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NO. 1275

A FORTRAN PROGRAM FOR CALCULATING CHEMICAL HAZARDS USING THE NATO STANAG 2103/ATP-45 ALGORITHM

by

Stanley B. Mellsen

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A FORTRAN PROGRAM FOR CALCULATING CHEMICAL HAZARDS USING THE NATO STANAG 2103/ATP-45 ALGORITHM

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ABSTRACT

A computer program has been written in Microsoft Fortran Version 4.1 to apply the algorithm of NATO Stanag 2103/ATP-45 Appendix E, First Preliminary Draft, April 1987. Downwind dosages obtained with the program by an IBM compatible personal computer are presented in graphical form.

LIST OF SYMBOLS

D (x,y,o)	total dosage at ground level at co-ordinates x,y, downwind from a point source, mg min m^{-3}
F_1, f_1, G, g, Fm, fm	Constants used in calculating diffusion parameters
Q	Effective initial source strength: input, kg, calculations, g
u	mean wind speed: input, kn, (knots) calculations, m s^{-1}
v_d	deposition velocity; specification, mm s^{-1} calculations, m s^{-1}
x	alongwind distance from point source: input, km, calculations, m
y	crosswind distance from point source: input, km, calculations, m
γ	dimensionless parameter related to deposition velocity
σ_y	diffusion parameter for crosswind horizontal direction, m
σ_z	vertical diffusion parameter, m

INTRODUCTION

The Military Agency for Standardization (MAS) of the North Atlantic Treaty Organization (NATO) has issued a draft for the algorithm to be used in calculating the maximum downwind hazard distances after attacks with chemical agents. The algorithm is provided under Standardization Agreement (STANAG) Number 2103 [1] associated with the document entitled "Reporting Nuclear Detonations, Biological and Chemical Attacks and Predicting and Warning of Associated Hazards and Hazard Areas - ATP-45". The algorithm is stated in the First Preliminary Draft of Annex E, ATP-45, Volume II dated April 1987.

The purpose of this report is to describe a computer program written in Microsoft FORTRAN Version 4.1 to apply the algorithm to calculate a set of sample results for dispersion over both land and sea for all atmospheric stability categories. Another purpose is to present the results in graphical form for convenient use. The validity of the algorithms is not appraised herein, but the program and results provided can be used for familiarization and as aids in improving the algorithm if changes are suggested. The computer program was developed on an IDM Research T286 computer with an Intel 80287 Coprocessor from which results were obtained almost instantaneously after the calculations were started.

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THE ALGORITHM

After an attack with chemical agents a certain amount of the agent will be dispersed in the air in the form of vapour or aerosols. This portion of the weapon payload is subject to atmospheric diffusion processes and will create danger to personnel downwind of the actual attack area. During actual cloud travel, portions of vapour and aerosol are removed from it by gravitational deposition, scavenging by vegetation and chemical processes. These effects may be accounted for by a surface depletion model. The solution provided for point source surface releases neglecting gravitational settling is given by the following equation [1]:

$$D(x,y,o) = \frac{Q}{\pi u \sigma_y \sigma_z} \exp\left(\frac{-y^2}{2\sigma_y^2}\right) \left[1-\sqrt{\pi}\,\gamma \exp(\gamma^2) \operatorname{erfc}(\gamma)\right] \tag{1}$$

with:

$$\gamma = \frac{v_d\, x}{u g \sigma_z \sqrt{2}} \tag{2}$$

g = exponent of $\sigma_z = Gx^g$
u = representative wind speed
v_d = deposition velocity, and
x = downwind distance from source

The deposition velocity is:

$$v_d\ (\text{land}) = 4\ \text{mm s}^{-1} \qquad v_d\ (\text{sea}) = 3\ \text{mm s}^{-1} \tag{3 a,b}$$

The diffusion parameters σ_y and σ_z are defined by the equations below [1].

$$\sigma_y^2 = \sigma_y\ \text{inst}^2 + \sigma_y\ \text{meander}^2 \tag{4}$$

$$\sigma_z = \sigma_z\ \text{inst} = Gx^g \tag{5}$$

$$\sigma_y\ \text{inst} = F_1 x^{f_1} \tag{6}$$

$$\sigma_y\ \text{meander} = F_m x^{f_m} \tag{7}$$

The stability categories, S, are defined as follows:

$$S = \begin{cases} 1 & \text{very unstable} \\ 2 & \text{unstable} \\ 3 & \text{slightly unstable} \\ 4 & \text{neutral} \\ 5 & \text{slightly stable} \\ 6 & \text{stable} \\ 7 & \text{very stable.} \end{cases}$$

The constants used for obtaining the diffusion parameters in equations (4) to (7) are given in Table I [1].

TABLE I - CONSTANTS FOR DIFFUSION PARAMETERS

LAND	SEA
$F_1 = 0.2997 \exp(0.2621S)$	$= 0.4570 \exp(-0.0863S)$
$f_1 = 0.89 - 0.07S$	$= 0.7$
$G = 0.1229 \exp(0.3295S)$	$= 0.9740 \exp(0.1750S)$
$g = 0.97 - 0.09\ S$	$= 0.68 - 0.06\ S$
$F_m = \left\| \begin{array}{l} 1.577\ u < 10 \text{ kts} \\ 1.130\ u \geq 10 \text{ kts} \end{array} \right.$	$= \left\| \begin{array}{l} 1.538\ u < 10 \text{ kts} \\ 1.038\ u \geq 10 \text{ kts} \end{array} \right.$
$f_m = 0.7$	$= 0.7$

SOLUTION OF THE ALGORITHM

The solution of equation (1) to obtain total dosage at some downwind point x, y is straightforward with the exception of calculation of the complementary error function, erfc (γ). This function and the error function, erf (γ), are defined and tabulated for various values of the argument in Reference 2. Various mathematical relationships involving these functions are also shown [2]. The present solution consists of calculating the error function using a numerical procedure called Gauss-Legendre quadrature [3] and applying the following relationship.

$$\operatorname{erfc}(\gamma) = 1 - \operatorname{erf}(\gamma) \tag{8}$$

This equation can be written in terms of the defining integrals as follows:

$$\frac{2}{\sqrt{\pi}} \int_{\gamma}^{\infty} e^{-t^2}\, dt = 1 - \frac{2}{\sqrt{\pi}} \int_{0}^{\gamma} e^{-t^2}\, dt \tag{9}$$

COMPUTER PROGRAM

A listing of the program which was written in Microsoft Fortran Version 4.1 is shown in Annex A, along with a set of input data and calculated results. The listing is annotated to describe the program step by step. The required units of the input data as described in the listing and shown in the output results conform to those listed in Annex E of the ATP-45 [1]. After the pertinent input data is read in knots, kilograms and kilometers, the units are automatically changed to meters per seconds, milligrams and meters. Next, the constants in Table I are calculated for the input stability category and choice of land or sea. Then the diffusion parameters given by equations (4) to (7) are calculated, followed by calculation of γ using equation (2).

The only quantity which remains to be calculated for substitution into equation (1) to obtain total dosage is the complementary error function, obtained through equation (8) from the error function. The error function is obtained by integrating the function e^{-x^2} using a function subprogram by which Gauss-Legendre quadrature is applied and multiplying the results by $2/\sqrt{\pi}$. The subprogram provides a choice of the number of Gauss-Legendre base points to be used in the calculation, depending upon the accuracy required. The choices available are 2,3,4,5,6,10 and 15 points [3]. Further description of the method is shown in the program listing and in greater detail in Reference 3. After the error function has been calculated, the complementary error function is calculated using equation (8). Then the total dosage is calculated using equation (2) and the results are available for printing.

RESULTS AND DISCUSSION

Total dosages were calculated for various downwind distances for each of the seven stability categories for dispersion over both land and sea. The results are shown for land in Figures 1 to 7 and for sea in Figures 8 to 14. Vapour source strength, Q, divided by total dosage, D is plotted against downwind distance for various wind spreads appropriate to each stability category. Plotting the variables in this manner results in nearly straight lines on log-log paper for the most unstable atmospheric conditions, and lines of increasing curvature as atmospheric stability increases. Each wind speed has a range of wind speeds shown along with it, for which the graph can be used for quick estimations. At any downwind distance from the source, the dosage is assumed to be accumulated during the full time interval of the cloud passage.

In writing the program some thought was given to the possibility of using a programmable pocket calculator. The feasibility of this is mostly dependent on the availability of the error function. Some calculators have a facility for calculating this function. For example, the Hewlett Packard HP 41C has an error function program in its Math/Stat Pack. For effective field application of a pocket calculator, it should be able to produce accurate results with short computing time. The Gauss-Legendre method used in the Fortran program could possibly be applied. The six point quadrature produced accurate results for at least the lowest four values of S. This was determined by experimenting with various numbers of points in the quadrature and comparing results to those of other workers [4]. However, the fifteen point quadrature was necessary to provide accurate results for the higher values of S. For the lowest wind speed of two knots, and the highest value of seven for S, the results are only accurate up to ten kilometers for both land and sea. Therefore, the graphs for these conditions are not plotted beyond ten kilometers as shown in Figures 7 and 14. For all other conditions the calculation method produced accurate results out to forty kilometers. Examination of the values of the error function shows why the results become unreliable for the lowest wind speed and highest value of S. The value of the error function approaches one as distance increases. Therefore the value of the complementary error function which is used in equation (1) approaches zero. For these small values, a more precise calculation is required to keep the percentage error low.

CONCLUSIONS

A Fortran Program written for an IBM compatible personal computer applies the algorithms of ATP 45 to give quick and accurate calculations for distances up to ten kilometers, under all wind speeds and stability categories, and for all but the lowest wind speed in a very stable atmosphere, for distances up to forty kilometers. However, one must remember that this paper does not intend to confirm how accurately the algorithms represent actual downwind cloud travel. It only provides a method for applying them as they are stated in Reference 1.

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REFRENCES

1. NATO STANAG No. 2103, "Reporting Nuclear Detonations, Biological and Chemical Attacks and Predicting and Warning of Associated Hazards and Hazard Area - ATP-45", Annex E, First Preliminary Draft, April 1987. UNCLASSIFIED.

2. Abramowitz, M. and Stegun, L.A. "Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables". US Department of Commerce, National Bureau of Standards Applied Mathematics Series 55, 1964.

3. Carnahan, Brice, Luther, H.A. and Wilkes "Applied Numerical Methods", John Wiley and Sons, Inc. 1969.

4. aufm Kampe, Welfhart, Amt für Wehrgeophysik, Traben-Trarbach, Federal Republic of Germany, Private Communication, 1985.

```
C        DOWNWIND CONCENTRATIONS FROM VAPOUR OR AERSOL
C        CALCULATED FROM ATP45 VOLUME II ALGORITHMS
C
C        THIS PROGRAM READS ATMOSPHERIC CONDITIONS AND STRENGTH
C        OF A POINT SOURCE AND CALCULATES DOWNWIND DOSAGES OVER
C        LAND OR SEA. THE ERROR FUNCTION WHICH IS NEEDED IS OBTAINED
C        USING THE FUNCTION GAUSS TO COMPUTE THE NUMERICAL APPROXIMATION
C        OF THE INTEGRAL OF FUNCTN(X)*DX BETWEEN INTEGRATION LIMITS
C        A AND B USING THE M POINT GAUSS-LEGENDRE QUADRATURE FORMULA. THE
C        PROGRAM PRINTS THE RESULTS, AND RETURNS TO READ A NEW SET OF
C        DOWNWIND COORDINATES USING THE SAME INITIAL CONDITIONS.
C
      IMPLICIT  DOUBLE PRECISION(A-H, O-Z)
      EXTERNAL FUNCTN
      REAL S
      OPEN (5,FILE='ATP45P.DAT')
      OPEN (6,FILE='ATP45P.OUT')
C
C     M IS THE NUMBER OF POINTS TO BE USED IN THE GAUSS-LEGENDRE QUADRATURE
C     LS = 1 FOR LAND. LS = 2 FOR SEA.
C     S IS ATMOSPHERIC STABILITY CATEGORY
C         1.0  VERY UNSTABLE
C         2.0  UNSTABLE
C         3.0  SLIGHTLY UNSTABLE
C         4.0  NEUTRAL
C         5.0  SLIGHTY STABLE
C         6.0  STABLE
C         7.0  VERY STABLE
C     U IS WIND SPEED IN KNOTS
C     Q IS VAPOUR OR AEROSOL SOURCE STRENGTH IN KILOGRAMS
C
      READ (5,100) M, LS, S, U, Q
C
C     OUTPUT HEADINGS AND INPUT DATA
C
      WRITE(6,200)
      WRITE(6,201) M, LS, S, U, Q
      WRITE(6,202)
      WRITE(6,203)
C
C     X IS ALONGWIND DISTANCE FROM SOURCE
C     Y IS CROSSWIND DISTANCE CENTRE FROM ALONGWIND DIRECTION
C
    1 READ (5,101,END=999) X, Y
C
C     CONVERT INPUT PARAMETER UNITS TO METRES, SECONDS AND MILLIGRAMS
C
      UMS = 0.5144*U
      QMG = 1000000.0*Q
      XM = 1000.0*X
      YM = 1000.0*Y
```

```
C
      IF (LS .GT. 1) GOTO 11
C
C     CONSTANTS FOR LAND
C
      FI = 0.2997*EXP(0.2621*S)
      FFI = 0.89 - 0.07*S
      G = 0.1229*EXP(0.3295*S)
      GG = 0.97 - 0.09*S
      FFM = 0.7
      FM = 1.577
      IF (U .LT. 10.0) GOTO 10
      FM = 1.130
   10 VD = 0.004
      GOTO 20
C
C     CONSTANTS FOR SEA
C
   11 FI = 0.4570*EXP(-0.0863*S)
      FFI = 0.7
      G = 0.9740*EXP(0.1750*S)
      GG = 0.68 - 0.06*S
      FFM = 0.7
      FM = 1.538
      IF (U .LT. 10.0) GOTO 15
      FM = 1.038
   15 VD = 0.003
C
C     STANDARD DEVIATIONS OF PLUME
C
   20 SIGYI = FI*XM**FFI
      SIGYM = FM*XM**FFM
      SIGY = SQRT(SIGYI**2 + SIGYM**2)
      SIGZ = G*XM**GG
C
C     UPPER LIMIT OF ERROR FUNCTION INTEGRAL
C
      GAMMA = VD*XM/(SQRT(2.0)*UMS*GG*SIGZ)
C
C     COMPLEMENTARY ERROR FUNCTION
C
      A = 0.0
      B = GAMMA
      AREA = GAUSS ( A, B, M, FUNCTN )
      PI = 3.14159265358979323846264
      ERF =(2.0/SQRT(PI))*AREA
      ERFC = 1.0 - ERF
C
C     DOWNWIND DOSAGE
C
```

```
      D1 = QMG/(PI*UMS*SIGY*SIGZ*60.0)
      D2 = EXP(-YM**2/(2.0*SIGY**2))
      D3 = 1.0 - SQRT(PI)*GAMMA*EXP(GAMMA**2)*ERFC
      D = D1*D2*D3
      QD = Q/D
C
C     OUTPUT RESULTS
C
      WRITE (6,204) X,Y,D,QD
C
      GO TO 1
C
C     ..... FORMATS FOR INPUT AND OUTPUT STATEMENTS .....
 100  FORMAT ( 2I5,F5.1,2F10.3)
 101  FORMAT ( 2F10.3)
 200  FORMAT ( '1',20X, 'DOWNWIND DOSAGES'/ )
 201  FORMAT ( 20X,'M =',I3/20X,'LS =',I3/20X,'S =',F5.1,/
     120X,'U =',F5.1,2X,'KNOTS'/20X,'Q =',F7.3,2X,'KG'/)
 202  FORMAT (/,12X,'X',14X,'Y',12X,'D',14X,'Q/D')
 203  FORMAT ( 7X,'KILOMETRES',6X,'KILOMETRES',4X,'MG MIN/CU M',
     13X,'KG/(MG MIN/CU M)'/)
 204  FORMAT ( 5X,F10.3,5X,F10.3,5X,F10.5,7X,F10.5)
C
 999  CLOSE (5)
      CLOSE (6)
      STOP
      END
C
      FUNCTION FUNCTN( X )
C
C     ..... THIS FUNCTION RETURNS EXP(-X**2) AS ITS VALUE .....
      DOUBLE PRECISION  X, FUNCTN
      FUNCTN = EXP(-X**2)
      RETURN
C
      END
      FUNCTION GAUSS( A, B, M, FUNCTN )
C
C         THE FUNCTION GAUSS USES THE M POINT GAUSS-LEGENDRE QUADRATURE
C         FORMULA TO COMPUTE THE INTEGRAL OF FUNCTN(X)*DX BETWEEN
C         INTEGRATION LIMITS A AND B.  THE ROOTS OF SEVEN LEGENDRE
C         POLYNOMIALS AND THE WEIGHT FACTORS FOR THE CORRESPONDING
C         QUADRATURES ARE STORED IN THE Z AND WEIGHT ARRAYS
C         RESPECTIVELY.  M MAY ASSUME VALUES 2,3,4,5,6,10, AND 15
C         ONLY.  THE APPROPRIATE VALUES FOR THE M POINT FORMULA ARE
C         LOCATED IN ELEMENTS Z(KEY(I))...Z(KEY(I+1)-1) AND
C         WEIGHT(KEY(I))...WEIGHT(KEY(I+1)-1) WHERE THE PROPER
C         VALUE OF I IS DETERMINED BY FINDING THE SUBSCRIPT OF THE
C         ELEMENT OF THE ARRAY NPOINT WHICH HAS THE VALUE M.  IF AN
C         INVALID VALUE OF M IS USED, A TRUE ZERO IS RETURNED AS THE
C         VALUE OF GAUSS.
C
```

```
      IMPLICIT DOUBLE PRECISION(A-H, O-Z)
      DOUBLE PRECISION  GAUSS, A, B, FUNCTN
      DIMENSION NPOINT(7), KEY(8), Z(24), WEIGHT(24)
C
C     ..... PRESET NPOINT, KEY, Z, AND WEIGHT ARRAYS .....
      DATA  NPOINT / 2, 3, 4, 5, 6, 10, 15 /
C
      DATA  KEY / 1, 2, 4, 6, 9, 12, 17, 25 /
C
      DATA  Z              / 0.577350269,0.0        ,0.774596669,
     1          0.339981044,0.861136312,0.0        ,0.538469310,
     2          0.906179846,0.238619186,0.661209387,0.932469514,
     3          0.148874339,0.433395394,0.679409568,0.865063367,
     4          0.973906529,0.0        ,0.201194094,0.394151347,
     5          0.570972173,0.724417731,0.848206583,0.937273392,
     6          0.987992518 /
C
      DATA  WEIGHT         / 1.0        ,0.888888889,0.555555556,
     1          0.652145155,0.347854845,0.568888889,0.478628671,
     2          0.236926885,0.467913935,0.360761573,0.171324493,
     3          0.295524225,0.269266719,0.219086363,0.149451349,
     4          0.066671344,0.202578242,0.198431485,0.186161000,
     5          0.166269206,0.139570678,0.107159221,0.070366047,
     6          0.030753242 /
C
C     ..... FIND SUBSCRIPT OF FIRST Z AND WEIGHT VALUE .....
      DO 1   I=1,7
        IF (M.EQ.NPOINT(I))  GO TO 2
    1 CONTINUE
C
C     ..... INVALID M USED .....
      GAUSS = 0.0
      RETURN
C
C     ..... SET UP INITIAL PARAMETERS .....
    2 JFIRST = KEY(I)
      JLAST = KEY(I+1) - 1
      C = (B-A)/2.0
      D = (B+A)/2.0
C
C     ..... ACCUMULATE THE SUM IN THE M POINT FORMULA .....
      SUM = 0.0
      DO 5  J=JFIRST,JLAST
        IF ( Z(J).EQ.0.0 )  THEN
          SUM = SUM + WEIGHT(J)*FUNCTN(D)
        ELSE
          SUM = SUM + WEIGHT(J)*(FUNCTN(Z(J)*C + D) + FUNCTN(-Z(J)
     1    *C + D))
        END IF
    5 CONTINUE
```

```
C
C     ..... MAKE INTERVAL CORRECTION AND RETURN .....
      GAUSS = C*SUM
      RETURN
C
      END
```

```
   4    1  1.0      2.0     1.0
  1.0         0.0
  5.0         0.0
  10.0        0.0
  40.0        0.0
```

```
1                        DOWNWIND DOSAGES

                        M =  4
                        LS =  1
                        S =  1.0
                        U =  2.0  KNOTS
                        Q =  1.000  KG

           X               Y               D                Q/D
      KILOMETRES      KILOMETRES     MG MIN/CU M     KG/(MG MIN/CU M)

         1.000           .000          .28161           3.55098
         5.000           .000          .02066          48.41128
        10.000           .000          .00667         150.00835
        40.000           .000          .00069        1457.16011
```

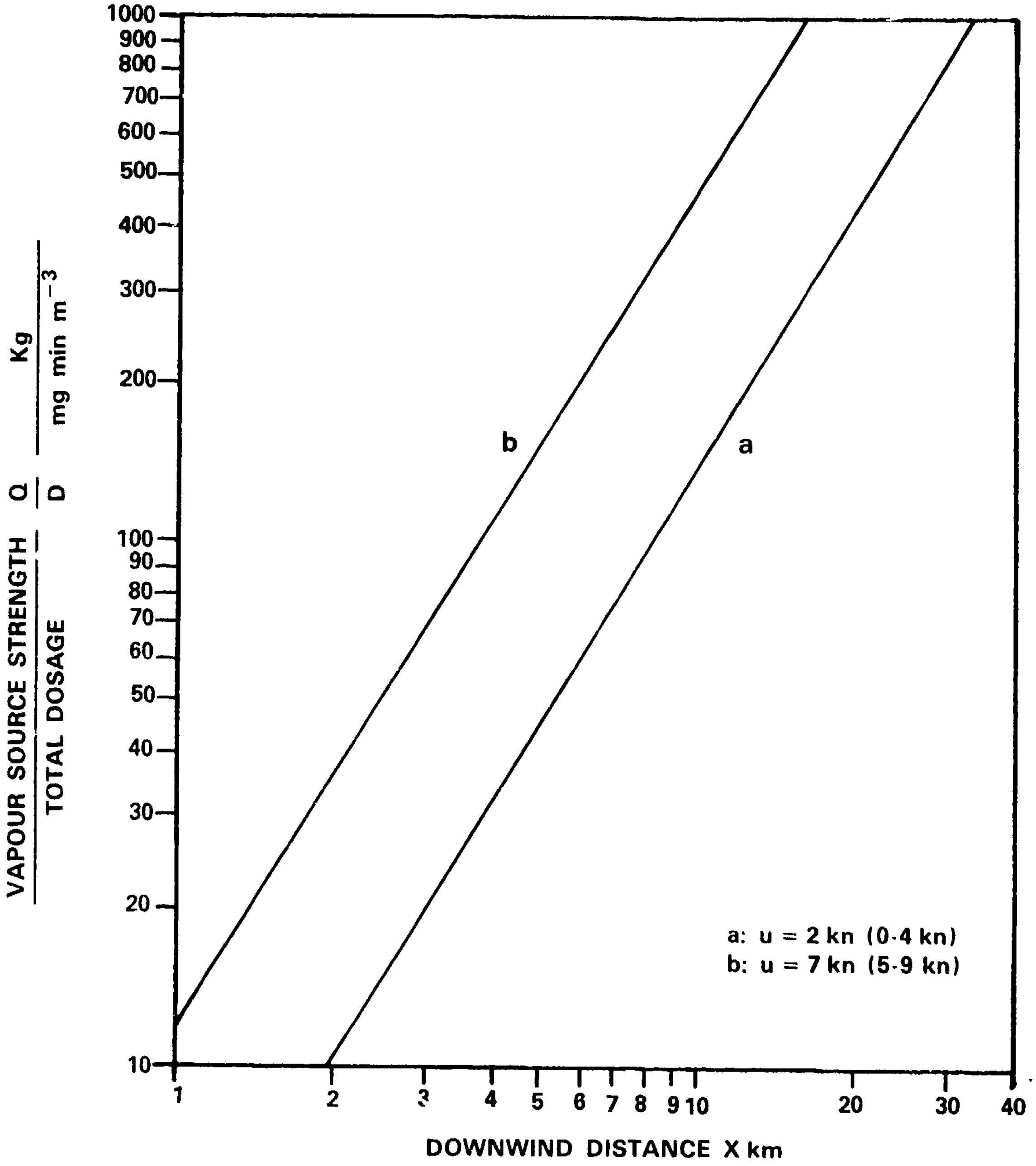

Figure 1

DISPERSION OVER LAND STABILITY CATEGORY S = 1

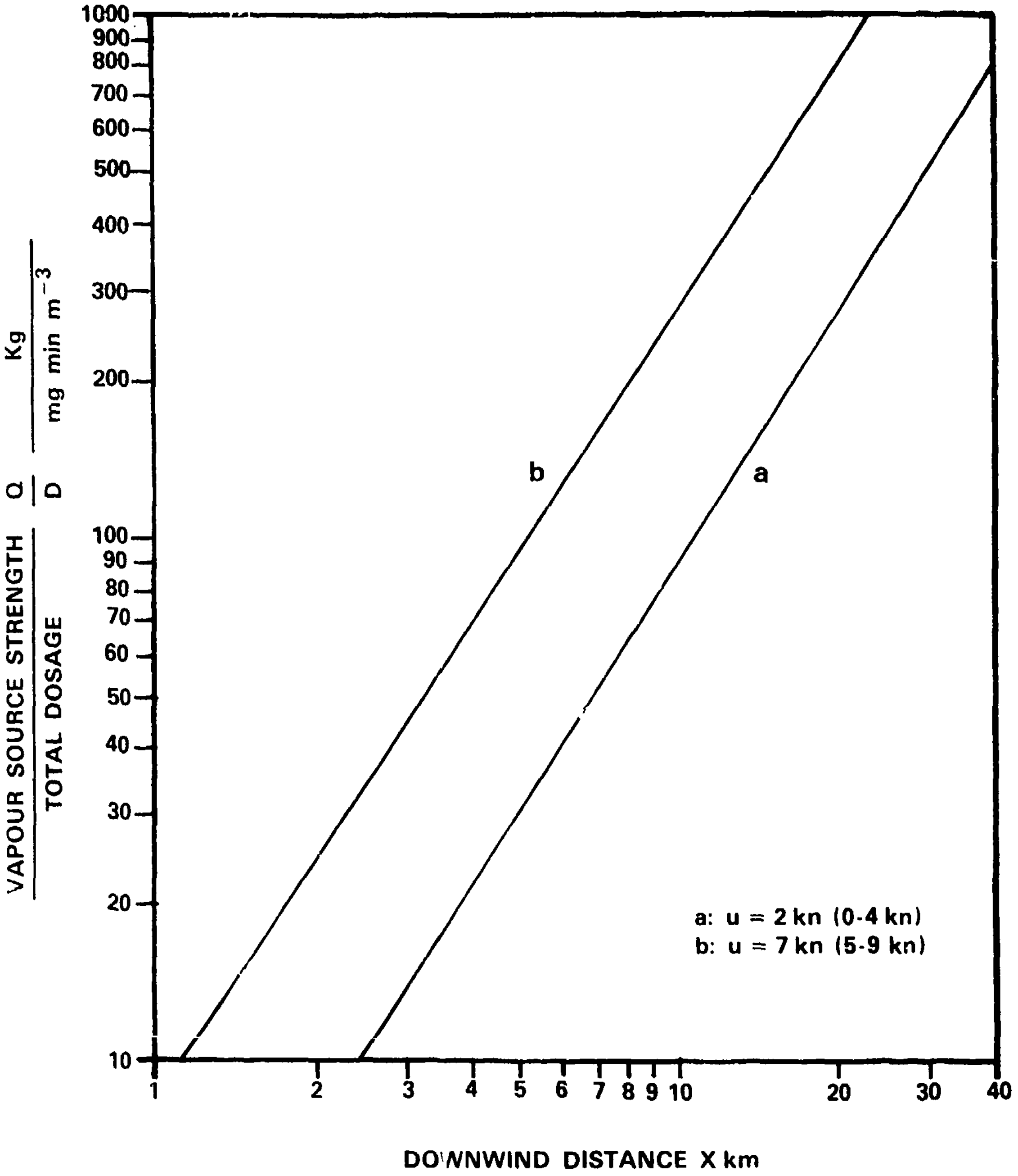

Figure 2

DISPERSION OVER LAND STABILITY CATEGORY S = 2

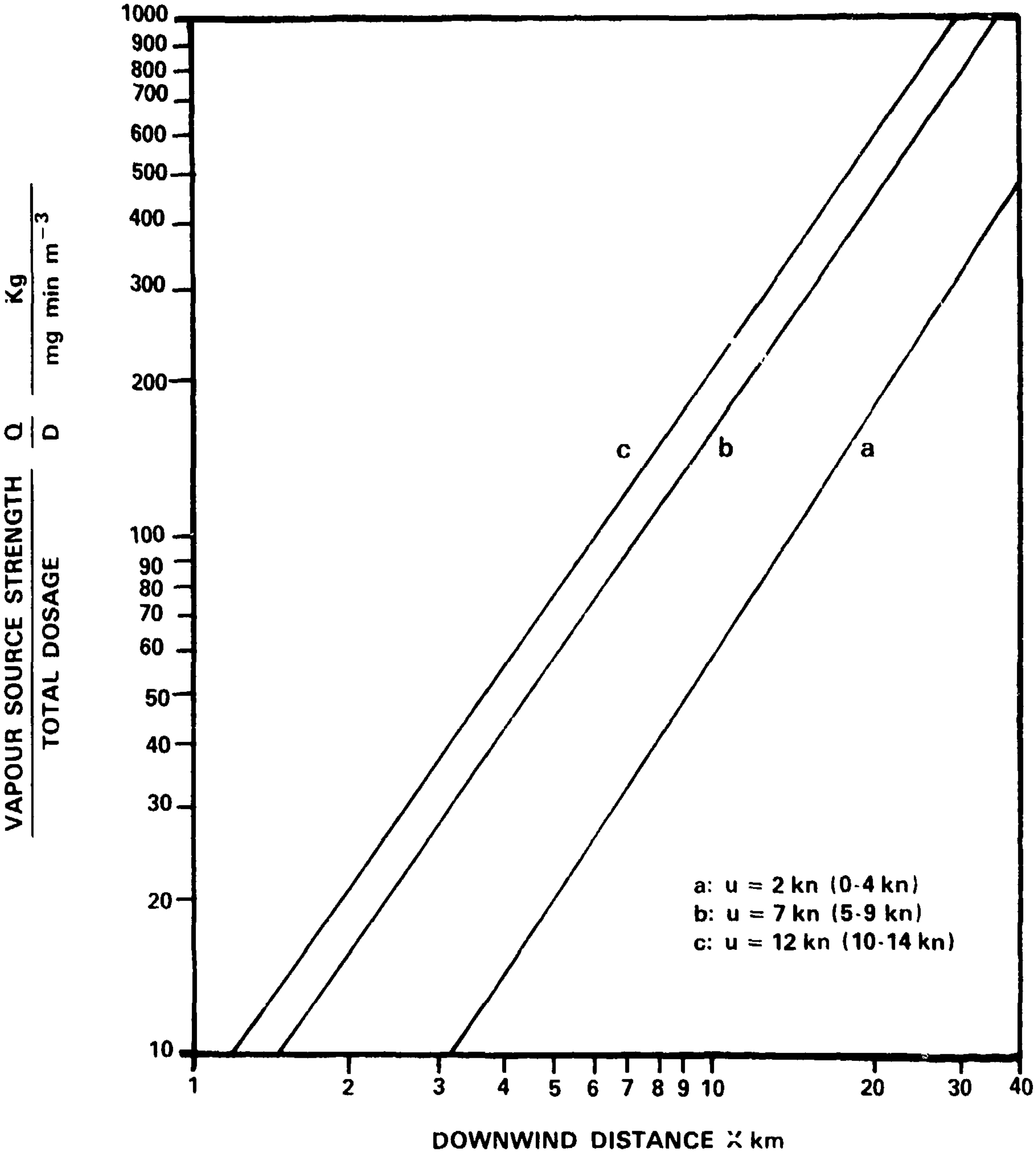

Figure 3

DISPERSION OVER LAND STABILITY CATEGORY S = 3

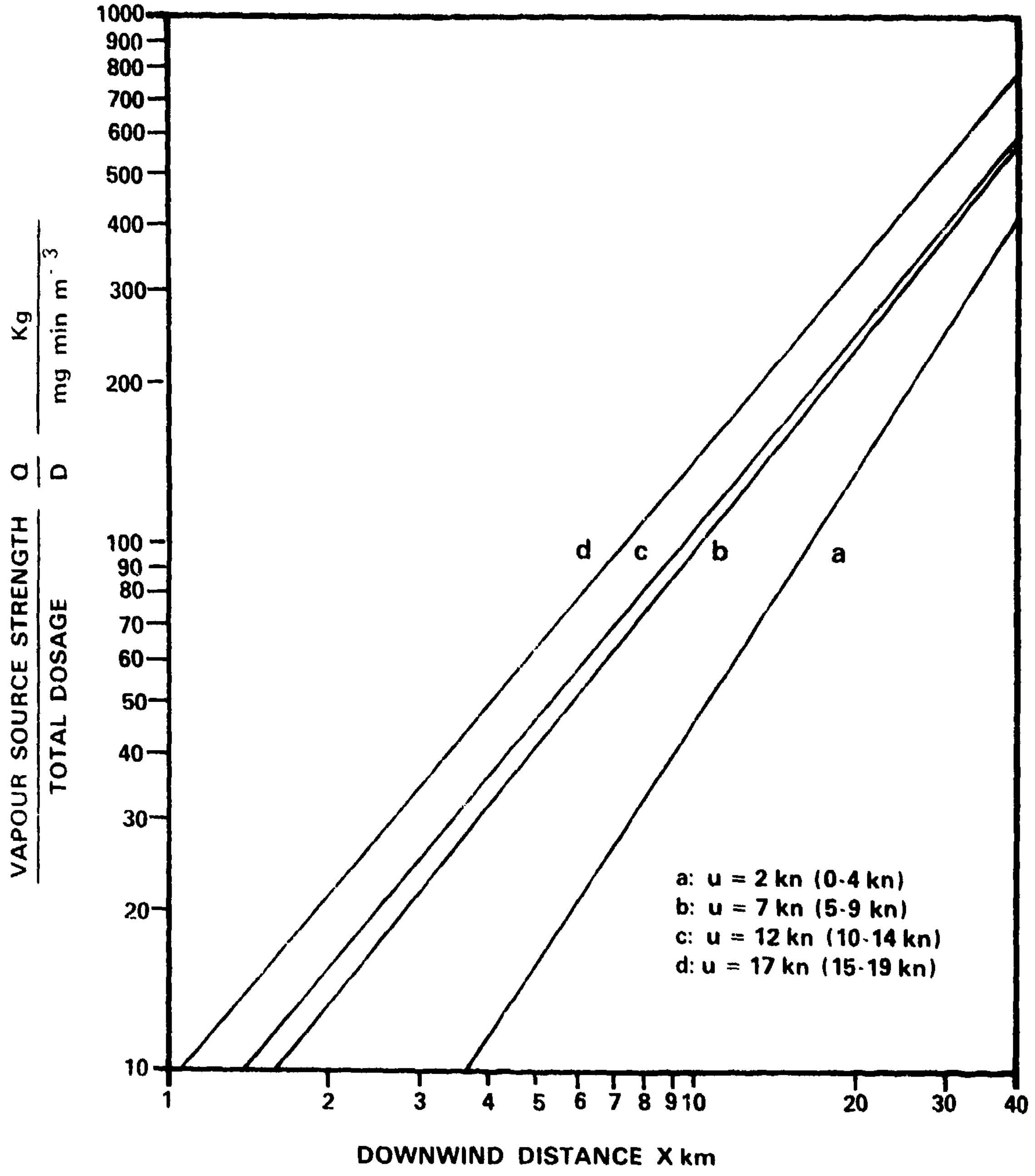

Figure 4

DISPERSION OVER LAND STABILITY CATEGORY S = 4

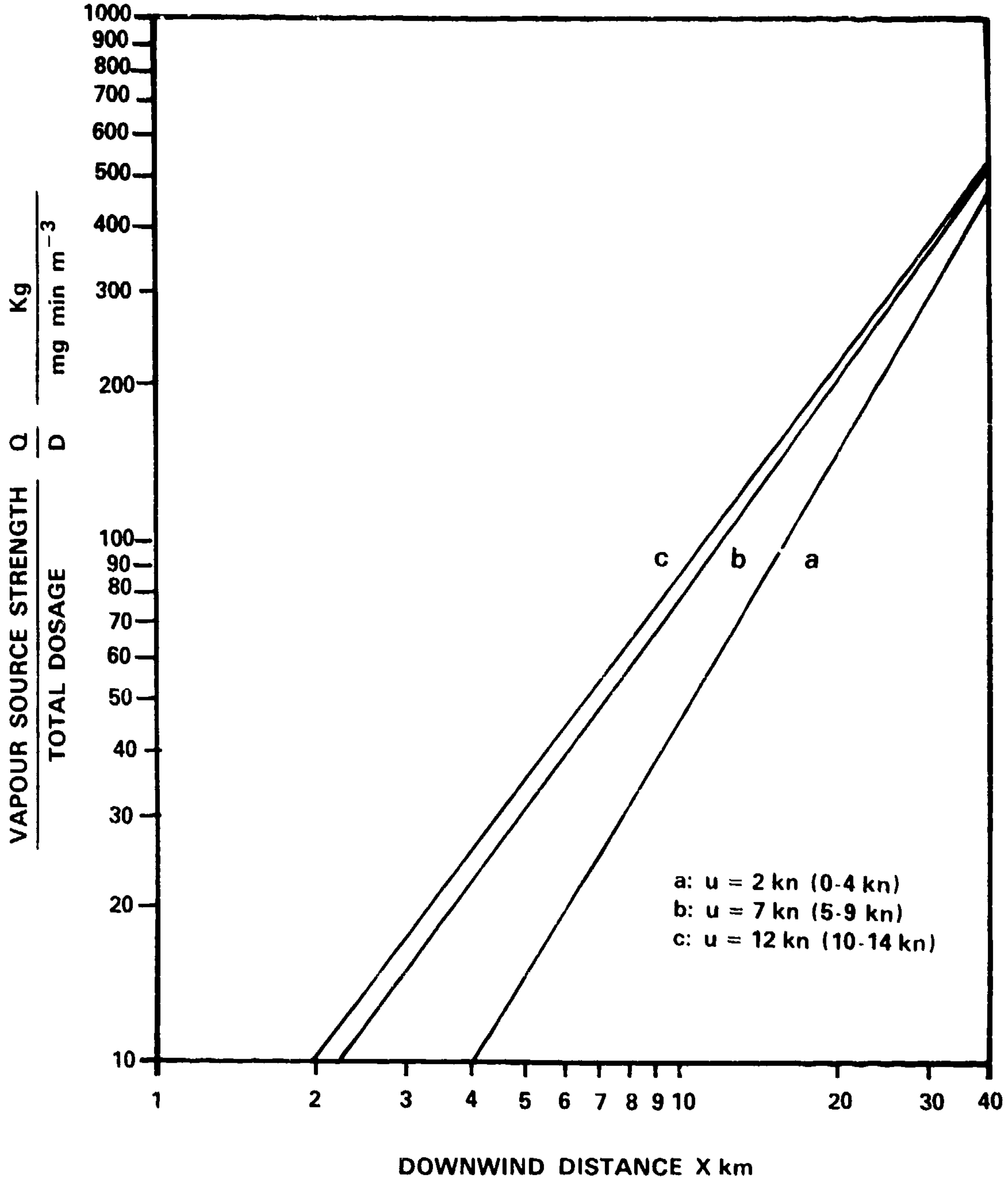

Figure 5

DISPERSION OVER LAND STABILITY CATEGORY S = 5

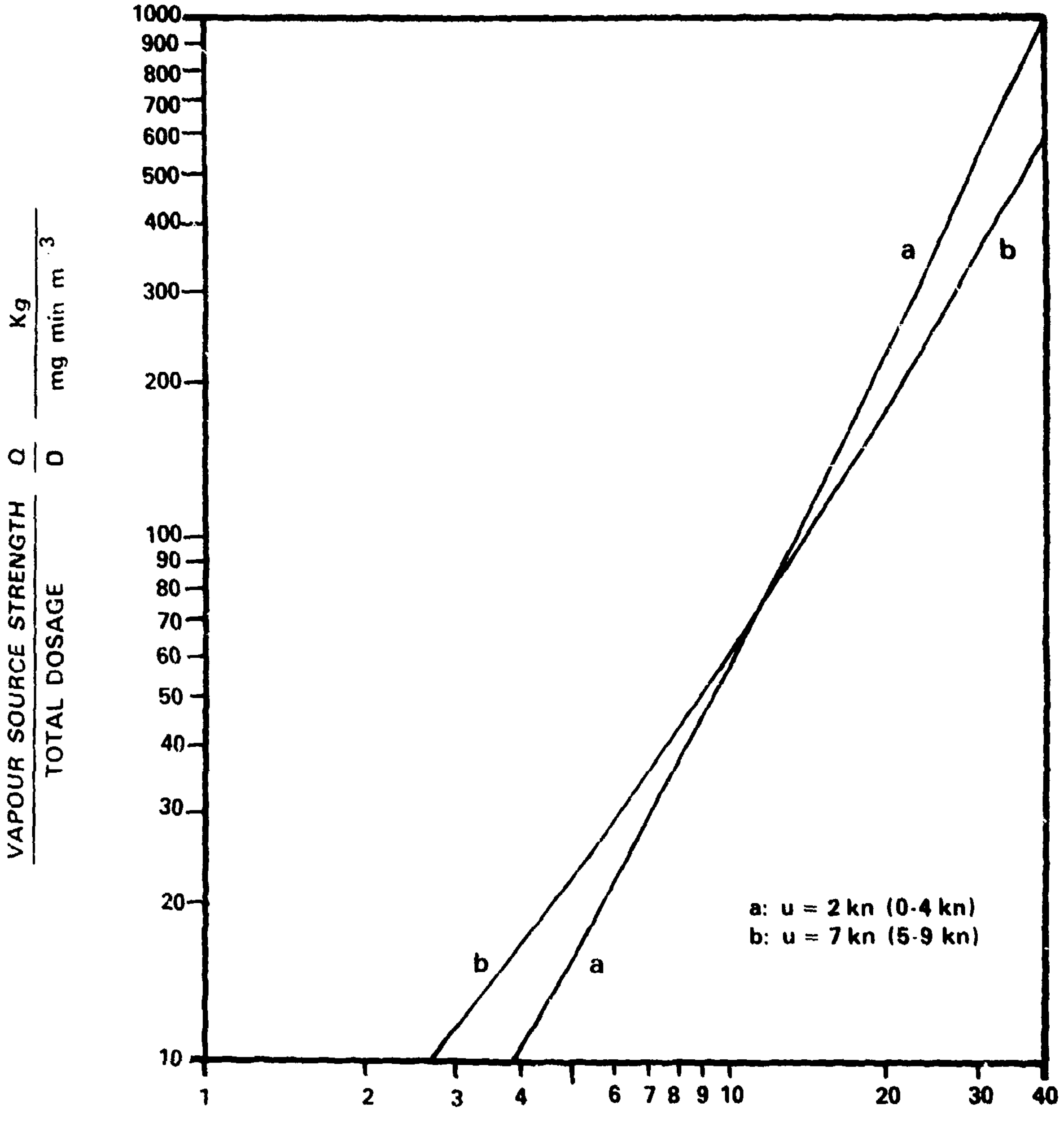

Figure 6

DISPERSION OVER LAND STABILITY CATEGORY S = 6

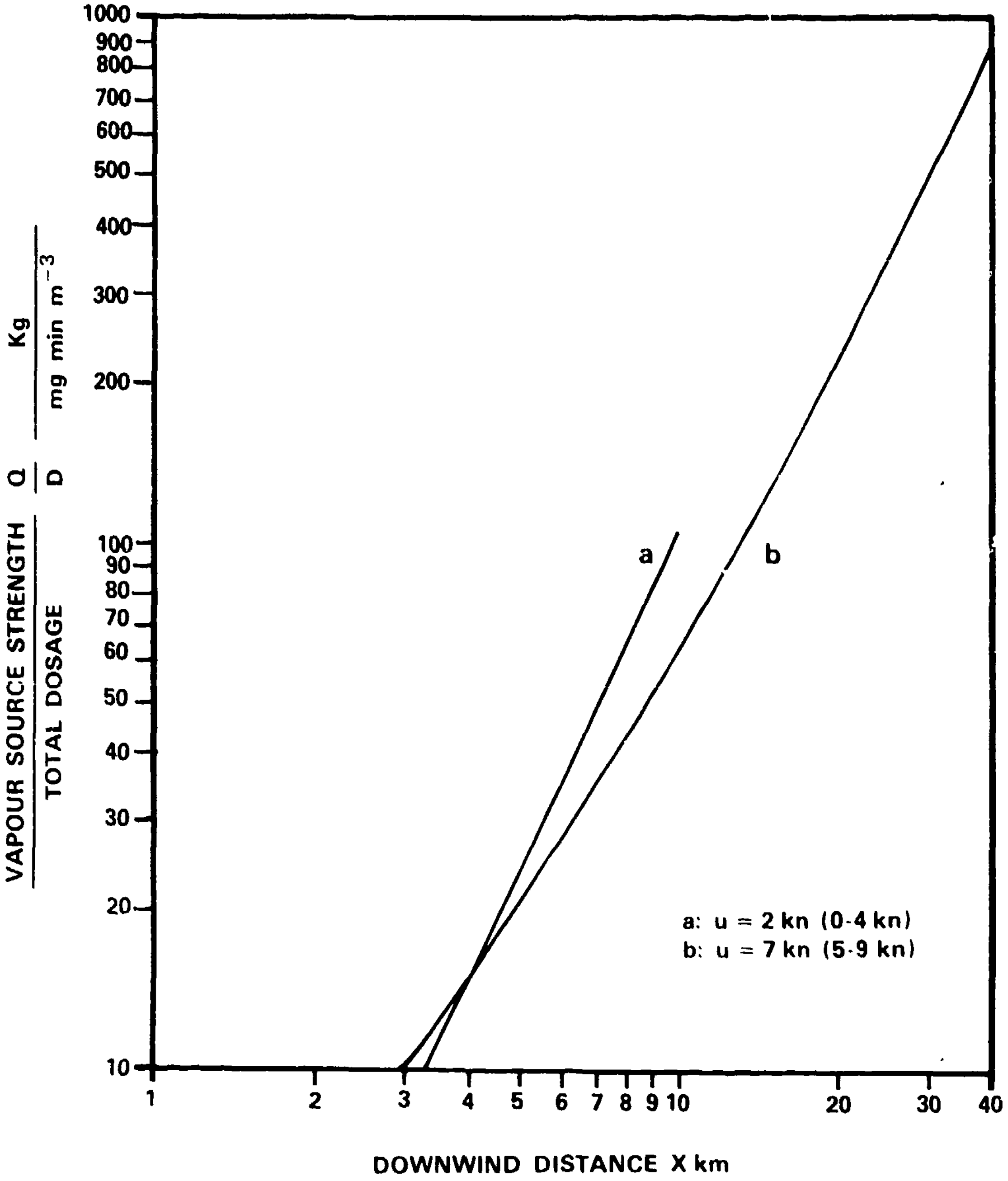

Figure 7

DISPERSION OVER LAND STABILITY CATEGORY S = 7

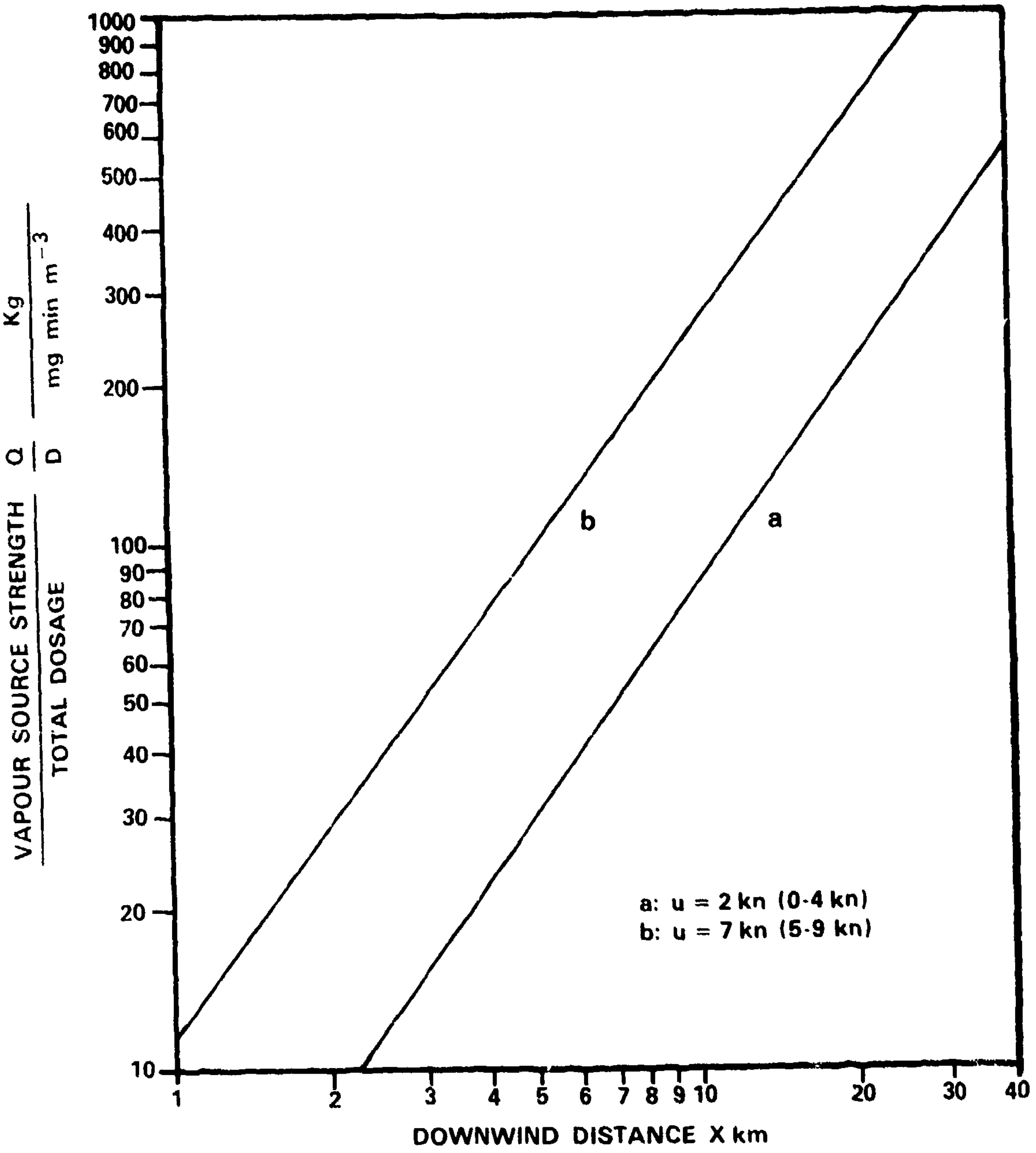

Figure 8

DISPERSION OVER LAND STABILITY CATEGORY S = 8

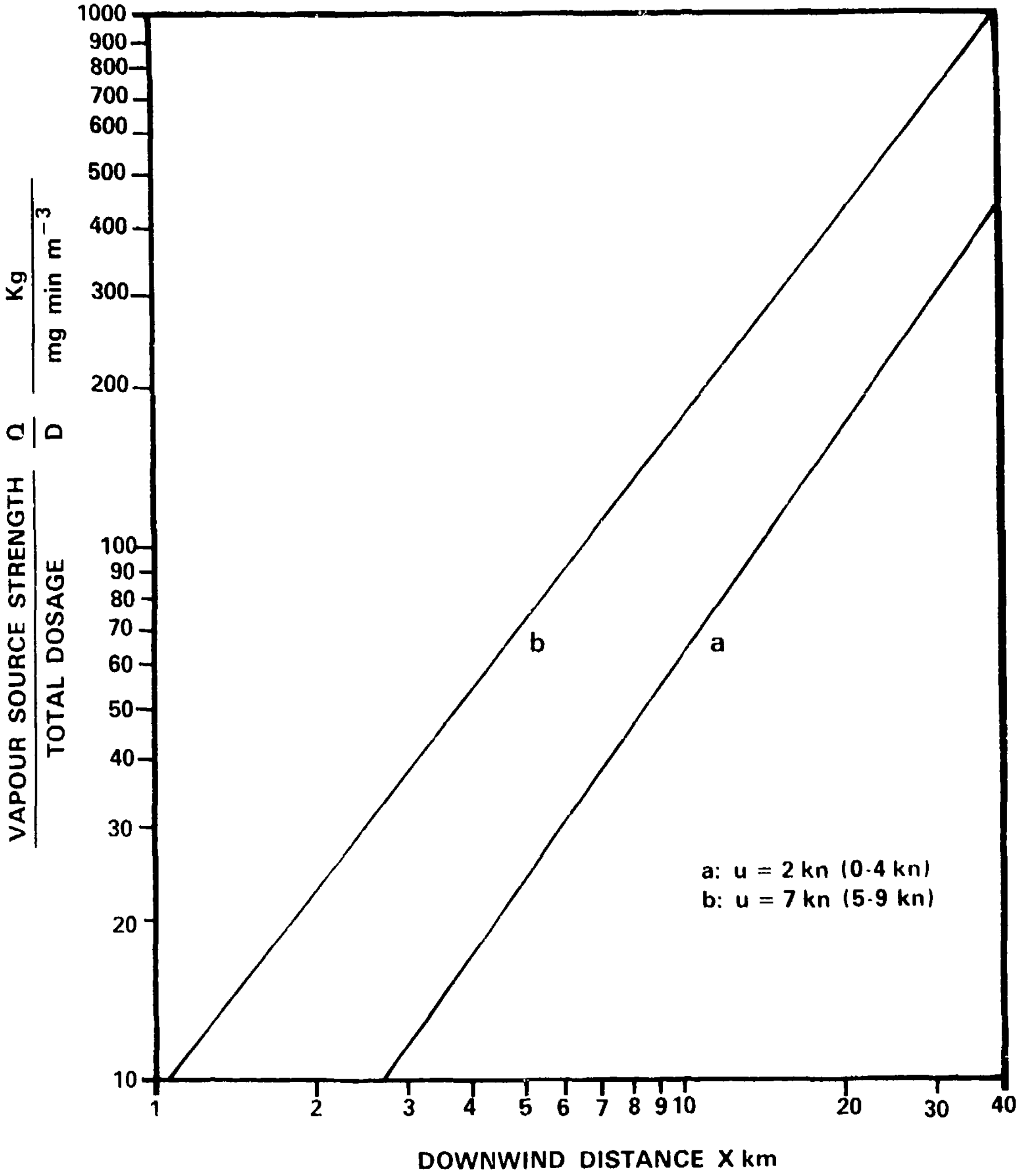

Figure 9

DISPERSION OVER LAND STABILITY CATEGORY S = 9

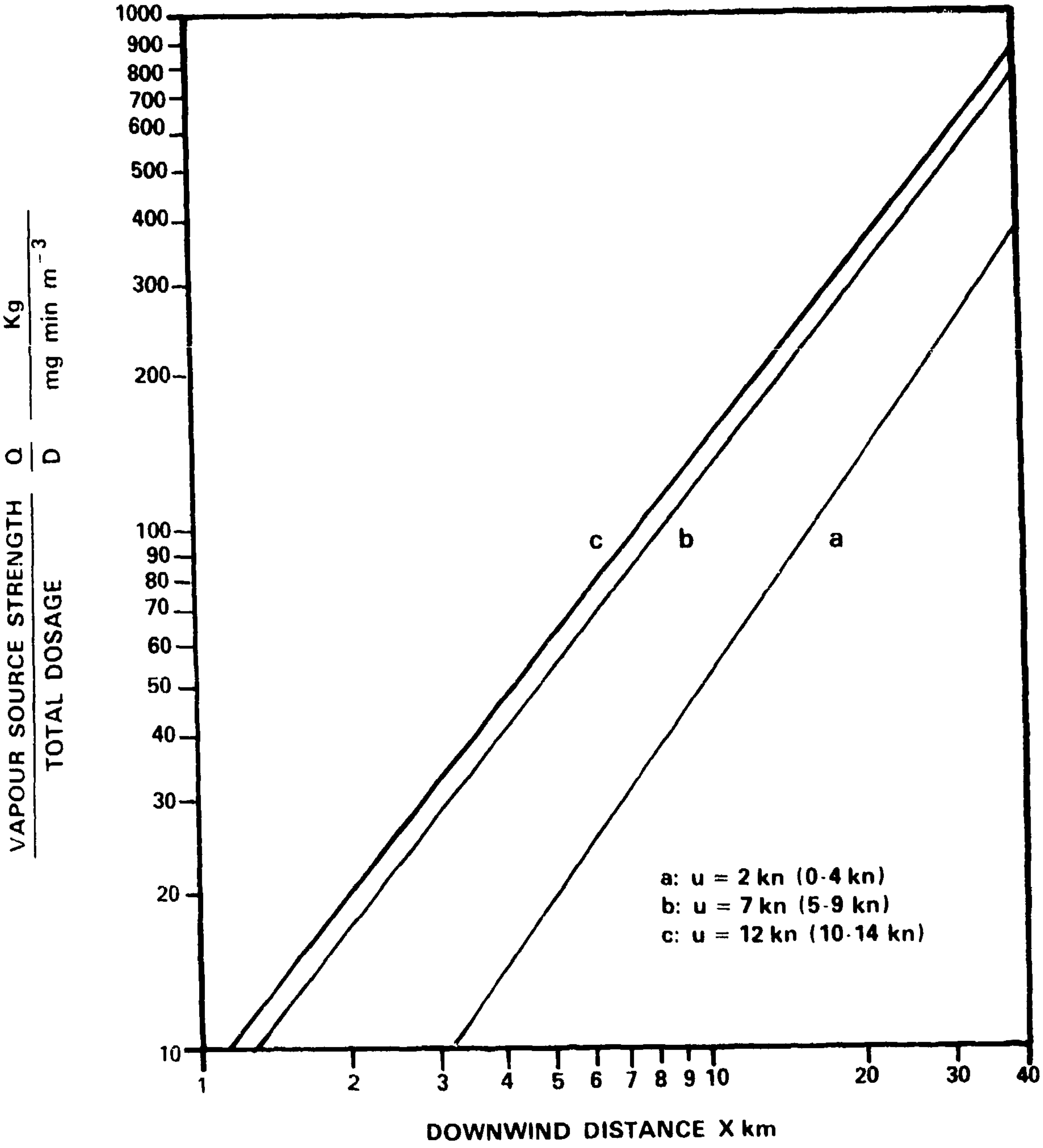

Figure 10

DISPERSION OVER LAND STABILITY CATEGORY S = 10

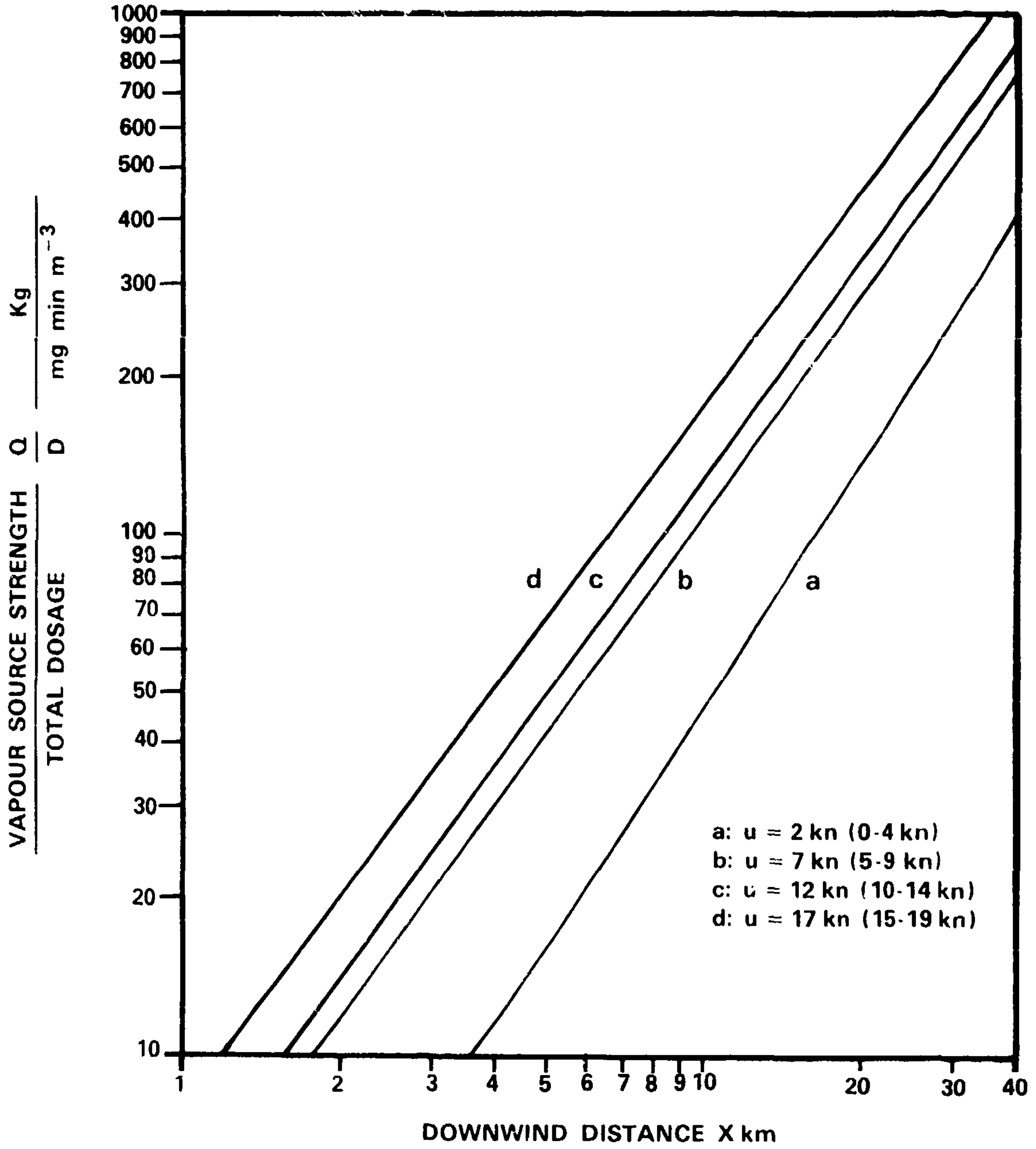

Figure 11

DISPERSION OVER LAND STABILITY CATEGORY S = 11

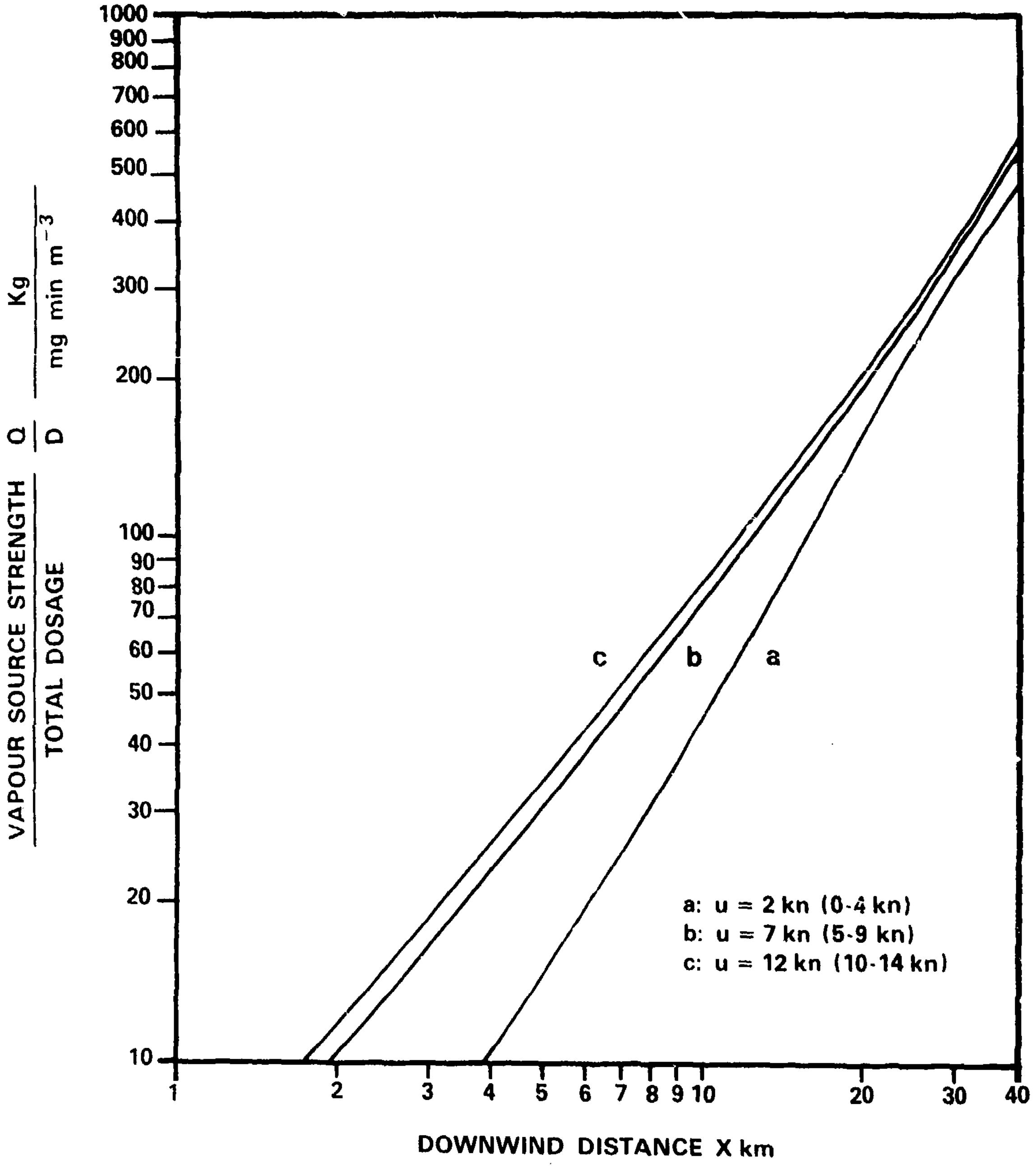

Figure 12

DISPERSION OVER LAND STABILITY CATEGORY S = 12

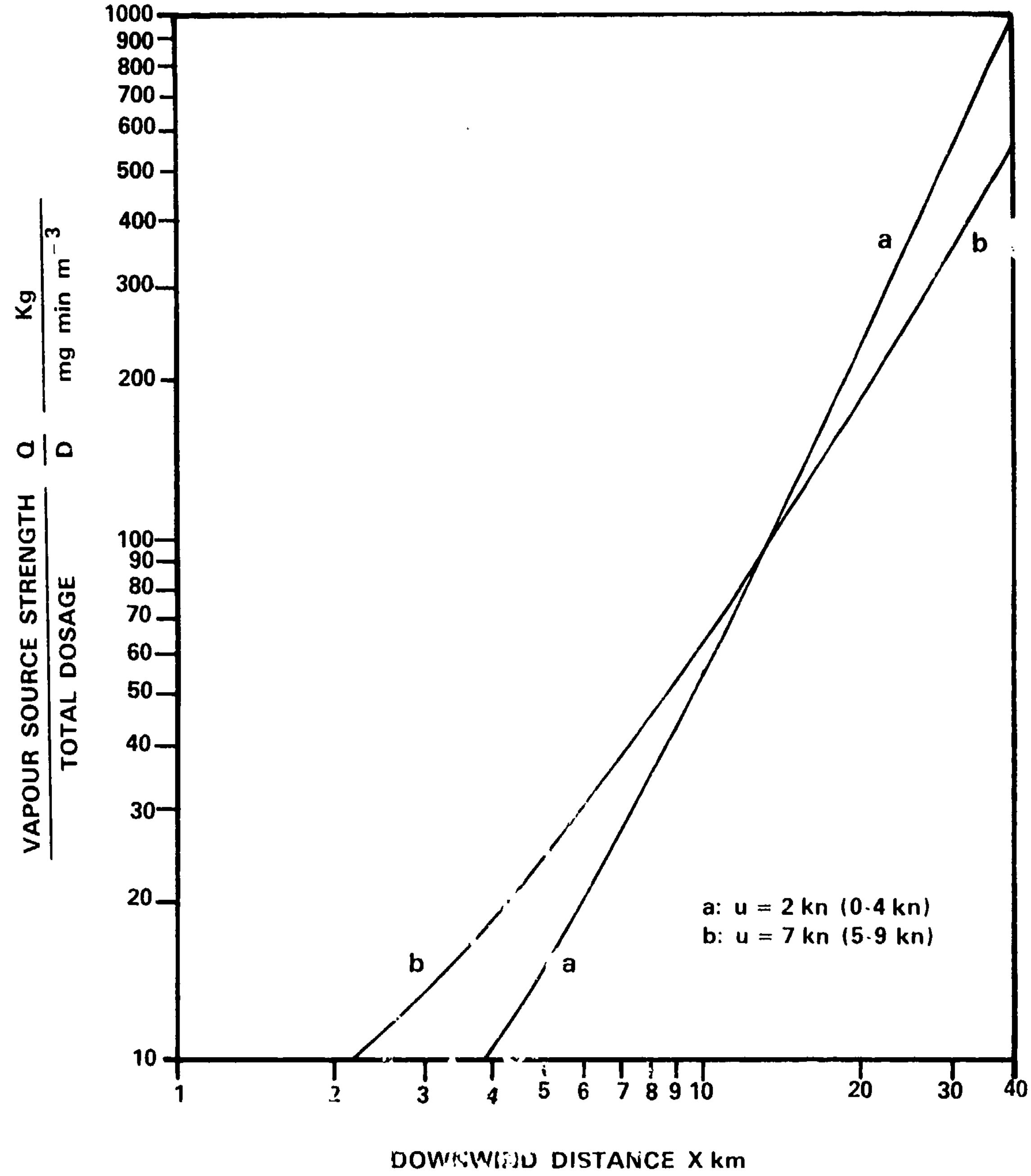

Figure 13

DISPERSION OVER LAND STABILITY CATEGORY S = 13

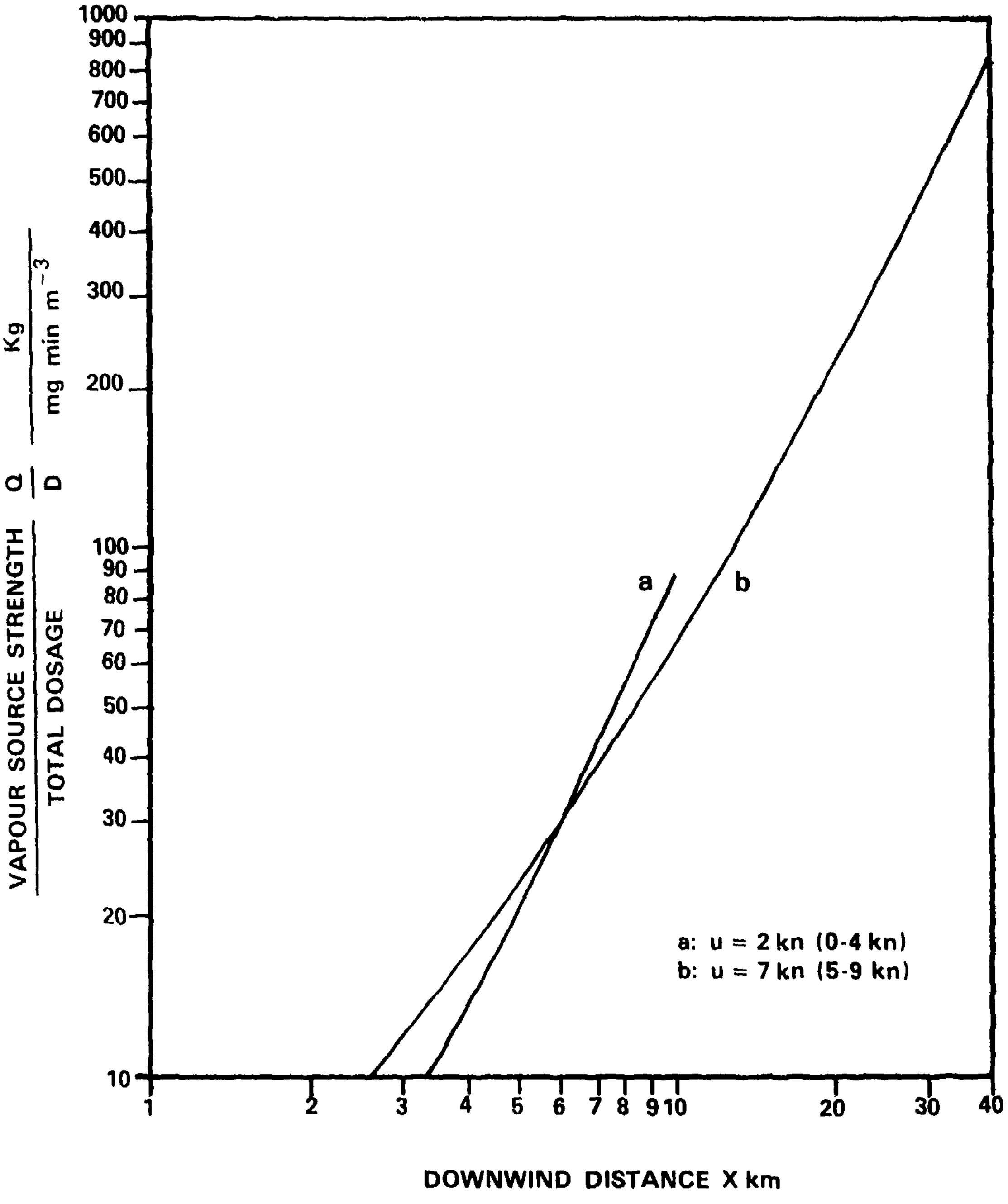

Figure 14

DISPERSION OVER LAND STABILITY CATEGORY S = 14

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(highest classification of Title, Abstract, Keywords)

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A FORTRAN PROGRAM FOR CALCULATING CHEMICAL HAZARDS USING THE NATO STANAG 2103/ATP-45 ALGORITHM

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