NOAA Western Region Computer Programs and
Problems NWS WRCP - No. 26

PROGRAM TO COMPUTE DOWNWIND CONCENTRATIONS FROM A TOXIC SPILL

Salt Lake City, Utah
February 1981

U.S. DEPARTMENT OF COMMERCE / National Oceanic and Atmospheric Administration / National Weather Service

PREFACE

This Western Region publication series is considered as a subset of our Technical Memorandum series. This series will be devoted exclusively to the exchange of information on and documentation of computer programs and related subjects. This series was initiated because it did not seem appropriate to publish computer program papers as Technical Memoranda; yet, we wanted to share this type of information with all Western Region forecasters in a systematic way. Another reason was our concern that in the developing AFOS-era there will be unnecessary and wasteful duplication of effort in writing computer programs in National Weather Service (NWS). Documentation and exchange of ideas and programs envisioned in this series hopefully will reduce such duplication. We also believe that by publishing the programming work of our forecasters, we will stimulate others to use these programs or develop their own programs to take advantage of the computing capabilities AFOS makes available.

We solicit computer-oriented papers and computer programs from forecasters for us to publish in this series. Simple and short programs should not be prejudged as unsuitable.

The great potential of the AFOS-era is strongly related to local computer facilities permitting meteorologists to practice in a more scientific environment. It is our hope that this new series will help in developing this potential into reality.

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1 Standard Format for Computer Series. June 1979
2 AFOS Crop and Soil Information Report Program. Ken Mielke, July 1979.
3 Decoder for Significant Level Transmissions of Raobs. John A. Jannuzzi, August 1979.
4 Precipitable Water Estimate. Elizabeth Morse, October 1979.
5 Utah Recreational Temperature Program. Kenneth M. Labas, November 1979.
6 Normal Maximum/Minimum Temperature Program for Montana. Kenneth Mielke, Dec. 1979.
7 Plotting of Ocean Wave Energy Spectral Data. John R. Zimmerman, Dec. 1979.
8 Raob Plot and Analysis Routines. John Jannuzzi, January 1980.
9 The SWAB Program. Morris S. Webb, Jr., April 1980. (PB 80-196041)
10 Flash-Flood Procedure. Donald P. Laurine and Ralph C. Hatch, April 1980. (PB 80-198658)
11 Program to Forecast Probability of Summer Stratus in Seattle Using the Durst Objective Method. John Zimmerman, May 1980.
12 Probability of Sequences of Wet and Dry Days. Hazen H. Bedke, June 1980. (PB80-223340)
13 Automated Montana Hourly Weather Roundup. Joe L. Johnston, July 1980. (PB81102576)
14 Lightning Activity Levels. Mark A. Mollner, July 1980. (PB81108300)
15 Two Fortran Applications of Wind-Driven Ekman Water Trnasport Theory: Upwelling Index and Storm Tide. Kent S. Short, July 1980. (PB81102568)
16 AFOS System Local Database Save and Rebuild Procedures or A Master Doomsday Program. Brian W. Finke, July 1980. (PB81108342)
17 AFOS/RDOS Translator Subroutine. Morris S. Webb, Jr., August 1980. (PB81108334)
18 AFOS Graphics Creation from Fortran. Alexander E. MacDonald
19 DATAKEYØ Repair Program. Paul D. Tolleson, August 1980. (PB81102543) (PB81-128035)
20 Contiguous File Transfer from the DPCM to the DCM. Paul D. Tolleson, September 19[illegible]
21 Freezing Level Program. Kenneth B. Mielke, September 1980. (PB81-128043)
22 Radar Boresighting Verification Program. Thomas E. Adler, November 1980.
23 Accessing the AFOS Database. Matthew Peroutka, January 1981.
24 AFOS Word Processor. Morris S. Webb, Jr., February 1981.
25 Automated Weather Log for Terminal Forecasting. John A. Jannuzzi, February 1981.

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PROGRAM TO COMPUTE DOWNWIND CONCENTRATIONS FROM A TOXIC SPILL

John Zimmerman

National Weather Service Forecast Office
Seattle, Washington
February 1981

UNITED STATES
DEPARTMENT OF COMMERCE / NATIONAL OCEANIC AND
ATMOSPHERIC ADMINISTRATION / National Weather
Service
Richard E. Hallgren, Director

This Technical Memorandum has been reviewed and is approved for publication by Scientific Services Division, Western Region.

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Scientific Services Division
Western Region Headquarters
Salt Lake City, Utah

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PROGRAM TO COMPUTE DOWNWIND CONCENTRATIONS FROM A TOXIC SPILL

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Seattle, Washington

I. General Information

A. Summary:

One of the unscheduled duties of the Air Pollution Focal Point is to provide meteorological assistnace in event of an accidental spill of toxic material. The immediate requirements of an on-site cleanup crew are for wind information at the location of the accident and wind forecasts for the next 12 to 24 hours. Site wind direction is obviously the most critical factor in determining what areas should be evacuated, if materials released into the atmosphere are toxic or othewise harmful.

Making an accurate forecast of surface winds in mountain-valley terrain of the Western Region is a difficult task and must be given first priority. The Air Pollution Focal Point should, first of all, provide good weather forecasts, especially wind forecasts.

On rare occasions, however, Weather Service meteorologists may be able to render additional assistance by using "AFOS" power. Normally, estimates of downwind concentrations from a toxic spill will be provided by the EPA meteorologist when such estimates are necessary. It is conceivable, especially during nonduty hours or on weekends, that the EPA meteorologist may be difficult to contact. Therefore, the following simple computer program was developed for such occasions when it is necessary to quickly estimate toxic air concentrations and no other experts are available.

Downwind pollutant concentration is computed assuming that the plume is a continuous point source and has a Gaussian distribution, i.e.,

$$X = \frac{Q}{2\pi\ \sigma y\ \sigma z\ u} \bullet \exp -\tfrac{1}{2} \left(\frac{y}{\sigma y}\right)^2 \bullet \{\exp[-\tfrac{1}{2} \left(\frac{z - H}{\sigma z}\right)^2 + \exp[-\tfrac{1}{2} \left(\frac{z + H}{\sigma z}\right)^2]\}$$

A complete description of the Gaussian plume model and its application can be found below in C. Reference. The dispersion coefficients used, sigma y (σy) and sigma z (σz), are given in Table I.

In the program the option is allowed of either entering a value of atmospheric stability or having a value computed based on the weather conditions. Five stability values are available, i.e.,

1. very unstable
2. unstable
3. slightly unstable
4. neutral
5. stable.

The weather parameters which are used to determine atmospheric stability are given in Table II.

Output of concentration X is given in grams per-cubic meter. The units for input of wind and height of release are in the usual English units, knots, and feet as shown in the sample run of the Application section. The computer program converts these units into meters per second and meters, respectively.

The release rate Q should be input in grams per second. Information on release rate Q will be difficult to obtain when an accidental spill occurs.

If a value of 1 is input for Q, however, then relative values of air concentration are obtained; that is, concentrations normalized with respect to Q. Relative concentration (x/Q) is useful in determining the relative values of concentration at different locations. In other words, if off axis plume concentrations are measured, concentrations can be found for other locations by using the ratios of relative concentration determined by computer. It is also possible to work backwards to determine the amount of material released by considering Q the unknown and along with actual measurements of air concentration, calculate Q from computed values of relative concentration, i.e.,

$$Q = \left(\frac{X}{Q\,X_m} \right)^{-1}$$

where $\frac{X}{Q}$ = relative concentration

X_m = measured concentration.

B. Environment:

This program is written in FORTRAN IV and is run on the Eclipse S/230 computer.

C. Reference:

Turner, D. B. (1969): Workbook of Atmospheric Dispersion Estimates. USDHEW PHS Environmental Health Series, Air Pollution PHS Publication No. 999-AP-26.

II. Application

A. Complete Program Description:

This computer program has been incorporated into an AFOS procedure called "SPILL". Input data are manually input into a preformat called GAS, which is shown in Figure 1. Procedure SPILL automatically calls preformat GAS to the ADM.

Table I. Dispersion Coefficients sigma y and sigma z

Stability Class	Crosswind Constant(1) a	Constants for Vertical Diffusion Parameter, σ_z(2) $x \le x_1$ b	$x \le x_1$ q	x_1 (Meters)	$x_1 \le x \le x_2$ b	$x_1 \le x \le x_2$ q	x_2 (Meters)	$x_2 \le x$ b	$x_2 \le x$ q
A	0.40	0.125	1.03	250	0.00883	1.51	500	0.000226	2.10
B	0.295	0.119	0.986	1000	0.0579	1.09	10,000	0.0579	1.09
C	0.20	0.111	0.911	1000	0.111	0.911	10,000	0.111	0.911
D	0.13	0.105	0.827	1000	0.392	0.636	10,000	0.948	0.540
E	0.098	0.100	0.778	1000	0.373	0.587	10,000	2.85	0.366

(1) $\sigma_y = ax^{0.903}$, Where x is Downwind Distance from Source; σ_y and x are in Meters.

(2) $\sigma_z = bx^q$; σ_z and x are in Meters.

Table II. Weather and Stability Categories

Surface Wind Speed (at 10 m), m sec^{-1}	Day: Incoming Solar Radiation — Strong	Day: Moderate	Day: Slight	Night: Thinly Overcast or Low Cloud	Night: Cloud
2	A	A-B	B		
2-3	A-B	B	C	E	F
3-5	B	B-C	C	D	E
5-6	C	C-D	D	D	D
6	C	D	D	D	D

The neutral class D, should be assumed for overcast conditions during day or night.

```
SEAMCPGAS
WOUS00 KSEA 221741

  INPUT DATA FOR PROGRAM SPILL TO COMPUTE DOWNWIND CONCENTRATIONS.
          HEIGHT OF SPILL       [        ] FEET
          RATE OF SPILL         [        ] GRAMS/SEC
          HEIGHT OF RECEPTOR [        ] FEET

        ...DOWNWIND LOCATIONS          ...CROSWIND LOCATIONS
          1. [       ] MILES            1. [       ] MILES
          2. [       ]   "              2. [       ]   "
          3. [       ]   "              3. [       ]   "
          4. [       ]   "              4. [       ]   "
          5. [       ]   "              5. [       ]   "
        WIND SPEED           [        ] KNOTS

        ...ATMOSPHERIC STABILITY IF KNOWN ENTER VALUE...
                   OTHERWISE ENTER 0 [ ]
        ...IF STABILITY UNKNOWN FILL IN BELOW...SKIP IF KNOWN...
           SKY NOT OVERCAST=0....SKY OVERCAST=1       [ ]
           OVERCAST THIN=0.......OVERCAST THICK=1    [ ]
           DAYTIME=0............NIGHTTIME=1          [ ]
           SOLAR RADIATION STRONG=1 MODERATE=2 SLIGHT=3  [ ]             [[
```

Figure 1. AFOS Preformat for Data Entry.

III. Procedures

A. Input/Output:

The following is an example of input data and resultant output on ADM.

```
TEMPORARY
WOUS00 KSEA 221736
..../....1..../....2..../....3..../....4..../....5..../....6..../
   INPUT DATA FOR PROGRAM SPILL TO COMPUTE DOWNWIND CONCENTRATIONS.
          HEIGHT OF SPILL      0.      FEET
          RATE OF SPILL        3.      GRAMS/SEC
          HEIGHT OF RECEPTOR   0.      FEET

         ...DOWNWIND LOCATIONS          ...CROSWIND LOCATIONS
           1.  .1      MILES             1.  0.      MILES
           2.  .5        "               2.  .25       "
           3.  1.        "               3.  .5        "
           4.  3.        "               4.  .75       "
           5.  15.       "               5.  1.        "
          WIND SPEED           14.     KNOTS

           ...ATMOSPHERIC STABILITY IF KNOWN ENTER VALUE...
                    OTHERWISE ENTER 0  4
           ...IF STABILITY UNKNOWN FILL IN BELOW...SKIP IF KNOWN...
              SKY NOT OVERCAST=0....SKY OVERCAST=1
              OVERCAST THIN=0.......OVERCAST THICK=1
              DAYTIME=0.............NIGHTTIME=1
              SOLAR RADIATION STRONG=1 MODERATE=2 SLIGHT=3
```

```
PORARY           EWOUS00 KSEA 221736
 WIND SPEED = 14.KNOTS                   ATMOSPHERIC STABILITY =   4
 MILES                                   MILES CROSSWIND
 DOWNWIND              0.00       0.25       0.50       0.75       1.00
      0.1        0.192E -3 0.000E  0 0.000E  0 0.000E  0 0.000E  0
      0.5        0.161E -4 0.279E-16 0.000E  0 0.000E  0 0.000E  0
      1.0        0.556E -5 0.240E -8 0.195E-18 0.000E  0 0.000E  0
      3.0        0.102E -5 0.353E -6 0.145E -7 0.704E-10 0.407E-13
     15.0        0.937E -7 0.884E -7 0.743E -7 0.555E -7 0.369E -7
```

B. Program Listing:

1. Procedure "SPILL".

2. Program Spill.

```
SEAPCDØØ4
WOUSØØ KSEA 181855
  DISPLAY    MODE     ACC/OV      COMMAND
   (1-4)     (D/M)    (R/A/O)     (ANY COMMAND; LAST LINE MUST BE END OF "NAME")
  -------    -----    -------     ----------------------------------------------
Ø1                                PURGE:TEMPORARY
Ø2                                PAUSE 5
Ø3   1         M        R         M:GAS
Ø4                                PAUSE 5
Ø5                                SAVE:TEMPORARY DPØF:TEMPORARY
Ø6                                PAUSE 5
Ø7                                RUN:@SPILLX@
Ø8                                PAUSE 2Ø
Ø9   1         D        R         DSP:DPØF:SPILL
1Ø                                END
11
12
13
14
15
16
17
18
```

Procedure "SPILL"

```
DIR DPØF
 DELETE DPØF:TOXICSPIL
 RENAME DPØF:TEMPORARY DPØF:TOXICSPIL
 DELETE DPØF:SPILL
 CRAND DPØF:SPILL
 DPØF:SPILL.SV
 DIR DPØ
```

File SPILLX

```
TYPE SPILL.FR
C     PROGRAM TO COMPUTE DOWNWIND CONCENTRATIONS FROM A TOXIC SPILL
C
      DIMENSION STA(5,5),SYA(5),SZA(5,3),SZB(5,3)
      DIMENSION CQ(5,5),XD(5),YD(5),AA(80)
       CALL OPEN(20,"TOXICSPIL",1,IER,500)
       READ(20,50)AA
50    FORMAT(80A1)
      READ(20,5)Z,Q,H
5     FORMAT(//,3(30X,F5.0,/),/)
       TYPE Z,Q,H
       Z=Z/3.2808
       H=H/3.2808
      DO 6 I=1,5
6     READ(20,7)XD(I),YD(I)
7     FORMAT(15X,F5.0,20X,F5.0)
      READ(20,8)U,KK,KS,KT,KD,KR
8     FORMAT(30X,F5.0,///,40X,I1,//,3(55X,I1,/),60X,I1)
      CALL CLOSE(20,IER)
      TYPE XD(1),YD(1),U,KK,KS,KT,KD,KR
       U=U/1.9425
       CALL OPEN(20,"SPILL1",1,IER,500)
       DO 4 I=1,5
      READ(20,9)(STA(I,J),J=1,5)
9     FORMAT(5F5.0)
4     CONTINUE
      CALL CLOSE(20,IER)
       IF(KK.NE.0)GO TO 40
       CALL STAB(U,KK,KS,KT,KD,KR,STA)
40    TYPE "1"
       CALL OPEN(20,"SPILL2",1,IER,500)
      READ(20,15)(SYA(I),I=1,5)
15    FORMAT(5F5.0)
      CALL CLOSE(20,IER)
      CALL OPEN(20,"SPILL3",1,IER,500)
       DO 11 J=1,3
      READ(20,16)(SZA(I,J),I=1,5)
16    FORMAT(5F10.0)
11    CONTINUE
      CALL CLOSE(20,IER)
      CALL OPEN(20,"SPILL4",1,IER,500)
       DO 12 J=1,3
      READ(20,16)(SZB(I,J),I=1,5)
12    CONTINUE
      CALL CLOSE(20,IER)
       TYPE "2"
      DO 10 QI=1,5
      DO 10 J=1,5
      CALL CHI(Z,H,U,KK,Q,I,J,C,XD,YD,SYA,SZA,SZB)
       CQ(I,J)=C
```

```
10  CONTINUE
      TYPE "3"
    CALL OPEN(20,"SPILL",3,IER,500)
      WRITE(20,50)AA
      U=U*1.9425
    WRITE(20,21)U,KK
    WRITE(10,21)U,KK
21  FORMAT("   WIND SPEED =",F4.0,"KNOTS","                              ATMOSPHERIC STABILITY
     WRITE(20,22)(YD(I),I=1,5)
      WRITE(10,22)(YD(I),I=1,5)
 22  FORMAT("   MILES                                           MILES CROSSWIND",/,
   1"   DOWNWIND      ",5F10.2)
      DO 30 I=1,5
     WRITE(20,23)XD(I),(CQ(I,J),J=1,5)
      WRITE(10,23) XD(I),(CQ(I,J),J=1,5)
 23  FORMAT(F11.1,5X,5E10.3)
30  CONTINUE
      STOP
      END

R
```

```
TYPE SPILL01.FR
      SUBROUTINE STAB(W,KK,KS,KT,KD,KR,STA)
      DIMENSION STA(5,5)
      IF(KS.NE.0)GO TO 60
      IF(U.LE.4)GO TO 11
      IF(U.LE.6)GO TO 12
      IF(U.LE.10)GO TO 13
      IF(U.LE.12)GO TO 14
      IS=5
      GO TO 20
   11 IS=1
      GO TO 20
   12 IS=2
      GO TO 20
   13 IS=3
      GO TO 20
   14 IS=4
   20 CONTINUE
      IF(KD.NE.0)GO TO 30
      JS=KR
      GO TO 40
  30  IF(KT.EQ.1)JS=4
      IF(KT.EQ.0)JS=5
   40 CONTINUE
      KK=STA(IS,JS)
       GO TO 70
  60  KK=4
   70 CONTINUE
      RETURN
      END
      R
```

```
TYPE SPILL02.FR
        SUBROUTINE CHI(Z,H,U,KK,Q,I,J,C,XD,YD,SYA,SZA,SZB)
        DIMENSION XD(5),YD(5),SYA(5),SZA(5,3),SZB(5,3)
        X=XD(I)*1609
        Y=YD(J)*1609
        IF(KK.NE.1)GO TO 30
        IF(X.GT.250)GO TO 10
        IX=1
        GO TO 100
   10   IF(X.GT.500)GO TO 20
        IX=2
        GO TO 100
  20    IX=3
  30    IF(X.GT.100)GO TO 40
        IX=1
        GO TO 100
  40    IF(X.GT.10000)GO TO 50
        IX=2
        GO TO 100
  50    IX=3
 100    CONTINUE
        SY=SYA(KK)*X**.903
        SZ=SZA(KK,IX)*X**SZB(KK,IX)
        A=Q/(6.2832*U*SY*SZ)
        B=.5*((Z-H)/SZ)**2+EXP(-.5*((Z+H)/SZ)**2)
        IF(B.GT.50)GO TO 200
        B=EXP(-B)
        C=.5*((Y/SY)**2)
        IF(C.GT.50)GO TO 200
        C=EXP(-C)
        C=A*B*C
        GO TO 300
  200  C=0
  300  RETURN
        END
R
```

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