIGTK PROFILE
      DIMENSION  A(42),HH(10),XX(10)
      DIMENSION RA(32),CA(32),RB(32),B(44),AK(5),AM(5),DY(4),CB(32)
      DATA HH(1),HH(2),XX(1),XX(2)/
     ,  8.0491409E-01,  8.1312835E-02,  5.2464762E-01,   1.6506801E+00/
      DATA A/
     ,  0.              ,  1.9999999E-01,  0.              , -1.8400000E-01,
     ,  0.              ,  1.5583999E-01,  0.              , -1.2166400E-01,
     ,  0.              ,  8.7708159E-02,  0.              , -5.8514124E-02,
     ,  0.              ,  3.6215730E-02,  0.              , -2.0849765E-02,
     ,  0.              ,  1.1196011E-02,  0.              , -5.6231896E-03,
     ,  0.              ,  2.6487634E-03,  0.              , -1.1732670E-03,
     ,  0.              ,  4.8995199E-04,  0.              , -1.9336308E-04,
     ,  0.              ,  7.2287745E-05,  0.              , -2.5655512E-05,
     ,  0.              ,  8.6620736E-06,  0.              , -2.7876379E-06,
     ,  0.              ,  8.5668736E-07,  0.              , -2.5184337E-07,
     ,  0.              ,  7.0936022E-08/
      Z=0.0
  401 X=XIN
      Y = YIN
      X2 = X*X
      Y2 = Y*Y
      IF (X-7.0) 200,201,201
  200 IF (Y-1.) 202,202,203
  203 RA(1) = 0.
      CA(1) = 0.
      RB(1) = 1.
      CB(1) = 0.
      RA(2 ) = X
      CA(2) = Y
      RB(2) = .5-X2+Y2
      CB(2) = -2.*X*Y
      CB1 = CB(2)
      CA1 = 0.
      UV1=0.
      DO 250 J=2,31
      JMINUS = J-1
      JPLUS = J+1
      FLOATJ = JMINUS
      RB1 =2.*FLOATJ+RB(2)
      RA1 = -FLOATJ*(2.*FLOATJ-1.)/2.
      RA(JPLUS)=RB1*RA(J)-CB1*CA(J)+RA1*RA(JMINUS)-CA1*CA(JMINUS)
      CA(JPLUS)=RB1*CA(J)+CB1*RA(J)+RA1*CA(JMINUS)+CA1*RA(JMINUS)
      RB(JPLUS)=RB1*RB(J)-CB1*CB(J)+RA1*RB(JMINUS)-CA1*CB(JMINUS)
      CB(JPLUS)=RB1*CB(J)+CB1*RB(J)+RA1*CB(JMINUS)+ CA1*RB(JMINUS)
```

```
      UV=(CA(JPLUS)*RB(JPLUS)-RA(JPLUS)*CB(JPLUS))/(RB(JPLUS)*RB(JPLUS)+
     1CB(JPLUS)*CB(JPLUS))
      IF (ABS(UV-UV1)-1.E-7)251,250,250
250   UV1=UV
251   VOIGTK=UV/1.772454
      RETURN
202   IF (X-2.) 301,301,302
301   AINT = 1.
      MAX = 12.+5.*X2
      DO 303  J=1,MAX
      K=J-1
      AJ = MAX-K
303   AINT = AINT*(-2.*X2)/(2.*AJ+1.)+1.
      U = -2.*X*AINT
      GO TO 304
302   IF (X-4.5) 305,306,306
305   B(43)=0.
      B(44) = 0.
      J = 42
      DO 307 K =1,42
      B(J) = .4*X*B(J+1)-B(J+2)+A(J)
307   J = J-1
      U = B(3)-B(1)
      GO TO 304
306   AINT =1.0
      MAX = 2.+40./X
      AMAX = MAX
      DO 308 K=1,MAX
      AINT = AINT*(2.*AMAX-1.)/(2.*X2)+1.
308   AMAX = AMAX -1.
      U = -AINT/X
304   V = 1.772454*EXP(-X2)
      H = .02
      JM = Y/H
      IF (JM) 310,311,310
311   H=Y
310   Z = 0.
      L = 0
      DY(1) = 0.
312   DY(2) = H/2.
      DY(3) = DY(2)
      DY(4) = H
318   AK(1) = 0.
      AM(1) = 0.
      DO 313 J=1,4
      YY = Z+DY(J)
      UU = U+.5*AK(J)
      VV = V+.5*AM(J)
      AK(J+1) = 2.*(YY*UU+X*VV)*H
      AM(J+1) = -2.*(1.+X*UU-YY*VV)*H
      IF (J-3) 313,314,313
```

```
314 AK(4)=2.*AK(4)
    AM(4) = AM(4)+AM(4)
313 CONTINUE
    Z=Z+H
    L = L+1
    U = U+.1666667*(AK(2)+2.*AK(3)+AK(4)+AK(5))
    V = V+.1666667*(AM(2)+AM(3)+AM(3)+AM(4)+AM(5))
    IF(JM) 315,320,315
315 IF (L-JM) 318,317,320
317 AJM = JM
    H = Y-AJM*H
    GO TO 312
320 VOIGTK= V/1.772454
    RETURN
201 F1 = 0.
    DO 330 J=1,2
330 F1=F1+HH(J)/(Y2+(X-XX(J))*(X-XX(J)))+HH(J)/(Y2+(X+XX(J))*(X+XX(J))
   1)
    VOIGTK= Y*F1/3.1415927
    RETURN
    END
```

METHOD C


```
$KIEL2
      REAL FUNCTION KIEL(X,Y)
      REAL L,LN2
      DATA EXPTEST/-675.84/
      DATA RTPI/1.772453851/
C *** KIELKOPF APPROXIMATION TO THE VOIGT PROFILE FUNCTION
C     J.O.S.A. AUGUST 1973 VOLUME 63 NUMBER 8
C     PAGES 987-994
C *** INPUT PARAMETERS ***
      DATA EPS/0.0990/
C *** CALCULATE THE VOIGT PARAMETER
      LN2=ALOG(2.0)
      A=Y/SQRT(LN2)
      ASQ=A*A
      PL=2.0/(1.0+EPS*LN2 + SQRT((1.0-EPS*LN2)**2 + 4.0*LN2/ASQ))
      PGSQ=(1.0/LN2)*(1.0-(1.0+EPS*LN2)*PL+ (EPS*LN2)*PL*PL)
      XK=X/SQRT(LN2)
      XSQ=XK*XK
C *** KLUGE TO AVOID CDC EXP(A) ERROR MESSAGES
      IF((-LN2*XSQ).GE.EXPTEST) GO TO 5
      G=0
      GO TO 6
    5 G=EXP(-LN2*XSQ)
    6 CONTINUE
      L=1.0/(1.0+XSQ)
      ETA=PL/(PL+PGSQ)
      E=(0.8029-0.4207*XSQ)/(1.0+0.2030*XSQ+0.07335*XSQ*XSQ)
      KIEL=(1.0-ETA)*G + ETA*L + ETA*(1.0-ETA)*E*(G-L)
C *** TEST FOR REGION AND CALCULATE
C     INTENSITY FUNCTION ACCORDINGLY
      IF(A.GE.1.5) GO TO 10
C *** REGION I ***
      T=1.0/(1.0+0.47047*A)
      FA=1.0/RTPI * (0.61686*T-0.16994*T*T +1.32554*T*T*T)
      GO TO 20
C *** REGION II (EXTENDED FRACTION) ***
   10 CONTINUE
      FA=1.0/(A+(0.5/(A+(1.0/(A+(1.5/(A+2.0)))))))
C *** NORMALISE VOIGT VALUE...V(X)=U(X)*I(X)
   20 KIEL=KIEL*FA
      RETURN
      END
```

METHOD D

```
$VOIGT
      FUNCTION VOIGT(X,Y)
C *** ALGORITHM FOR RAPID COMPUTATION OF THE VOIGT PROFILE, BY S. R. DRAYSON,
C *** J.Q.S.R.T., VOL. 16, PP. 611-614, 1976.
C *** ROUTINE COMPUTES THE VOIGT FUNCTION   Y/PI*INTEGRAL FROM  ***
C ***  - TO + INFINITY OF EXP(-T*T )/(Y*Y+(X-T)*(X-T))DT         ***
      DIMENSION B(22), RI(15), XN(15), YN(15), D0(25), D1(25), D2(25),
     1            D3(25), D4(25), HN(25), XX(3), HH(33), C(21)
      REAL NBY2(19)
      LOGICAL TRU
      DATA B(1),B(2)/0.,.709360E-7/, XN/10.,9.,2*8.,7.,6.,5.,4.,7*3./,
     1     YN/3*.6,.5,2*.4,4*.3,1.,.9,.8,2*.7/, H/.201/,
     2     XX/.5246476,1.65068,.7071068/, (HH(I),I=1,3)/.2562121,
     3     .2588268E-1,.2820948/, NBY2/9.5,9.,8.5,8.,7.5,7.,6.5,6.,5.5,
     4     5.,4.5,4.,3.5,3.,2.5,2.,1.5,1.,.5/, C/.7093602E-7,
     5      -.2518434E-6,.8566874E-6,-.2787638E-5,.866074E-5,
     6      -.2565551E-4,.7228775E-4,-.1933631E-3,.4899520E-3,
     7      -.1173267E-2,.2648762E-2,-.5623190E-2,.1119601E-1,
     8      -.2084976E-1,.3621573E-1,-.5851412E-1,.8770816E-1,
     9      -.121664,.15584,-.184,.2/
      DATA TRU/.FALSE./
      IF(TRU) GO TO 104
C
C *** REGION I.  COMPUTE DAWSON FUNCTION AT MESH POINTS ***
C
      TRU = .TRUE.
      DO 101 I=1,15
  101 RI(I) = -I/2.
      DO 103 I=1,25
      HN(I) = H*(I-.5)
      CO = 4.*HN(I)*HN(I)/25. - 2.
C
        DO 102 J=2,21
  102   B(J+1) = CO*B(J) - B(J-1) + C(J)
C
      D0(I) = HN(I)*(B(22) - B(21))/5.
      D1(I) = 1. - 2.*HN(I)*D0(I)
      D2(I) = (HN(I)*D1(I) + D0(I))/RI(2)
      D3(I) = (HN(I)*D2(I) + D1(I))/RI(3)
  103 D4(I) = (HN(I)*D3(I) + D2(I))/RI(4)
C
  104 IF(X-5.) 105,112,112
  105 IF(Y-1.) 110,110,106
  106 IF(X.GT.1.85*(3.6-Y)) GO TO 112
C
C *** REGION II.  CONTINUED FRACTION.  COMPUTE NUMBER OF TERMS NEEDED. ***
C
```

```
      IF(Y.LT.1.45) GO TO 107
      I = Y + Y
      GO TO 108
  107 I = 11.*Y
  108 J = X + X + 1.85
      MAX = XN(J)*YN(I) + .46
      MIN = MIN0(16,21-2*MAX)
C
C *** EVALUATE CONTINUED FRACTION. ***
C
      UU = Y
      VV = X
      DO 109 J=MIN,19
      U = NBY2(J)/(UU*UU + VV*VV)
      UU = Y + U*UU
  109 VV = X - U*VV
      VOIGT = UU/(UU*UU + VV*VV)/1.772454
      RETURN
C
  110 Y2 = Y*Y
      IF(X+Y.GE.5.) GO TO 113
C
C *** REGION I.  COMPUTE DAWSON FUNCTION AT X FROM TAYLOR SERIES. ***
C
      N = X/H
      DX = X - HN(N+1)
      U = (((D4(N+1)*DX + D3(N+1))*DX + D2(N+1))*DX + D1(N+1))*DX +
     1                                                          D0(N+1)
      V = 1. - 2.*X*U
C
C *** TAYLOR SERIES EXPASION ABOUT Y = 0.0   ***
C
      VV = EXP(Y2 - X*X)*COS(2.*X*Y)/1.128379 - Y*V
      UU = -Y
      MAX = 5. + (12.5 - X)*.8*Y
C
      DO 111 I=2,MAX,2
      U = (X*V + U)/RI(I)
      V = (X*U + V)/RI(I+1)
      UU = -UU*Y2
  111 VV = VV + V*UU
C
      VOIGT = 1.128379*VV
      RETURN
C
C
  112 Y2 = Y*Y
      IF(Y.LT.11. -.6875*X) GO TO 113
C
C *** REGION IIIB.  2-POINT GAUSS-HERMITE QUADRATURE. ***
C
```

```
      U = X - XX(3)
      V = X + XX(3)
      VOIGT = Y*(HH(3)/(Y2 + U*U) + HH(3)/(Y2 + V*V))
      RETURN
C
C *** REGION IIIA.  4-POINT GAUSS-HERMITE QUADRATURE. ***
C
  113 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)
     1                                               + HH(2)/(Y2+VV*VV))
      RETURN
      END
```

METHOD E

```
$ZVOIGT
      FUNCTION ZVOIGT(X,Y)
C *** FAST CALCULATIONAL ALGORITHM FOR THE VOIGT PROFILE
C JQSRT VOL 18 PP555-558
C PIERLUISSI AND VANDERWOOD
C U.T. AT EL PASO
      DIMENSION AN(30)
      DATA AN/1.0,-.33333333,0.1,-.238095238E-01,
     1 4.62962963E-03,-7.57575757E-04,1.068376068E-04,-1.322751323E-05,
     2 1.45891691E-6,-1.450385222E-7,1.312253296E-8,-1.089222104E-9,
     3 8.350702795E-11,-5.947794014E-12,3.955429516E-13,
     4 -2.46682701E-14,1.448326465E-15,-8.032735012E-17,
     5 4.221407289E-18,-2.107855192E-19,1.002516493E-20,
     6 -4.551846759E-22,1.977064754E-23,-8.230149299E-25,
     7 3.289260349E-26,-1.264107899E-27,4.67848352E-29,
     8 -1.669761793E-30,5.754191644E-32,-1.916942862E-33/
      DATA A1/.46131350/
      DATA B4/2.72474500/
      DATA PISQ/1.128379167/
      DATA A2/0.19016350/
      DATA A3/0.09999216/
      DATA A4/1.78449270/
      DATA A5/0.002883894/
      DATA A6/5.52534370/
      DATA B1/0.51242424/
      DATA B2/0.27525510/
      DATA B3/0.05176536/
C
      S=X*X-Y*Y
      T=2.0*X*Y
C *** REGION SELECTION
      IF(Y.GE.5.0.OR.X.GE.5.0)GO TO 111
      IF(Y.GE.1.8.OR.X.GE.3.0)GO TO 112
C *** REGION I ***
      XSER=Y
      YSER=-X
      XN=Y
      YN=-X
      X2=-S
      Y2=-T
      N=6.842*X+8.0
      IF(N.GT.29) N=29
      IF(X.EQ.0.0) N=15
      DO 10 I10=1,N
      XNEW=XN*X2-YN*Y2
      YNEW=Y2*XN+YN*X2
      XSER=XSER+XNEW*AN(I10+1)
```

```
      YSER=YSER+YNEW*AN(I10+1)
      XN=XNEW
      YN=YNEW
   10 CONTINUE
      ZVOIGT=EXP(-S)*(COS(-T)*(1.0-PISQ*XSER)+PISQ*SIN(-T)*YSER)
      RETURN
C *** REGION II ***
  112 R=T*T
      T=T*X
      F=S-A6
      G=S-A4
      H=S-A2
      ZVOIGT=A1*((T-H*Y)/(H*H+R))+A3*((T-G*Y)/(G*G+R))+
     1   A5*((T-F*Y)/(F*F+R))
      RETURN
C *** REGION III ***
  111 R=T*T
      T=T*X
      F=S-B2
      G=S-B4
      ZVOIGT=B1*((T-F*Y)/(F*F+R))+B3*((T-G*Y)/(G*G+R))
      RETURN
      END
```

METHOD F

```
 $LORZ
      REAL FUNCTION LORZ(X,Y)
      DATA RPI/0.5641896/
      LORZ=Y*RPI/(X*X+Y*Y)
      RETURN
      END
```

METHOD G

```
$DOPL
      FUNCTION DOPL(X,Y)
      DOPL=EXP(-X*X)
      RETURN
      END
```

```
MODULE CIMATS BEGIN MAINPROG;$XREF;$SOURCE(1,80);$NOCHECK;$OPT=3;
/*        ATTEMPT AT 32-BIT MATH ON VECTORIZED VOIGT PROFILE            */
   LITERALLY '161' TOPX;
   LITERALLY '20' TOPY;
   EXTERNAL PROCEDURE(REAL,REAL)Q3CLOCKS;
PROCEDURE MAINPROG;
   REAL XX,VALUE;
   SHORT REAL YY;
   REAL ZVAL;
   REAL CPU,W;
   INTEGER NY,NX,I,J;
   SHORT REAL VECTOR[TOPX] X,PROFILE;
   SHORT REAL VECTOR[TOPY] Y;
   INITIAL(NY=TOPY);
   INITIAL(Y=\0.1,0.2,0.3,0.4,0.5,0.6,0.7,0.8,0.9,
   1.0,2.0,3.0,4.0,5.0,6.0,7.0,8.0,9.0,10.0,11.0\);
   INITIAL(NX=TOPX);
/*  SET UP SAMPLE SPACE        */
   X:=IOTA(0.0,0.25,TOPX);
/*  TIMING LOOP   */
   CALL Q3CLOCKS(CPU,W);
   FOR I:=1 TO NY DO
           YY:=Y[I];
           PROFILE:=VOIGTZ(X,YY);
   ENDF;
   CALL Q3CLOCKS(CPU,W);
   PRINT(CPU)$' VOIGTZ CPU SECS = 'F10.4//$;
/*        PRINT LOOP           */
   FOR I:= 1 TO NY DO
           YY:=Y[I];
           PROFILE:=VOIGTZ(X,YY);
        PRINT(YY,X,PROFILE)$5X,2F10.4,//(5E15.5)$;
   ENDF;
 ENDP;
 FUNCTION VOIGTZ(X,Y)RETURNS (SHORT REAL VECTOR[TOPX]);
 /* FAST CALCULATIONAL ALGORITHM FOR THE VOIGT PROFILE
  J.Q.S.R.T. VOL 18 PPG 555-558
  PIERLUISSI AND VANDERWOOD UNIV OF TEX AT EL PASO       */
   SHORT REAL VECTOR[30] AN;
   SHORT REAL A1,A2,A3,A4,A5,A6;
   SHORT REAL Y;
   SHORT REAL VECTOR[TOPX]X,ZV,S,T;
   INTEGER L1,U1,L2,U2,L3,U3;
   INTEGER JV;
   SHORT REAL B1,B2,B3,B4;
   SHORT REAL PISQ;
   SHORT REAL XSER,YSER,XN,YN,XNEW,YNEW;
   SHORT REAL X2,Y2;
   SHORT REAL VECTOR[TOPX]R,G,H,F;
   INTEGER N,I10;
   INITIAL(AN=\1.0,-.33333333,0.1,-.238095238E-01,
     4.62962963E-03,-7.57575757E-04,1.068376068E-04,-1.322751323E-05,
     1.458916981E-6,-1.450385222E-7,1.312253296E-8,-1.089222104E-9,
     8.350702795E-11,-5.947794014E-12,3.955429516E-13,
     -2.466827010E-14,1.448326486E-15,-8.032735012E-17,
     4.221407289E-18,-2.107855192E-19,1.002516493E-20,
     -4.551846759E-22,1.977064754E-23,-8.230149299E-25,
     3.289260349E-26,-1.264107899E-27,4.678483528E-29,
     -1.669761793E-30,5.754191644E-32,-1.916942862E-33\);
   INITIAL(A1=0.46131350);
   INITIAL(A2=0.19016350);
   INITIAL(A3=0.09999216);
   INITIAL(A4=1.78449270);
   INITIAL(A5=0.002883894);
   INITIAL(A6=5.52534370);
   INITIAL(B1=0.51242424);
   INITIAL(B2=0.27525510);
   INITIAL(B3=0.05176536);
   INITIAL(B4=2.72474500);
   INITIAL(PISQ=1.128379167);                               */
/*
   S:=X*X-Y*Y;
   T:=2.0*X*Y;
/*  PRESET BOUNDS ON KNOWN X VECTOR   */
/*  THESE ARE DEFAULTS FOR REGION III    */
   L1:=1;
   L2:=1;
   L3:=1;
   U1:=0;
   U2:=0;
   U3:=TOPX;                                                */
/*     SIMPLE REGION SELECTION
/*    PERFORM BOUNDS CALCULATION FOR VECTOR OPS IN          */
      VARIOUS REGIONS
   IF(Y)=5.0) THEN GO TO REG3;
   ENDI;
/* SET UP REGION II / REGION III BREAK POINT  */
/* BREAKPOINT IS AT X=5.0                     */
   U2:=SELGE(X,5.0)
   L3:=U2+1
   IF(Y)=1.8) THEN  /* WE HAVE R2 AND R3 TO BOUND*/
       GO TO REG2;
   ENDI;
/* WE HAVE ALL 3 REGIONS TO CONTEND WITH  */
/*  SET REGION I/REGION II BRKPT AT X=3.0     */
     U1:=SELGE(X,3.0);
     L2:=U1+1;                                              */
/*                                                          */
/*     REGION I                                              */
/*
 FOR JV:=1 TO U1 DO
   XSER:=Y;
   YSER:=-X[JV];
   XN:=Y;
   YN:=-X[JV];
   X2:=-S[JV];
   Y2:=-T[JV];
   N:=TRUNC(5.842*X[JV]+8.0);
   IF(N>29) THEN N:=29;
   ENDI;
   IF(X[JV]=0.0) THEN N:=15;
   ENDI;
   FOR I10:=1 TO N DO
          XNEW:=XN*X2-YN*Y2;
          YNEW:=Y2*XN+YN*X2;
          XSER:=XSER+XNEW*AN[I10+1];
          YSER:=YSER+YNEW*AN[I10+1];
          XN:=XNEW;
          YN:=YNEW;
   ENDF;
   ZV[JV]:=EXP(-S[JV])*(COS(-T[JV])*(1.0-PISQ*XSER)+PISQ*SIN(-T[JV])*YSER);
 ENDF;                                                      */
/*                                                          */
/*      REGION II
```

```
/*                                                          */
REG2: R[L2:U2]:=T[L2:U2]*T[L2:U2];
    T[L2:U2]:=T[L2:U2]*X[L2:U2];
    F[L2:U2]:=S[L2:U2]-A6;
    G[L2:U2]:=S[L2:U2]-A4;
    H[L2:U2]:=S[L2:U2]-A2;
    ZV[L2:U2]:=A1*((T[L2:U2]-H[L2:U2]*Y)/(H[L2:U2]*H[L2:U2]+R[L2:U2]))
    +A3*((T[L2:U2]-G[L2:U2]*Y)/(G[L2:U2]*G[L2:U2]+R[L2:U2]))+
         A5*((T[L2:U2]-F[L2:U2]*Y)/(F[L2:U2]*F[L2:U2]+R[L2:U2]));
/*                                                          */
/*    REGION III                                            */
/*                                                          */
REG3:R[L3:U3]:=T[L3:U3]*T[L3:U3];
    T[L3:U3]:=T[L3:U3]*X[L3:U3];
    F[L3:U3]:=S[L3:U3]-B2;
    G[L3:U3]:=S[L3:U3]-B4;
    ZV[L3:U3]:=B1*((T[L3:U3]-F[L3:U3]*Y)/(F[L3:U3]*F[L3:U3]+R[L3:U3]))
     +B3*((T[L3:U3]-G[L3:U3]*Y)/(G[L3:U3]*G[L3:U3]+R[L3:U3]));
/*    RETURN ENTIRE PROFILE VECTOR.......                   */
    RETURN(ZV);
ENDFN;
ENDM;
END OF FILE
??
```