

Final Report
Multivariate Analysis of Petroleum
Weathering in the Marine Environment -
Sub Arctic

Volume II - Appendices

SCIENCE APPLICATIONS, INC.

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Final Report

Multivariate Analysis of Petroleum
Weathering in the Marine Environment -
Sub Arctic

Volume II - Appendices

Submitted by:

James R. Payne, Bruce E. Kirstein, G. Daniel McNabb, Jr.,
James L. Lambach, Robert Redding, Randolph E. Jordan,
Wilson Hom, Celso de Oliveira, Gary S. Smith, Daniel M. Baxter,
and Russel Gaegel (NOAA Kasitsna Bay laboratory manager)

James R. Payne, Principal Investigator
Division of Environmental Chemistry and Geochemistry
Science Applications, Inc.
La Jolla, CA 92038

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BACKGROUND

The Appendices contained in this volume (II) are an integral component of the Oil Weathering Program Final Report. They document the complete Oil Weathering Model Computer Code; contain the Oil Weathering Model User's Manual; provide detailed descriptions of analytical methods not otherwise covered in Volume I, and present the results of X-ray defraction analyses on selected SPM samples and the analyses of subtidal sediments examined in support of another NOAA research unit. Originally it was our desire to bind these appendices with the Technical Results in Volume I, but the length of the document made it too large to conveniently use in that format. Therefore, the report was divided into two separate documents; however, this volume should be archived with the technical portion (Volume I) and delivered to persons requesting the results of this study for easy referral. For reference, the following five pages present the Table of Contents for Volume I.

Appendices A through E herein present detailed code listings for various components of the overall weathering model. Appendix A lists the entire computer code as it existed in December, 1983. Appendix B includes the Oil Weathering Model User's Manual which was published as a separate document in July, 1983. Appendix C includes a code description for component-specific dissolution. Appendix D includes a code listing for dispersed oil-concentration profiles with a time varying oil flux, and Appendix E includes a code listing for dispersed oil concentration profiles with a constant oil flux. Appendix F presents analytical methods utilized throughout the oil weathering program, and Appendix G includes the results of X-ray diffraction analyses completed by Technology of Materials Company on suspended particulate material used for oil/SPM adsorption studies. Finally, because the information on long-term fate of sedimented oil is pertinent to the overall goals of this program, the results of our collaborative efforts with Drs. Griffiths and Morita of Oregon State University are included as Appendix H.

The facts, conclusions and issues appearing in this report are based on results of an Alaskan environmental studies program managed by the Outer Continental Shelf Environmental Assessment Program (OCSEAP) of the National Oceanic and Atmospheric Administration (NOAA), U.S. Department of Commerce, and primarily funded by the Minerals Management Service (MMS), U.S. Department of Interior, through interagency agreement.

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APPENDIX A

CODE LISTING FOR OPEN-OCEAN OIL-WEATHERING CALCULATIONS

APPENDIX A

```

00010 C ***** CUTVP2.FOR *****
00020 C
00030 C THIS IS THE OPEN-OCEAN OIL-WEATHERING CODE AND
00040 C THE OIL PHASE IS CONSIDERED WELL-STIRRED ALL THE
00050 C TIME.
00060 C
00070 C THIS VERSION OF THE OIL-WEATHERING CODE DIFFERS
00080 C FROM CUTVP1 IN THE VISCOSITY CALCULATION.
00090 C
00100 C JANUARY, 1983
00110 C
00120 C GET YOUR OUTPUT FROM CUTVP2.OUT/FILE:FORTRAN
00130 C THE PLOT FILE IS CUTVP2.PLT
00140 C THE TYPE FILE IS CUTVP2.TYP
00150 C
00160 REAL*4 MW,MW1,KH,MTCA,MTCA,MASS,MOLES,KOIL,KAIR,KA,KB
00170 1,MK3,MK4,MK3L,MK4L
00180 COMMON /COIL/ MW1,TC1,VC1,PC1,CNUM1,VIS1
00190 COMMON /SPILL/ MTC(30),VP(30),VLOG(30),RHO(30),MW(30)
00200 1,SPGR(30),FRACTS,STEN,EB,DISPER,Z,TERM2,SPREAD,KMTC
00210 COMMON /PCODE/ VSLEAD,MK4,IOU,IPU,ITY
00220 COMMON /MOOSE/ WINDS,C1,C2,C3,C4
00230 DIMENSION TB(30),API(30),A(30),B(30),TBL(6,30),APIL(6,30)
00240 1,TC(30),PC(30),CNUM(30),TIG(30),HVAPI(30),HVAPZ(30)
00250 2,VOLL(6,30),VOL(30),MOLES(30),MTCA(30),VIS(30),VISC(30)
00260 3,VLOCK(30),HLAW(30),VC(30),APIBL(6),NC(30)
00270 4,NCTS(6),NS(30),ITEML(6),ISAMPL(6)
00280 DIMENSION ANAMEL(5),ANAMEL(6,5),C1L(6),C2L(6),C4L(6)
00290 1,STENL(6),VISZL(6),MK3L(6),MK4L(6)
00300 DATA (ANAMEL(1,J),J=1,5)/'PRUDH','OE BA','Y, AL','ASKA '
00310 1,
00320 DATA (ANAMEL(2,J),J=1,5)/'COOK ','INLET','ALA','SKA '
00330 1,
00340 DATA (ANAMEL(3,J),J=1,5)/'WILMI','NGTON','CAL','IFORN'
00350 1,'IA '
00360 DATA (ANAMEL(4,J),J=1,5)/'MURBA','N, AB','U DHA','BI '
00370 1,
00380 DATA (ANAMEL(5,J),J=1,5)/'LAKE ','CHICO','T, LO','UISIA'
00390 1,'NA '
00400 DATA (ANAMEL(6,J),J=1,5)/'LIGHT','DIES','EL CU','T '
00410 1,
00420 DATA APIBL/27.35,4.19,4.40,5.54,7.38,9/
00430 DATA ITEMIL/9,7,94,99999,221,1/
00440 DATA ISAMPL/71011,72025,71052,99999,54062,2/
00450 DATA NCTS/15,16,13,16,16,11/
00460 C
00470 C FOR CRUDE OIL THE RESIDUUM CUT IS ASSIGNED A NORMAL
00480 C BOILING POINT OF 850.
00490 C
00500 DATA (TBL(1,J),J=1,30)/167.,212.,257.,302.,347.,392.,
00510 1,437.,482.,527.,580.,638.,685.,738.,790.,850.,15*0./
00520 DATA (TBL(2,J),J=1,20)/122.,167.,212.,257.,302.,347.,
00530 1,392.,437.,482.,527.,580.,638.,685.,738.,790.,850.,
00540 2,4*0./
00550 DATA (TBL(3,J),J=1,20)/212.,257.,302.,347.,392.,437.,
00560 1,482.,527.,580.,638.,685.,738.,850.,7*0./
00570 DATA (TBL(4,J),J=1,20)/122.,167.,212.,257.,302.,347.,
00580 1,392.,437.,482.,527.,580.,638.,685.,738.,790.,850.,
00590 2,4*0./
00600 DATA (TBL(5,J),J=1,20)/122.,167.,212.,257.,302.,347.,
00610 1,392.,437.,482.,527.,580.,638.,685.,738.,790.,850.,
00620 2,4*0./
00630 DATA (TBL(6,J),J=1,11)/313.,342.,366.,395.,415.,438.,461.,
00640 1,479.,501.,518.,538./
00650 DATA (APIL(1,J),J=1,30)/72.7,64.2,56.7,51.6,47.6,45.2
00660 1,41.5,37.8,34.8,30.6,29.1,26.2,24.,22.5,11.4,15*0./

```

```

00670 DATA (APIL(2,J),J=1.20)/89.2.77.2.65.39.5.55.4.50.8
00680 1.46.5.43.39.6.37.32.8.31.3.28.7.26.6.25.11.6.4*0./
00690 DATA (APIL(3,J),J=1.20)/68.6.58.7.53.48.1.43.2.38.8
00700 1.35.4.32.3.26.8.24.5.22.3.20.3.8.9.7*0./
00710 DATA (APIL(4,J),J=1.20)/96.7.86.2.70.6.62.3.55.7.51.6
00720 1.48.5.45.6.43.40.35.8.34.30.28.4.26.6.16.7.4*0./
00730 DATA (APIL(5,J),J=1.20)/92.4.81.68.9.62.1.57.2.52.5
00740 1.48.8.45.2.41.7.38.2.34.4.33.2.30.6.28.9.26.1.18.1.4*0./
00750 DATA (APIL(6,J),J=1.11)/49.6.47.3.46.44.38.6.38.8.37.2
00760 1.35.4.33.9.33.1.32.2/
00770 DATA (VOLL(1,J),J=1.30)/2.1.2.6.3.5.3.6.3.7.3.5.4.3.4.8
00780 1.5.2.8.6.5.6.8.6.0.7.4.36.3.15*0./
00790 DATA (VOLL(2,J),J=1.20)/2.4.2.5.5.9.6.1.5.1.5.2.4.9
00800 1.5.1.5.2.5.3.3.5.2.7.4.2.4.2.25.6.4*0./
00810 DATA (VOLL(3,J),J=1.20)/2.3.2.4.2.4.2.5.2.8.3.6.4.4
00820 1.5.3.4.7.6.3.4.1.5.5.53.3.7*0./
00830 DATA (VOLL(4,J),J=1.20)/1.7.2.9.4.9.6.6.8.6.5.5.7
00840 1.5.6.6.4.9.5.7.5.6.6.5.6.5.6.19.3.4*0./
00850 DATA (VOLL(5,J),J=1.20)/7.5.8.2.9.7.11.9.1.8.3.7.2
00860 1.7.2.7.4.6.9.3.5.3.1.6.1.4.1.9.2.4*0./
00870 DATA (VOLL(6,J),J=1.11)/4.78.9.57.9.09.9.57.9.57.9.57
00880 1.9.57.9.57.9.57.9.57.9.57/
00890 C
00900 C C1L, C2L, AND C4L ARE THE MOUSSE FORMATION CONSTANTS.
00910 C C1L IS THE VISCOSITY CONSTANT.
00920 C C2L IS THE INVERSE OF THE MAXIMUM WATER IN OIL WEIGHT
00930 C FRACTION. C4L IS THE WATER INCORPORATION RATE.
00940 C
00950 DATA C1L/0.62.0.62.0.63.0.64.0.65.0.65/
00960 DATA C2L/1.42.3.33.1.43.5.-1.-1./
00970 DATA C4L/0.001.0.001.0.01.0.001.0.0./
00980 C
00990 C FOR THE DISPERSION PROCESS, KA IS THE CONSTANT IN THE
01000 C SEA SURFACE DISPERSION EQUATION. KB IS THE CONSTANT IN
01010 C THE DROPLET FRACTION EQUATION. STENL(6) IS THE LIBRARY
01020 C OIL-WATER SURFACE TENSION IN DYNES/CM.
01030 C
01040 DATA KA.KB.STENL/0.108.50.30.30.30.30.30.30./
01050 DATA VISZL/35.35.195.15.13.5.11.5/
01060 DATA MK3L/9000.9000.9000.9000.9000.3000./
01070 DATA MK4L/10.5.7.4.15.3.10.5.2.2./
01080 YI(X)=((1.-X)**0.38)/(X**X)
01090 OPEN(UNIT=32,DIALOG='DSKD:CUTVP2.OUT')
01100 OPEN(UNIT=34,DIALOG='DSKD:CUTVP2.PLT')
01110 OPEN(UNIT=35,DIALOG='DSKD:CUTVP2.TYP')
01120 IOU=32
01130 IPU=34
01140 ITY=35
01150 C
01160 C FILL IN SOME LIBRARY IDENTIFICATIONS.
01170 C
01180 10 TYPE 20
01190 20 FORMAT(1X,'ENTER THE NUMBER OF TBP CUTS TO BE CHARACTERIZED
01200 1 ON 12')
01210 TYPE 30
01220 30 FORMAT(1X,'IF YOU HAVE NO INPUT DATA JUST ENTER 99')
01230 TYPE 40
01240 40 FORMAT(1X,'A 99 ENTRY WILL USE A LIBRARY EXAMPLE')
01250 ICODE=1
01260 ACCEPT 50, NCUTS
01270 50 FORMAT(12)
01280 LSWTCH=NCUTS
01290 C
01300 C LSWTCH=99 IS USED TO INDICATE THAT A LIBRARY CRUDE WAS
01310 C CHOSEN.
01320 C

```

```

01330      IF(NCUTS.NE.99) GO TO 120
01340      C
01350      C      USING A LIBRARY CRUDE.
01360      C
01370      TYPE 60
01380      60      FORMAT(1X,'CHOOSE A CRUDE ACCORDING TO:')
01390      DO 80 I=1,6
01400      TYPE 70, I,(ANAMEL(I,J),J=1,5)
01410      70      FORMAT(1X,I1,' = ',5A5)
01420      80      CONTINUE
01430      ACCEPT 90, IC
01440      90      FORMAT(I1)
01450      APIB=APIBL(IC)
01460      ITEN=ITEML(IC)
01470      ISAMP=ISAMPL(IC)
01480      NCUTS=NCTS(IC)
01490      ICODE=2
01500      DO 100 J=1,5
01510      ANAME(J)=ANAMEL(IC,J)
01520      100      CONTINUE
01530      TYPE 110, (ANAME(J),J=1,5)
01540      110      FORMAT(/,1X,'YOU CHOSE: ',5A5)
01550      GO TO 200
01560      C
01570      C      USER IS ENTERING THE CRUDE DATA.
01580      C
01590      120      TYPE 130
01600      130      FORMAT(1X,'ENTER THE NAME OF THE CRUDE')
01610      ACCEPT 140, (ANAME(1),I=1,5)
01620      140      FORMAT(10A5)
01630      TYPE 150
01640      150      FORMAT(1X,'ENTER AN IDENTIFICATION NUMBER FOR
1 THIS CRUDE ON 15')
01650      ACCEPT 160, ITEM
01660      160      FORMAT(I5)
01670      TYPE 170
01680      170      FORMAT(1X,'ENTER A SAMPLE NUMBER ON 15')
01690      ACCEPT 160, ISAMP
01700      TYPE 180
01710      180      FORMAT(1X,'ENTER THE BULK API GRAVITY')
01720      ACCEPT 230, APIB
01730      TYPE 190
01740      190      FORMAT(/,1X,'YOU MUST ENTER THE TRUE BOILING POINT
1 CUT DATA STARTING ',/1X,'WITH THE MOST VOLATILE CUT
2 AND GOING TO THE BOTTOM OF THE BARREL',/)
01750      C
01760      C      CALCULATE THE BULK DENSITY OF THE CRUDE AT 60/60.
01770      C
01780      C
01790      C
01800      C
01810      200      DCRUDE=141.5/(APIB+131.5)
01820      DCRUDE=0.983*DCRUDE
01830      C
01840      C      TRANSFER CRUDE INPUT DATA TO THE VARIABLES USED IN
01850      C      THE CALCULATIONS.
01860      C
01870      DO 270 I=1,NCUTS
01880      GO TO (210,260), ICODE
01890      210      TYPE 220, I
01900      C
01910      C      ENTER THE CRUDE CUT DATA.
01920      C
01930      220      FORMAT(1X,'ENTER THE BOILING POINT AT 1 ATM IN DEG F
1 FOR CUT',I3)
01940      ACCEPT 230, TB(I)
01950      230      FORMAT(F10.0)
01960      TYPE 240, I
01970      240      FORMAT(1X,'ENTER API GRAVITY FOR CUT',I3)

```

```

01996      ACCEPT 230, API(I)
02000      TYPE 250, I
02010 250    FORMAT(1X, 'ENTER VOLUME PER CENT FOR CUT', 13)
02020      ACCEPT 230, VOL(I)
02030      GO TO 270
02040      C
02050      C      TRANSFER CRUDE CUT INPUT DATA FROM THE LIBRARY.
02060      C
02070 260    TB(I)=TBL(IC,I)
02080      API(I)=APIL(IC,I)
02090      VOL(I)=VOLL(IC,I)
02100 270    CONTINUE
02110      C
02120      C      DISPLAY THE CUTS BACK TO THE USER.
02130      C
02140 280    TYPE 290
02150 290    FORMAT(/, 1X, 'CUT', 5X, 'TB', 10X, 'API', 8X, 'VOL')
02160      DO 310 I=1, NCUTS
02170      TYPE 300, I, TB(I), API(I), VOL(I)
02180 300    FORMAT(1X, 12, 5X, F5.1, 7X, F4.1, 6X, F5.1)
02190 310    CONTINUE
02200      TYPE 320
02210 320    FORMAT(1X, 'DO YOU WANT TO CHANGE ANY?')
02220 330    ACCEPT 340, ANS
02230 340    FORMAT(A1)
02240      IF(ANS.EQ.'N') GO TO 420
02250      C
02260      C      ALLOW THE INPUT TO BE CHANGED.
02270      C
02280      TYPE 350
02290 350    FORMAT(1X, 'ENTER THE CUT NUMBER TO BE CHANGED ON 12')
02300      ACCEPT 50, N
02310      TYPE 360
02320 360    FORMAT(1X, 'ENTER 1 TO CHANGE TB, 2 FOR API, 3 FOR VOL')
02330      ACCEPT 370, IC
02340 370    FORMAT(I1)
02350      TYPE 380
02360 380    FORMAT(1X, 'ENTER THE CHANGED DATA')
02370      GO TO (390, 400, 410), IC
02380 390    ACCEPT 230, TB(N)
02390      GO TO 280
02400 400    ACCEPT 230, API(N)
02410      GO TO 280
02420 410    ACCEPT 230, VOL(N)
02430      GO TO 280
02440 420    DO 430 I=2, NCUTS
02450      IM1=I-1
02460      IF(TB(I).LT.TB(IM1)) GO TO 440
02470 430    CONTINUE
02480      GO TO 460
02490 440    TYPE 450, I, IM1
02500 450    FORMAT(/, 1X, 'THE BOILING POINT OF CUT ', 12
02510      1, ' IS LESS THAN CUT ', 12, /, 1X, 'AND THIS ORDER IS NOT
02520      2 ACCEPTABLE. SO START OVER', /)
02530      GO TO 10
02540      C
02550      C      ALWAYS RENORMALIZE THE INPUT VOLUMES TO 100%.
02560      C
02570 460    VTOTAL=0.
02580      DO 470 I=1, NCUTS
02590      VTOTAL=VTOTAL+VOL(I)
02600 470    CONTINUE
02610      DO 480 I=1, NCUTS
02620      VOL(I)=100.*VOL(I)/VTOTAL
02630 480    CONTINUE
02640      C

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02650 C      NOW CHARACTERIZE ALL THE CUTS.  IF THE LAST CUT IS
02660 C      RESIDUUM DO NOT CHARACTERIZE IT BUT USE A VAPOR
02670 C      PRESSURE OF 0. AND A MOLECULAR WEIGHT OF 600.
02680 C
02690 C      MW(NCUTS)=600.
02700 C      VP(NCUTS)=0.
02710 C
02720 C      NV=1 MEANS NO RESIDUUM CUT PRESENT.
02730 C      NV=2 MEANS A RESIDUUM IS PRESENT.
02740 C
02750 C      NV=1
02760 C      NC1=NCUTS
02770 C      DO 550 I=1,NCUTS
02780 C      APIN=API(I)
02790 C      SPGR(I)=141.5/(API(I)+131.5)
02800 C      SPCR(I)=0.983*SPGR(I)
02810 C      TBN=TB(I)
02820 C
02830 C      THE RESIDUUM CUT IS IDENTIFIED BY A NORMAL BOILING
02840 C      POINT OF 850.  LOOP AROUND THE NV=2 SWITCH IF A
02850 C      RESIDUUM IS PRESENT.  NC1 IS THE NUMBER OF PSEUDO COMPONENTS
02860 C      WITH FINITE VAPOR PRESSURES.
02870 C
02880 C      IF(TBN.LT.850.) GO TO 490
02890 C      NV=2
02900 C      NC1=NCUTS-1
02910 490 C      CALL CHAR(APIN,TBN,AN,BN,NSN,NV)
02920 C
02930 C      THE CHARACTERIZATION SUBROUTINE RETURNS THE LOG10 OF THE
02940 C      KINEMATIC VISCOSITY (CENTISTOKES) AT 122 DEG F.
02950 C
02960 C      VISK(I)=10.**VIS1
02970 C      VLOCK(I)=ALOG(VISK(I))
02980 C      GO TO (500,550), NV
02990 C
03000 C      STORE THE CUT INFORMATION FOR A NON-RESIDUUM CUT.
03010 C
03020 500 C      NS(I)=NSN
03030 C      A(I)=AN
03040 C      B(I)=BN
03050 C      MW(I)=MW1
03060 C      TC(I)=TC1
03070 C      TC(I)=TC(I)+459.
03080 C      VC(I)=VC1
03090 C      PC(I)=PC1
03100 C      CNUM(I)=CNUM1
03110 C
03120 C      FIND THE TEMPERATURE AT WHICH THE VAPOR PRESSURE IS 10 MMHG
03130 C      BY USING NEWTON-RAPHSON WITH TB AS THE FIRST GUESS.
03140 C
03150 C      NC(I)=0
03160 C      YTEN=ALOG10(0.01315/PC(I))
03170 C      X=(TB(I)+459.)/TC(I)
03180 510 C      EX=EXP(-20.*(X-B(I))**2)
03190 C      Y=-A(I)*(1.-X)/X-EX
03200 C      YOBJ=Y-YTEN
03210 C      VP(I)=PC(I)*10.**Y
03220 C      TEST=ABS(VP(I)-0.01315)
03230 C      IF(TEST.LT.0.001315) GO TO 540
03240 C      NC(I)=NC(I)+1
03250 C      IF(NC(I).GT.20) GO TO 520
03260 C      DY=A(I)/(X*X)+40.*(X-B(I))*EX
03270 C      BI=YOBJ-DY*X
03280 C      X=-BI/DY
03290 C      GO TO 510
03300 C

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03310 C      UNSUCCESSFUL EXIT FROM NEWTON-RAPHSON
03320 C
03330 520 TYPE 530, I,X,Y
03340 530 FORMAT(IX,'T10 FAILURE FOR',I4,' AT T = ',1PE10.3,' WHERE
03350 1 LOG10(P) = ',1PE10.3)
03360 GO TO 2130
03370 C
03380 C      SUCCESSFUL EXIT FROM NEWTON-RAPHSON
03390 C
03400 540 T10(I)=X*TC(I)
03410 C
03420 C      CALCULATE THE HEAT OF VAPORIZATION AT 10 MMHG WITH THE
03430 C      CLAPEYRON EQUATION AND USE WATSON'S METHOD FOR THE
03440 C      VAPOR PRESSURE BELOW 10 MMHG. SEE CAMSON AND WATSON,
03450 C      1944, NATIONAL PETROLEUM NEWS, R-258 TO R-264.
03460 C
03470 TR2=T10(I)/TC(I)
03480 EX=92.12*(TR2-B(I))*EXP(-20.*(TR2-B(I))**2)
03490 HVAP=1.987*T10(I)*T10(I)*(2.303*A(I)/(TR2*TR2)+EX)/TC(I)
03500 HVAP1(I)=HVAP/MW(I)
03510 HVAPZ(I)=HVAP/(1.-TR2)**0.38
03520 550 CONTINUE
03530 C
03540 C      END OF TRUE-BOILING-POINT CUTS CHARACTERIZATION
03550 C
03560 WRITE (10U,560) (ANAME(I),I=1,5)
03570 560 FORMAT(1H1,'SUMMARY OF TBP CUTS CHARACTERIZATION FOR:
03580 1,5A5)
03590 WRITE (10U,570)
03600 570 FORMAT(1X,'CODE VERSION IS CUTVP2 OF FEBRUARY 83')
03610 WRITE (10U,580) ITEM,ISAMP
03620 580 FORMAT(IX,'ITEM ',I5,' SAMPLE ',I5)
03630 WRITE (10U,590)
03640 590 FORMAT(1X,'TB',7X,'API',6X,'SPGR',7X,'VOL',8X,'MW',8X
03650 1,'TC',8X,'PC',8X,'VC',8X,'A',9X,'B',8X,'T10',7X,'VIS'
03660 2,4X,'NC NS')
03670 DO 610 I=1,NCUTS
03680 WRITE (10U,600) I,TB(I),API(I),SPGR(I),VOL(I),MW(I),TC(I)
03690 1,PC(I),VC(I),A(I),B(I),T10(I),VISC(I),NC(I),NS(I)
03700 600 FORMAT(IX,12,12(1X,1PE9.2),2(1X,12))
03710 610 CONTINUE
03720 WRITE (10U,620) APIB
03730 620 FORMAT(1X,'BULK API GRAVITY = ',F5.1)
03740 WRITE (10U,630)
03750 630 FORMAT(1X,'TB = NORMAL BOILING TEMPERATURE, DEG F')
03760 WRITE (10U,640)
03770 640 FORMAT(IX,'API = API GRAVITY')
03780 WRITE (10U,650)
03790 650 FORMAT(IX,'VOL = VOLUME PER CENT OF TOTAL CRUDE')
03800 WRITE (10U,660)
03810 660 FORMAT(IX,'MW = MOLECULAR WEIGHT')
03820 WRITE (10U,670)
03830 670 FORMAT(IX,'TC = CRITICAL TEMPERATURE, DEG RANKINE')
03840 WRITE (10U,680)
03850 680 FORMAT(IX,'PC = CRITICAL PRESSURE, ATMOSPHERES')
03860 WRITE (10U,690)
03870 690 FORMAT(IX,'VC = CRITICAL VOLUME, CC/MOLE')
03880 WRITE (10U,700)
03890 700 FORMAT(IX,'A AND B ARE PARAMETERS IN THE VAPOR PRESSURE
03900 1 EQUATION')
03910 WRITE (10U,710)
03920 710 FORMAT(IX,'T10 IS THE TEMPERATURE IN DEG R WHERE THE VAPOR
03930 1 PRESSURE IS 10 MM HG')
03940 WRITE (10U,720)
03950 720 FORMAT(IX,'VIS IS THE KINEMATIC VISCOSITY IN CENTISTOKES
03960 1 AT 122 DEG F')

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03970      WRITE (10U,730)
03980 730    FORMAT(1X,'NC = ERROR CODE. SHOULD BE LESS THAN 20')
03990      WRITE (10U,740)
04000 740    FORMAT(1X,'NS = ERROR CODE. SHOULD BE EQUAL TO 1')
04010      WRITE (10U,750) NCUTS
04020 750    FORMAT(1X,'IGNORE THE ERROR CODES FOR COMPONENT NUMBER ',12
04030      1,' IF IT IS A RESIDUUM')
04040 760    WRITE (IPU,770) ITEM,ISAMP
04050 770    FORMAT(2I5)
04060      WRITE (IPU,780) (ANAME(I),I=1,5)
04070 780    FORMAT(5A5)
04080      C
04090      C      THE CUTVP2.PLT PLOT FILE IS WRITTEN AS:
04100      C      1. ITEM AND SAMPLE NUMBER ON 215
04110      C      2. THE CRUDE NAME ON 5A5
04120      C      3. NCUTS ON 15
04130      C      4. BOILING POINT IN DEG F OF EACH CUT ON
04140      C      10(1X,1PE10.3)
04150      C      5. TEMPERATURE IN DEG F OF EVAPORATION, XPRINT
04160      C      WIND SPEED IN KNOTS, WINDS
04170      C      KA AND KB IN THE DISPERSION EQUATION,
04180      C      SURFACE TENSION IN DYNES/CM, STEN
04190      C      VOLUME OF THE SPILL IN BARRELS, BBL
04200      C      C1, C2, AND C4 IN THE MOUSSE EQUATION,
04210      C      KMTCC, MASS TRANSFER COEFFICIENT CODE (FLOATED),
04220      C      ALL ON 10(1X,1PE10.3)
04230      C      6. NUMBER OF CUTS+1 ON 15
04240      C      7. TIME, MASS OF CUTS, AREA ON 10(1X,1PE10.3)
04250      C      8. TOTAL MASS FRACTION REMAINING IN THE OIL
04260      C      SLICK FOR EACH TIME STEP PRINTED ON
04270      C      10(1X,1PE10.3)
04280      C
04290      C      ITEMS 6 AND 7 ABOVE ARE WRITTEN FOR EACH TIME STEP
04300      C      WITH THE FIRST TIME STEP BEING ZERO. WHEN THE
04310      C      VERY LAST TIME STEP IS WRITTEN THEN ITEM 8 IS WRITTEN.
04320      C
04330      C      THE NUMBER OF LINES WRITTEN ON THE CUTVP2.PLT PLOT FILE
04340      C      REFERS TO THE NUMBER OF 'TIMES' WRITTEN THROUGH
04350      C      ITEMS 6 AND 7 ABOVE.
04360      C
04370      WRITE (IPU,790) NCUTS
04380 790    FORMAT(15)
04390      WRITE (IPU,800) (TB(I),I=1,NCUTS)
04400 800    FORMAT(10(1X,1PE10.3))
04410      TYPE 810
04420 810    FORMAT(1X,'ENTER THE TEMPERATURE IN DEG F FOR
04430      1 THE VAPOR PRESSURE CALCULATION')
04440      ACCEPT 230, XSAVE
04450      C
04460      C      TK IS THE ABSOLUTE TEMPERATURE IN DEG K.
04470      C
04480      TK=(XSAVE-32.)/1.8+273.
04490      XPRINT=XSAVE
04500      C
04510      C      CALCULATE AN ABSOLUTE TEMPERATURE IN DEG RANKINE.
04520      C
04530      XSAVE=XSAVE+459.
04540      C
04550      C      CALCULATE THE VAPOR PRESSURE AT THE INPUT TEMPERATURE.
04560      C
04570      C      AT THIS POINT IF THE INPUT TEMPERATURE IS LESS THAN THE
04580      C      10-MMHG TEMPERATURE USE THE WATSON-CLAPEYRON EQUATION.
04590      C
04600      C      THE WATSON-CLAPEYRON EQUATION IS:
04610      C
04620      C       $LN(P2/P1) = (HVAPZ/(R*TC))*INTEGRAL$ 

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05290 C
05300 930 TYPE 940
05310 940 FORMAT(1X,'ENTER THE SPILL SIZE IN BARRELS')
05320 ACCEPT 230, BBL
05330 TYPE 950
05340 950 FORMAT(1X,'ENTER NUMBER OF HOURS FOR OIL WEATHERING TO OCCUR')
05350 ACCEPT 230, X2
05360 IF(LSWTCH.EQ.99) GO TO 980
05370 TYPE 960
05380 960 FORMAT(1X,'SINCE YOU DID NOT USE A LIBRARY CRUDE.')
05390 TYPE 970
05400 970 FORMAT(1X,'YOU MUST ENTER THE FOLLOWING THREE MOUSSE
05410 1 FORMATION CONSTANTS')
05420 GO TO 1000
05430 980 TYPE 990
05440 990 FORMAT(1X,'DO YOU WANT TO ENTER MOUSSE FORMATION CONS
05450 1TANTS?')
05460 ACCEPT 340, ANS
05470 IF(ANS.EQ.'N') GO TO 1060
05480 C
05490 C TO SPECIFY NO MOUSSE. ENTER C2 = 0
05500 C
05510 1000 TYPE 1010
05520 1010 FORMAT(1X,'1. ENTER THE MAXIMUM WEIGHT FRACTION WATER
05530 1 IN OIL')
05540 ACCEPT 230, C2
05550 IF(C2.GT.0.) GO TO 1030
05560 C
05570 C SET C2=-1. IF A MOUSSE CANNOT BE FORMED AND LOOP OUT.
05580 C
05590 C2=-1.
05600 TYPE 1020
05610 1020 FORMAT(/,1X,'SINCE A 0% WATER CONTENT WAS SPECIFIED
05620 1. THE REMAINING TWO MOUSSE',/,1X,'CONSTANTS ARE NOT
05630 2 NEEDED')
05640 GO TO 1070
05650 1030 C2=1./C2
05660 TYPE 1040
05670 1040 FORMAT(1X,'2. ENTER THE MOUSSE-VISCOSITY CONSTANT
05680 1, TRY 0.65')
05690 ACCEPT 230, C1
05700 TYPE 1050
05710 1050 FORMAT(1X,'3. ENTER THE WATER INCORPORATION RATE CONSTANT
05720 1, TRY 0.001')
05730 ACCEPT 230, C4
05740 GO TO 1070
05750 1060 C1=C1L(IC)
05760 C2=C2L(IC)
05770 C4=C4L(IC)
05780 1070 IF(LSWTCH.EQ.99) GO TO 1100
05790 TYPE 1080
05800 1080 FORMAT(/,1X,'YOU MUST ALSO ENTER AN OIL-WATER SURFACE
05810 1 TENSION (DYNES/CM')
05820 TYPE 1090
05830 1090 FORMAT(1X,'FOR DISPERSION. TRY 30.')
05840 GO TO 1130
05850 1100 TYPE 1110
05860 1110 FORMAT(1X,'DO YOU WANT TO ENTER AN OIL-WATER SURFACE
05870 1 TENSION (DYNES/CM)?')
05880 ACCEPT 340, ANS
05890 IF(ANS.EQ.'N') GO TO 1140
05900 TYPE 1120
05910 1120 FORMAT(1X,'TRY 30.')
05920 1130 ACCEPT 230, STEN
05930 GO TO 1150
05940 1140 STEN=STENL(IC)

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05950 C
05960 C      START THE MASS-TRANSFER COEFFICIENT SPECIFICATION.
05970 C
05980 1150 TYPE 1160
05990 1160 FORMAT(1X,'ENTER THE MASS-TRANSFER COEFFICIENT CODE: 1
06000 1, 2, OR 3 WHERE:')
06010 TYPE 1170
06020 1170 FORMAT(1X,'1=USER SPECIFIED OVER-ALL MASS-TRANSFER COEF
06030 FICIENT')
06040 TYPE 1180
06050 1180 FORMAT(1X,'2=CORRELATION MASS-TRANSFER COEFFICIENT BY
06060 1 MACKAY & MATSUGU')
06070 TYPE 1190
06080 1190 FORMAT(1X,'3=INDIVIDUAL-PHASE MASS-TRANSFER COEFFICIENTS')
06090 ACCEPT 370, KNTC
06100 C
06110 C      NOW ENTER THE WIND SPEED IN KNOTS AND CONVERT TO METER/SEC
06120 C      AND METER/HOUR.
06130 C
06140 TYPE 1200
06150 1200 FORMAT(1X,'ENTER THE WIND SPEED IN KNOTS')
06160 ACCEPT 230, WINDS
06170 C
06180 C      NEVER LET THE WIND SPEED DROP BELOW 2 KNOTS. A ZERO WIND
06190 C      SPEED DESTROYS THE MASS-TRANSFER CALCULATION AND WILL
06200 C      YIELD A ZERO MASS-TRANSFER COEFFICIENT.
06210 C
06220 IF(WINDS.LT.2.) WINDS=2.
06230 WINDMS=0.514*WINDS
06240 WINDMH=1853.*WINDS
06250 C
06260 C      NOW CALCULATE THE INITIAL GRAM MOLES FOR EACH COMPONENT TO
06270 C      GET THE INTEGRATION STARTED.
06280 C
06290 1210 BM=0.159*BBL
06300 TMOLES=0.
06310 DO 1220 I=1,NCUTS
06320 AMASS=1582.*SPCR(I)*BBL*VOL(I)
06330 MOLES(I)=AMASS/MW(I)
06340 TMOLES=TMOLES+MOLES(I)
06350 C
06360 C      RHO IS THE DENSITY IN GM MOLES/CUBIC METER.
06370 C
06380 RHO(I)=100.*MOLES(I)/(BM*VOL(I))
06390 1220 CONTINUE
06400 C
06410 C      CALCULATE THE MEAN MOLECULAR WEIGHT OF THE CRUDE
06420 C
06430 WTMOLE=0.
06440 DO 1230 I=1,NCUTS
06450 WTMOLE=WTMOLE+MW(I)*MOLES(I)/TMOLES
06460 1230 CONTINUE
06470 WRITE (10U,1240) WTMOLE
06480 1240 FORMAT(/,1X,'MEAN MOLECULAR WEIGHT OF THE CRUDE = ',1PE10.3)
06490 C
06500 C      IF MWSCTH=1, WEATHER THE OIL.
06510 C      IF MWSCTH=2, EXIT.
06520 C
06530 GO TO (1250,2110) MWSCTH
06540 C
06550 C      SPECIFY SLICK SPREADING.
06560 C
06570 1250 SPREAD=0.
06580 TYPE 1260
06590 1260 FORMAT(1X,'DO YOU WANT THE SLICK TO SPREAD?')
06600 ACCEPT 340, ANS

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06610      IF(ANS.EQ.'N') GO TO 1270
06620      SPREAD=1.
06630      GO TO 1290
06640      C
06650      C      CALCULATE AN AREA IN SAME WAY IT WILL BE CALCULATED
06660      C      AS THE SLICK WEATHERS. Z=THICKNESS IN METERS.
06670      C
06680      1270 TYPE 1280
06690      1280 FORMAT(1X,'SINCE THE SLICK DOES NOT SPREAD, ENTER
06700      1 A STARTING THICKNESS IN CM')
06710      ACCEPT 230, Z
06720      Z=Z/100.
06730      GO TO 1300
06740      C
06750      C      THE SLICK ALWAYS STARTS AT 2-CM THICKNESS.
06760      C
06770      1290 Z=0.02
06780      1300 VOLUM=0.
06790      DO 1310 I=1,NCUTS
06800      VOLUM=VOLUM+MOLES(I)/RHO(I)
06810      1310 CONTINUE
06820      C
06830      C      CALCULATE THE INITIAL AREA AND DIAMETER.
06840      C
06850      AREA=VOLUM/Z
06860      DIA=SQRT(AREA/0.785)
06870      C
06880      C      THE MASS-TRANSFER COEFFICIENT CAN BE CALCULATED ACCORDING TO:
06890      C
06900      C      1. A USER-SPECIFIED OVER-ALL MASS-TRANSFER COEFFICIENT.
06910      C
06920      C      2. THE MASS-TRANSFER COEFFICIENT CORRELATION ACCORDING
06930      C      TO MACKAY AND MATSUGU, 1973, CAN. J. CHE. V51,
06940      C      P434-439.
06950      C
06960      C      3. INDIVIDUAL OIL- AND AIR-PHASE MASS-TRANSFER COEFFI-
06970      C      CIENTS BASED ON SOME REAL ENVIRONMENTAL DATA SUCH
06980      C      AS THAT OF LISS AND SLATER. SCALE THE AIR-PHASE
06990      C      VALUE WITH RESPECT TO WIND SPEED ACCORDING TO
07000      C      GARRATT, 1977, MONTHLY WEATHER REVIEW, V105,
07010      C      P915-920.
07020      C
07030      C      TEMP IS R*T AND USED TO CHANGE THE UNITS ON THE MASS-
07040      C      TRANSFER COEFFICIENT.
07050      C
07060      1320 TEMP=(8.2E-05)*TK
07070      GO TO (1330,1370,1450), KMTIC
07080      C
07090      C      USER SPECIFIED OVER-ALL MASS-TRANSFER COEFFICIENT.
07100      C
07110      1330 TYPE 1340
07120      1340 FORMAT(1X,'ENTER THE OVER-ALL MASS-TRANSFER COEFFICIENT
07130      1, CM/HR. TRY 10')
07140      ACCEPT 230, UMTIC
07150      WRITE (10U,1350) UMTIC
07160      1350 FORMAT(1H1,'OVER-ALL MASS-TRANSFER COEFFICIENT WAS USER
07170      1-SPECIFIED AT .1PE10.3.' CM/HR BY INPUT CODE 1')
07180      C
07190      C      CONVERT CM/HR TO GM-MOLES/(HR)(ATM)(M**2) SINCE VAPOR
07200      C      PRESSURE IS THE DRIVING FORCE FOR MASS TRANSFER.
07210      C
07220      UMTIC=UMTIC/TEMP/100.
07230      DO 1360 I=1,NC1
07240      MTC(I)=UMTIC
07250      1360 CONTINUE
07260      GO TO 1530

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07270 C
07280 C      USE THE MACKAY AND MATSUGU MASS-TRANSFER COEFFICIENT.
07290 C
07300 1370 TERM1=0.015*WINDMH**0.78
07310 IF(SPREAD.EQ.0.) GO TO 1330
07320 TERM2=DIA**(-0.11)
07330 GO TO 1390
07340 C
07350 C      IF THE SLICK DOES NOT SPREAD BASE THE DIAMETER DEPENDENCE
07360 C      ON 1000 METERS AND DIVIDE THE RESULT BY 0.7
07370 C
07380 1380 TERM2=0.65
07390 C
07400 C      KH INCLUDES THE SCHMIDT NUMBER FOR CUMENE.
07410 C
07420 1390 KH=TERM1*TERM2
07430 WRITE (10U,1400) KMTG
07440 1400 FORMAT(1H1,'OVER-ALL MASS-TRANSFER COEFFICIENTS BY INPUT
07450 1 CODE',12)
07460 WRITE (10U,1410) KH
07470 1410 FORMAT(/,1X,'OVER-ALL MASS-TRANSFER COEFFICIENT FOR CUMENE = '
07480 1,1PE10.3,' M/HR',/)
07490 WRITE (10U,1420)
07500 1420 FORMAT(3X,'CUT',12X,'M/HR',7X,'GM-MOLES/(HR)(ATM)(M**2)')
07510 DO 1440 I=1,NC1
07520 C
07530 C      THE MASS-TRANSFER COEFFICIENT IS CORRECTED FOR THE
07540 C      DIFFUSIVITY OF COMPONENT I IN AIR. THE SQRT IS USED
07550 C      (I.E. LISS AND SLATER). BUT THE 1/3 POWER COULD ALSO
07560 C      BE USED (I.E. THE SCHMIDT NUMBER).
07570 C
07580 MTCA(I)=KH*0.93*SQRT((MW(I)+29.)/MW(I))
07590 C
07600 C      MTC(I) IS THE OVER-ALL MASS-TRANSFER COEFFICIENT DIVIDED
07610 C      BY R*T. R=82.06E-06 (ATM)(M**3)/(G-MOLE)(DEG K)
07620 C
07630 MTC(I)=MTCA(I)/TEMP
07640 WRITE (10U,1430) I,MTCA(I),MTC(I)
07650 1430 FORMAT(2X,13.2(10X,1PE10.3))
07660 1440 CONTINUE
07670 GO TO 1530
07680 C
07690 C      USER SPECIFIED INDIVIDUAL-PHASE MASS-TRANSFER
07700 C      COEFFICIENTS.
07710 C
07720 1450 TYPE 1460
07730 1460 FORMAT(1X,'ENTER THE OIL-PHASE MASS-TRANSFER COEFFICIENT
07740 1 IN CM/HR. TRY 10')
07750 ACCEPT 230, KOIL
07760 TYPE 1470
07770 1470 FORMAT(1X,'ENTER THE AIR-PHASE MASS-TRANSFER COEFFICIENT
07780 1 IN CM/HR. TRY 1000')
07790 ACCEPT 230, KAIR
07800 TYPE 1480
07810 1480 FORMAT(1X,'ENTER THE MOLECULAR WEIGHT OF THE COMPOUND
07820 1 FOR K-AIR ABOVE. TRY 200')
07830 ACCEPT 230, DATMW
07840 C
07850 C      SCALE K-AIR ACCORDING TO WIND SPEED (GARRATT, 1977).
07860 C      SO THAT AS THE WIND SPEED GOES UP THE MASS TRANSFER
07870 C      GOES UP, I.E., THE CONDUCTANCE INCREASES.
07880 C
07890 KAIR=KAIR*(1.+0.089*WINDMS)
07900 RKAIR=1./KAIR
07910 C
07920 C      CALCULATE R*T IN ATM*CM**3/GM-MOLE

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07930 C
07940 RT=82.06*TK
07950 HTERM=WTMOLE/(DCRUDE*RT)
07960 WRITE (IOU,1400) KMTC
07970 C
07980 C WRITE THE USERS INPUT, WIND SPEED, AND HENRYS LAW
07990 C TERM TO THE OUTPUT.
08000 C
08010 WRITE (IOU,1490) KAIR,KOIL,DATAMW
08020 1490 FORMAT(/,1X,'K-AIR = ',1PE10.3,' AND K-OIL = ',1PE10.3
08030 1, ' CM/HR. BASED ON A MOLECULAR WEIGHT OF ',1PE10.3)
08040 WRITE (IOU,1500) WINDMS
08050 1500 FORMAT(1X,'WIND SPEED = ',1PE10.3,' M/S')
08060 WRITE (IOU,1510) HTERM
08070 1510 FORMAT(1X,'THE HENRYS LAW CONVERSION TERM FOR OIL = '
08080 1,1PE10.3,' 1/ATM')
08090 WRITE (IOU,1420)
08100 C
08110 C CLACULATE THE OVER-ALL MASS-TRANSFER COEFFICIENT BASED
08120 C ON GAS-PHASE CONCENTRATIONS FOR EACH CUT.
08130 C
08140 DO 1520 I=1,NC1
08150 HLAW(I)=HTERM*VP(I)
08160 MTCA(I)=REAIR+HLAW(I)/KOIL
08170 C
08180 C NOW TAKE THE INVERSE TO OBTAIN CM/HR AND THEN MULTIPLY
08190 C BY 0.01 TO GET M/HR.
08200 C
08210 MTCA(I)=0.01/MTCA(I)
08220 C
08230 C CORRECT FOR MOLECULAR WEIGHT ACCORDING TO LISS & SLATER.
08240 C 1974, NATURE, V247, P181-184.
08250 C
08260 MTCA(I)=MTCA(I)*SQRT(DATAMW/MW(I))
08270 MTC(I)=MTCA(I)/TEMP
08280 C
08290 C AND WRITE THE OVER-ALL MASS-TRANSFER COEFFICIENT
08300 C IN M/HR AND MOLE/HR*ATM*M*M.
08310 C
08320 WRITE (IOU,1430) I,MTCA(I),MTC(I)
08330 1520 CONTINUE
08340 1530 SPCRB=141.5/(APIB+131.5)
08350 MASS=0.1582*BBL*SPCRB
08360 WRITE (IOU,1540) BBL,MASS
08370 1540 FORMAT(/,1X,'FOR THIS SPILL OF ',1PE10.3,' BARRELS, THE
08380 1 MASS IS ',1PE10.3,' METRIC TONNES')
08390 VOLUMB=VOLUM/0.159
08400 WRITE (IOU,1550) VOLUM,VOLUMB
08410 1550 FORMAT(/,1X,'VOLUME FROM SUMMING THE CUTS = ',1PE8.1,' M**3
08420 1, OR ',1PE10.3,' BARRELS')
08430 GO TO (1530,1560,1580), KMTC
08440 1560 WRITE (IOU,1570) WINDS,WINDMH
08450 1570 FORMAT(/,1X,'WIND SPEED = ',1PE10.3,' KNOTS, OR ',1PE10.3
08460 1, ' M/HR')
08470 1580 WRITE (IOU,1590) DIA,AREA
08480 1590 FORMAT(/,1X,'INITIAL SLICK DIAMETER = ',1PE10.3,' M, OR AREA
08490 1 = ',1PE10.3,' M**2')
08500 IF(SPREAD.GT.0.) GO TO 1610
08510 WRITE (IOU,1600)
08520 1600 FORMAT(/,1X,'THIS SLICK DOES NOT SPREAD FOR THIS CALCULATION')
08530 C
08540 C CALCULATE THE KINEMATIC VISCOSITY OF THE CRUDE AT 122
08550 C DEG F AND THE ENTERED ENVIRONMENTAL TEMPERATURE.
08560 C USE THE VISCOSITY MIXING RULE OF (MOLE FRACTION)*(LOG),
08570 C SEE PAGE 460 OF REID, PRAUSNITZ & SHERWOOD IN
08580 C THE BOOK 'THE PROPERTIES OF GASES AND LIQUIDS'

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08590 C
08600 1610 VISMIX=0.
08610 DO 1620 I=1,NCUTS
08620 VISMIX=VISMIX+MOLES(I)*VLOGK(I)/TMOLES
08630 1620 CONTINUE
08640 VISMIX=EXP(VISMIX)
08650 WRITE (100,1630) VISMIX
08660 1630 FORMAT(/,1X,'KINEMATIC VISCOSITY OF THE BULK CRUDE FROM
08670 1 THE CUTS = ',1PE8.1,' CENTISTOKES AT 122 DEG F')
08680 VISMIX=0.
08690 C
08700 C SCALE THE VISCOSITY WITH TEMPERATURE ACCORDING TO
08710 C ANDRADE.
08720 C
08730 EXPT=EXP(1923.*(1./XSAVE-0.001721))
08740 DO 1640 I=1,NCUTS
08750 VIS(I)=VISK(I)*EXPT
08760 VLOG(I)=ALOG(VIS(I))
08770 VISMIX=VISMIX+MOLES(I)*VLOG(I)/TMOLES
08780 1640 CONTINUE
08790 VISMIX=EXP(VISMIX)
08800 WRITE (100,1650) VISMIX,XPRINT,EXPT
08810 1650 FORMAT(/,1X,'KINEMATIC VISCOSITY OF THE BULK CRUDE FROM THE
08820 1 CUTS = ',1PE8.1,' AT T = ',0PF3.1,' DEG F. SCALE
08830 2 FACTOR = ',1PE8.1)
08840 C
08850 C IMPORTANT NOTE: THE VISCOSITY PREDICTION OF THE WHOLE
08860 C CRUDE FROM CUT INFORMATION IS NOT GOOD AT ALL. SO THE
08870 C VISCOSITY INFORMATION CALCULATED ABOVE IS NOT USED IN
08880 C THIS VERSION OF THE CODE, BUT IT COULD BE IF A GOOD
08890 C MIXING RULE IS EVER DETERMINED.
08900 C THEREFORE, FOR THE TIME BEING, THE VISCOSITY OF THE WHOLE
08910 C WEATHERED CRUDE IS CALCULATED ACCORDING TO MACKAY.
08920 C
08930 C NOW LOAD THE VISCOSITY INFORMATION IN THE FORM
08940 C OF THREE CONSTANTS:
08950 C 1. THE VISCOSITY IN CP AT 25 DEG C
08960 C 2. THE ANDRADE-VISCOSITY-SCALING CONSTANT
08970 C WITH RESPECT TO TEMPERATURE. SEE GOLD &
08980 C OGLE, 1969, CHEM. ENG., JULY 14, P121-123
08990 C 3. THE VISCOSITY AS AN EXPONENTIAL FUNCTION OF
09000 C THE FRACTION OF OIL WEATHERED
09010 C
09020 IF(LSWTCH.EQ.99) GO TO 1670
09030 TYPE 1660
09040 1660 FORMAT(1X,'SINCE A LIBRARY CRUDE WAS NOT USED
09050 1. ',1X,'ENTER THE FOLLOWING THREE VISCOSITY CONSTANTS')
09060 GO TO 1690
09070 1670 TYPE 1680
09080 1680 FORMAT(1X,'DO YOU WANT TO ENTER VISCOSITY CONSTANTS?')
09090 ACCEPT 340, ANS
09100 IF(ANS.EQ.'N') GO TO 1730
09110 1690 TYPE 1700
09120 1700 FORMAT(1X,'1. ENTER THE BULK CRUDE VISCOSITY
09130 1 AT 25 DEG C, CENTIPOISE, TRY 35.')
09140 ACCEPT 230, VISZ
09150 TYPE 1710
09160 1710 FORMAT(1X,'2. ENTER THE VISCOSITY TEMPERATURE SCALING
09170 1 CONSTANT (ANDRADE), TRY 9000.')
09180 ACCEPT 230, MK3
09190 TYPE 1720
09200 1720 FORMAT(1X,'3. ENTER THE VISCOSITY-FRACTION-OIL
09210 1-WEATHERED CONSTANT, TRY 10.5')
09220 ACCEPT 230, MK4
09230 GO TO 1740
09240 C

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09250 C      USE THE LIBRARY VISCOSITY DATA
09260 C
09270 1730 VISZ=VISZL(IC)
09280 MK3=MK3L(IC)
09290 MK4=MK4L(IC)
09300 C
09310 C      INSERT VISCOSITY CALCULATION ACCORDING TO MASS
09320 C      FRACTION EVAPORATED. THIS IS THE VISCOSITY
09330 C      MODIFICATION RELATIVE TO CUTVP1
09340 C
09350 1740 VSLEAD=VISZ*EXP(MK3*(1./TK-0.003357))
09360 WRITE (100,1730) VISZ,MK3,MK4,VSLEAD
09370 1750 FORMAT(/,1X,'VISCOSITY ACCORDING TO MASS EVAPORATED:
09380 1 VIS25C =',1PE9.2,'. ANDRADE =',1PE9.2
09390 2.,', FRACT WEATHERED =',1PE9.2,'. VSLEAD =',1PE9.2
09400 3.,', CP')
09410 C2P=1./C2
09420 WRITE (100,1960) C1,C2P,C4
09430 NEQ=NCUTS
09440 C
09450 C      SET UP THE DISPERSION PROCESS CONSTANTS.
09460 C      CALCULATE THE FRACTION OF THE SEA SURFACE SUBJECT TO
09470 C      DISPERSIONS/HOUR.
09480 C
09490 TYPE 1760
09500 1760 FORMAT(1X,'DO YOU WANT THE WEATHERING TO OCCUR WITH
09510 1 DISPERSION?')
09520 ACCEPT 340,ANS
09530 FRACTS=0.
09540 IF(ANS.EQ.'N') GO TO 1810
09550 TYPE 1770
09560 1770 FORMAT(1X,'DO YOU WANT TO ENTER THE DISPERSION
09570 1 CONSTANTS?')
09580 ACCEPT 340,ANS
09590 IF(ANS.EQ.'N') GO TO 1800
09600 TYPE 1780
09610 1780 FORMAT(1X,'ENTER THE WIND SPEED CONSTANT. TRY 0.1')
09620 ACCEPT 230,KA
09630 TYPE 1790
09640 1790 FORMAT(1X,'ENTER THE CRITICAL DROPLET SIZE CONSTANT
09650 1. TRY 50')
09660 ACCEPT 230,KB
09670 1800 FRACTS=KA*(1.+WINDMS)**2
09680 1810 WRITE (100,1820) FRACTS
09690 1820 FORMAT(/,1X,'THE FRACTIONAL SLICK AREA SUBJECT TO
09700 1 DISPERSION IS',1PE8.1,' PER HOUR')
09710 IF(ANS.EQ.'N') GO TO 1840
09720 WRITE (100,1830) KA,KB,STEN
09730 1830 FORMAT(1X,'THE DISPERSION PARAMETERS USED: KA = '
09740 1.1PE9.2,'. KB = ',1PE9.2,'. SURFACE TENSION = ',1PE9.2
09750 2.,' DYNES/CM')
09760 C
09770 C      PRINT EVERY XP TIME INCREMENT (HOURS).
09780 C      X1 IS THE STARTING TIME = 0.
09790 C      X2 IS THE NUMBER OF HOURS FOR WEATHERING TO OCCUR.
09800 C
09810 1840 XP=1.
09820 X1=0.
09830 MOLES(NCUTS+1)=AREA
09840 C
09850 C      PRINT AN OUTPUT FILE FOR 80 COLUMN OUTPUT, THIS IS
09860 C      THE CUTVP2.TYP FILE.
09870 C
09880 WRITE (ITY,1850) (ANAME(J),J=1,5)
09890 1850 FORMAT(/,1X,'OIL WEATHERING FOR ',5A5)
09900 WRITE (ITY,570)

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09910      WRITE (ITY,1860) XPRINT,WINDS
09920 1860  FORMAT(1X,'TEMPERATURE= ',F5.1,' DEG F. WIND SPEED= '
09930      1,F5.1,' KNOTS')
09940      WRITE (ITY,1870) BBL
09950 1870  FORMAT(1X,'SPILL SIZE= ',1PE10.3,' BARRELS')
09960      WRITE (ITY,1880) KMTC
09970 1880  FORMAT(1X,'MASS-TRANSFER COEFFICIENT CODE=',13)
09980      WRITE (ITY,1890)
09990 1890  FORMAT(/,1X,'FOR THE OUTPUT THAT FOLLOWS. MOLES
10000      1=GRAM MOLES')
10010      WRITE (ITY,1900)
10020 1900  FORMAT(1X,'GMS=GRAMS, VP=VAPOR PRESSURE IN ATMOSPHERES')
10030      WRITE (ITY,1910)
10040 1910  FORMAT(1X,'BP=BOILING POINT IN DEG F, API=GRAVITY')
10050      WRITE (ITY,1920)
10060 1920  FORMAT(1X,'MW=MOLECULAR WEIGHT')
10070      WRITE (ITY,1930)
10080 1930  FORMAT(/,2X,'CUT',3X,'MOLES',6X,'GMS',8X,'VP',8X,'BP'
10090      1,7X,'API',5X,'MW')
10100      DO 1950 I=1,NCUTS
10110      GMS=MOLES(I)*MW(I)
10120      IMW=MW(I)
10130      WRITE (ITY,1940) I,MOLES(I),GMS,VP(I),TB(I),API(I),IMW
10140 1940  FORMAT(3X,12.5(1X,1PE9.2),1X,13)
10150 1950  CONTINUE
10160      WRITE (ITY,1960) C1,C2P,C4
10170 1960  FORMAT(/,1X,'MOUSSE CONSTANTS: MOONEY=',1PE9.2
10180      1,' MAX H2O=',0PF5.2,' WIND**2=',1PE9.2)
10190      WRITE (ITY,1970) KA,KB,STEN
10200 1970  FORMAT(1X,'DISPERSION CONSTANTS: KA=',1PE9.2
10210      1,' KB=',1PE9.2,' S-TENSION=',1PE9.2)
10220      WRITE (ITY,1980) VISZ,MK3,MK4
10230 1980  FORMAT(1X,'VIS CONSTANTS: VIS25C=',1PE9.2
10240      1,' ANDRADE =',1PE9.2,' FRACT =',1PE9.2)
10250      WRITE (ITY,1990)
10260 1990  FORMAT(/,1X,'FOR THE OUTPUT THAT FOLLOWS. TIME=HOURS')
10270      WRITE (ITY,2000)
10280 2000  FORMAT(1X,'BBL=BARRELS, SPCR=SPECIFIC GRAVITY, AREA=M*M')
10290      WRITE (ITY,2010)
10300 2010  FORMAT(1X,'THICKNESS=CM. W=PERCENT WATER IN OIL (
10310      1MOUSSE)')
10320      WRITE (ITY,2020)
10330 2020  FORMAT(1X,'DISP=DISPERSION RATE IN GMS/M*M/HR')
10340      WRITE (ITY,2030)
10350 2030  FORMAT(1X,'ERATE=EVAPORTION RATE IN GMS/M*M/HR')
10360      WRITE (ITY,2040)
10370 2040  FORMAT(1X,'M/A=MASS PER M*M OF OIL IN THE SLICK')
10380      WRITE (ITY,2050)
10390 2050  FORMAT(1X,'I=FIRST CUT WITH GREATER THAN 1% (MASS)
10400      1 REMAINING')
10410      WRITE (ITY,2060)
10420 2060  FORMAT(1X,'J=FIRST CUT WITH GREATER THAN 50% (MASS)
10430      1 REMAINING')
10440      IF(FRACTS.NE.0.) GO TO 2080
10450      WRITE (ITY,2070)
10460 2070  FORMAT(1X,'DISPERSION WAS TURNED OFF')
10470 2080  IF(SPREAD.NE.0.) GO TO 2100
10480      WRITE (ITY,2090)
10490 2090  FORMAT(/,1X,'SPREADING WAS TURNED OFF')
10500      C
10510      C      WRITE SOME INFORMATION TO THE PLOT FILE.
10520      C
10530 2100  TCODE=KMTC
10540      C
10550      C      XPRINT IS THE ENVIRONMENTAL TEMPERATURE. DEG F.
10560      C

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10570      WRITE (IPU,800) XPRINT,WINDS,KA,KB,STEN,BBL,C1,C2,C4
10580      1,TCODE
10590      C
10600      C      TO THIS POINT IT WAS JUST GETTING READY. NOW
10610      C      INTEGRATE IT.
10620      C
10630      CALL BRKC4(MOLES,X1,X2,XP,NEQ)
10640      2110 TYPE 2120
10650      2120 FORMAT(1X,'DO IT AGAIN?')
10660      ACCEPT 340,ANS
10670      IF(ANS.EQ.'Y') GO TO 760
10680      2130 CONTINUE
10690      END
10700      SUBROUTINE CHAR(API,TB,A,B,NS,NV)
10710      REAL*4 MW1
10720      COMMON /COIL/ MW1,TC1,VC1,PC1,CNUM1,VIS1
10730      DIMENSION C(2,6),T(2,6),P(4),V(2,6)
10740      DATA ((C(I,J),J=1,6),I=1,2)/6.241E+01,-4.595E-02,-2.836E-01
10750      1.3.256E-03,4.578E-04,5.279E-04
10760      2.4.268E+02,-1.007,-7.449,1.38E-02,1.047E-03,2.621E-02/
10770      DATA ((T(I,J),J=1,6),I=1,2)/4.055E+02,1.337,-2.662,-2.169E-03
10780      1.-4.943E-04,1.454E-02
10790      2.412,2.1.276,-2.865,-2.888E-03,-3.707E-04,2.888E-02/
10800      DATA P/1.237E-02,0.2516,4.039E-02,-4.024E-02/
10810      DATA ((V(I,J),J=1,6),I=1,2)/-0.4488,-9.344E-04,0.01583
10820      1.-5.219E-05,5.268E-06,1.336E-04
10830      2.-0.6019,1.793E-03,-3.159E-03,-5.1E-06,9.067E-07,3.522E-05/
10840      C
10850      C      THIS SUBROUTINE CHARACTERIZES A CUT OF CRUDE OIL WITH RESPECT
10860      C      TO VAPOR PRESSURE. THE INPUT REQUIRED IS API GRAVITY AND THE
10870      C      BOILING POINT AT 1 ATMOSPHERE. THE OUTPUT IS A SWITCH NS
10880      C      WHERE NS=1 MEANS THE VAPOR PRESSURE EQUATION CAN BE USED DOWN TO
10890      C      10MM HG AND NS=2 MEANS THE CLAPEYRON EQUATION SHOULD BE USED.
10900      C
10910      C      THE VAPOR PRESSURE EQUATION IS:
10920      C
10930      C      LOG10(PR) = -A*(1.-TR)/TR - EXP(-20*(TR-B)**2)
10940      C
10950      C      WHERE PR = REDUCED PRESSURE, TR = REDUCED TEMPERATURE AND
10960      C      A AND B ARE RETURNED BY THIS SUBROUTINE.
10970      C
10980      C      API = GRAVITY, TB = BOILING POINT AT 1 ATMOSPHERE IN DEG F.
10990      C      CALCULATE CRITICAL TEMPERATURE AND MOLECULAR WEIGHT.
11000      C
11010      C      API2=API*API
11020      C      TB2=TB*TB
11030      C      CROSS=API*TB
11040      C      I=1
11050      C      IF(API.GT.35.) I=2
11060      C      VIS1=V(I,1)+V(I,2)*TB+V(I,3)*API+V(I,4)*CROSS+V(I,5)*TB2
11070      C      1+V(I,6)*API2
11080      C      GO TO (10.30), NV
11090      10 I=1
11100      C      IF(TB.GT.500.) I=2
11110      C      MW1=C(I,1)+C(I,2)*TB+C(I,3)*API+C(I,4)*CROSS+C(I,5)*TB2
11120      C      1+C(I,6)*API2
11130      C      TC1=T(I,1)+T(I,2)*TB+T(I,3)*API+T(I,4)*CROSS+T(I,5)*TB2
11140      C      1+T(I,6)*API2
11150      C      TCK=(TC1+459.)/1.8
11160      C
11170      C      CALCULATE THE VISCOSITY OF THE CUT.
11180      C
11190      C      I=1
11200      C      IF(API.GT.35.) I=2
11210      C      VIS1=V(I,1)+V(I,2)*TB+V(I,3)*API+V(I,4)*CROSS+V(I,5)*TB2
11220      C      1+V(I,6)*API2

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11230 C
11240 C      CALCULATE THE CARBON NUMBER
11250 C
11260 CNUM1=(MW1-2.)/14.
11270 X=ALOG10(CNUM1)
11280 C
11290 C      CALCULATE B FOR THE VAPOR PRESSURE EQUATION
11300 C
11310 BPRIME=P(1)+X*(P(2)+X*(P(3)+X*P(4)))
11320 B=BPRIME-0.02
11330 C
11340 C      CALCULATE THE CRITICAL VOLUME. CC/GMOLE
11350 C
11360 VW=1.88+2.44*CNUM1
11370 VC1=VW/0.044
11380 C
11390 C      CALCULATE THE CRITICAL PRESSURE IN ATMOSPHERES
11400 C
11410 PCP=20.8*TCK/(VC1-8.)
11420 PC1=PCP+10.
11430 TR=(TB+459.)/(TC1+459.)
11440 PR=1./PC1
11450 NS=1
11460 IF (TR.LE.B) GO TO 20
11470 A=(ALOG10(PR)+EXP(-20.*(TR-B)**2))*TR/(TR-1.)
11480 GO TO 30
11490 20 NS=2
11500 30 RETURN
11510 END
11520 SUBROUTINE BRKG4(Y,X1,X2,XP,NEQ)
11530 REAL*4 K1,K2,K3,K4,MTC,MW,MWU,KB,MK4
11540 COMMON /SPILL/ MTC(30),VP(30),VLOG(30),RHO(30),MW(30)
11550 1,SPGR(30),FRACTS,STEN,KB,DISPER,Z,TERM2,SPREAD,KMTC
11560 COMMON /PCODE/ VSLEAD,MK4,IOU,IPU,ITY
11570 COMMON /TALK/ MWU(30),NEQ1,NEQ2,NEQ3
11580 DIMENSION Y(30),YARG(30),K1(30),K2(30),K3(30),K4(30)
11590 1,GONE(200),YSAVE(30),YF(30),YMSAVE(30),YM(30),YM1(30)
11600 C
11610 C      RUNGA-KUTTA 4-TH ORDER NUMERICAL INTEGRATION FOR SIMULTANEOUS
11620 C      DIFFERENTIAL EQUATIONS. SEE C.R. WYLIE, PAGES 108-117 OR
11630 C      D. GREENSPAN, PAGES 113-115.
11640 C
11650 C      THIS SUBROUTINE DOES THE PRINTING. THE INITIAL AND FINAL VALUES
11660 C      ARE ALWAYS PRINTED. PRINT THE RESULTS EVERY XP INCREMENT
11670 C      IN X.
11680 C
11690 C      THE USER MUST WRITE SUBROUTINE FXYZ WHICH CALCULATES THE
11700 C      K1, K2, K3, AND K4 VECTORS AS A FUNCTION OF X AND THE
11710 C      CURRENT Y VECTOR. INTEGRATION FOLLOWS THE REFERENCES AND
11720 C      WAS TESTED ON PROBLEM 3, PAGE 116 IN WYLIE.
11730 C
11740 C      THE FIRST NCUTS POSITIONS IN THE Y VECTOR ARE THE MOLES
11750 C      OF THE COMPONENTS. POSITION NCUTS+1 IS THE AREA OF THE
11760 C      SLICK. POSITION NCUTS+2 IS THE MASS LOST FROM THE SLICK
11770 C      BY DISPERSION ALONE. POSITION NCUTS+3 IS THE MASS LOST
11780 C      FROM THE SLICK BY EVAPORATION ALONE.
11790 C
11800 C      LINE KEEPS TRACK OF HOW MANY LINES ARE WRITTEN TO THE
11810 C      PLOT FILE. NEQ1 IS THE NUMBER OF COMPONENTS+1. NS IS
11820 C      A ROUTING SWITCH TO CHANGE THE PRINT INTERVAL. IN IS
11830 C      AN INPUT ROUTING SWITCH TO DELETE RAPIDLY CHANGING
11840 C      COMPONENTS. GONE(LINE) IS THE MASS FRACTION REMAINING
11850 C      AT TIME STEP LINE. INT IS A SWITCH TO INDICATE WHEN THE
11860 C      INTEGRATION HAS STARTED; INT=1, NOT STARTED; INT=2,
11870 C      STARTED. ITP IS A HEADER PRINT SWITCH FOR THE
11880 C      80-COLUMN FILE.

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11890 C      INT=1
11900      ITYP=1
11910      LINE=0
11920      NEQ1=NEQ+1
11930      NEQ2=NEQ+2
11940      NEQ3=NEQ+3
11950      NS=1
11960      IN=1
11970      IKEEP=1
11980      GONE(1)=1.
11990      DISPER=0.
12000
12010 C
12020 C      TOTAL IS THE INITIAL NUMBER OF MOLES.
12030 C      TSAVE IS THE INITIAL MASS.
12040 C
12050      TOTAL=0.
12060      TSAVE=0.
12070      DO 10 I=1,NEQ
12080 C
12090 C      CALCULATE AND SAVE THE INITIAL CONDITIONS.
12100 C
12110      YSAVE(I)=Y(I)
12120      YMSAVE(I)=Y(I)*MW(I)
12130      MWU(I)=MW(I)
12140      TSAVE=TSAVE+YMSAVE(I)
12150      TOTAL=TOTAL+Y(I)
12160 10 C      CONTINUE
12170 C
12180 C      SAVE THE INITIAL AREA.
12190 C
12200      YMSAVE(NEQ1)=Y(NEQ1)
12210 C
12220 C      INITIALIZE THE MASS LOST BY DISPERSION ALONE AND
12230 C      EVAPORATION ALONE.
12240 C
12250      Y(NEQ2)=0.
12260      Y(NEQ3)=0.
12270 C
12280 C      NDEL IS THE NUMBER OF COMPONENTS DELETED BECAUSE THEY
12290 C      EVAPORATE TOO FAST. NFAST IS THE CURRENT ARRAY LOCATION
12300 C      OF THE FASTEST MOVING COMPONENT.
12310 C
12320      NDEL=0
12330      NFAST=0
12340      X=X1
12350 C
12360 C      INITIALIZE THE PRINT SWITCH TO FORCE A PRINT AND
12370 C      SUBSEQUENT CALCULATIONS THE FIRST TIME THROUGH.
12380 C
12390      XW=-1.
12400      WRITE (10U,20)
12410 20  FORMAT(/,1X,'COUNT THE CUTS IN THE FOLLOWING OUTPUT FROM LEFT
12420      1 TO RIGHT',/)
12430      WRITE (10U,30)
12440 30  FORMAT(1X,'THE INITIAL GRAM MOLES IN THE SLICK ARE:')
12450      WRITE (10U,40) (Y(I),I=1,NEQ)
12460 40  FORMAT(11(1X,1PE10.3))
12470      WRITE (10U,50)
12480 50  FORMAT(/,1X,'THE INITIAL MASSES (GRAMS) IN THE SLICK ARE
12490      1:')
12500      WRITE (10U,40) (YMSAVE(I),I=1,NEQ)
12510      WRITE (10U,60) TSAVE
12520 60  FORMAT(1X,'THE TOTAL MASS FROM THESE CUTS IS '
12530      1,1PE10.3,' GRAMS')
12540      WRITE (10U,70)

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12550 70  FORMAT(/)
12560 C
12570 C
12580 C
12590 C
12600 C
12610 C
12620 C
12630 C
12640 C
12650 C
12660 C
12670 80  NFAST=NFAST+1
12680 90  CALL FXYZ(X,Y,K1,NEQ)
12690 C
12700 C
12710 C
12720 C
12730 C
12740 C
12750 C
12760 C
12770 C
12780 C
12790 C
12800 C
12810 C
12820 C
12830 100 IF(H.GT.0.05) GO TO 130
12840 C
12850 C
12860 C
12870 C
12880 C
12890 C
12900 C
12910 C
12920 C
12930 C
12940 C
12950 C
12960 C
12970 C
12980 C
12990 C
13000 C
13010 C
13020 C
13030 C
13040 C
13050 C
13060 C
13070 C
13080 C
13090 C
13100 C
13110 C
13120 C
13130 C
13140 C
13150 C
13160 110 CONTINUE
13170 C
13180 C
13190 C
13200 C

```

CALCULATE DY/DX AND SET THE STEP SIZE TO APPROXIMATE
 A 5% CHANGE IN THE MOST RAPIDLY CHANGING Y. WHEN THIS
 Y DECREASES BY A FACTOR OF 20, RESET THE STEP SIZE
 ACCORDING TO THE NEXT Y.
 SOME Y'S WILL CHANGE SO FAST THAT THEY WILL BE GONE
 IN A FEW MINUTES. THESE ARE DELETED BEFORE INTEGRATION
 STARTS AND NOTED ON THE PRINTED RESULTS.

INITIALIZE OR INCREMENT NFAST.

THE TIME UNIT IS HOUR.
 SET THE STEP SIZE TO $H=0.05*Y/(DY/DX)$.

$H=0.05*Y(NFAST)/K1(NFAST)$
 $YOLD=Y(NFAST)$
 $H=ABS(H)$
 $H2=H/2$.
 GO TO (100,170). IN

IF THERE IS A RAPIDLY MOVING COMPONENT AT THE BEGINNING
 ITS STEP SIZE WILL BE VERY SMALL. DO NOT LET THE
 STEP SIZE BE LESS THAN 0.05 HOUR.

IF(H.GT.0.05) GO TO 130

Y(NFAST) CHANGES TOO FAST TO CALCULATE. DELETE IT AND MOVE
 EVERYBODY ONE SPACE TO THE LEFT.

WHEN YOU MOVE THE AREA BE SURE TO SUBTRACT THE CONTRIBUTION
 OF THE CUT JUST DELETED.

ISTART=1
 NFAST=1
 NDEL=NDEL+1

DECREASE THE NUMBER OF COMPONENTS BY 1

$NEQ=NEQ-1$
 $NEQ1=NEQ+1$
 $NEQ2=NEQ+2$
 $NEQ3=NEQ+3$
 $NEQ4=NEQ+4$
 $AD=Y(1)/RHO(1)/Z$
 DO 110 I=1,NEQ

SHIFT THE ARRAYS.

$I1=I+1$
 $Y(I)=Y(I1)$
 $VP(I)=VP(I1)$
 $MTG(I)=MTG(I1)$
 $YSAVE(I)=YSAVE(I1)$
 $VLOG(I)=VLOG(I1)$
 $RHO(I)=RHO(I1)$
 $MWU(I)=MWU(I1)$
 $YMSAVE(I)=YMSAVE(I1)$

BE SURE AND DO THE LAST THREE POSITIONS WHEN SHIFTING
 $Y(NEQ1)=Y(NEQ2)-AD$


```

13210      Y(NEQ2)=Y(NEQ3)
13220      Y(NEQ3)=Y(NEQ4)
13230      WRITE (10U,120) NDEL
13240      120  FORMAT(1X,'CUT '.12,' GOES AWAY IN MINUTES. THEREFORE IT WAS
13250      1 DELETED AND THE CUTS RENUMBERED'./)
13260      WRITE (1TY,120) NDEL
13270      GO TO 90
13280      130  IN=2
13290      GO TO (140,160) ITYP
13300      140  ITYP=2
13310      WRITE (1TY,150)
13320      150  FORMAT(/.1X,'TIME'.2X,'BBL'.3X,'SPCR'.2X,'AREA'.2X
13330      1,'THICKNESS 'W'.2X,'DISP'.4X,'ERATE'.4X,'M/A ' I ' J')
13340      C
13350      C      THE COMPONENTS THAT MOVE TOO FAST TO CONSIDER (AT TIME
13360      C      ZERO) HAVE BEEN DELETED AND THE ARRAYS SHIFTED.
13370      C
13380      160  NEQ1=NEQ+1
13390      NEQ2=NEQ+2
13400      NEQ3=NEQ+3
13410      C
13420      C      NEVER LET THE STEP SIZE BE GREATER THAN 0.5
13430      C
13440      170  IF(H.GT.0.5) H=0.5
13450      WRITE (10U,180) H,NFAST
13460      180  FORMAT(/.2X,'STEP SIZE OF '.1PE10.3.' IS BASED ON CUT '.13./)
13470      C
13480      C      CHECK THE PRINT SWITCH.
13490      C
13500      190  IF(X.LT.XW) GO TO 380
13510      C
13520      C      INCREMENT THE PRINT SWITCH AND CALCULATE INTERMEDIATE
13530      C      RESULTS NOT CARRIED WITH THE INTEGRATION.
13540      C
13550      XW=X+XP
13560      YTOT=0.
13570      TMASS=0.
13580      DO 200 I=1,NEQ
13590      YF(I)=Y(I)/YSAVE(I)
13600      YTOT=YTOT+Y(I)
13610      YM(I)=Y(I)*MWU(I)
13620      YMI(I)=YM(I)
13630      TMASS=TMASS+YM(I)
13640      YH(I)=YM(I)/YMSAVE(I)
13650      200  CONTINUE
13660      YMI(NEQ1)=Y(NEQ1)
13670      C
13680      C      CALCULATE THE MEAN MOLECULAR WEIGHT OF THE SLICK.
13690      C
13700      WMEANS=0.
13710      DO 210 I=1,NEQ
13720      WMEANS=WMEANS+MWU(I)*Y(I)/YTOT
13730      210  CONTINUE
13740      LINE=LINE+1
13750      WRITE (10U,220) X,LINE
13760      220  FORMAT(2X,'TIME = '.1PE8.1.' HOURS. MASS FRACTION OF EACH
13770      1 CUT REMAINING:'.65X.13)
13780      WRITE (10U,230) (YM(I),I=1,NEQ)
13790      230  FORMAT(14(1X,1PE8.1))
13800      CHECK=TMASS+Y(NEQ2)+Y(NEQ3)
13810      WRITE (10U,240) TMASS,Y(NEQ2),Y(NEQ3),CHECK
13820      240  FORMAT(2X,'MASS REMAINING = '.1PE10.3.' MASS DISPERSED
13830      1 = '.1PE10.3.' MASS EVAPORATED = '.1PE10.3.'
13840      2. SUM = '.1PE10.3)
13850      WRITE (1PU,250) NEQ1
13860      250  FORMAT(15)

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13870      WRITE (IPU,260) X.(YM1(I),I=1,NEQ1)
13880 260    FORMAT(10(1X,1PE10.3))
13890      C
13900      C      WHEN THE FRACTION REMAINING OF COMPONENT I GETS LOW.
13910      C      SET ITS VAPOR PRESSURE AND MOLES EQUAL TO ZERO.
13920      C
13930      DO 270 I=ISTART,NEQ
13940      IF(YF(I).GT.1.0E-08) GO TO 270
13950      IKEEP=I+1
13960      VP(I)=0.
13970      Y(I)=0.
13980 270    CONTINUE
13990      ISTART=IKEEP
14000      NFAST=IKEEP
14010      GONE(LINE)=TMASS/TSAVE
14020      ZP=Z*100.
14030      WRITE (IOU,280) GONE(LINE),Y(NEQ1),ZP,WMEANS
14040 280    FORMAT(2X,'FRACTION (BASED ON MASS) REMAINING IN THE SLICK
14050      1='1PEB.1.',AREA='1PEB.1.'M**2,THICKNESS='
14060      2.1PEB.1.'CM,MOLE WT='.0PF5.1)
14070      C
14080      C      WIO IS THE MOUSSE CALCULATION.
14090      C
14100      CALL WIO(X,W,VTERM)
14110      C
14120      C      VISCP1 IS THE VISCOSITY OF THE PARENT OIL WITH NO WATER
14130      C      INCORPORATED.
14140      C      VISCP1 IS IN CENTIPOISE. FEVAP IS THE FRACTION OF OIL
14150      C      EVAPORATED. NOTE THAT FEVAP IS NOT
14160      C      1 - (FRACTION REMAINING) BECAUSE DISPERSION LOSSES
14170      C      WOULD BE INCLUDED. THE FRACTION EVAPORATED MUST
14180      C      CORRECT FOR THE LOSS DUE TO DISPERSION.
14190      C
14200      FEVAP=1.0-GONE(LINE)
14210      FEVAP=FEVAP/YM(NEQ)
14220      VISCP1=VSLEAD*EXP(MK4*FEVAP)
14230      C
14240      C      VTERM IS THE VISCOSITY MULTIPLIER FROM THE MOUSSE
14250      C      CALCULATION.
14260      C
14270      VISCP=VISCP1*VTERM
14280      C
14290      C      CALCULATE THE BULK SPGR.
14300      C
14310      BSPGR=0.
14320      DO 290 I=ISTART,NEQ
14330      BSPGR=BSPGR+SPGR(I)*Y(I)/YTOT
14340 290    CONTINUE
14350      VISQT=SQRT(VISCP/10.)
14360      C
14370      C      CALCULATE THE DISPERSION FACTOR.
14380      C
14390      FB=1./(1.+KB*VISQT*Z*STEN/0.024)
14400      DISPER=FRAC*FB
14410      WRITE (IOU,300) W,VISCP,DISPER
14420 300    FORMAT(2X,'WEIGHT FRACTION WATER IN OIL = '1PEB.1.',VIS
14430      1COSITY = '1PEB.1.'CENTISTOKES,DISPERSION TERM = '
14440      2.1PEB.1.'WEIGHT FRACTION/HR')
14450      CVOLUM=Y(NEQ1)*Z
14460      TBBL=CVOLUM/0.159
14470      CVOLUM=(1.0E+06)*CVOLUM
14480      CSPGR=TMASS/CVOLUM
14490      WAREA=(1.0E+06)*Z*CSPGR
14500      WDISP=WAREA*DISPER
14510      IF(INT.EQ.1) ERATE=0.
14520      ERATE=ERATE/Y(NEQ1)

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14530      WRITE (10U,310) WAREA,CSPGR,TBBL,WDISP,ERATE
14540 310    FORMAT(2X,'MASS/AREA=.1PE8.1,' GMS/M*M, 'SPGR='
14550      1.1PE8.1,' TOTAL VOLUME=.1PE8.1,' BBL, 'DISPERSION='
14560      2.1PE8.1,' GMS/M*M/HR, 'EVAP RATE=.1PE8.1,' GMS/M*M/HR')
14570 C
14580 C      PRINT AN OUTPUT FILE FOR 80 COLUMN OUTPUT.
14590 C
14600      DO 320 J=1,NEQ
14610      JCUT=J
14620      IF(YM(J).GT.0.5) GO TO 330
14630 320    CONTINUE
14640 330    DO 340 I=1,NEQ
14650      ICUT=I
14660      IF(YM(I).GT.0.01) GO TO 350
14670 340    CONTINUE
14680 350    IX=X
14690      IW=W*100.
14700      WRITE (1TY,360) IX,TBBL,CSPGR,Y(NEQ1),ZP,IW,WDISP
14710      1,ERATE,WAREA,ICUT,JCUT
14720 360    FORMAT(1X,13.1PE8.1,0PF5.2,2(1PE8.1),1X,13
14730      1.3(1PE8.1),12,13)
14740      WRITE (10U,70)
14750 C
14760 C      INCREASE XP TO 10 HOURS AFTER 50 HOURS OF WEATHERING.
14770 C
14780      GO TO (370,380), NS
14790 370    IF(X.LT.50.) GO TO 380
14800      NS=2
14810      XP=10.
14820 C
14830 C      TAKE A STEP IN TIME
14840 C
14850 380    XARG=X
14860      DO 390 I=1,NEQ3
14870      YARG(I)=Y(I)
14880 390    CONTINUE
14890 C
14900 C      INT IS A SWITCH TO INDICATE THAT THE INTEGRATION WAS
14910 C      INITIATED.
14920 C
14930      INT=2
14940      CALL FXYZ(XARG,YARG,K1,NEQ)
14950      XARG=X+H2
14960      DO 400 I=1,NEQ3
14970      YARG(I)=Y(I)+H*K1(I)/2.
14980 400    CONTINUE
14990 C
15000 C      SAVE THE EVAPORATION RATE FROM THE FIRST TIME
15010 C      THE DERIVATIVES ARE CALCULATED.
15020 C
15030      ERATE=K1(NEQ3)
15040      CALL FXYZ(XARG,YARG,K2,NEQ)
15050      DO 410 I=1,NEQ3
15060      YARG(I)=Y(I)+H*K2(I)/2.
15070 410    CONTINUE
15080      CALL FXYZ(XARG,YARG,K3,NEQ)
15090      XARG=X+H
15100      DO 420 I=1,NEQ3
15110      YARG(I)=Y(I)+H*K3(I)
15120 420    CONTINUE
15130      CALL FXYZ(XARG,YARG,K4,NEQ)
15140      DO 430 I=1,NEQ3
15150      Y(I)=Y(I)+H*(K1(I)+2.*(K2(I)+K3(I))+K4(I))/6.
15160 430    CONTINUE
15170 C
15180 C      IF 10 PER CENT BY MOLES OR LESS OF THE SLICK IS LEFT, STOP

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15190 C      THE CALCULATION BECAUSE STRANGE THINGS HAPPEN CLOSE TO
15200 C      ZERO OIL.
15210 C
15220      REMAIN=0.
15230      DO 440 I=1,NEQ
15240      REMAIN=REMAIN+Y(I)
15250 440    CONTINUE
15260      TEST=REMAIN/TOTAL
15270      IF(TEST.GT.0.1) GO TO 470
15280      WRITE (10U,450)
15290 450    FORMAT(/,1X,'THE SLICK (MOLES) HAS DECREASED TO 10%
15300      1 OR LESS. THEREFORE THE CALCULATION WAS STOPPED.')
15310      WRITE (1TY,460)
15320 460    FORMAT(/,1X,'SLICK DECREASED TO 10% MASS **STOP**')
15330      GO TO 310
15340 C
15350 C      RECALCULATE THE OVER-ALL MASS-TRANSFER COEFFICIENTS OUTSIDE
15360 C      THE DERIVATIVE SUBROUTINE. THE DIAMETER DEPENDENCE IS VERY
15370 C      SLOW. TERM2 IS THE OLD DIA**(-0.11). SO DIVIDE THE OLD
15380 C      COEFFICIENT BY TERM2 AND MULTIPLY IN THE NEW ONE.
15390 C
15400 C      WHEN YOU CHANGE THE WIND SPEED WITH RESPECT TO TIME.
15410 C      CHANGE THE MASS-TRANSFER COEFFICIENT HERE. DIVIDE
15420 C      OUT THE OLD WIND TERM AND MULTIPLY IN THE NEW ONE.
15430 C      ALSO. IF THE TEMPERATURE CHANGES. RECALCULATE THE
15440 C      VAPOR PRESSURE HERE. THIS APPLIES ONLY TO MACKAY
15450 C      AND MATSUGU.
15460 C
15470 470    GO TO (500,480,500), KMTG
15480 480    DIA=SQRT(Y(NEQ1)/0.785)
15490      TNEW=DIA**(-0.11)
15500      ADJUST=TNEW/TERM2
15510      DO 490 I=1,NEQ
15520      MTC(I)=MTC(I)*ADJUST
15530 490    CONTINUE
15540      TERM2=TNEW
15550 C
15560 C      CHECK TO SEE IF THE INTEGRATION IS COMPLETED.
15570 C
15580 500    IF(X.GE.X2) GO TO 510
15590      X=XARG
15600 C
15610 C      CHECK TO SEE IS THE FIRST NON-ZERO MOLES HAS FALLEN TO
15620 C      0.01 OF ITS STARTING VALUE. IF IT HAS. RECALCULATE THE
15630 C      STEP SIZE ON THE NEXT NON-ZERO COMPONENT. NOTE THAT
15640 C      A COMPONENT IS NOT ZEROED UNTIL ITS MOLE NUMBER HAS
15650 C      FALLEN TO LESS THAN 1.0E-08.
15660 C
15670      TEST=ABS(Y(NFAST)/YOLD)
15680      IF(TEST.LT.0.01) GO TO 80
15690      GO TO 190
15700 510    NDEL=NDEL+1
15710      WRITE (10U,520) NDEL
15720 520    FORMAT(/,1X,'THE CUT NUMBERING BEGINS WITH',13,' BASED ON
15730      1 THE ORIGINAL CUT NUMBERS',/)
15740      LINE=LINE+1
15750      WRITE (10U,530) X,LINE
15760 530    FORMAT(1X,'THE FINAL MASS FRACTIONS FOR THE SLICK AT '
15770      1,1PEB,1,' HOURS ARE:',65X,13)
15780      TYPE 540, LINE
15790 540    FORMAT(1X,'NUMBER OF LINES WRITTEN TO CUTVP2.PLT = ',14)
15800      TMASS=0.
15810      DO 550 I=1,NEQ
15820      YM(I)=Y(I)*MWU(I)
15830      TMASS=TMASS+YM(I)
15840      YM1(I)=YM(I)

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15850      YM(I)=YM(I)/YMSAVE(I)
15860 550    CONTINUE
15870      YM1(NEQ1)=Y(NEQ1)
15880      GONE(LINE)=TMASS/TSAVE
15890      WRITE (IOU,40) (YM(I),I=1,NEQ)
15900      WRITE (IPU,250) NEQ1
15910      WRITE (IPU,260) X.(YM1(I),I=1,NEQ1)
15920      WRITE (IPU,260) (GONE(I),I=1,LINE)
15930      ZP=Z*100.
15940      WRITE (IOU,280) GONE(LINE),Y(NEQ1),ZP,WMEANS
15950      CHECK=TMASS+Y(NEQ2)+Y(NEQ3)
15960      WRITE (IOU,240) TMASS,Y(NEQ2),Y(NEQ3),CHECK
15970      WRITE (IOU,560)
15980 560    FORMAT(/,IX,'*****')
15990      1*****',/)
16000      RETURN
16010      END
16020      SUBROUTINE FXYZ(XARG,MOLES,K,NEQ)
16030      REAL*4 MOLES,K,MTC,MW,MWU,KB
16040      COMMON /SPILL/ MTC(30),VP(30),VLOG(30),RHO(30),MW(30)
16050      1,SPGR(30),FRACTS,STEN,KB,DISPER,Z,TERM2,SPREAD,KMTC
16060      COMMON /TALK/ MWU(30),NEQ1,NEQ2,NEQ3
16070      DIMENSION MOLES(30),K(30),TMPVP(30),TMPDS(30)
16080      C
16090      C      THE VECTOR BEING INTEGRATED RESIDES IN MOLES(I).
16100      C      POSITIONS I=1 THROUGH I=NEQ ARE THE PSEUDO COMPONENTS.
16110      C      POSITION NEQ1=NEQ+1 IS THE AREA.
16120      C      POSITION NEQ2=NEQ+2 IS THE MASS LOST BY DISPERSION ALONE.
16130      C      POSITION NEQ3=NEQ+3 IS THE MASS LOST BY EVAPORATION ALONE.
16140      C
16150      C
16160      SUM=0.
16170      DO 10 I=1,NEQ
16180      SUM=SUM+MOLES(I)
16190 10    CONTINUE
16200      DO 20 I=1,NEQ
16210      C
16220      C      CALCULATE THE MOLE DERIVATIVES.
16230      C
16240      TMPVP(I)=MTC(I)*MOLES(NEQ1)*VP(I)*MOLES(I)/SUM
16250      TMPDS(I)=DISPER*MOLES(I)
16260      K(I)=TMPVP(I)+TMPDS(I)
16270      K(I)=-K(I)
16280 20    CONTINUE
16290      VOL=0.
16300      DO 30 I=1,NEQ
16310      VOL=VOL+MOLES(I)/RHO(I)
16320      CONTINUE
16330      C
16340      C      CALCULATE THE AREA DERIVATIVE.
16350      C
16360      Z=VOL/MOLES(NEQ1)
16370      K(NEQ1)=(5.4E+05)*(Z**1.33)*MOLES(NEQ1)**0.33
16380      K(NEQ1)=SPREAD*K(NEQ1)
16390      C
16400      C      CALCULATE THE MASS LOST FROM THE SLICK DUE TO
16410      C      EVAPORATION ALONE AND THEN DISPERSION ALONE.
16420      C
16430      K(NEQ2)=0.
16440      K(NEQ3)=0.
16450      DO 40 I=1,NEQ
16460      K(NEQ3)=K(NEQ3)+TMPVP(I)*MWU(I)
16470      K(NEQ2)=K(NEQ2)+TMPDS(I)*MWU(I)
16480 40    CONTINUE
16490      RETURN
16500      END

```

```

16510 SUBROUTINE WIO(TIME,W,VTERM)
16520 COMMON /MOOSE/ WINDS,C1,C2,C3,C4
16530 WFUNC(W)=(1.0-C2*W)*EXP(-2.5*W/(1.0-C1*W))
16540 VIS(W)=EXP(2.5*W/(1.0-C1*W))
16550 DATA WSAVE,C4SAVE/-1.,-1./
16560 C
16570 C THIS IS THE WATER-IN-OIL (MOUSSE) ROUTINE.
16580 C W IS THE FRACTIONAL WATER CONTENT IN THE OIL.
16590 C WINDS IS THE WIND SPEED IN KNOTS.
16600 C TIME IS IN HOURS.
16610 C C1 IS A VISCOSITY CONSTANT = 0.65
16620 C C2 IS AN OIL-COALESCEING CONSTANT AND IS OIL
16630 C DEPENDENT, AND IS THE INVERSE OF THE MAXIMUM WEIGHT
16640 C FRACTION WATER IN OIL.
16650 C C3 IS A WATER INCORPORATION RATE (1./HR), USUALLY 0.01*U*U
16660 C
16670 C THE PREDICTION EQUATION FOR W IS IMPLICIT AND IS
16680 C SOLVED BY TRIAL AND ERROR.
16690 C
16700 C REFERENCE: CHAPTER 4 BY MACKAY IN OIL SPILL PROCESSES
16710 C AND MODELS.
16720 C
16730 C DECEMBER, 1981
16740 C
16750 C IERR IS THE ERROR CODE.
16760 C IERR=1 IS A NORMAL EXIT. IERR=2 IS A PROBLEM IN THE
16770 C TRIAL-AND-ERROR ROUTINE. IERR=3 IS A STEADY-STATE
16780 C MOUSSE EXIT.
16790 C
16800 C IF THE OIL DOES NOT FORM MOUSSE, C2 WAS SET TO -1.
16810 C
16820 C IF(C2.GT.0.) GO TO 10
16830 C
16840 C NO MOUSSE FOR THIS OIL. SET TERMS AND RETURN.
16850 C
16860 C W=0.
16870 C VTERM=1.
16880 C GO TO 90
16890 10 IERR=1
16900 C
16910 C CHECK TO SEE IF THE WIND OR INCORPORATION RATE CONSTANT
16920 C CHANGED.
16930 C
16940 C IF(WINDS.EQ.WSAVE.AND.C4.EQ.C4SAVE) GO TO 20
16950 C WSAVE=WINDS
16960 C C4SAVE=C4
16970 C U2=WINDS*WINDS
16980 C C3=C4*U2
16990 20 EX=C3*TIME
17000 C IF(EX.GT.20.) GO TO 80
17010 C TEST=EXP(-EX)
17020 C
17030 C BRACKET THE TIME WITH TWO VALUES OF W.
17040 C
17050 C W=0.
17060 C WMAX=1./C2
17070 C WSTEP=WMAX/10.
17080 30 W=W+WSTEP
17090 C TRY=WFUNC(W)
17100 C IF(TRY.LT.TEST) GO TO 40
17110 C IF(W.LT.WMAX) GO TO 30
17120 C IERR=2
17130 C GO TO 90
17140 C
17150 C NOW DO INTERVAL HALVING TO FIND W.
17160 C

```

17170	40	NTRY=0
17180		WR=W
17190		WL=W-WSTEP
17200	50	W=(WR+WL)/2.
17210		TRY=WFUNC(W)
17220		IF(TRY.LT.TEST) GO TO 60
17230		WL=W
17240		GO TO 70
17250	60	WR=W
17260	70	NTRY=NTRY+1
17270		IF(NTRY.LT.10) GO TO 50
17280		VTERM=VIS(W)
17290		GO TO 90
17300	80	IERR=3
17310	90	CONTINUE
17320		RETURN
17330		END

APPENDIX B

APPENDIX B

Contract No. NA80RAC00018
Research Unit No. 597

OIL-WEATHERING COMPUTER PROGRAM
USER'S MANUAL

for

MULTIVARIATE ANALYSIS OF PETROLEUM
WEATHERING IN THE MARINE ENVIRONMENT -
SUB ARCTIC

Submitted to:

Outer Continental Shelf Environmental Assessment Program
National Oceanic and Atmospheric Administration

Submitted by:

Bruce E. Kirstein, James R. Payne,
Robert T. Redding

James R. Payne, Principal Investigator
Division of Environmental Chemistry and Geochemistry
Science Applications, Inc.
La Jolla, California 92038

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SCIENCE APPLICATIONS, LA JOLLA, CALIFORNIA
ALBUQUERQUE • ANN ARBOR • ARLINGTON • ATLANTA • BOSTON • CHICAGO • HUNTSVILLE
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P.O. Box 2351, 1200 Prospect Street, La Jolla, California 92037

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ABSTRACT

The Open-Ocean Oil-Weathering User's Manual is written to provide specific instructions on the use the computer code CUTVP2.FOR. This code calculates crude oil properties and the weathering of oil for a set of environmental parameters. The use of the code requires knowledge about the physical properties of crude oil and the weathering of oil. In order to aid the user, the code has been written to ask the user for specific input and provide examples of input. The best way to learn to use the code is to access the computer and work through some of the examples presented in this manual.

OIL-WEATHERING COMPUTER PROGRAM USER'S MANUAL

Model Overview

The open-ocean oil-weathering code is written in FORTRAN as a stand-alone code that can be easily installed on any machine. All the trial-and-error routines, integration routines, and other special routines are written in the code so that nothing more than the normal system functions such as EXP are required. The code is user-interactive and requests input by prompting questions with suggested input. Therefore, the user can actually learn about the nature of crude oil and its weathering by using this code.

The open-ocean oil-weathering model considers the following weathering processes:

- o evaporation
- o dispersion (oil into water)
- o mousse (water into oil)
- o spreading

These processes are used to predict the mass balance and composition of oil remaining in the slick as a function of time and environmental parameters. Dissolution of oil into the water column is not considered because this weathering process is not significant with respect to the over-all material balance of the oil slick.

An important assumption required in order to write material balance equations for evaporation is the state of mixedness of the oil in the slick. The open-ocean oil-weathering model is based on the assumption that the oil is well mixed. This might not always be true but data have been taken and interpreted as if the oil is well mixed. Thus, experimental results based on this

assumption must be used in the same way mathematically. There is growing thought based on physical observations (not compositional) that the oil is not always well mixed. As the oil weathers its viscosity increases (measured and known to be true) resulting in a slab-like oil phase. Clearly, the mass transfer within the oil will change drastically in going from a well-mixed to a slab-like phase.

The other three processes noted above are not explicitly component specific as is evaporation. However, the dispersion process is a function of the oil viscosity; oil viscosity is a function of composition. Thus the dispersion process does depend on the evaporation process. Mousse formation also alters the oil viscosity but the present knowledge of this process does not point to any quantifiable compositional dependence. The spreading of the slick results in an ever-increasing area for mass transfer.

The composition of the oil is described in terms of pseudocomponents that are obtained by fractionating the oil in a true-boiling-point distillation column. This procedure yields cuts of the oil which are characterized by boiling point and density. This information is then used to calculate many more parameters about the cut. The most important calculated parameters pertain to vapor pressure and molecular weight. The evaporation process is driven by vapor pressures, and system partial pressures are calculated assuming Raoult's law.

Model Description

The pseudocomponents characterization of crude oil for the open-ocean oil-weathering model is described in detail (Payne, Kirstein, et al., 1983). The specific detail presented in the oil characterization can vary depending upon exactly which literature references are used. Those references used to write the current open-ocean oil-weathering model are all essentially contained in a standard text (Hougen, Watson and Ragatz, 1965).

The pseudocomponent evaporation model and the over-all mass-transfer coefficient required for evaporation has also been described in detail (Payne, Kirstein, et al., 1983). The fundamental process of evaporation is described in many texts, such as Mass Transfer Operations (Treybal, 1955) and in papers in the open literature. A paper on this subject relevant to oil weathering is that by Liss and Slater (Liss and Slater, 1974).

The equation which describes slick spreading has also been described (Payne, Kirstein, et al., 1983). The spreading equation is based on observations due to Mackay (Mackay, et al., 1980) and is not based on the many publications which describe oil spreading due to gravity-viscosity-surface tension. The phenomenological approach to oil spreading does not pertain to a rough ocean surface, and the empirical approach at least reflects reality.

The viscosity prediction used in early oil-weathering model calculations is based on a (mole fraction)^{0.5}(cut viscosity) summation (Reid, et al., 1977). This viscosity prediction has been found to be inadequate in that the predicted viscosity is always too low. This viscosity prediction has been replaced with one due to Tebeau and Mackay (Tebeau, Mackay, et al., 1981) where the viscosity at 25°C is a function of the fraction of oil evaporated on a dispersion-free basis. The functional relationship is $\exp(K_4 F)$ where K_4 is an oil-dependent constant and F is the fraction evaporated. The viscosity is scaled with respect to temperature according to the Andrade equation (Gold and Olge, 1969).

The prediction of water-in-oil emulsification is based on three parameters (Mackay, et al., 1980) appearing in the following equation:

$$(1 - K_2 W) \exp \left[\frac{-2.5W}{1 - K_1 W} \right] \equiv \exp \left[-K_3 t \right]$$

where W is the weight fraction water in the oil-water mixture, K_1 is a constant in a viscosity equation due to Mooney (Mooney, 1951), K_2 is a

coalescing-tendency constant, and K_3 is a lumped water incorporation rate constant. The viscosity equation due to Mooney is

$$\mu = \mu_0 \exp \left[\frac{-2.5W}{1-K_1W} \right]$$

where μ_0 is the parent oil viscosity. K_1 is usually around 0.62 to 0.65 and apparently does not change much with respect to different types of oils. The constant K_2 above must satisfy the relation $K_2W < 1$ in order for the water incorporation rate term (right-hand side) to be > 0 . Thus, K_2 is the inverse of the maximum weight fraction water in the mixture. K_3 is the water incorporation rate constant and is a function of wind speed in knots.

The dispersion (oil into water) weathering process is described by two equations (Mackay, et al., 1980). These equations are

$$F = K_a (U + 1)^2$$

$$F_B = (1 + K_b \mu^{0.5} \delta x)$$

where F is the fraction of sea surface subject to dispersions per second, U is the wind speed in m/sec and K_a is constant. F_B is the fraction of droplets of oil below a critical size which do not return to the slick, K_b is a constant, μ is the viscosity in centipoise, x is the slick thickness in meter, and δ is the surface tension in dynes/cm. The mass fraction that leaves the slick as dispersed droplets is $F_B \cdot F$ and this fraction applies to each cut of oil.

User Input Description

The initial input required to perform an oil-weathering calculation is the distillation characterization of the crude oil. The desired input is termed a true-boiling-point (TBP) distillation and consists of distillate cuts

of the oil with each cut characterized by its average boiling point and API gravity. For a description of the TBP distillation see Van Winkle (Van Winkle, 1967). An example of a TBP distillation is shown in Table 1 for a typical crude oil.

TBP distillations of crude oils are not always readily available. The more common inspection on crude oil is termed an ASTM (D-86) distillation. The ASTM distillation (Perry, R. H., and C. H. Chilton, 1973) differs in that the ASTM distillation is essentially a flask distillation and thus has no more than a few theoretical plates. The TBP distillation (ASTM D-2982, 1977) is performed in a column with greater than 15 theoretical plates and at high reflux ratios. The high degree of fractionation in this distillation yields an accurate component distribution for the crude oil (mixture). Another type of crude oil inspection available is the equilibrium flash vaporation (EFV) which differs from both the ASTM and TBP distillation in that the vapor is allowed to equilibrate with the liquid, and the quantity vaporized reported. In the distillations vapor is continuously removed from the still pot.

Both the ASTM distillation and EFV can be converted to a TBP distillation (API, 1964). However, at the present the ASTM D-86 distillation results can be used directly in the oil-weathering calculations because it is a reasonable approximation to the TBP-distillation result at the light end of the barrel. The differences between the two distillations at the heavy end of the barrel are noticeable but since the heavy ends of the barrel do not evaporate in oil weathering, this difference is of little consequence.

Currently the best sources of distillation data are "Evaluation of World's Important Crudes" (O&GJ, 1973) where a tremendous number of distillations and other characterizations are reported. The distillations reported are a mix of ASTMs and TBPs. Another excellent source of distillation data is "Analyses of 800 Crude Oils from United States Oilfields" (Coleman, et al., 1978). The distillations reported by Coleman are not TBP distillations but are essentially ASTM distillations and can be used in the oil-weathering

TABLE 1. Example of True Boiling Point (TBP) Distillation of Crude Oil (from Van Winkle, 1967).

<u>% Distilled</u>	<u>T, °F</u>	<u>API Gravity</u>
0	105	first drop
5	230	63.5
10	300	46.7
20	392	39.0
30	458	34.5
40	505	32.0
50	542	30.8
60	585	27.5
70	640	23.5
80	720	20.4
90	880	13.1
99	1090	----

calculations when the boiling points are all converted to one atmosphere total pressure. The reason parts of the ASTM or TBP distillations are conducted at sub-atmospheric pressure is that cracking begins to occur in the still pot at temperatures around 700°F. Thus, the data reported by Coleman are around atmospheric pressure up to 527°F, and for fractions boiling above this temperature the distillation is performed at 40-mm Hg. In order for the entire distillation to be used as input to the oil-weathering calculation, the cut data must be converted to one atmosphere total pressure. The procedure for converting sub-atmospheric boiling points to atmospheric boiling points is described in many places (Edmister and Okamoto, 1959; ASTM D-2892, 1977; API, 1964). An example of the sub-atmospheric boiling-point conversion is shown in Table 2 for Prudhoe Bay Crude Oil. The reported distillation pressure for Prudhoe Bay crude oil in Table 2 which is near atmospheric but not exactly at one atmosphere is not critical for the oil-weathering calculations.

An example of the use of the distillation data as input for the oil-weathering calculation is shown in Table 3. This table is an actual computer display of what the user sees beginning with the EXecute command. In this example the user is using data that is programmed into data statements and will not have to enter the distillation characterization data. The TBP cuts echoed to the user in Table 3 were obtained from the data of Coleman (Coleman, et al., 1978) in Table 2, and illustrate the transfer of these data to the oil-weathering calculation. Notice that cut 1 (fraction 1) in Table 2 has been deleted and the cuts renumbered. The reason cut 1 was deleted is because it is not the first cut with any measurable volume. Also note that the residuum cut is assigned a boiling point of $\geq 850^{\circ}\text{F}$. This assigned boiling point is fictitious and used to indicate that this cut is indeed a residuum.

A similar example of the use of distillation data from Coleman (Coleman, et al., 1978) is illustrated in Tables 4 and 5. Table 4 again is the published data and Table 5 illustrates how these data appear as input to the oil-weathering calculation.

TABLE 2. Distillation Data for Prudhoe Bay Crude Oil Showing Conversion of Sub-Atmosphere Boiling Points to Atmospheric Boiling Points (see text) (Coleman, et al, 1978).

Prudhoe Bay field
Sukorski, Triassic
8,890 - 9,008 feet

Alaska
North Slope

GENERAL CHARACTERISTICS

Gravity, specific, 0.893 Gravity, ° API, 27.0 Pour point, ° F, 15
Sulfur, percent, 0.82 Color, brownish black
Viscosity, Saybolt Universal at 77° F, 111 sec; 100° F, 84 sec Nitrogen, percent, 0.230

DISTILLATION, BUREAU OF MINES ROUTINE METHOD

Branch 1—Distillation at atmospheric pressure, 741 mm. Hg
First drop, 81 ° F

Fraction No.	Cut temp. ° F	Percent	Area percent	Sp. gr. 60/60° F	° API at 60° F	C. I.	Refractive index, n _D at 20° C	Viscosity, centipoise at 100° F	S. U. vis. 100° F	Cloud point, ° F
1	138									
2	140	2.1	2.1	0.693	72.7	-	1.38591	127.9		
3	142	2.6	4.7	.723	64.2	23	1.40312	139.0		
4	147	3.5	8.2	.732	56.7	27	1.41922	141.9		
5	149	3.6	11.8	.773	51.6	30	1.43082	147.0		
6	147	3.7	15.5	.790	47.6	31	1.43922	149.6		
7	148	3.5	19.0	.801	45.2	30	1.44626	152.1		
8	147	4.3	23.3	.818	41.5	33	1.45528	154.7		
9	148	4.8	28.1	.836	37.8	36	1.46565	157.0		
10	157	5.0	33.1	.851	34.8	38	1.47467	160.5		

Branch 2—Distillation continued at 40 mm. Hg

Fraction No.	Cut temp. ° F	Percent	Area percent	Sp. gr. 60/60° F	° API at 60° F	C. I.	Refractive index, n _D at 20° C	Viscosity, centipoise at 100° F	S. U. vis. 100° F	Cloud point, ° F
11	168	2.8	35.9	0.873	30.6	45	1.48218	161.5	40	10
12	167	6.5	42.4	.881	29.1	45	1.48650	168.6	45	30
13	168	6.8	49.2	.897	26.2	49	1.49477	169.4	58	50
14	167	6.0	55.2	.910	24.0	52			93	70
15	178	7.4	62.6	.919	22.5	53			176	90
Residue		34.3	98.9	.990	11.4					

Other notes: Conversion: Residue, 11.6 percent; dist. 4.7 percent.

Residue:

APPROXIMATE SUMMARY

Sulfur, percent, -
Nitrogen, percent, -

	Percent	Sp. gr.	° API	Viscosity
Light ends	4.7	0.710	67.9	
Total distillate and residue	19.0	0.762	54.2	
Kerosene distillate	4.3	.818	41.5	
Gas oil	18.4	.860	33.1	
Heaviest lubricating distillate	11.0	.887	28.0-23.9	40-100
Medium lubricating distillate	8.1	.911	23.9-22.0	100-200
Viscous lubricating distillate	1.8	.922	22.0-21.6	Above 200
Residue	34.3	.990	11.4	
Thermaxene loss	1.1			

Fraction No.	Cut Temperature, °F at 1 Atmosphere
10	580
11	638
12	685
13	738
14	790

Residuum

TABLE 3. Distillation Cut Data as Used in Oil-Weathering Calculation (data obtained from Table 2)

.EX
 LINK: Loading
 [LNKXCT CUTVP2 execution]
 ENTER THE NUMBER OF TBP CUTS TO BE CHARACTERIZED ON I2
 IF YOU HAVE NO INPUT DATA JUST ENTER 99
 A 99 ENTRY WILL USE A LIBRARY EXAMPLE
 99

CHOOSE A CRUDE ACCORDING TO:

- 1 = PRUDHOE BAY, ALASKA
- 2 = COOK INLET, ALASKA
- 3 = WILMINGTON, CALIFORNIA
- 4 = MURBAN, ABU DHABI
- 5 = LAKE CHICOT, LOUISIANA
- 6 = LIGHT DIESEL CUT

1

YOU CHOSE: PRUDHOE BAY, ALASKA

CUT	TB	API	VOL
1	167.0	72.7	2.1
2	212.0	64.2	2.6
3	257.0	56.7	3.5
4	302.0	51.6	3.6
5	347.0	47.6	3.7
6	392.0	45.2	3.5
7	437.0	41.5	4.3
8	482.0	37.8	4.8
9	527.0	34.8	5.0
10	580.0	30.6	2.8
11	638.0	29.1	6.5
12	685.0	26.2	6.8
13	738.0	24.0	6.0
14	790.0	22.5	7.4
15	850.0	11.4	36.3

DO YOU WANT TO CHANGE ANY?

Y

TABLE 4. Distillation Data for Wilmington Field Crude Oil (Coleman, et al, 1978)

Wilmington field
Beverly, Lower Miocene
and Puente, Miocene

California
Los Angeles County

GENERAL CHARACTERISTICS

Gravity, specific: 0.938 Gravity, ° API: 17.4 Pour point, ° F: below 1
Sulfur, percent: 1.57 Color: brownish black
Viscosity, Saybolt Universal at 100° F: 470 mcs. 130° F: 222 mcs. Nitrogen, percent: 0.597

DISTILLATION, BUREAU OF MINES ROUTINE METHOD

Stage 1—Distillation at atmospheric pressure: 738
First drop: 118 ° F

Fraction No.	Dist. temp. ° F	Percent	Sum percent	No. of drops	° API	C. I.	Refractive index at 20° C	Specific gravity at 15.6° C	N. U. vis. at 100° F	Cloud temp. ° F
1	133									
2	147									
3	212	2.3	2.3	0.707	68.6	-	1.39794	122.7		
4	257	2.4	4.7	.744	58.7	24	1.41215	125.7		
5	288	2.4	7.1	.767	51.0	27	1.42308	127.1		
6	347	2.5	9.6	.788	48.1	30	1.43480	128.8		
7	388	2.8	12.4	.810	43.2	34	1.44651	133.3		
8	427	3.6	16.0	.831	38.8	39	1.45771	148.6		
9	468	4.4	20.4	.848	35.4	41	1.46754	150.5		
10	527	5.3	25.7	.864	32.3	44	1.47736	152.9		

Stage 2—Distillation continued at 48 mm. Hg

11	388	4.7	30.4	0.894	26.8	55	1.48843	155.3	42	Below 5
12	427	6.3	36.7	.907	24.5	57	1.49898	163.8	56	do.
13	468	4.1	40.8	.920	22.3	60			87	do.
14	527	5.5	46.3	.932	20.3	62			172	do.
15	572									
Residue		53.3	99.6	1.008	8.9					

Carbon residue, Conradson: Residue, 8.6 percent; grade, 4.2 percent.

Residue:

Sulfur, percent:

Nitrogen, percent: 1.043

APPROXIMATE SUMMARY

	Percent	° API	Viscosity
Light naphtha	2.3	0.707	68.6
Total gasoline and naphtha	12.4	0.763	51.4
Kerosene distillate	-	-	-
Gas oil	18.8	.843	32.5
Heaviest lubricating distillate	8.3	.901-.922	25.5-22.0
Medium lubricating distillate	5.6	.922-.936	22.0-19.7
Viscous lubricating distillate	1.2	.936-.939	19.7-19.2
Residue	53.3	1.008	8.9
Distillate loss	.4		

1/ Distillation discontinued at 527° F.

TABLE 5. Distillation Data for Wilmington Field Crude Oil Illustrating Use in Oil-Weathering Calculations (See Table 4 for published data).

```
.EX CUTVP2.FOR
LINK: Loading
[LNKXCT CUTVP2 execution]
ENTER THE NUMBER OF TBP CUTS TO BE CHARACTERIZED ON I2
IF YOU HAVE NO INPUT DATA JUST ENTER 99
A 99 ENTRY WILL USE A LIBRARY EXAMPLE
99
CHOOSE A CRUDE ACCORDING TO:
1 = PRUDHOE BAY, ALASKA
2 = COOK INLET, ALASKA
3 = WILMINGTON, CALIFORNIA
4 = MURBAN, ABU DHABI
5 = LAKE CHICOT, LOUISIANA
6 = LIGHT DIESEL CUT
3
YOU CHOSE: WILMINGTON, CALIFORNIA

CUT      TB      API      VOL
1      212.0    68.6     2.3
2      257.0    58.7     2.4
3      302.0    53.0     2.4
4      347.0    48.1     2.5
5      392.0    43.2     2.8
6      437.0    38.8     3.6
7      482.0    35.4     4.4
8      527.0    32.3     5.3
9      580.0    26.8     4.7
10     638.0    24.5     6.3
11     685.0    22.3     4.1
12     738.0    20.3     5.5
13     850.0     8.9    53.3
DO YOU WANT TO CHANGE ANY?
N
ENTER THE TEMPERATURE IN DEG F FOR THE VAPOR PRESSURE CALCULATION
32.
THE TBP CUTS HAVE BEEN CHARACTERIZED
DO YOU WANT TO WEATHER THIS CRUDE?
N
DO IT AGAIN?
N
```

The distillation cut data can be entered by the user. An example of this entering procedure is illustrated using the TBP data for a gasoline cut (O&GJ, 1973, page 57) which is presented in Table 6. The user's entries to the oil-weathering calculation is shown in Table 7. Each time an input is required the user is prompted with an appropriate question. Since it is impossible to enter many numbers into the oil-weathering calculation without an error, the distillation cut data are always echoed to the user for review. In the event an input error is discovered or it is desired to change an entry, the user's response to DO YOU WANT TO CHANGE ANY? is yes. The error recovery is illustrated in Table 8 where the gasoline-cut data from Table 6 is entered. Note the input error for TB (boiling temperature) for cut 3 where 22.8 was entered instead of 228. The user is prompted for the error-recovery information and the final data is echoed to the user. In the event another error is to be corrected, a "YES" would be entered in response to the very last question in Table 8.

After entering the distillation-cut data, the user is asked for a temperature in degrees Fahrenheit. This temperature is used to calculate the vapor pressure of each cut as previously described (J. R. Payne, B. E. Kirstein, et al., 1983). At this point the calculation can be stopped and the crude oil characterization is all that will have been calculated. However, in order to "weather the crude", the user types "YES" in response to DO YOU WANT TO WEATHER THIS CRUDE?

The user input required for an oil-weathering calculation begins with a YES in response to the question DO YOU WANT TO WEATHER THIS CRUDE? The user is then prompted for the spill size in barrels and the number of hours for oil weathering to occur. The input responses presented in Table 9 follow the specification of a library crude (i.e., programmed into the code) such as those illustrated in Tables 3 or 5.

After specifying the spill size and number of hours for weathering to occur, and a library crude has been specified, the user is prompted for mousse-formation constants and an oil-water surface tension. By responding NO

TABLE 6. True Boiling Point Distillation Data for a Gasoline Cut (O&GJ, 1973, page 57).

<u>Cut</u>	<u>Cut temp, °F</u>	<u>Vol %</u>	<u>API Gravity</u>
1	137	1.5	71.6
2	196	2.1	59.7
3	228	2.0	55.0
4	256	2.0	53.8
5	283	2.0	49.6

TABLE 7. Illustration of User Input of Data for a Gasoline Cut (See Table 6 for "published" data).

```
.EX CUTVP2.FOR
LINK:  Loading
[LINKXCT CUTVP2 execution]
ENTER THE NUMBER OF TBP CUTS TO BE CHARACTERIZED ON 12
IF YOU HAVE NO INPUT DATA JUST ENTER 99
A 99 ENTRY WILL USE A LIBRARY EXAMPLE
5
ENTER THE NAME OF THE CRUDE
GASOLINE CUT
ENTER AN IDENTIFICATION NUMBER FOR THIS CRUDE ON 15
11111
ENTER A SAMPLE NUMBER ON 15
22222
ENTER THE BULK API GRAVITY
55.

YOU MUST ENTER THE TRUE BOILING POINT CUT DATA STARTING
WITH THE MOST VOLATILE CUT AND GOING TO THE BOTTOM OF THE BARREL

ENTER THE BOILING POINT AT 1 ATM IN DEG F FOR CUT  1
137.
ENTER API GRAVITY FOR CUT  1
71.6
ENTER VOLUME PER CENT FOR CUT  1
1.5
ENTER THE BOILING POINT AT 1 ATM IN DEG F FOR CUT  2
196.
ENTER API GRAVITY FOR CUT  2
59.7
ENTER VOLUME PER CENT FOR CUT  2
2.1
ENTER THE BOILING POINT AT 1 ATM IN DEG F FOR CUT  3
228.
ENTER API GRAVITY FOR CUT  3
55.
ENTER VOLUME PER CENT FOR CUT  3
2.
ENTER THE BOILING POINT AT 1 ATM IN DEG F FOR CUT  4
256.
ENTER API GRAVITY FOR CUT  4
53.8
ENTER VOLUME PER CENT FOR CUT  4
2.
ENTER THE BOILING POINT AT 1 ATM IN DEG F FOR CUT  5
283.
ENTER API GRAVITY FOR CUT  5
49.6
ENTER VOLUME PER CENT FOR CUT  5
2.

CUT      TB      API      VOL
1      137.0    71.6    1.5
2      196.0    59.7    2.1
3      228.0    55.0    2.0
4      256.0    53.8    2.0
5      283.0    49.6    2.0

DO YOU WANT TO CHANGE ANY?
N
ENTER THE TEMPERATURE IN DEG F FOR THE VAPOR PRESSURE CALCULATION
32.
THE TBP CUTS HAVE BEEN CHARACTERIZED
DO YOU WANT TO WEATHER THIS CRUDE?
N
DO IT AGAIN?
N
```

TABLE 8. Illustration of Input-Error Recovery (Note error for cut 3 boiling temperature).

ENTER THE BOILING POINT AT 1 ATM IN DEG F FOR CUT 5
283.

ENTER API GRAVITY FOR CUT 5
49.6

ENTER VOLUME PER CENT FOR CUT 5
2.

CUT	TB	API	VOL
1	137.0	71.6	1.5
2	196.0	59.7	2.1
3	22.8	55.0	2.0
4	256.0	53.8	2.0
5	283.0	49.6	2.0

DO YOU WANT TO CHANGE ANY?
Y

ENTER THE CUT NUMBER TO BE CHANGED ON I2
3

ENTER 1 TO CHANGE TB, 2 FOR API, 3 FOR VOL%
1

ENTER THE CHANGED DATA
228.

CUT	TB	API	VOL
1	137.0	71.6	1.5
2	196.0	59.7	2.1
3	228.0	55.0	2.0
4	256.0	53.8	2.0
5	283.0	49.6	2.0

DO YOU WANT TO CHANGE ANY?
N

TABLE 9. Illustration of User Input for Oil-Weathering Calculation with a Library-Specified Crude

ENTER THE TEMPERATURE IN DEG F FOR THE VAPOR PRESSURE CALCULATION
32.
THE TBP CUTS HAVE BEEN CHARACTERIZED
DO YOU WANT TO WEATHER THIS CRUDE?
YES
ENTER THE SPILL SIZE IN BARRELS
10000.
ENTER NUMBER OF HOURS FOR OIL WEATHERING TO OCCUR
240.
DO YOU WANT TO ENTER MOUSSE FORMATION CONSTANTS?
NO
DO YOU WANT TO ENTER AN OIL-WATER SURFACE TENSION (DYNES/CM)?
NO
ENTER THE MASS-TRANSFER COEFFICIENT CODE: 1, 2, OR 3 WHERE:
1=USER SPECIFIED OVER-ALL MASS-TRANSFER COEFFICIENT
2=CORRELATION MASS-TRANSFER COEFFICIENT BY MACKAY & MATSUGU
3=INDIVIDUAL-PHASE MASS-TRANSFER COEFFICIENTS
2
ENTER THE WIND SPEED IN KNOTS
10.
DO YOU WANT THE SLICK TO SPREAD?
YES
DO YOU WANT TO ENTER VISCOSITY CONSTANTS?
NO
DO YOU WANT THE WEATHERING TO OCCUR WITH DISPERSION?
YES
DO YOU WANT TO ENTER THE DISPERSION CONSTANTS?
NO
NUMBER OF LINES WRITTEN TO CUTVP2.PLT = 71
DO IT AGAIN?
YES

to these prompts the calculation procedure will use library constants for the specified crude. The user is then prompted for mass-transfer coefficient information. The mass-transfer coefficient is for the evaporation weathering process, not dissolution. There are three possible mass-transfer coefficient input specifications, and the one recommended is 2 as illustrated in Table 9. The next entry is wind speed which is in knots and should be less than 40 knots because oil-weathering processes at and above this wind speed are not quantified. Also, the lowest wind speed used in the calculation is 2 knots and any value entered lower than this is reset to 2.

After specifying the wind speed the user specifies if the slick is to spread (YES) or not (NO). Viscosity constants can then be entered if desired for a library crude, and finally the dispersion process (oil into water) can be specified as occurring (YES) or not (NO) along with the dispersion constants. At this point all input information has been supplied and the calculation proceeds.

The preceding input description illustrates a straight-forward use of the information programmed in the oil-weathering code. Illustrations of how the programmed information can be changed is presented in the following discussion. Altering the programmed information allows other crudes or petroleum cuts to be entered into the calculation, or actual spills and experiments can be analyzed to find the best physical properties or rate constants which predict observed data.

The first input information that can be changed by the user is the mousse-formation constants as illustrated in Table 10. The mousse constants appear in an equation which quantifies the rate of water incorporation into the oil with respect to time. This rate equation is (Mackay, et al., 1980)

$$(1 - K_2 W) \exp \left[\frac{-2.5W}{1 - K_1 W} \right] \equiv \exp \left[-K_3 t \right]$$

TABLE 10. Illustration of User-Specified Mousse-Formation Constants

DO YOU WANT TO ENTER MOUSSE FORMATION CONSTANTS?
YES
1. ENTER THE MAXIMUM WEIGHT FRACTION WATER IN OIL
.60
2. ENTER THE MOUSSE-VISCOSITY CONSTANT, TRY 0.65
.65
3. ENTER THE WATER INCORPORATION RATE CONSTANT, TRY 0.001
.001
DO YOU WANT TO ENTER AN OIL-WATER SURFACE TENSION (DYNES/CM)?
YES
.001
30.

where W is the weight fraction water in mousse. K_1 is a constant in the viscosity equation, K_2 is a coalescing-tendency constant and K_3 is a lumped water incorporation rate constant. K_1 appears in a stand-alone equation for the apparent viscosity of the emulsion as (Mooney, 1951)

$$\mu = \mu_0 \exp \left[\frac{-2.5W}{1-K_1W} \right]$$

where μ_0 is the parent oil viscosity. K_1 is usually around 0.62 to 0.65 and apparently does not change much with respect to different types of oils.

The constant K_2 must satisfy the relation $K_2W < 1$ in order for the water incorporation rate to be > 0 . Thus, K_2 is the inverse of the maximum weight fraction water in mousse. K_3 is the water incorporation rate constant and is a function of wind speed in knots. Currently the oil-weathering code calculates K_3 from

$$K_3 = 0.001 (\text{WIND SPEED})^2$$

and the constant actually entered by the user is the 0.001 constant above.

Thus, referring to Table 10, the first mousse formation constant entered is the maximum weight fraction water in the mousse. The reciprocal of this number is used for K_1 . The second constant entered is the viscosity constant in Mooney's equation and this number should be 0.62 to 0.65 unless experimental evidence suggests otherwise. The third constant entered is the multiplier of the $(\text{wind speed})^2$ which then yields K_3 . This number is around 0.001 as indicated. Note that the prompting for input also prints suggested values for each constant.

The next input parameter that the user can change is the mass-transfer coefficient for evaporation. The input illustration in Table 9 uses the correlation mass transfer coefficient as developed by Mackay and Matsugu (Mackay and Matsugu, 1973). Table 11 illustrates the three possible input

TABLE 11. Illustrations of Three Input Options for the Mass Transfer Coefficient for Evaporation

ENTER THE MASS-TRANSFER COEFFICIENT CODE: 1, 2, OR 3 WHERE:
1=USER SPECIFIED OVER-ALL MASS-TRANSFER COEFFICIENT
2=CORRELATION MASS-TRANSFER COEFFICIENT BY MACKAY & MATSUGU
3=INDIVIDUAL-PHASE MASS-TRANSFER COEFFICIENTS

1

ENTER THE WIND SPEED IN KNOTS

10.

DO YOU WANT THE SLICK TO SPREAD?

YES

ENTER THE OVER-ALL MASS-TRANSFER COEFFICIENT, CM/HR, TRY 10

10.

ENTER THE MASS-TRANSFER COEFFICIENT CODE: 1, 2, OR 3 WHERE:
1=USER SPECIFIED OVER-ALL MASS-TRANSFER COEFFICIENT
2=CORRELATION MASS-TRANSFER COEFFICIENT BY MACKAY & MATSUGU
3=INDIVIDUAL-PHASE MASS-TRANSFER COEFFICIENTS

2

ENTER THE WIND SPEED IN KNOTS

10.

DO YOU WANT THE SLICK TO SPREAD?

YES

DO YOU WANT TO ENTER VISCOSITY CONSTANTS?

NO

DO YOU WANT THE WEATHERING TO OCCUR WITH DISPERSION?

NO

ENTER THE MASS-TRANSFER COEFFICIENT CODE: 1, 2, OR 3 WHERE:
1=USER SPECIFIED OVER-ALL MASS-TRANSFER COEFFICIENT
2=CORRELATION MASS-TRANSFER COEFFICIENT BY MACKAY & MATSUGU
3=INDIVIDUAL-PHASE MASS-TRANSFER COEFFICIENTS

3

ENTER THE WIND SPEED IN KNOTS

10.

DO YOU WANT THE SLICK TO SPREAD?

YES

ENTER THE OIL-PHASE MASS-TRANSFER COEFFICIENT IN CM/HR, TRY 10

10.

ENTER THE AIR-PHASE MASS-TRANSFER COEFFICIENT IN CM/HR, TRY 1000

1000.

ENTER THE MOLECULAR WEIGHT OF THE COMPOUND FOR K-AIR ABOVE, TRY 200

200.

options for the evaporation mass transfer coefficient. The first input option shown in Table 11 allows the user to input the mass transfer coefficient directly in contrast to the second input option where the coefficient is calculated as a function of wind speed and slick diameter. In the third input option the user can enter individual-phase mass transfer coefficients. In this last option the entered coefficient is scaled according to the square root of the molecular of each cut to yield a coefficient specific to each cut (Liss and Slater, 1974). The coefficient in this last option is also scaled according to wind speed according to Garratt's drag coefficient (Garratt, 1977).

After specifying the mass-transfer coefficient options the user can specify if the slick is to spread or not. This option is illustrated in Table 12 by entering YES or NO to the prompt. In this particular illustration the user has specified that the slick does not spread. This option is useful for investigating evaporation from spills on solid surfaces such as ice or land. When the no-spreading option is selected the user is prompted for a starting thickness. In the illustration in Table 12 the entered thickness is 3 cm.

The final physical property optional input that can be specified by the user is the viscosity. The viscosity-prediction for the bulk weathered oil is important when dispersion of oil into water occurs since viscosity appears in the rate equation for dispersion. The current method of viscosity prediction is based on the viscosity of the initial crude at 25°C, a temperature-scaling constant, and a fraction-oil-weathered constant. The viscosity predicted is for oil only, and must not be interpreted as that viscosity when on water-in-oil emulsion is present.

The viscosity at 25°C is scaled to other temperatures by the Andrade equation (Gold and Olge, 1969) which is

$$\ln \frac{\mu_1}{\mu_0} = B \left(\frac{1}{T_1} - \frac{1}{T_0} \right)$$

TABLE 12. Illustration of the 'No-Spreading' Option and Starting Thickness Specification

ENTER THE MASS-TRANSFER COEFFICIENT CODE: 1, 2, OR 3 WHERE:
1=USER SPECIFIED OVER-ALL MASS-TRANSFER COEFFICIENT
2=CORRELATION MASS-TRANSFER COEFFICIENT BY MACKAY & MATSUGU
3=INDIVIDUAL-PHASE MASS-TRANSFER COEFFICIENTS

2

ENTER THE WIND SPEED IN KNOTS

10.

DO YOU WANT THE SLICK TO SPREAD?

NO

SINCE THE SLICK DOES NOT SPREAD, ENTER A STARTING THICKNESS IN CM.

3.

and the temperature-scaling constant is B. The viscosity of the weathered oil is calculated according to $\exp(K_4 F)$ where F is the fraction weathered (Tebeau, Mackay, et al., 1982) i.e., fresh crude oil has $F = 0$. As weathering proceeds, the parent oil viscosity increase exponentially with respect to F.

The user can enter the three viscosity constants by answering YES to the prompt illustrated in Table 13. In this illustration suggested input viscosity constants are printed along with the prompt.

The constants which appear in the dispersion process can also be specified by the user. The dispersion of oil into the water column is described by two equations (Mackay, et al., 1980):

$$F = K_a (U + 1)^2$$

and

$$F_B = (1 + K_b \mu^{0.5} \delta \chi)^{-1}$$

where F is the fraction of sea surface subject to dispersion per second, U is the wind speed in m/sec and K_a is a constant, typically 0.1 hr^{-1} . F_B is the fraction of droplets of oil below a critical size which do not return to the slick, K_b is a constant, around 50, μ is the viscosity in centipoise, χ is the slick thickness in meter, and δ is the surface tension in dynes/cm. The mass fraction that leaves the slick as dispersed droplets is $F_B \cdot F$ and this fraction applies to each cut of oil. Table 14 illustrates the user input of the constants K_a and K_b .

TABLE 13. Illustration of Viscosity-Constant Input Options

ENTER THE MASS-TRANSFER COEFFICIENT CODE: 1, 2, OR 3 WHERE:
1=USER SPECIFIED OVER-ALL MASS-TRANSFER COEFFICIENT
2=CORRELATION MASS-TRANSFER COEFFICIENT BY MACKAY & MATSUGU
3=INDIVIDUAL-PHASE MASS-TRANSFER COEFFICIENTS

2

ENTER THE WIND SPEED IN KNOTS

10.

DO YOU WANT THE SLICK TO SPREAD?

YES

DO YOU WANT TO ENTER VISCOSITY CONSTANTS?

YES

1. ENTER THE BULK CRUDE VISCOSITY AT 25 DEG C, CENTIPOISE, TRY 35.

40.

2. ENTER THE VISCOSITY TEMPERATURE SCALING CONSTANT (ANDRADE), TRY 9000.

9000.

3. ENTER THE VISCOSITY-FRACTION-OIL-WEATHERED CONSTANT, TRY 10.5

10.5

DO YOU WANT THE WEATHERING TO OCCUR WITH DISPERSION?

YES

DO YOU WANT TO ENTER THE DISPERSION CONSTANTS?

TABLE 14. Illustration of Dispersion Constants Input

DO YOU WANT TO ENTER VISCOSITY CONSTANTS?
NO
DO YOU WANT THE WEATHERING TO OCCUR WITH DISPERSION?
YES
DO YOU WANT TO ENTER THE DISPERSION CONSTANTS?
YES
ENTER THE WIND SPEED CONSTANT, TRY 0.1
.2
ENTER THE CRITICAL DROPLET SIZE CONSTANT, TRY 50
70.
NUMBER OF LINES WRITTEN TO CUTVP2.PLT = 71
DO IT AGAIN?
NO

Output Description

The output generated by the oil-weathering code is written to three disk files: CUTVP2.OUT, CUTVP2.TYP and CUTVP2.PLT. These files contain the calculated results in various forms. The CUTVP2.OUT file is 130 columns wide and intended to be printed on an appropriate high speed printer. The CUTVP2.TYP file is 80 columns wide and intended for printing on portable terminals. The CUTVP2.TYP file is an abbreviated version of CUTVP2.OUT. The CUTVP2.PLT is a numbers-only raw data file and intended to be read by a plotting routine or other data processing routines.

An example of the CUTVP2.OUT file (130 column) is presented in Table 15a where the calculated results for an oil-weathering calculation at 32°F for Prudhoe Bay crude is presented. The first page of this output is crude characterization information calculated according to previous descriptions (J. R. Payne, B. E. Kirstein, et al., 1983), and page two is the result of the vapor pressure calculation for each cut of the crude. Page three presents the input parameters and constants, and the beginning of the results of the oil-weathering calculation. The information presented for various times is self explanatory but some care must be taken in order to identify the cuts at each time step. There are cases where the first cuts can be so volatile that they evaporate away immediately (< 1 hour). In this case the cut(s) will be deleted from the calculation and the remaining cuts renumbered.

Table 15b illustrates the output where a cut has been deleted because it evaporates too fast to be considered in the calculation. The cut renumbering occurs immediately before the time integration begins and will always be noted on the output before the time = 0 print. The user must know that a cut has been deleted or interpretation of the results will be shifted by one (or more) cut. The deletion of a cut is also noted before the final mass fractions are printed by telling the user the number of the first cut printed. This is illustrated in Table 15b (final page) where it is noted that the cut numbering begins with 2.

Examples of the 80-column output is presented in Tables 16a and 16b for weathering Prudhoe Bay crude oil at 32 and 60°F. The output in Tables 16a and 16b was generated at the same time as the output in Tables 15a and 15b. Note that the output in Tables 16a and 16b is essentially a condensed, self-contained, version of the calculated results.

Most of the output information is self explanatory as illustrated in Tables 15a and 15b. These two tables are examples of calculated results at two different temperatures for Prudhoe Bay crude oil. Currently some of the information printed is not used. Refer to Table 15a (page 3) which begins at the top of the page with: OVER-ALL MASS-TRANSFER COEFFICIENTS BY INPUT CODE 2. On this page of the output the two lines beginning with KINEMATIC VISCOSITY present information that is not used. This viscosity information was used early in program development and found not to be applicable for predicting the viscosity of weathered crude. The viscosity of weathered crude is now calculated according to the fraction weathered, as previously described in the input description and noted here by the parameters printed immediately below the kinematic viscosity information.

Accessing the Computer

Currently the oil-weathering code resides on a DEC System-10® at Science Applications, Inc. in La Jolla, California. Table 17 presents a description of the commands to execute the code that pertain to this specific installation. Accessing the DEC-10 from anywhere in the United States can be accomplished through TELENET. The TELENET access procedure is described in Appendix A. Once access to DEC-10 has been obtained the system will then ask for a project-programmer number (PPN) which in the example in Table 17 is 4601,4601. The password must then be typed in. The typed password will not show up at the terminal. The current password must be obtained by calling SAI. Once logged in the code can be executed by typing EX CUTVP2.FOR. The code will then execute and the user will be prompted for input. After an oil-weathering calculation is finished the FORTRAN code will ask the user: DO

IT AGAIN? By replying NO a normal exit and file closing will be accomplished. The system will then print CPU time and elapsed time. In order to obtain the calculated results the user must instruct the system to print or type the results from the appropriate disk files. To obtain 130-column detailed output the user types PRINT CUTVP2.OUT. The output will be printed at SAI's La Jolla facility and it must then be picked up by the user. By typing TYPE CUTVP2.TYP the user will obtain the 80-column abbreviated output file at his terminal. To log off the computer type BYE.

There will be times when the connection to the DEC-10 will be lost during execution or while the user is doing something else. When this happens the job becomes detached but can be picked up again by the user. When computer access is obtained the user must login using the same PPN and PASSWORD. The system will then type to the user the detached job number, program name, and status. The user will then be asked if he wants to attach. The attach procedure is illustrated in Table 18.

A listing of the open-ocean oil-weathering code is presented in Appendix 2.

TABLE 15a: Illustration of Output from Oil-Weathering Calculations; Prudhoe Bay
Crude Oil Characterization.

SUMMARY OF TBP CUTS CHARACTERIZATION FOR: PRUDHOE BAY, ALASKA

CODE VERSION IS OUTVPS OF FEBRUARY 83
ITEM % SAMPLE T1011

ITEM	TS	API	SPCR	VOL	MW	TO	PO	VO	A	B	T10	V10	NO	MS
1	1.67E+02	7.37E+01	6.61E-01	2.15E+00	9.92E+01	9.31E+02	8.63E+01	8.68E+02	8.23E+00	1.08E-01	4.60E+02	4.14E-01	3	1
2	2.12E+02	6.42E+01	7.11E-01	2.40E+00	1.03E+02	9.68E+02	8.48E+01	8.87E+02	8.31E+00	2.11E-01	4.96E+02	4.92E-01	3	1
3	2.67E+02	5.47E+01	7.09E-01	3.53E+00	1.14E+02	1.04E+03	8.81E+01	9.86E+02	8.39E+00	2.34E-01	5.81E+02	6.01E-01	3	1
4	3.02E+02	5.16E+01	7.68E-01	5.61E+00	1.28E+02	1.09E+03	8.86E+01	9.41E+02	8.49E+00	2.34E-01	5.81E+02	6.01E-01	3	1
5	3.47E+02	4.74E+01	7.77E-01	8.74E+00	1.43E+02	1.14E+03	8.82E+01	9.01E+02	8.77E+00	2.38E-01	6.04E+02	6.43E-01	3	1
6	3.92E+02	4.52E+01	7.87E-01	8.84E+00	1.61E+02	1.18E+03	8.82E+01	7.40E+02	8.91E+00	2.38E-01	6.43E+02	1.20E+00	3	1
7	4.37E+02	4.18E+01	8.04E-01	4.08E+00	1.78E+02	1.23E+03	8.82E+01	7.40E+02	8.91E+00	2.38E-01	6.43E+02	1.20E+00	3	1
8	4.82E+02	3.78E+01	8.22E-01	4.08E+00	1.96E+02	1.27E+03	8.82E+01	7.40E+02	8.91E+00	2.38E-01	6.43E+02	1.20E+00	3	1
9	5.27E+02	3.48E+01	8.38E-01	2.83E+00	2.12E+02	1.32E+03	8.82E+01	7.40E+02	8.91E+00	2.38E-01	6.43E+02	1.20E+00	3	1
10	5.88E+02	3.06E+01	8.56E-01	2.83E+00	2.36E+02	1.37E+03	8.82E+01	7.40E+02	8.91E+00	2.38E-01	6.43E+02	1.20E+00	3	1
11	6.08E+02	2.91E+01	8.62E-01	6.08E+00	2.73E+02	1.42E+03	8.82E+01	7.40E+02	8.91E+00	2.38E-01	6.43E+02	1.20E+00	3	1
12	6.88E+02	2.62E+01	8.82E-01	6.08E+00	2.99E+02	1.46E+03	8.82E+01	7.40E+02	8.91E+00	2.38E-01	6.43E+02	1.20E+00	3	1
13	7.88E+02	2.40E+01	8.94E-01	6.08E+00	3.85E+02	1.51E+03	8.82E+01	7.40E+02	8.91E+00	2.38E-01	6.43E+02	1.20E+00	3	1
14	7.98E+02	2.38E+01	9.03E-01	7.48E+00	3.74E+02	1.55E+03	8.82E+01	7.40E+02	8.91E+00	2.38E-01	6.43E+02	1.20E+00	3	1
15	8.88E+02	1.14E+01	9.70E-01	5.67E+01	6.08E+02	1.60E+03	8.82E+01	7.40E+02	8.91E+00	2.38E-01	6.43E+02	1.20E+00	3	1

BULK API GRAVITY = 27.0

TS = NORMAL BOILING TEMPERATURE, DEG F
API = API GRAVITY
VOL = VOLUME PER CENT OF TOTAL CRUDE
MW = MOLECULAR WEIGHT
TC = CRITICAL TEMPERATURE, DEG RANKINE
PO = CRITICAL PRESSURE, ATMOSPHERES
VO = CRITICAL VOLUME, CC/MOLE

A AND B ARE PARAMETERS IN THE VAPOR PRESSURE EQUATION
T10 IS THE TEMPERATURE IN DEG R WHERE THE VAPOR PRESSURE IS 10 MM HG
V10 IS THE KINEMATIC VISCOSITY IN CENTISTOKES AT 132 DEG F
NO = ERROR CODE, SHOULD BE LESS THAN 25
MS = ERROR CODE, SHOULD BE EQUAL TO 1
ICNONE, THE ERROR CODES FOR COMPONENT NUMBER IS IF IT IS A RESIDUUM

TABLE 15a (Continued): Output from Oil-Weathering Calculations;
 Prudhoe Bay Crude Oil Vapor Pressures at
 32° F.

CRUDE OIL CHARACTERIZATION AND PSEUDOCOMPONENT EVAPORATION MODEL
 IDENTIFICATION: PRUDHOE BAY, ALASKA

ITEM 9. SAMPLE 71011
 VAPOR PRESSURE IN ATMOSPHERES AT 3.200E+01 DEG F

VP	
1	3.784E-02
2	1.086E-02
3	2.584E-03
4	5.643E-04
5	1.123E-04
6	1.955E-05
7	3.176E-06
8	4.635E-07
9	6.603E-08
10	5.303E-09
11	2.092E-10
12	1.422E-11
13	4.512E-13
14	8.824E-15

MEAN MOLECULAR WEIGHT OF THE CRUDE = 2.739E+02

TABLE 15a (Continued) : Output from Oil-Weathering Calculations; Prudhoe Bay Crude Oil, Mass-Transfer Coefficients, Problem Specifications, and Beginning of Calculated Results at 32°F.

OVER-ALL MASS-TRANSFER COEFFICIENTS BY INPUT CODE 2

OVER-ALL MASS-TRANSFER COEFFICIENT FOR CUMENE = 1.926×10^{-4} M/HR

CUT	MHR	CM-HOLES/ (HR) (ATH) (M#2)
1	2.662E+01	9.312E+02
2	2.681E+01	9.074E+02
3	2.607E+01	8.964E+02
4	1.904E+01	8.064E+02
5	1.965E+01	8.776E+02
6	1.946E+01	8.693E+02
7	1.932E+01	8.600E+02
8	1.919E+01	8.574E+02
9	1.910E+01	8.551E+02
10	1.890E+01	8.479E+02
11	1.883E+01	8.410E+02
12	1.876E+01	8.302E+02
13	1.060E+01	8.342E+02
14	1.059E+01	8.306E+02

FOR THIS SPILL OF 1.080E+03 BARRELS, THE MASS IS 1.412E+02 METRIC TONNES

VOLUME FROM SUMMING THE CUTS = 1.6E+02 M**3, ON 1.000E+03 BARRELS

WIND SPEED = 1.000E+01 KNOTS, OR 1.853E+04 M/HR

INITIAL SLICK DIAMETER = 1.006E+02 M, OR AREA = 7.950E+03 M**2

KINEMATIC VISCOSITY OF THE BULK CRUDE FROM THE CUTS = $4.9E+00$ CENTISTOKES AT 122 DEG F

KINEMATIC VISCOSITY OF THE BULK CRUDE FROM THE CUTS = 8.9E+00 AT T = 32.0 DEG F, SCALE FACTOR = 1.8E+00

VISCOSITY ACCORDING TO MASS EVAPORATED, VIS25C = 3.50E+01, ANDRADE = 9.00E+03, FRACT WEATHERED = 1.00E+01, VSLEAD = 3.30E+02 CP

MOUSSE CONSTANTS: MOONEY* 6.20E-01, MAX IIS0= 0.70, WIND**2= 1.00E-03

THE FRACTIONAL SLICK AREA SUBJECT TO DISPERSION IS 4.1E+00 PER HOUR

THE DISPERSION PARAMETERS USED: $K_A = 1.00E-01$, $K_B = 5.00E+01$, SURFACE TENSION = $3.00E+01$ DYNES/CM

COUNT THE CUTS IN THE FOLLOWING OUTPUT FROM LEFT TO RIGHT

THE INITIAL GRAM HOLES IN THE SLICK ARE:

	2.563E+04	2.911E+04	3.638E+04	3.423E+04
	3.211E+04	2.566E+04	2.846E+04	9.420E+04

THE INITIAL HASSES (GRAMS) IN THE SLICK AREA;

2.200E+06	2.956E+06	4.133E+06	4.375E+06
9.594E+06	0.505E+06	1.069E+07	5.652E+07

THE TOTAL MASS FROM THESE CUTS IS 1.395 ± 0.01 CHANS

STEP SIZE OF 9.191E-02 IS BASED ON CUT

TIME = 0.0E+00 HOURS, MASS FRACTION OF EACH CUT REMAINING:

[illegible]

MASS REMAINING = 1.395E+00, MASS DISPERSED = 0.000E+00, MASS EVAPORATED = 0.000E+00, SUM = 1.395E+00

WEIGHT FRACTION WATER IN OIL, = 6.9E-06, VISCOSITY = 5.5E+02 CENTISTOYES, DISPERSIONAL POWER = 2.4E+01, THICKNESS = 2.0E+00 CM, MOLE WT=279.9

MASS/AREA = 1.0E+04 GHS/N*H, SPCR = 0.0E+01, TOTAL VOLUME = 1.0E+03 DM., DISPERSION = 7.7E+00 GHS/N*H/DM, EVAP RATE = 0.0E+00
 0.0E+02 CENTISTOKES, DISPERSION TPEH = 4.4E+04 WEIGHT FRACTION/HR

[illegible]

TIME = 1.0E+00 HOURS, MASS FRACTION OF EACH CUT REMAINING:

[illegible]

TABLE 15a (Continued): Output from Oil-Weathering Calculations; Prudhoe Bay Crude Oil, Time versus Calculated Results at 32°F.

MASS REMAINING = 1.362E+08, MASS DISPENSED = 6.123E+04, MASS EVAPORATED = 3.299E+06, SUM = 1.395E+08 FRACTION (BASED ON MASS) REMAINING IN THE SLICK = 9.0E-01, AREA = 3.1E+04 M**2, THICKNESS = 5.0E-01 CM, MOLE WT=286.7 WEIGHT FRACTION WATER IN OIL = 2.9E-02, VISCOSITY = 7.6E+02 CENTISTOKES, DISPERSION TERM = 1.5E-03 WEIGHT FRACTION/HR MASS/AREA = 4.4E+03 GMS/M**2, SPGR = 8.8E-01, TOTAL VOLUME = 9.7E+02 BBL, DISPERSION = 6.6E+00 GMS/M**2/HR, EVAP RATE = 9.9E+01 GMS/M**2/HR									
TIME = 2.0E+00 HOURS, MASS FRACTION OF EACH CUT REMAINING: 1.0E-02 3.1E-01 7.6E-01 9.4E-01 9.9E-01 1.0E+00 1.0E+00 1.0E+00 1.0E+00 1.0E+00 4 1.0E+00									
MASS REMAINING = 1.337E+08, MASS DISPENSED = 2.678E+03, MASS EVAPORATED = 5.585E+06, SUM = 1.395E+08 FRACTION (BASED ON MASS) REMAINING IN THE SLICK = 9.0E-01, AREA = 4.3E+04 M**2, THICKNESS = 3.5E-01 CM, MOLE WT=293.6 WEIGHT FRACTION WATER IN OIL = 3.0E-02, VISCOSITY = 9.7E+02 CENTISTOKES, DISPERSION TERM = 1.9E-03 WEIGHT FRACTION/HR MASS/AREA = 3.1E+03 GMS/M**2, SPGR = 8.9E-01, TOTAL VOLUME = 9.5E+02 BBL, DISPERSION = 5.9E+00 GMS/M**2/HR, EVAP RATE = 4.2E+01 GMS/M**2/HR									
STEP SIZE OF 5.591E-02 IS BASED ON CUT 2									
TIME = 3.0E+00 HOURS, MASS FRACTION OF EACH CUT REMAINING: 1.1E-04 1.2E-01 6.0E-01 8.9E-01 9.7E-01 9.9E-01 1.0E+00 1.0E+00 1.0E+00 1.0E+00 5 1.0E+00									
MASS REMAINING = 1.319E+08, MASS DISPENSED = 5.228E+03, MASS EVAPORATED = 7.094E+06, SUM = 1.395E+08 FRACTION (BASED ON MASS) REMAINING IN THE SLICK = 9.0E-01, AREA = 5.2E+04 M**2, THICKNESS = 2.9E-01 CM, MOLE WT=301.4 WEIGHT FRACTION WATER IN OIL = 7.4E-02, VISCOSITY = 1.2E+03 CENTISTOKES, DISPERSION TERM = 2.1E-03 WEIGHT FRACTION/HR MASS/AREA = 2.9E+03 GMS/M**2, SPGR = 8.9E-01, TOTAL VOLUME = 9.3E+02 BBL, DISPERSION = 5.0E+00 GMS/M**2/HR, EVAP RATE = 2.5E+01 GMS/M**2/HR									
STEP SIZE OF 4.679E-02 IS BASED ON CUT 2									
TIME = 4.1E+00 HOURS, MASS FRACTION OF EACH CUT REMAINING: 7.3E-06 3.5E-02 4.5E-01 0.4E-01 9.6E-01 9.9E-01 9.9E-01 9.9E-01 9.9E-01 9.9E-01 6 9.9E-01									
MASS REMAINING = 1.303E+08, MASS DISPENSED = 8.003E+03, MASS EVAPORATED = 0.237E+06, SUM = 1.395E+08 FRACTION (BASED ON MASS) REMAINING IN THE SLICK = 9.4E-01, AREA = 6.0E+04 M**2, THICKNESS = 2.5E-01 CM, MOLE WT=309.0 WEIGHT FRACTION WATER IN OIL = 9.7E-02, VISCOSITY = 1.4E+03 CENTISTOKES, DISPERSION TERM = 2.2E-03 WEIGHT FRACTION/HR MASS/AREA = 2.2E+03 GMS/M**2, SPGR = 8.9E-01, TOTAL VOLUME = 9.2E+02 BBL, DISPERSION = 4.9E+00 GMS/M**2/HR, EVAP RATE = 1.0E+01 GMS/M**2/HR									
STEP SIZE OF 4.020E-02 IS BASED ON CUT 2									
TIME = 5.1E+00 HOURS, MASS FRACTION OF EACH CUT REMAINING: 6.0E-08 9.4E-03 3.3E-01 7.0E-01 9.3E-01 9.0E-01 9.9E-01 9.9E-01 9.9E-01 9.9E-01 7 9.9E-01									
MASS REMAINING = 1.293E+08, MASS DISPENSED = 1.101E+06, MASS EVAPORATED = 9.124E+06, SUM = 1.395E+08 FRACTION (BASED ON MASS) REMAINING IN THE SLICK = 9.5E-01, AREA = 6.6E+04 M**2, THICKNESS = 2.2E-01 CM, MOLE WT=309.1 WEIGHT FRACTION WATER IN OIL = 1.2E-01, VISCOSITY = 1.7E+03 CENTISTOKES, DISPERSION TERM = 2.3E-03 WEIGHT FRACTION/HR MASS/AREA = 2.0E+03 GMS/M**2, SPGR = 8.9E-01, TOTAL VOLUME = 9.1E+02 BBL, DISPERSION = 4.3E+00 GMS/M**2/HR, EVAP RATE = 1.2E+01 GMS/M**2/HR									
STEP SIZE OF 3.578E-02 IS BASED ON CUT 2									
TIME = 6.1E+00 HOURS, MASS FRACTION OF EACH CUT REMAINING: 3.0E-10 2.1E-03 2.3E-01 7.2E-01 9.3E-01 9.0E-01 9.9E-01 9.9E-01 9.9E-01 9.9E-01 8 9.9E-01									
MASS REMAINING = 1.283E+08, MASS DISPENSED = 1.401E+06, MASS EVAPORATED = 9.071E+06, SUM = 1.395E+08 FRACTION (BASED ON MASS) REMAINING IN THE SLICK = 9.2E-01, AREA = 7.2E+04 M**2, THICKNESS = 2.0E-01 CM, MOLE WT=312.0 WEIGHT FRACTION WATER IN OIL = 1.4E-01, VISCOSITY = 1.9E+03 CENTISTOKES, DISPERSION TERM = 2.4E-03 WEIGHT FRACTION/HR MASS/AREA = 1.8E+03 GMS/M**2, SPGR = 8.9E-01, TOTAL VOLUME = 9.0E+02 BBL, DISPERSION = 4.2E+00 GMS/M**2/HR, EVAP RATE = 9.3E+00 GMS/M**2/HR									
STEP SIZE OF 3.078E-02 IS BASED ON CUT 2									
TIME = 7.1E+00 HOURS, MASS FRACTION OF EACH CUT REMAINING: 0.0E+00 4.3E-04 1.6E-01 6.7E-01 9.1E-01 9.7E-01 9.9E-01 9.9E-01 9.9E-01 9.9E-01 9 9.9E-01									

TABLE 15a (Continued): Output from Oil-Weathering Calculations; Prudhoe Bay Crude Oil, Final Time Step at 320F.

TITLE = 8.2E+01 HOURS, MASS FRACTION OF EACH CUT REMAINING.
 @ .0E+00 @ .0E+00 @ .9E+00 2.7E-00 2.9E-02 4.9E-01 8.7E-01 8.9E-01 8.9E-01 8.9E-01 8.9E-01 8.9E-01
 0.9E-01
 MASS REMAINING = 1.08E+08, MASS DISPENSED = 1.40E+07, SUM = 1.09E+08
 MASS FRACTION REMAINING IN THE SLICK= 7.6E-01, AREA= 2.4E+03 M**2, THICKNESS= 4.9E-02 CM, MOLE WT= 91.9
 WATERSHED FRACTION WATER IN OIL = 7.9E-01, VISCOSITY = 2.2E+05 CENTISTOKES, DISPERSION TERM = 0.9E-04 WEIGHT FRACTION HUM
 DENSITY= 1.0E+01 GMS/M**3, SPEC GRAV= 1.0E+01 GMS/M**3, TOTAL VOLUME= 7.3E+02 BBL, DISPERSION= 4.0E-01 GMS/M**HR, EVAP RATE= 1.8E-01 GMS/M**HR

STEP SIZE OF 5.000E-01 IS BASED ON CUT 5

TIME = 9.2E+01 HOURS, MASS FRACTION OF EACH CUT REMAINING:

0.0E+00	0.0E+00	9.0E+00	9.1E-10	1.3E-02	4.4E-01	7.8E-01	0.6E-01	0.8E-01	0.8E-01	0.0E-01	0.8E-01	0.8E-01
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MASS REMAINING = 1.040E+08, MASS DISPERSED = 1.49E+07, MASS EVAPORATED = 2.05E+07, SUM = 1.055E+08

MASS FRACTION (BASED ON THE SLICK= 7.0E-01, AREA= 2.5E+05 M*2, THICKNESS= 4.0E-02 CM, MOLE WT=350.5

WEIGHT FRACTION WATER IN OIL = 7.0E-01, VISCOSITY = 2.6E+05 CENTISTOKES, DISPERSION TERM = 0.8E-04 WEIGHT FRACTION/HR

WATER/AREA = 4.2E+02 GMS/M*HR, SUCH= 9.1E-01 TOTAL VOLUME= 7.2E+02 DBL, DISPERSION= 3.7E-01 GMS/HR*HR, EVAP RATE= 1.5E-01 GMS/HR*HR

[illegible]

TABLE 15b: Output from Oil-Weathering Calculations; Prudhoe Bay
Crude Oil Vapor Pressures at 60°F.

CRUDE OIL CHARACTERIZATION AND PSEUDOCOMPONENT EVAPORATION MODEL
IDENTIFICATION: PRUDHOE BAY, ALASKA

ITEM 9, SAMPLE 71011
VAPOR PRESSURE IN ATMOSPHERES AT 6.000E+01 DEG F

VP

1	8.843E-02
2	2.830E-02
3	8.209E-03
4	2.004E-03
5	4.492E-04
6	8.934E-05
7	1.662E-05
8	2.801E-06
9	4.596E-07
10	4.453E-08
11	2.257E-09
12	1.879E-10
13	7.774E-12
14	2.070E-13

MEAN MOLECULAR WEIGHT OF THE CRUDE = 2.739E+02

TABLE 15.b (Continued) Output from Oil-Weathering Calculations; Prudhoe Bay Crude Oil, Mass-Transfer Coefficients, Problem Specifications, and Beginning of Calculated Results at 60°F (Note deletion of cut 1 and renumbering of cuts).

OVER-ALL MASS-TRANSFER COEFFICIENTS BY INPUT CODE 2
 OVER-ALL MASS-TRANSFER COEFFICIENT FOR CUMENE = 1.926E+01 M/HR

CUT	M/HR	CM-MOLES/(HR)(ATH)(M**2)
1	2.962E+01	8.716E+02
2	2.931E+01	8.805E+02
3	2.907E+01	8.481E+02
4	1.904E+01	8.806E+02
5	1.965E+01	8.803E+02
6	1.946E+01	8.226E+02
7	1.932E+01	8.165E+02
8	1.919E+01	8.112E+02
9	1.910E+01	8.071E+02
10	1.890E+01	8.022E+02
11	1.805E+01	7.965E+02
12	1.876E+01	7.900E+02
13	1.860E+01	7.893E+02
14	1.859E+01	7.889E+02

FOR THIS SPILL OF 1.000E+03 BARRELS, THE MASS IS 1.412E+02 METRIC TONNES
 VOLUME FROM SUMMING THE CUTS = 1.6E+02 M**3, OR 1.000E+03 BARRELS
 WIND SPEED = 1.000E+01 KNOTS, OR 1.853E+04 M/HR
 INITIAL SLICK DIAMETER = 1.006E+02 M, OR AREA = 7.950E+03 M**2
 KINEMATIC VISCOSITY OF THE BULK CRUDE FROM THE CUTS = 4.9E+00 CENTISTOKES AT 122 DEG F
 KINEMATIC VISCOSITY OF THE BULK CRUDE FROM THE CUTS = 7.2E+00 AT T = 60.0 DEG F, SCALE FACTOR = 1.5E+00
 VISCOSITY ACCORDING TO MASS EVAPORATED: VIS2BC = 3.50E+01, ANDRADE = 9.00E+03, FRACT WEATHERED = 1.05E+01, VSLEAD = 9.30E+01 CP
 MOUSE CONSTANTS: MOONEY= 6.20E-01, MAX H2O= 0.70, WIND**2= 1.00E-03
 THE FRACTIONAL SLICK AREA SUBJECT TO DISPERSION IS 4.1E+00 PER HOUR
 THE DISPERSION PARAMETERS USED: KA = 1.00E-01, KB = 5.00E+01, SURFACE TENSION = 3.00E+01 DYNES/CM
 COUNT THE CUTS IN THE FOLLOWING OUTPUT FROM LEFT TO RIGHT
 THE INITIAL GRAM MOLES IN THE SLICK ARE:
 2.505E+04 2.911E+04 3.603E+04 3.423E+04 3.210E+04 2.743E+04 3.100E+04 3.219E+04 3.140E+04 1.625E+04 3.309E+04
 3.211E+04 2.566E+04 2.846E+04 9.420E+04
 THE INITIAL MASSES (GRAMS) IN THE SLICK ARE:
 2.200E+06 2.956E+06 4.100E+06 4.075E+06 4.596E+06 4.407E+06 5.530E+06 6.300E+06 6.690E+06 3.043E+06 9.005E+06
 9.594E+06 0.503E+06 1.069E+07 5.652E+07
 THE TOTAL MASS FROM THESE CUTS IS 1.395E+08 GRAMS

CUT 1 GOES AWAY IN MINUTES, THEREFORE IT WAS DELETED AND THE CUTS RENUMBERED

STEP SIZE OF 1.279E-01 IS BASED ON CUT 1

TIME = 0.0E+00 HOURS, MASS FRACTION OF EACH CUT REMAINING:
 1.0E+00 1.0E+00 1.0E+00 1.0E+00 1.0E+00 1.0E+00 1.0E+00 1.0E+00 1.0E+00 1.0E+00 1.0E+00
 MASS REMAINING = 1.372E+00, MASS DISPERSION = 0.000E+00, MASS EVAPORATED = 0.000E+00, SUM = 1.372E+00
 FRACTION (BASED ON MASS) REMAINING IN THE SLICK 9.0E-01, AREA = 7.40E+03 M**2, THICKNESS = 2.0E+00 CM, RUIE MC=200, Z
 WEIGHT FRACTION WATER IN OIL = 6.9E-03, VISCOSITY 1.0E+02 CENTISTOKES, DISPERSION TEMP 0E+04 MIGHT FRACTION/HR
 MASS/AREA= 1.0E+04 GMS/PPH, SPCH= 0.0E-01, TOTAL VOLUME= 9.4E+02 BBL, DISPERSION= 1.7E+01 GMS/PPH/HR, EVAP RATE= 0.0E+00 GMS/PPH/HR

TIME = 1.0E+00 HOURS, MASS FRACTION OF EACH CUT REMAINING:
 0.31E-01 7.4E-01 9.3E-01 9.8E-01 1.0E+00 1.0E+00 1.0E+00 1.0E+00 1.0E+00 1.0E+00 1.0E+00

TABLE 16a: Illustration of 80-Column Output from Open-Ocean Oil-Weathering Code, Prudhoe Bay Crude Oil at 32°F.

OIL WEATHERING FOR PRUDHOE BAY, ALASKA

CODE VERSION IS CUTVP2 OF FEBRUARY 83
 TEMPERATURE= 32.0 DEG F, WIND SPEED= 10.0 KNOTS
 SPILL SIZE= 1.000E+03 BARRELS
 MASS-TRANSFER COEFFICIENT CODE= 2

FOR THE OUTPUT THAT FOLLOWS, MOLES=GRAM MOLES
 GMS=GRAMS, VP=VAPOR PRESSURE IN ATMOSPHERES
 BP=BOILING POINT IN DEG F, API=GRAVITY
 MW=MOLECULAR WEIGHT

CUT	MOLES	GMS	VP	BP	API	MW
1	2.56E+04	2.29E+06	3.78E-02	1.67E+02	7.27E+01	89
2	2.91E+04	2.96E+06	1.09E-02	2.12E+02	6.42E+01	101
3	3.63E+04	4.14E+06	2.58E-03	2.57E+02	5.67E+01	113
4	3.42E+04	4.37E+06	5.64E-04	3.02E+02	5.16E+01	127
5	3.21E+04	4.60E+06	1.12E-04	3.47E+02	4.76E+01	143
6	2.74E+04	4.41E+06	1.96E-05	3.92E+02	4.52E+01	160
7	3.11E+04	5.53E+06	3.18E-06	4.37E+02	4.15E+01	177
8	3.22E+04	6.31E+06	4.63E-07	4.82E+02	3.78E+01	195
9	3.15E+04	6.69E+06	6.60E-08	5.27E+02	3.48E+01	212
10	1.63E+04	3.84E+06	5.30E-09	5.80E+02	3.06E+01	236
11	3.31E+04	9.01E+06	2.09E-10	6.38E+02	2.91E+01	272
12	3.21E+04	9.59E+06	1.42E-11	6.85E+02	2.62E+01	298
13	2.57E+04	8.59E+06	4.51E-13	7.38E+02	2.40E+01	334
14	2.85E+04	1.07E+07	8.82E-15	7.90E+02	2.25E+01	375
15	9.42E+04	5.65E+07	0.00E+00	8.50E+02	1.14E+01	600

MOUSSE CONSTANTS: MOONEY= 6.20E-01, MAX H2O= 0.70, WIND**2= 1.00E-03
 DISPERSION CONSTANTS: KA= 1.00E-01, KB= 5.00E+01, S-TENSION= 3.00E+01
 VIS CONSTANTS: VIS25C= 3.50E+01, ANDRADE = 9.00E+03, FRACT = 1.05E+01

FOR THE OUTPUT THAT FOLLOWS, TIME=HOURS
 BBL=BARRELS, SPCR=SPECIFIC GRAVITY, AREA=M*M
 THICKNESS=CM, W=PERCENT WATER IN OIL (MOUSSE)
 DISP=DISPERSION RATE IN GMS/M*M/HR
 ERATE=EVAPORTION RATE IN GMS/M*M/HR
 M/A=MASS PER M*M OF OIL IN THE SLICK
 I=FIRST CUT WITH GREATER THAN 1% (MASS) REMAINING
 J=FIRST CUT WITH GREATER THAN 50% (MASS) REMAINING

TIME	BBL	SPCR	AREA	THICKNESS	W	DISP	ERATE	M/A	I	J
0	1.0E+03	0.88	7.9E+03	2.0E+00	0	7.7E+00	0.0E+00	1.8E+04	1	1
1	9.7E+02	0.88	3.1E+04	5.0E-01	2	6.6E+00	9.9E+01	4.4E+03	1	2
2	9.5E+02	0.89	4.3E+04	3.5E-01	4	5.9E+00	4.2E+01	3.1E+03	1	3
3	9.3E+02	0.89	5.2E+04	2.9E-01	7	5.3E+00	2.5E+01	2.5E+03	2	3
4	9.2E+02	0.89	6.0E+04	2.5E-01	9	4.9E+00	1.6E+01	2.2E+03	2	4
5	9.1E+02	0.89	6.6E+04	2.2E-01	11	4.5E+00	1.2E+01	2.0E+03	3	4
6	9.0E+02	0.89	7.2E+04	2.0E-01	14	4.2E+00	9.5E+00	1.8E+03	3	4
7	9.0E+02	0.89	7.7E+04	1.8E-01	16	3.9E+00	7.7E+00	1.6E+03	3	4
8	8.9E+02	0.89	8.3E+04	1.7E-01	18	3.7E+00	6.3E+00	1.5E+03	3	4
9	8.8E+02	0.90	8.7E+04	1.6E-01	20	3.4E+00	5.2E+00	1.4E+03	3	4
10	8.8E+02	0.90	9.2E+04	1.5E-01	22	3.2E+00	4.4E+00	1.4E+03	3	5
11	8.7E+02	0.90	9.6E+04	1.4E-01	24	3.0E+00	3.8E+00	1.3E+03	3	5
12	8.7E+02	0.90	1.0E+05	1.4E-01	26	2.9E+00	3.3E+00	1.2E+03	3	5
13	8.6E+02	0.90	1.0E+05	1.3E-01	27	2.7E+00	2.9E+00	1.2E+03	4	5
14	8.6E+02	0.90	1.1E+05	1.3E-01	29	2.6E+00	2.6E+00	1.1E+03	4	5
15	8.5E+02	0.90	1.1E+05	1.2E-01	31	2.4E+00	2.4E+00	1.1E+03	4	5
16	8.5E+02	0.90	1.1E+05	1.2E-01	32	2.3E+00	2.2E+00	1.1E+03	4	5
17	8.4E+02	0.90	1.2E+05	1.1E-01	34	2.2E+00	2.0E+00	1.0E+03	4	5
18	8.4E+02	0.90	1.2E+05	1.1E-01	35	2.1E+00	1.8E+00	9.9E+02	4	5
19	8.4E+02	0.90	1.2E+05	1.1E-01	37	2.0E+00	1.7E+00	9.6E+02	4	5
20	8.3E+02	0.90	1.3E+05	1.0E-01	38	1.9E+00	1.6E+00	9.4E+02	4	5

TABLE 16b: Illustration of 80-Column Output from Open-Ocean Oil-Weathering Code, Prudhoe Bay Crude Oil at 60°F. (Note deletion of cut 1 at beginning out of weathering output).

OIL WEATHERING FOR PRUDHOE BAY, ALASKA

CODE VERSION IS CUTVP2 OF FEBRUARY 83
 TEMPERATURE= 60.0 DEG F, WIND SPEED= 10.0 KNOTS
 SPILL SIZE= 1.000E+03 BARRELS
 MASS-TRANSFER COEFFICIENT CODE= 2

FOR THE OUTPUT THAT FOLLOWS, MOLES=GRAM MOLES
 GMS=GRAMS, VP=VAPOR PRESSURE IN ATMOSPHERES
 BP=BOILING POINT IN DEG F, API=GRAVITY
 MW=MOLECULAR WEIGHT

CUT	MOLES	GMS	VP	BP	API	MW
1	2.56E+04	2.29E+06	8.84E-02	1.67E+02	7.27E+01	89
2	2.91E+04	2.96E+06	2.83E-02	2.12E+02	6.42E+01	101
3	3.63E+04	4.14E+06	8.21E-03	2.57E+02	5.67E+01	113
4	3.42E+04	4.37E+06	2.00E-03	3.02E+02	5.16E+01	127
5	3.21E+04	4.60E+06	4.49E-04	3.47E+02	4.76E+01	143
6	2.74E+04	4.41E+06	8.93E-05	3.92E+02	4.32E+01	160
7	3.11E+04	5.53E+06	1.66E-05	4.37E+02	4.15E+01	177
8	3.22E+04	6.31E+06	2.80E-06	4.82E+02	3.78E+01	195
9	3.15E+04	6.69E+06	4.60E-07	5.27E+02	3.48E+01	212
10	1.63E+04	3.84E+06	4.45E-08	5.80E+02	3.06E+01	236
11	3.31E+04	9.01E+06	2.26E-09	6.38E+02	2.91E+01	272
12	3.21E+04	9.59E+06	1.88E-10	6.85E+02	2.62E+01	298
13	2.57E+04	8.59E+06	7.77E-12	7.38E+02	2.40E+01	334
14	2.85E+04	1.07E+07	2.07E-13	7.90E+02	2.25E+01	375
15	9.42E+04	5.65E+07	0.00E+00	8.50E+02	1.14E+01	600

MOUSSE CONSTANTS: MOONEY= 6.20E-01, MAX H2O= 0.70, WIND**2= 1.00E-03
 DISPERSION CONSTANTS: KA= 1.08E-01, KB= 5.00E+01, S-TENSION= 3.00E+01
 VIS CONSTANTS: VIS25C= 3.50E+01, ANDRADE = 9.00E+03, FRACT = 1.05E+01

FOR THE OUTPUT THAT FOLLOWS, TIME=HOURS
 BBL=BARRELS, SPGR=SPECIFIC GRAVITY, AREA=M*M
 THICKNESS=CM, W=PERCENT WATER IN OIL (MOUSSE)
 DISP=DISPERSION RATE IN GMS/M*M/HR
 ERATE=EVAPORTION RATE IN GMS/M*M/HR
 M/A=MASS PER M*M OF OIL IN THE SLICK
 I=FIRST CUT WITH GREATER THAN 1% (MASS) REMAINING
 J=FIRST CUT WITH GREATER THAN 50% (MASS) REMAINING
 CUT 1 GOES AWAY IN MINUTES, THEREFORE IT WAS DELETED AND THE CUTS RENUMBERED

TIME	BBL	SPGR	AREA	THICKNESS	W	DISP	ERATE	M/A	I	J
0	9.8E+02	0.88	7.8E+03	2.0E+00	0	1.7E+01	0.0E+00	1.8E+04	1	1
1	9.5E+02	0.89	3.1E+04	4.9E-01	2	1.5E+01	1.2E+02	4.3E+03	1	2
2	9.2E+02	0.89	4.2E+04	3.4E-01	5	1.3E+01	5.3E+01	3.1E+03	1	3
3	9.0E+02	0.89	5.1E+04	2.8E-01	7	1.1E+01	2.9E+01	2.5E+03	2	3
4	8.9E+02	0.90	5.9E+04	2.4E-01	9	1.0E+01	1.9E+01	2.1E+03	2	3
5	8.7E+02	0.90	6.5E+04	2.1E-01	12	9.1E+00	1.3E+01	1.9E+03	2	4
6	8.6E+02	0.90	7.1E+04	1.9E-01	14	8.3E+00	1.0E+01	1.7E+03	3	4
7	8.5E+02	0.90	7.6E+04	1.8E-01	16	7.7E+00	8.1E+00	1.6E+03	3	4
8	8.4E+02	0.90	8.1E+04	1.7E-01	18	7.1E+00	6.7E+00	1.5E+03	3	4
9	8.3E+02	0.90	8.5E+04	1.6E-01	20	6.5E+00	5.6E+00	1.4E+03	3	4
10	8.3E+02	0.90	9.0E+04	1.5E-01	22	6.0E+00	4.7E+00	1.3E+03	3	4
11	8.2E+02	0.90	9.4E+04	1.4E-01	24	5.6E+00	4.0E+00	1.2E+03	3	5
12	8.1E+02	0.90	9.8E+04	1.3E-01	26	5.2E+00	3.5E+00	1.2E+03	3	5
13	8.1E+02	0.90	1.0E+05	1.3E-01	27	4.9E+00	3.1E+00	1.1E+03	3	5
14	8.0E+02	0.90	1.0E+05	1.2E-01	29	4.5E+00	2.8E+00	1.1E+03	3	5
15	7.9E+02	0.90	1.1E+05	1.2E-01	31	4.2E+00	2.5E+00	1.1E+03	4	5
16	7.9E+02	0.90	1.1E+05	1.1E-01	33	4.0E+00	2.2E+00	1.0E+03	4	5
17	7.8E+02	0.90	1.1E+05	1.1E-01	34	3.7E+00	2.1E+00	9.8E+02	4	5
18	7.8E+02	0.90	1.2E+05	1.0E-01	36	3.5E+00	1.9E+00	9.5E+02	4	5
20	7.7E+02	0.90	1.2E+05	1.0E-01	37	3.3E+00	1.7E+00	9.2E+02	4	5

TABLE 17: Execution of Open-Ocean Oil-Weathering Code on SAI's
DEC-10 System. Underlined Characters are Entered by User.

connecting to host system.

Science App Inc 701a.20 09:50:19 TTY31 system 1256

Connected to Node LJASYN(2) Line # 57

Please LOGIN or ATTACH

.LOG

JOB 58 Science App Inc 701a.20 TTY31

PPN:4601,4601

Password:

09:50 8-Mar-83 Tue

.EX CUTVP2.FOR

LINK: Loading

[LNKXCT CUTVP2 execution]

DO IT AGAIN?

N

CPU time 1.75 Elapsed time 2:19.85

EXIT

.PRINT CUTVP2.OUT

[Printer Job CUTVP2 queued, request #6115, limit 35]

.TYPE CUTVP2.TYP

OIL WEATHERING FOR LIGHT DIESEL CUT

CODE VERSION IS CUTVP2 OF FEBRUARY 83

TEMPERATURE= 32.0 DEG F, WIND SPEED= 10.0 KNOTS

SPILL SIZE= 1.000E+04 BARRELS

MASS-TRANSFER COEFFICIENT CODE= 2

.BYE

Charge.... 0.1 J 3.7 CP 614 RD 61 WR= \$ 0.67

Job 58 User OIL-WEATHER [4601,4601]

Lossed-off TTY31 at 9:54:29 on 8-Mar-83

Runtime: 0:00:03, KCS:97, Connect time: 0:04:02

Disk Reads:648, Writes:66, Blocks saved:279

TABLE 18. Illustration of Procedure to Attach to a Job

.log 1234,1234

JOB 29 Science App Inc 701.17e TTY25

Password: <cr>

Other jobs detached with same PPN:

Job 73 <program name> running

Do you want to ATTACH to this job? [Y]<cr>

ATTACH 73[1234,1234]

[LGNATJ Attaching to job 73 running <program name> in user mode]

<cr>

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Attachment 1

HOW TO USE TELENET

HOW TO USE TELENET INFORMATION FOR TERMINAL USERS

WELCOME TO TELENET

The Telenet public network makes it possible for terminal users to dial up a computer anywhere in the country at rates that are many times lower than long distance telephone rates.

Once you have become an authorized user of any of the computer centers on the network, you simply dial a local Telenet telephone number to make your connection. No prior arrangements with Telenet are necessary.

We think you will find the Telenet public network easy to use and highly reliable. If you are a new user, we suggest that you read through this entire writeup first. If you have any questions, the Customer Service Desk, (800) 336-0437, will be happy to help answer them.

TELENET SIGN-ON PROCEDURE

The instructions below explain how to connect to your computer through Telenet if you are using an ASCII-type terminal. In the examples, <cr> = carriage return and _ (underscore) = space. All other messages are automatically typed by Telenet.

STEPS

1. Turn on the terminal and coupler.
2. Dial the nearest Telenet access number. When you hear a high-pitched tone, place the telephone receiver into the acoustic coupler.
3. Type two carriage returns.
4. Telenet will give you a port identification number and ask you to identify your terminal. Your response to "TERMINAL=" is a carriage return or appropriate terminal type such as DECW<cr> for DECwriter or D1<cr> for a CRT or TI745.
5. The La Jolla Computer Center will require an identification code and password before accepting your connection. In this case, after Telenet prompts with an @, type ID, skip a space, and type your ID code, followed by a carriage return.

Example:

@ID_LAJOLLA<cr>

Type in your password:

Password=nnnnnn<cr> ; call 454-3811 ext 2731 for the password

6. After Telenet prompts with an @, type a C, skip a space and type the network address of your computer, followed by a carriage return.

Example:

@C_714_20<cr> (for DEC-10)

7. Telenet will respond with a connection message. You are now ready to begin your conversation with the computer.

Example:

<cr>

SAI banner

PLEASE LOGIN OR ATTACH

LOG_P,PN<cr>

Password.....<cr>

If the wrong password is typed, the response is .KJOB.

8. To disconnect from your computer, log off as usual.

Hang up the phone to disconnect from Telenet.

* * * *

DO NOT USE TELENET 800 DIALIN DATA ACCESS. This in watts service costs SAI far more than the cost allocated to computer users.

* * * *

CUSTOMER SERVICE

TELEPHONE 800-336-0437 (From Virginia 800-572-0408)

Telenet's Customer Service Desk is available to assist users around the clock, seven days a week. Important: If you are reporting a problem with a network connection, be sure to give the port identification number which you received at call set-up time. If you are not sure what this number is, use the STAT network command (see page 5).

You may also contact Customer Service from your terminal. Follow exactly the same procedure given for connecting to any network address.

CUSTOMER SERVICE NETWORK ADDRESS - 202 CS

This is a receive-only terminal on which you should leave your name, telephone number, and a brief description of your problem. Your message will be responded to promptly by telephone.

If you would like general information about Telenet and its services, please contact their corporate headquarters or any of the regional sales offices listed below:

Boston	(617)	890-0202
Chicago	(312)	298-2188
Los Angeles	(213)	477-2048
New York	(212)	594-8644
Orange County, CA	(714)	891-4481
San Francisco	(415)	854-5845
Washington	(202)	637-7920

EXPLANATION OF NETWORK MESSAGES

Messages that appear at call set-up time:

- 0 A Telenet prompt character that indicates that the network is waiting for a command.
- TERMINAL = A request to enter your terminal model identifier.
- ? The network does not understand your command. Check to see if you have made a typing error. If not, contact Telenet Customer Service.

Messages that appear after you have requested a computer connection:

- CONNECTED Your computer connection has been established. Follow normal log-in procedures.
- BUSY,
CONNECTIONS
UNAVAILABLE All computer ports are temporarily in use. Try again in a few minutes. If this condition persists, notify your computer center.
- NOT AVAILABLE
NOT RESPONDING
NOT OPERATING Your computer is not currently available to network users. Check with your computer center to see when service will be resumed.
- ILLEGAL ADDRESS Non-existent network address. Check for a typing error.
- ILLEGAL DESTINATION ADDRESS
ILLEGAL SOURCE ADDRESS You are not recognized as an authorized user of this computer system. No connection can be made by Telenet.
- SUBPROCESS UNAVAILABLE The application program requested is not available at this time.
- NOT REACHABLE Indicates a temporary network problem. Report condition to Telenet Customer Service.
- REFUSED COLLECT CONNECTION You must obtain a "caller paid" identification code and password in order to access this system. Check with your computer center.
- STILL CONNECTED Your terminal is still actively connected to this address. If you wish to resume your session, enter the CONT command.

STILL PENDING

You have a request still pending for connection to the address given. If you wish to connect to a different network address, you must disconnect with the D command.

DISCONNECTED

This message normally appears when you have logged off your computer or when you have given the D command to the network. If it appears by itself, it indicates your connection has been reset due to a problem. Follow normal connection procedures to continue your session. See Sign-On Procedure, Step 5, page 1.

NETWORK COMMANDS

- C To request a connection to a computer address. The command is followed by a space, the computer address and a carriage return.
- D<cr> To disconnect from your computer system. This command is used in cases where the computer does not automatically send a DISCONNECTED message at logout time.
- <cr>Q<cr> To interrupt your computer session to return to network command mode.
- CONT<cr> To return to your computer session after you have been in Telenet command mode.
- FULL<cr> To echo keyboard input on ASCII terminals.
- HALF<cr> To stop the network from echoing keyboard input on ASCII terminals.
- STAT<cr> To determine the identification number of the Telenet port you are using.
- TAPE<cr> To signify that your input will be paper tape or cassette. After you have set up the computer utility program for tape transmission, return to Telenet command mode. Type the TAPE command. Then start your tape. When the tape is completed, depress the BREAK key.
- TERM = To change the terminal identifier specified at call set-up time. The command is followed by a new two or four-character terminal identifier and a carriage return.

LAST UPDATE: 08/09/82

* NEW TELENET CENTRAL OFFICE
NEW 1200 BAUD ACCESS AVAILABLE
& NEW TELENET CENTRAL OFFICE ADDED CURRENT MONTH
\$ NEW 1200 BAUD ACCESS AVAILABLE ADDED CURRENT MONTH
% NEW-LEAD NUMBER/NUMBER CHANGED

GTE/TELENET PROVIDES LOCAL NETWORK ACCESS IN THESE U.S. CITIES OF 50,000 POPULATION OR MORE. IN-WATS ACCESS IS AVAILABLE IN OTHER LOCATIONS. 1200 BPS ACCESS NUMBERS REQUIRE THE USE OF BELL 212- OR VADIC 3405- COMPATIBLE MODEMS, AS NOTED.
(B) = BELL 212, (V) = VADIC 3405, (B/V) = EITHER BELL 212 OR VADIC 3405.

< > INDICATES THE ACTUAL LOCATION OF TELENET FACILITIES. IN SOME CASES, LOCAL ACCESS MAY REQUIRE EXTENDED METRO TELEPHONE SERVICE OR INVOLVE MESSAGE UNIT CHARGES.

TELENET CUSTOMER SERVICE:

CONTINENTAL USA -- 800/336-0437
IN VIRGINIA -- 800/572-0408
OUTSIDE CONTINENTAL USA -- 703/442-2200

TELEMAIL CUSTOMER SERVICE: 703/442-1900

	300 BPS	1200 BPS
AL%205 BESSEMER	326-3420 <BIRMINGHAM>	(B/V) 326-3420
AL%205 BIRMINGHAM	326-3420	(B/V) 326-3420
AL%205 FLORENCE	766-9101	(B/V) 766-9101
AL 205 HUNTSVILLE	539-2281	(B/V) 539-2281
AL%205 MOBILE	432-1680	(B/V) 432-1680
AL 205 MONTGOMERY	265-1500	(B/V) 265-1500
AL%205 SHEFFIELD	766-9101 <FLORENCE>	(B/V) 766-9101
AK 907 ANCHORAGE	276-0271	(B/V) 276-0271
AK 907 JUNEAU	586-9700	(B/V) 586-9700
AR%501 LITTLE ROCK	372-4616	(B/V) 372-4616
AZ%802 MESA	254-0244 <PHOENIX>	(B/V) 254-0244
AZ%802 PHOENIX	254-0244	(B/V) 254-0244
AZ%802 SCOTTSDALE	254-0244 <PHOENIX>	(B/V) 254-0244
AZ%802 TEMPE	254-0244 <PHOENIX>	(B/V) 254-0244
AZ 802 TUCSON	745-1666	(B/V) 745-1666
CA 213 ALHAMBRA	507-0909 <GLENDALE>	(B/V) 507-0909
CA 714 ANAHEIM	558-8061 <SANTA ANA>	(B/V) 558-7078
CA 805 BAKERSFIELD	327-8146	(B/V) 327-8146
CA 415 BURLINGAME	595-0360 <SAN CARLOS>	(B/V) 591-0726
CA%213 CANOGA PARK	306-2984 <MARINA DEL REY>	(B/V) 306-2984
CA%714 COLTON	824-9000	(B/V) 824-9000
CA%408 CUPERTINO	294-9119 <SAN JOSE>	(B/V) 294-9119
CA%714 ES CONDIDO	743-1210	(B/V) 743-1210
CA 213 EL MONTE	507-0909 <GLENDALE>	(B/V) 507-0909
CA 714 FULLERTON	558-8061 <SANTA ANA>	(B/V) 558-7078
CA 209 FRESNO	233-0961	(B/V) 233-0961
CA 714 GARDEN GROVE	898-9820	(B/V) 898-9820
CA%213 GLENDALE	507-0909	(B/V) 507-0909

CA 415 HAYWARD	881-1382		
CA 213 HOLLYWOOD	689-9040	<LOS ANGELES>	(B/V) 624-2251
CA#213 HOLLYWOOD	937-3580	<LOS ANGELES>	(B/V) 937-3580
CA 714 HUNTINGTON BEACH	558-8061	<SANTA ANA>	(B/V) 558-7078
CA 213 INGLEWOOD	689-9040	<LOS ANGELES>	(B/V) 624-2251
CA#213 INGLEWOOD	937-3580	<LOS ANGELES>	(B/V) 937-3580
CA 213 LOS ANGELES	689-9040		(B/V) 624-2251
CA#213 LOS ANGELES	937-3580		(B/V) 937-3580
CA 415 LOS ALTOS	856-9930	<PALO ALTO>	(B/V) 856-9995
CA 213 LONG BEACH	549-5150	<SAN PEDRO>	(B/V) 548-6141
CA%213 MARINA DEL REY	306-2984		(B/V) 306-2984
CA 209 MODESTO	576-2852		(B/V) 576-2852
CA 415 MOUNTAIN VIEW	856-9930	<PALO ALTO>	(B/V) 856-9995
CA 714 NEWPORT BEACH	558-8061	<SANTA ANA>	(B/V) 558-7078
CA%415 OAKLAND	836-4911		(B/V) 836-4911
CA 805 OXNARD	659-4660	<VENTURA>	(B/V) 656-6760
CA 415 PALO ALTO	856-9930		(B/V) 856-9995
CA 213 PASADENA	507-0909	<GLENDALE>	(B/V) 507-0909
CA 415 REDWOOD CITY	595-0360	<SAN CARLOS>	(B/V) 591-0726
CA%714 RIVERSIDE	824-9000	<COLTON>	(B/V) 824-9000
CA%916 SACRAMENTO	448-6262		(B/V) 448-6262
CA%408 SALINAS	443-4940		(B/V) 443-4940
CA%714 SAN BERNADINO	824-9000	<COLTON>	(B/V) 824-9000
CA%415 SAN CARLOS	591-0726		(B/V) 591-0726
CA 714 SAN DIEGO	231-1922		(B/V) 233-0233
CA 415 SAN FRANCISCO	362-6200		(B/V) 956-5777
CA%408 SAN JOSE	294-9119		(B/V) 294-9119
CA 415 SAN MATEO	595-0360	<SAN CARLOS>	(B/V) 591-0726
CA 213 SAN PEDRO	549-5150		(B/V) 548-6141
CA 714 SANTA ANA	558-8061		(B/V) 558-7078
CA 805 SANTA BARBARA	682-5361		(B/V) 682-5361
CA%408 SANTA CLARA	294-9119	<SAN JOSE>	(B/V) 294-9119
CA%213 SANTA MONICA	306-2984	<MARINA DEL REY>	(B/V) 306-2984
CA%408 SUNNYVALE	294-9119	<SAN JOSE>	(B/V) 294-9119
CA 213 TORRANCE	549-5150	<SAN PEDRO>	(B/V) 548-6141
CA 213 WOODLAND HILLS	992-0144		
CA 415 WOODSIDE	856-9930	<PALO ALTO>	(B/V) 856-9995
CA%805 VENTURA	656-6760		(B/V) 656-6760
CO#303 AURORA	773-8500	<DENVER>	(B/V) 694-2710
CO#303 BOULDER	773-8500	<DENVER>	(B/V) 741-4000
CO%303 COLORADO SPRINGS	634-5678		(B/V) 694-2710
CO#303 DENVER	773-8500		(B/V) 741-4000
CO#303 LAKEWOOD	773-8500	<DENVER>	(B/V) 635-5361
CT 203 DANBURY	794-9075		(B/V) 694-2710
CT 203 GREENWICH	348-0787	<STAMFORD>	(B/V) 741-4000
CT 203 HARTFORD	522-0344		(B/V) 794-9075
CT%203 MILFORD	624-5954	<NEW HAVEN>	(B/V) 348-0787
CT%203 NEW HAVEN	624-5954		(B/V) 247-9479
CT%203 STAMFORD	348-0787		(B/V) 624-5954
CT 203 WEST HARTFORD	522-0344	<HARTFORD>	(B/V) 348-0787
DC%202 WASHINGTON	429-7896		(B/V) 247-9479
			(B/V) 429-7800

DE 302 WILMINGTON	454-7710	(B/V)	454-7710
FL 813 CLEARWATER	323-4026	(B/V)	323-4026
FL 305 FT. LAUDERDALE	764-4505	(B/V)	764-4505
FL%904 JACKSONVILLE	356-2264	(B/V)	356-2264
FL%305 MIAMI	372-0230	(B/V)	372-0230
FL 305 ORLANDO	422-4088	(B/V)	422-4088
FL 813 ST PETERSBURG	323-4026	(B/V)	323-4026
FL*904 TALLAHASSEE	224-6824	(B/V)	224-6824
FL 813 TAMPA	224-9920	(B/V)	223-1088
FL 305 W PALM BEACH	833-8691		
GA 404 ATLANTA	577-8911	(B/V)	523-0834
GA 912 SAVANNAH	236-2605		
HI 808 HONOLULU	524-8110	(B)	524-8221
IA 319 CEDAR RAPIDS	384-0911	(B/V)	364-0911
IA 402 COUNCIL BLUFFS	341-7733	(B/V)	341-7733
IA 515 DES MOINES	288-4403	(B/V)	288-4403
ID 208 BOISE	343-0611	(B/V)	343-0611
IL 312 ARLINGTON HEIGHTS	938-0500	(B/V)	938-0600
IL 217 CHAMPAIGN	384-6428	(B/V)	384-6428
IL 312 CHICAGO	938-0500	(B/V)	938-0600
IL 312 CICERO	938-0500	(B/V)	938-0600
IL 314 EAST ST LOUIS	421-4990	(B/V)	421-4990
IL 312 OAK PARK	938-0500	(B/V)	938-0600
IL 309 PEORIA	637-8570	(B/V)	637-8570
IL 312 SKOKIE	938-0500	(B/V)	938-0600
IL 217 SPRINGFIELD	753-1373	(B/V)	753-1373
IL 217 URBANA	384-6428	(B/V)	384-6428
IN*812 EVANSVILLE	424-5250	(B/V)	424-5250
IN*219 FT. WAYNE	426-4022	(B/V)	426-4022
IN 219 GARY	882-8800	(B/V)	882-8800
IN 317 INDIANAPOLIS	635-9630	(B/V)	634-5708
IN 219 MISHAWKA	233-7104	(B/V)	233-7104
IN 219 OSCEOLA	233-7104	(B/V)	233-7104
IN 219 SOUTH BEND	233-7104	(B/V)	233-7104
KS 816 KANSAS CITY	221-9900	(B/V)	221-9900
KS 913 TOPEKA	233-9880	(B/V)	233-9880
KS 316 WICHITA	262-5669	(B/V)	262-5669
KY*502 BOWLING GREEN	843-9026	(B/V)	843-9026
KY%502 FRANKFORT	875-3920	(B/V)	875-3920
KY 606 LEXINGTON	233-0312		
KY%502 LOUISVILLE	589-5580	(B/V)	589-5580
LA 504 BATON ROUGE	343-0753		
LA 318 MONROE	387-6330		
LA%504 NEW ORLEANS	524-4094	(B/V)	524-4094
LA 318 SHREVEPORT	221-5833	(B/V)	221-5833
ME 207 AUGUSTA	623-5136	(B/V)	623-5136
MD 301 ANNAPOLIS	266-8888		
MD 301 BALTIMORE	962-5010	(B/V)	727-6060
MD%202 BETHESDA	429-7898	(B/V)	429-7800
MD 301 DUNDALK	962-5010	(B/V)	727-6060
MD%202 ROCKVILLE	429-7898	(B/V)	429-7800
MD%202 SILVER SPRING	429-7898	(B/V)	429-7800
MD 301 TOWSON	962-5010	(B/V)	727-6060
MA 617 ARLINGTON	338-1400	(B/V)	338-7495
MA 617 BOSTON	338-1400	(B/V)	338-7495

MA 617 BROOKLINE	338-1400	<BOSTON>	(B/V)	338-7495
MA 617 CAMBRIDGE	338-1400	<BOSTON>	(B/V)	338-7495
MA 413 CHICOPEE	781-3811	<SPRINGFIELD>	(B/V)	781-3811
MA 413 HOLYOKE	781-3811	<SPRINGFIELD>	(B/V)	781-3811
MA#617 LEXINGTON	863-1550		(B/V)	863-1550
MA 617 MEDFORD	338-1400	<BOSTON>	(B/V)	338-7495
MA 617 NEWTON	338-1400	<BOSTON>	(B/V)	338-7495
MA 617 QUINCY	338-1400	<BOSTON>	(B/V)	338-7495
MA 617 SOMERVILLE	338-1400	<BOSTON>	(B/V)	338-7495
MA 413 SPRINGFIELD	781-3811		(B/V)	781-3811
MA 617 WALTHAM	338-1400	<BOSTON>	(B/V)	338-7495
MA%617 WORCESTER	755-4740		(B/V)	755-4740
MI 313 ANN ARBOR	996-0351		(B/V)	996-5995
MI 616 BATTLE CREEK	968-0929		(B/V)	968-0929
MI 313 DETROIT	964-5538		(B/V)	964-2989
MI 313 FLINT	233-3050		(B/V)	233-3050
MI 616 GRAND RAPIDS	458-1200		(B/V)	774-0966
MI 616 KALAMAZOO	385-0160			
MI%517 LANSING	372-5400		(B/V)	484-2067
MI 517 SAGINAW	790-5166			
MI%313 WARREN	575-9480		(B/V)	575-9480
MN%218 DULUTH	722-1719		(B/V)	722-1719
MN%612 MINNEAPOLIS	341-2459		(B/V)	341-2459
MN%612 ST. PAUL	341-2459	<MINNEAPOLIS>	(B/V)	341-2459
MO 314 FLORISSANT	421-4990	<ST. LOUIS>	(B/V)	421-4990
MO 616 KANSAS CITY	221-9900		(B/V)	221-9900
MO 314 ST. LOUIS	421-4990		(B/V)	421-4990
MS#601 JACKSON	969-0036		(B/V)	969-0036
MT 406 HELENA	443-0000			
NE*402 LINCOLN	475-8392		(B/V)	475-8392
NE 402 OMAHA	341-7733		(B/V)	341-7733
NH 603 CONCORD	224-8110		(B/V)	224-1024
NH 603 PORTSMOUTH	431-2302			
NV 702 LAS VEGAS	733-2158		(B/V)	737-6861
NJ 609 ATLANTIC CITY	348-0561			
NJ 201 BAYONNE	623-6818	<NEWARK>	(B/V)	623-0469
NJ 201 JERSEY CITY	623-6818	<NEWARK>	(B/V)	623-0469
NJ 609 MARLTON	596-1500		(B/V)	596-1500
NJ 201 MORRISTOWN	455-0275		(B/V)	455-0275
NJ 201 NEW BRUNSWICK	246-1090			
NJ 201 NEWARK	623-6818		(B/V)	623-0469
NJ 201 PASSAIC	777-0952			
NJ 201 PATERSON	684-7560		(B/V)	684-7560
NJ*609 PRINCETON	683-1312		(B/V)	683-1312
NJ 609 TRENTON	989-8847		(B/V)	989-8847
NJ 201 UNION CITY	623-6818	<NEWARK>	(B/V)	623-0469
NM 505 ALBUQUERQUE	243-7701		(B/V)	243-4479
NY 518 ALBANY	445-9111		(B/V)	465-8444
NY 607 BINGHAMTON	772-6642		(B/V)	772-6642
NY 716 BUFFALO	847-0600		(B/V)	847-1440
NY#516 DEER PARK	667-5566		(B/V)	667-5566
NY 516 HEMPSTEAD	292-0320		(B/V)	292-3800
NY#212 NEW YORK	785-2540		(B/V)	785-3860
	736-0099		(B/V)	947-9600
NY%914 POUGHKEEPSIE	473-2240		(B/V)	473-2240

NY 716 ROCHESTER	454-3430		(B/V) 454-1020
NY 518 SCHENECTADY	445-9111	<ALBANY>	(B/V) 465-8444
NY 315 SYRACUSE	472-5503		(B/V) 472-5583
NY 518 TROY	445-9111	<ALBANY>	(B/V) 465-8444
NY 315 UTICA/ROME	797-0920		(B/V) 797-0920
NY 914 WHITE PLAINS	328-9199		(B/V) 328-9199
NC 704 ASHEVILLE	253-3517		(B/V) 253-3517
NC 704 CHARLOTTE	374-0371		(B/V) 332-3131
			(B/V) 377-6865
NC 919 DAVIDSON	549-8311	<RESEARCH TRI. PARK>	(B/V) 549-8139
NC 919 DURHAM	549-8311	<RESEARCH TRI. PARK>	(B/V) 549-8139
NC 919 GREENSBORO	273-2851		(B/V) 273-2851
NC 919 HIGH POINT	899-2253		(B/V) 889-2253
NC 919 RALEIGH	549-8311	<RESEARCH TRI. PARK>	(B/V) 549-8139
NC 919 RESEARCH TRI. PARK	549-8311		(B/V) 549-8139
NC 919 WINSTON-SALEM	725-2126		(B/V) 725-2126
OH 216 AKRON	762-9791		(B/V) 762-9791
OH 216 CANTON	452-0903		
OH%513 CINCINNATI	579-0390		(B/V) 579-0390
OH%216 CLEVELAND	575-1658		(B/V) 575-1658
OH 814 COLUMBUS	463-9340		(B/V) 463-9340
OH%513 DAYTON	461-5254		(B/V) 461-5254
OH 216 EUCLID	241-0940	<CLEVELAND>	(B/V) 696-4225
OH 216 KENT	678-5115		
OH 216 PARMA	241-0940	<CLEVELAND>	(B/V) 696-4225
OH%419 TOLEDO	255-7881		(B/V) 255-7881
OH 216 YOUNGSTOWN	743-2296		(B/V) 743-2296
OK 405 BETHANY	232-4546	<OKLAHOMA CITY>	(B/V) 232-4546
OK 405 NORMAN	232-4546	<OKLAHOMA CITY>	(B/V) 232-4546
OK 405 OKLAHOMA CITY	232-4546		(B/V) 232-4546
OK 405 STILLWATER	624-1112		
OK 918 TULSA	584-3247		(B/V) 584-3247
OR 503 PORTLAND	295-3000		(B/V) 295-3028
OR 503 SALEM	378-7712		(B/V) 378-7712
PA 215 ALLENTOWN	435-3330		(B/V) 435-3330
PA 814 ERIE	453-7561		(B/V) 453-6859
PA%717 HARRISBURG	236-6882		(B/V) 236-6882
PA 814 JOHNSTOWN	535-7576		(B/V) 535-8541
PA 215 KING OF PRUSSIA	337-4300		(B/V) 337-4300
PA 412 PENN HILLS	288-9950	<PITTSBURGH>	(B/V) 288-9974
PA 215 PHILADELPHIA	574-0620		(B/V) 574-9462
PA 412 PITTSBURGH	288-9950		(B/V) 288-9974
PA 717 SCRANTON	961-5321		
PA 215 UPPER DARBY	574-0620	<PHILADELPHIA>	(B/V) 574-9462
PA 717 YORK	846-6550		(B/V) 846-6550
RI%401 PROVIDENCE	751-7912		(B/V) 751-7912
RI%401 WARWICK	751-7912	<PROVIDENCE>	(B/V) 751-7912
SC%803 CHARLESTON	722-4303		(B/V) 722-4303
SC%803 COLUMBIA	254-0695		(B/V) 254-0695
SC%803 GREENVILLE	233-3486		(B/V) 233-3486
SD 805 PIERRE	224-6188		(B/V) 224-6188
TN%615 CHATTANOOGA	756-1161		(B/V) 756-1161
TN 615 KNOXVILLE	523-5500		(B/V) 523-5500
TN%901 MEMPHIS	521-0215		(B/V) 521-0215
TN 615 NASHVILLE	244-8310		(B/V) 244-5099

TX%915 ABILENE	876-8545	(B/V) 876-8545
TX 512 AUSTIN	928-1130	(B/V) 928-1130
TX 512 CORPUS CHRISTI	884-9030	(B/V) 884-9030
TX 214 DALLAS	748-0127	(B/V) 748-6371
TX 915 EL PASO	532-7907	(B/V) 532-7907
TX 817 FORT WORTH	336-7791	(B/V) 332-4307
TX 713 GALVESTON	762-3308	(B/V) 762-3308
TX%713 HOUSTON	227-1018	(B/V) 227-1018
TX%512 LACKLAND	225-8004	(B/V) 225-8004
TX%713 NEDERLAND	724-6717	(B/V) 724-6717
TX%915 SAN ANGELO	944-7621	(B/V) 944-7621
TX%512 SAN ANTONIO	225-8004	(B/V) 225-8004
UT%801 SALT LAKE CITY	359-0149	(B/V) 359-0149
VA%202 ALEXANDRIA	429-7896	(B/V) 429-7800
VA%202 ANNANDALE	429-7896	(B/V) 429-7800
VA 804 CHESAPEAKE	625-1186	(B/V) 625-1186
VA%202 FAIRFAX	429-7896	(B/V) 429-7800
VA%202 FALLS CHURCH	429-7896	(B/V) 429-7800
VA 703 HERNDON	435-3333	
VA 804 NEWPORT NEWS	596-6600	(B/V) 596-6600
VA 804 NORFOLK	625-1186	(B/V) 625-1186
VA 804 PORTSMOUTH	625-1186	(B/V) 625-1186
VA 804 RICHMOND	788-9902	(B/V) 788-9902
VA%202 SPRINGFIELD	429-7896	(B/V) 429-7800
VA%202 VIENNA	429-7896	(B/V) 429-7800
VA 804 VIRGINIA BEACH	625-1186	(B/V) 625-1186
VT*802 BURLINGTON	864-7942	(B/V) 864-7942
VT 802 MONTPELIER	229-4966	
WA%206 AUBURN	939-9982	(B/V) 939-9982
WA 206 BELLEVUE	447-9012	(B/V) 625-9612
WA 206 LONGVIEW	577-5835	
WA 206 SEATTLE	447-9012	
WA%509 SPOKANE	455-4071	(B/V) 625-9612
WA%206 TACOMA	627-1791	(B/V) 455-4071
WA 509 WENATCHEE	662-1901	(B/V) 627-1791
WI 608 MADISON	251-5904	(B/V) 662-1901
WI 414 MILWAUKEE	271-2560	(B/V) 257-5010
WV 304 CHARLESTON	345-6471	(B/V) 271-3914
WY%307 CHEYENNE	638-4421	(B/V) 345-6471
IN-WATS 800	424-9494	(B/V) 638-4421
		(B/V) 424-9494

APPENDIX C

CODE DESCRIPTION FOR COMPONENT-SPECIFIC DISSOLUTION

APPENDIX C. COMPONENT-SPECIFIC DISSOLUTION:
COMPUTER CODE DESCRIPTION

In order to make the analytical solutions (as described in Section 4.5) for the component-specific dissolution usable they have been programmed in FORTRAN to allow easy investigation of the results. This appendix presents the details of input-output information, examples of code usage, and a code listing.

Tables 1 through 3 present details on how the code is used. Table 1 is an illustration of the input procedure. All the required input is prompted from the keyboard and echoed back to the user. An input error can be corrected by answering yes to the question following the echo.

The output presented in Table 2 is the result of the input in Table 1. Reasonable estimates of the input parameters are used in this example from which an important conclusion can be drawn. The important parameters are the (vertical) eddy diffusivity = $185 \text{ cm}^2/\text{sec}$ (Pelto, 1982), the over-all mass-transfer coefficient = 1 cm/hr (Cohen, Mackay and Shin, 1980), and the ocean depth = 5 meters. The calculated concentration profiles are always quite flat from top to bottom while the average water column concentration increases by a factor of 5 from the first hour to the fifth. This indicates that the over-all mass transfer coefficient is controlling the rate at which the entire water column is gaining mass of the transferring species. Increasing the over-all mass-transfer from 1 cm/hr to 10 cm/hr and keeping all other parameters the same results in approximately 10 times more mass in the water column over the same time frame as illustrated by the results in Table 3. As a result of this example it is evident that the over-all mass-transfer coefficient is important and appears to be controlling the rate at which mass enters the water column.

Table 1: EXAMPLE OF INPUT FOR PROGRAM DISOLV TO CALCULATE MASS TRANSFER BETWEEN OIL SLICK AND WATER COLUMN

```
.EX DISOLV.FOR
LINK: Loading
[LINKXCT DISOLV execution]

ENTER THE EDDY DIFFUSIVITY, CM*CM/SEC, TRY 100
185.

ENTER THE SLICK THICKNESS, TRY 1 CM
1.

ENTER THE OCEAN DEPTH, TRY 20 METERS
5.

ENTER THE OIL/WATER PARTITION COEFFICIENT, UNITLESS, TRY 1000
2500.

ENTER THE OIL-WATER OVER-ALL MASS-TRANSFER COEFFICIENT, TRY 1 CM/HR
1.

ENTER THE INITIAL OIL-PHASE CONCENTRATION, GM/CC, TRY 0.001
.005

ENTER THE NUMBER OF TERMS IN THE SERIES, ON I3, TRY 100
100

ENTER THE NUMBER OF INTERVAL HALVINGS TO USE, ON I2, TRY 20
20

ENTER VALUE FOR LEAD EXPONENTIAL FOR STEADY STATE APPROXIMATION,
TRY 0.01
.01

1. EDDY DIFFUSIVITY      = 1.85D+02 CM*CM/SEC
2. SLICK THICKNESS      = 1.00 CM
3. OCEAN DEPTH          = 5.0 METERS
4. OIL/WATER PARTITION = 2.50D+03 UNITLESS
5. MASS TRANSFER K      = 1.00D+00, CM/HR
6. INITIAL OIL CONC.   = 5.00D-03 GM/CC
7. NTERM = 100
8. NHALF = 20
9. STEADY STATE APPROXIMATION = 1.00D-02

WANT TO CHANGE ANY?
NO

DO IT AGAIN?
NO

CPU time 1.73   Elapsed time 2:05.10
```

TABLE 2: EXAMPLE OF CALCULATED WATER COLUMN CONCENTRATIONS FOR OVER-ALL MASS TRANSFER COEFFICIENT = 1 cm/hr

WELL-STIRRED OIL GLASS IN CONTACT WITH A DIFFUSION GLASS
 EASY DIFFUSIVITY = 1.000E-02 CM/HR. OIL SLICK THICKNESS = 1.00 CM. OCEAN DEPTH = 5.0 METERS
 OIL/WATER PARTITION COEFFICIENT = 2.500E+03 UNITLESS. OIL/WATER OVER-ALL MASS TRANSFER COEFFICIENT = 1.000E-02 CM/HR
 INITIAL EFFLUENT OIL-PHASE CONCENTRATION = 5.000E+03 CM/CM. NUMBER OF YEARS IN THE SERIES = 10. NUMBER OF INTERVALS BETWEEN
 SIZE OF LEAD EXPONENTIAL TO APPROXIMATE STEADY STATE = 1.00E-02

DIMENSIONLESS CONCENTRATIONS AT VARIOUS TIMES AND DEPTHS FOLLOW

METERS	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	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HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER	CONC.	HOURS	BARREL	WATER
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Mass transfer within the 5-meter water column is quite fast as indicated by the relatively flat concentration profiles.

The over-all mass-transfer coefficient appears to control the rate at which dissolved mass enters the water column. The over-all mass-transfer for this problem is based on water-phase concentrations since water-phase concentrations are of interest. This coefficient is based on the individual phase coefficients and a thermodynamic equilibrium expression relating the concentrations in each phase. This thermodynamic equilibrium expression is typically called a Henry's Law coefficient or partition coefficient (Leo, et al, 1971). The general relationships for the quantities of interest in the oil/water system are (Treybal, 1955):

$$C_{oil} = MC_{water}$$

$$\frac{1}{k_{oil}} = \frac{1}{k_{oil}} + \frac{m}{k_{water}}$$

$$\frac{1}{k_{water}} = \frac{1}{mk_{oil}} + \frac{1}{k_{water}}$$

where K stands for the over-all mass-transfer coefficient based on the phase identified in the subscript and k stands for the individual-phase coefficient.

For the oil/water system transferring molecular species will have m on the order of >1000 (unitless) which implies that the substance is quite soluble in oil and sparingly soluble in water. Since the over-all mass-transfer coefficient of interest is K_{water} , this yields

$$\frac{1}{k_{water}} = \frac{1}{1000k_{oil}} + \frac{1}{k_{water}}$$

Based on published work k_{water} is somewhat less than k_{oil} , but for sparingly soluble substances, such as naphthalene, the above expression becomes:

$$\frac{1}{K_{\text{water}}} = \frac{1}{k_{\text{water}}}$$

since the reciprocal of mk_{oil} is quite small. Typical values for K_{water} range from 1 to 10 cm/hr (Cohen, et al, 1980). In general, since the transferring substances of interest are quite soluble in oil relative to water, the water phase resistance usually is the controlling resistance to mass transfer. Thus, the mass transfer coefficient in the water phase (under the oil slick) is the area of interest in improving prediction capabilities and understanding.

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APPENDIX - CODE TO CALCULATE WATER COLUMN CONCENTRATIONS
OF DISSOLVE OIL SPECIES

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00010      IMPLICIT REAL*8 (A-H,O-Z)
00020      REAL*8 L,LCM,LCM2,M,KZ,KZS,KH,KPRME,MOIL,NWATER
00030      REAL*8 LTIME
00040      COMMON /TRANS/ KH,HCAP
00050      DIMENSION ALPHA(300),ALPHA2(300),P(300),CWP(300)
00060      DIMENSION CTD(11,10),XP(11),TIMEP(10),COIL(10)
00070      DIMENSION WATER(10),NWATER(10),MOIL(10),FLUX(10)
00080      DIMENSION A2P(300)
00090      DATA PIE,ETEST/3.1415926536D0,30.D0/
00100      OPEN(UNIT=32,DIALOG='DSKD:DISOLV.OUT')
00110      IOU=32
00120      C
00130      C
00140      C      THIS CODE CALCULATES THE WATER-COLUMN CONCENTRATION
00150      C      OF A SPECIFIC COMPOUND DISSOLVING INTO THE WATER
00160      C      FROM AN OIL SLICK
00170      C
00180      C      OCTOBER, 1982
00190      C
00200      10      TYPE 10
00210      10      FORMAT(/,1X,'ENTER THE EDDY DIFFUSIVITY, CM*CM/SEC
00220      10      1, TRY 100')
00230      20      ACCEPT 20, DW
00240      20      FORMAT(F10.0)
00250      30      TYPE 30
00260      30      FORMAT(/,1X,'ENTER THE SLICK THICKNESS, TRY 1 CM')
00270      30      ACCEPT 20, DELTA
00280      40      TYPE 40
00290      40      FORMAT(/,1X,'ENTER THE OCEAN DEPTH, TRY 20 METERS')
00300      40      ACCEPT 20, L
00310      50      TYPE 50
00320      50      FORMAT(/,1X,'ENTER THE OIL/WATER PARTITION COEFFICIENT
00330      50      1, UNITLESS, TRY 1000')
00340      50      ACCEPT 20, M
00350      60      TYPE 60
00360      60      FORMAT(/,1X,'ENTER THE OIL-WATER OVER-ALL MASS-
00370      60      1TRANSFER COEFFICIENT, TRY 1 CM/HR')
00380      60      ACCEPT 20, KZ
00390      70      TYPE 70
00400      70      FORMAT(/,1X,'ENTER THE INITIAL OIL-PHASE CONCENTRATION
00410      70      1, CM/CC, TRY 0.001')
00420      70      ACCEPT 20, CZ
00430      80      TYPE 80
00440      80      FORMAT(/,1X,'ENTER THE NUMBER OF TERMS IN THE SERIES
00450      80      1, ON 13, TRY 100')
00460      90      ACCEPT 90, NTERM
00470      90      FORMAT(I3)
00480      100      TYPE 100
00490      100      FORMAT(/,1X,'ENTER THE NUMBER OF INTERVAL HALVINGS
00500      100      1 TO USE, ON 12, TRY 20')
00510      110      ACCEPT 90, NHALF
00520      110      TYPE 110
00530      110      FORMAT(/,1X,'ENTER VALUE FOR LEAD EXPONENTIAL
00540      110      1 FOR STEADY STATE APPROXIMATION,./
00550      110      2,1X,'TRY 0.01')
00560      120      ACCEPT 20, ELEAD
00570      120      TYPE 130, DW
00580      130      FORMAT(/,1X,'1. EDDY DIFFUSIVITY      = ',1PD9.2,' CM*CM
00590      130      1/SEC')
00600      140      TYPE 140, DELTA
00610      140      FORMAT(1X,'2. SLICK THICKNESS      = ',F5.2,' CM')
00620      150      TYPE 150, L
00630      150      FORMAT(1X,'3. OCEAN DEPTH      = ',F5.1,' METERS')
00640      160      TYPE 160, M
00650      160      FORMAT(1X,'4. OIL/WATER PARTITION = ',1PD9.2,' UNIT
00660      160      1LESS')
00670      170      TYPE 170, KZ

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00670 170 FORMAT(1X,'5. MASS TRANSFER K      = '.1PD9.2', CM
00680 1/HR')
00690 TYPE 180, CZ
00700 180 FORMAT(1X,'6. INITIAL OIL CONC.    = '.1PD9.2', CM/CC')
00710 TYPE 190, NTERM
00720 190 FORMAT(1X,'7. NTERM = ',13)
00730 TYPE 200, NHALF
00740 200 FORMAT(1X,'8. NHALF = ',13)
00750 TYPE 210, ELEAD
00760 210 FORMAT(1X,'9. STEADY STATE APPROXIMATION = '.1PD9.2)
00770 TYPE 220
00780 220 FORMAT(/,1X,'WANT TO CHANGE ANY?')
00790 ACCEPT 230, ANS
00800 230 FORMAT(A1)
00810 IF(ANS.EQ.'N') GO TO 350
00820 TYPE 240
00830 240 FORMAT(/,1X,'ENTER THE LINE NUMBER TO BE CHANGED')
00840 ACCEPT 250, LINE
00850 250 FORMAT(I1)
00860 GO TO (260,270,280,290,300,310,320,330,340) LINE
00870 260 TYPE 10
00880 ACCEPT 20, DW
00890 GO TO 120
00900 270 TYPE 30
00910 ACCEPT 20, DELTA
00920 GO TO 120
00930 280 TYPE 40
00940 ACCEPT 20, L
00950 GO TO 120
00960 290 TYPE 50
00970 ACCEPT 20, M
00980 GO TO 120
00990 300 TYPE 60
01000 ACCEPT 20, KZ
01010 GO TO 120
01020 310 TYPE 70
01030 ACCEPT 20, CZ
01040 GO TO 120
01050 320 TYPE 80
01060 ACCEPT 90, NTERM
01070 GO TO 120
01080 330 TYPE 100
01090 ACCEPT 90, NHALF
01100 GO TO 120
01110 340 TYPE 110
01120 ACCEPT 20, ELEAD
01130 GO TO 120
01140 C
01150 C      CALCULATE THE PARAMETERS
01160 C
01170 350 KZS=KZ/3600.D0
01180 H=KZS/DW
01190 LCM=100.D0*L
01200 LCM2=LCM*LCM
01210 HCAP=LCM*H
01220 KPRME=LCM/(M*DELTA)
01230 TDL=DW/LCM2
01240 HCAP2=HCAP*HCAP
01250 OSUM=2.D0*KPRME*HCAP2
01260 WSUM=2.D0*HCAP2
01270 FLEAD=2.D0*DW*HCAP2/LCM
01280 CLEAD=1.D0/(1.D0+KPRME)
01290 XSTEP=LCM/10.D0
01300 ESIZE=DLOG(ELEAD)
01310 ESIZE=DABS(ESIZE)
01320 WRITE (100,360)

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01330 360 FORMAT(1H1,5X,'WELL-STIRRED OIL SLAB
01340 1 IN CONTACT WITH A DIFFUSION SLAB')
01350 WRITE (10U,370) DW,DELTA,L
01360 370 FORMAT(1X,'EDDY DIFFUSIVITY = ',1PD10.3
01370 1,' CM*CM/SEC, OIL SLICK THICKNESS = ',0PF3.2
01380 2,' CM, OCEAN DEPTH = ',F5.1,' METERS')
01390 WRITE (10U,380) M,KZ
01400 380 FORMAT(1X,'OIL/WATER SPECIES PARTITION COEFFICIENT =
01410 1,1PD10.3,' UNITLESS, OIL-WATER OVER-ALL MASS TRANSFER
01420 2 COEFFICIENT = ',1PD10.3,' CM/HR')
01430 WRITE (10U,390) CZ,NTERM,NHALF
01440 390 FORMAT(1X,'INITIAL SPECIES OIL-PHASE CONCENTRATION
01450 1 = ',1PD10.3,' CM/CC, NUMBER OF TERMS IN THE SERIES =
01460 2,13,' NUMBER OF INTERVAL HALVINGS = ',13)
01470 WRITE (10U,400) ELEAD
01480 400 FORMAT(1X,'SIZE OF LEAD EXPONENTIAL TO
01490 1 APPROXIMATE STEADY STATE = ',1PD9.2)
01500 C
01510 C CALCULATE THE ROOTS OF THE TRANSCENDENTAL FUNCTION,
01520 C ONE ROOT PER PIE
01530 C
01540 C THE TRANSCENDENTAL FUNCTION IS:
01550 C
01560 C  $F(X) = X \cdot \cotangent(X) - (X^2 - KH) / HCAP$ 
01570 C
01580 CNSUM=0.D0
01590 P1=KPRME*HCAP*HCAP*(1.D0+KPRME)
01600 P2=HCAP*HCAP+HCAP-2.D0*KPRME*HCAP
01610 WRITE (10U,410) P2,P1
01620 410 FORMAT(/,1X,'P = ALPHA**4 + ',1PD13.6,
01630 1,'*ALPHA**2 + ',1PD13.6)
01640 KH=KPRME*HCAP
01650 WRITE (10U,420) HCAP,KPRME,KH
01660 420 FORMAT(/,1X,'HCAP = ',1PD10.3,' K-PRIME = ',1PD10.3
01670 1,' KH = ',1PD10.3)
01680 CNORM=CZ/M
01690 CNORM6=(1.D+06)*CNORM
01700 DELTCZ=DELTA*CZ
01710 CNORML=CNORM*LCM
01720 FLEAD=FLEAD*CNORM
01730 WRITE (10U,430) CNORM,CNORM6
01740 430 FORMAT(/,1X,'THE NORMALIZING CONCENTRATION IS '
01750 1,1PD10.3,' CM/CC, OR ',1PD10.3,' PPM')
01760 WRITE (10U,440) DELTCZ
01770 440 FORMAT(/,1X,'INITIAL MASS/AREA OF TRANSPORTABLE
01780 1 SPECIES = ',1PD9.2,' GRAM/CM*CM')
01790 DO 470 N=1,NTERM
01800 AN=DFLOAT(N)
01810 AN1=DFLOAT(N-1)
01820 XL=AN*PIE
01830 XL1=XL
01840 XU=AN*PIE
01850 XU1=XU
01860 DO 460 I=1,NHALF
01870 XT=(XL+XU)/2.D0
01880 TEST=F(XT)
01890 IF(TEST.LT.0.D0) GO TO 450
01900 XL=XT
01910 GO TO 460
01920 450 XU=XT
01930 460 CONTINUE
01940 C
01950 C CALCULATE OTHER PERTINENT QUANTITIES INVOLVING
01960 C THE ALPHA ROOTS
01970 C
01980 ALPHA(N)=XT

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01990      CALPHA=DCOS(XT)
02000      ALPHA2(N)=XT*XT
02010      P(N)=ALPHA2(N)*(ALPHA2(N)+P2)+P1
02020      A2P(N)=ALPHA2(N)/P(N)
02030      CWP(N)=(ALPHA2(N)-KH)/(P(N)*CALPHA)
02040      CMSUM=CMSUM+1.D0/P(N)
02050  470    CONTINUE
02060      CL6=CNORM6*CLEAD
02070      WRITE (100,480) CLEAD,CL6
02080  480    FORMAT(//,5X,'THE CONSTANT TERM IN THE CONCENTRATION
02090 1 EXPRESSIONS IS = ',1PD9.2,' UNITLESS, OR ',1PD9.2
02100 2,' PPM')
02110      WRITE (100,490)
02120  490    FORMAT(5X,'WHICH IS THE STEADY STATE WATER CON
02130 1CENTRATION')
02140      DTIME=ESIZE/ALPHA2(1)
02150      STIMES=LCM2*DTIME/DW
02160      STIMEH=STIMES/3600.D0
02170      WRITE (100,500) STIMES,STIMEH
02180  500    FORMAT(/,5X,'STEADY STATE TIME = ',1PD10.3,' SEC
02190 1, OR ',1PD10.3,' HOURS')
02200      CMSUM=2.D0*KPRME*HCAP*HCAP*CMSUM
02210      CMZERO=CLEAD+CMSUM
02220      WRITE (100,510) CMZERO
02230  510    FORMAT(/,5X,'THE TIME=0 DIMENSIONLESS CONCENTRATION
02240 1 IN THE OIL = ',1PD13.6)
02250  C
02260  C      NOW COMPUTE SOME CONCENTRATION PROFILES AT TIMES
02270  C      BEFORE STEADY STATE
02280  C
02290      XSTEP=L/10.D0
02300      TSLOC=(DLOG10(DTIME))/10.D0
02310      TSCALE=LCM2/(3600.D0*DW)
02320      LTIME=0.D0
02330      DO 570 ITIME=1,10
02340      LTIME=LTIME+TSLOC
02350      TIME=10.D0**LTIME
02360      TIMEP(ITIME)=TSCALE*TIME
02370      X=0.D0
02380      DO 540 JX=1,11
02390      XARG=1.D0-X/L
02400      SUM=0.D0
02410      DO 520 N=1,NTERM
02420      XCARG=ALPHA(N)*XARG
02430      COSINE=DCOS(XCARG)
02440      EARG=ALPHA2(N)*TIME
02450      IF(EARG.GT.ETEST) GO TO 530
02460      SUM=SUM+CWP(N)*COSINE*DEXP(-EARG)
02470  520    CONTINUE
02480  530    SUM=CLEAD-2.D0*HCAP*SUM
02490      CTD(JX,ITIME)=SUM
02500      XP(JX)=X
02510      X=X+XSTEP
02520  540    CONTINUE
02530  C
02540  C      CALCULATE THE OIL CONCENTRATION ALSO FOR THE GIVEN
02550  C      TIME, AND THE AVERAGE WATER CONCENTRATION
02560  C
02570      SUM=0.D0
02580      FSUM=0.D0
02590      DO 550 N=1,NTERM
02600      EARG=ALPHA2(N)*TIME
02610      IF(EARG.GT.ETEST) GO TO 560
02620      EXTERM=DEXP(-EARG)
02630      SUM=SUM+EXTERM/P(N)
02640      FSUM=FSUM+A2P(N)*EXTERM

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02650 550 CONTINUE
02660 560 COIL(ITIME)=CLEAD+OSUM*SUM
02670 WATER(ITIME)=CLEAD-WSUM*SUM
02680 FLUX(ITIME)=FLEAD*FSUM
02690 570 CONTINUE
02700 WRITE (100,580)
02710 580 FORMAT(//,5X,'DIMENSIONLESS CONCENTRATIONS AT
02720 1 VARIOUS TIMES AND DEPTHS FOLLOW')
02730 WRITE (100,590)
02740 590 FORMAT(/,5X,'METERS',3X,'HOURS',9(6X,'HOURS'))
02750 WRITE (100,600) (TIMEP(I),I=1,10)
02760 600 FORMAT(10X,10(2X,1PD9.2),/)
02770 DO 630 JX=1,11
02780 WRITE (100,610) XP(JX),(CTD(JX,I),I=1,10)
02790 610 FORMAT(5X,F5.1,10(2X,1PD9.2))
02800 DO 620 I=1,10
02810 CTD(JX,I)=CNORM6*CTD(JX,I)
02820 620 CONTINUE
02830 630 CONTINUE
02840 WRITE (100,640) (COIL(I),I=1,10)
02850 640 FORMAT(/,6X,'OIL',/,5X,'CONC.',10(2X,1PD9.2))
02860 WRITE (100,650) (WATER(I),I=1,10)
02870 650 FORMAT(/,4X,'AVERAGE',/,5X,'WATER',/,5X,'CONC.',
02880 1,10(2X,1PD9.2))
02890 WRITE (100,660)
02900 660 FORMAT(//,5X,'ACTUAL CONCENTRATIONS IN PPM
02910 1 AT VARIOUS TIMES AND DEPTHS')
02920 WRITE (100,590)
02930 WRITE (100,600) (TIMEP(I),I=1,10)
02940 DO 670 JX=1,11
02950 WRITE (100,610) XP(JX),(CTD(JX,I),I=1,10)
02960 670 CONTINUE
02970 C
02980 C CALCULATE THE OVER-ALL MASS BALANCE TO SEE THAT
02990 C ALL THE MASS IS ACCOUNTED FOR
03000 C
03010 CZ6=CZ*(1.D+06)
03020 DO 680 I=1,10
03030 MOIL(I)=DELT CZ*COIL(I)
03040 HWATER(I)=CNORM1*WATER(I)
03050 COIL(I)=CZ6*COIL(I)
03060 WATER(I)=CNORM6*WATER(I)
03070 680 CONTINUE
03080 WRITE (100,640) (COIL(I),I=1,10)
03090 WRITE (100,650) (WATER(I),I=1,10)
03100 WRITE (100,690)
03110 690 FORMAT(/,1X,'THE MASSES THAT FOLLOW ARE IN GRAMS
03120 1/CM*CM, THE FLUX IS IN GRAMS/CM*CM/SEC')
03130 WRITE (100,700) (MOIL(I),I=1,10)
03140 700 FORMAT(/,4X,'MASS IN',/,6X,'OIL',1X
03150 1,10(2X,1PD9.2))
03160 WRITE (100,710) (HWATER(I),I=1,10)
03170 710 FORMAT(/,4X,'MASS IN',/,5X,'WATER',10(2X,1PD9.2))
03180 WRITE (100,720) (FLUX(I),I=1,10)
03190 720 FORMAT(/,3X,'MASS FLUX',/,2X,'AT SURFACE'
03200 1,1PD9.2,9(2X,1PD9.2))
03210 TYPE 730
03220 730 FORMAT(/,1X,'DO IT AGAIN?')
03230 ACCEPT 230,ANS
03240 IF(ANS.EQ.'Y') GO TO 120
03250 END
03260 DOUBLE PRECISION FUNCTION F(X)
03270 IMPLICIT REAL*8 (A-H,O-Z)
03280 REAL*8 KH
03290 COMMON /TRANS/ KH,RCAP
03300 SINE=DSIN(X)
03310 COSINE=DCOS(X)
03320 F=X*COSINE/SINE-(X*X-KH)/RCAP
03330 RETURN
03340 END

```

APPENDIX D

CODE LISTING FOR DISPERSED-OIL CONCENTRATION
PROFILES WITH A TIME VARYING FLUX

The computer code listing and user's instructions in this Appendix are for the calculation of dispersed-oil concentrations in the water column for a time-varying flux (Section 4.9). The user's instructions presented in the following example prompt the user for specific input and provides sample input.

TABLE 1. Example of Input for Calculation of Dispersed-Oil concentration profiles for a time-varying flux.

```
.EX DSFLUX.FOR
LINK: Loading
[LINKXCT DSFLUX execution]

DO YOU WANT DETAILED INPUT INSTRUCTIONS?
YES

THIS CODE CALCULATES THE WATER-COLUMN CONCENTRATION OF DISPERSED OIL.
YOU MUST ENTER THE FLUX AT THE SURFACE IN THE FORM OF  $A \times \exp(-B \times \text{TIME})$ .
YOU CAN ENTER THE FLUX AS A SUM OF THESE EXPONENTIALS.
AN EXAMPLE DERIVED FROM THE OIL-WEATHERING CODE FOR A
DISPERSION FLUX (20-KNOT WIND) FITTED WITH TWO EXPONENTIALS IS:
A(1)=6.4D-08 GM/CM*CM/SEC
B(1)=2.03D-06 INVERSE SECONDS
A(2)=5.1D-07
B(2)=3.19D-05
FOR THE NUMBER OF TERMS IN THE SERIES, USE 100

ENTER THE VERTICAL DIFFUSIVITY, CM*CM/SEC
185.

ENTER THE OCEAN DEPTH, METERS
50.

ENTER THE MAXIMUM TIME, HOURS
24.

ENTER THE NUMBER OF TERMS IN THE SERIES ON I3
100

DO YOU WANT PREVIOUSLY STORED DISPERSION RATE COEFFICIENTS TO BE USED
FOR A 10-, 20-, OR 40-KNOT WIND?
YES

ENTER 10, 20 OR 40 FOR THE WIND SPEED YOU WANT
20.

1. VERTICAL K = 1.850D+02 CM*CM/SEC
2. OCEAN DEPTH = 50.0 METERS
3. MAXIMUM TIME = 24. HOURS
4. NUMBER OF TERMS IN THE SERIES = 100
5. NUMBER OF EXPONENTIAL FITS = 2

6. A(1) = 6.400D-08 GM/CM*CM/SEC
7. B(1) = 2.030D-06 1/SEC
8. A(2) = 5.100D-07 GM/CM*CM/SEC
9. B(2) = 3.190D-05 1/SEC

WANT TO CHANGE ANY?
NO

DO IT AGAIN?
NO

CPU time 2.21 Elapsed time 1:08.18
```

TABLE 2. Code Listing for Calculating the Dispersed-oil Concentration Profiles with a Time-Varying Flux.

```

00010      IMPLICIT REAL*8 (A-H,O-Z)
00020      REAL*8 K,L,L2,KP2L,KP2LN
00030      DIMENSION AI(5),BI(5),C(10,10,5),ABL(5),TIME(10)
00040      1,SINGLE(5),SQRTBK(5),SQRTKB(5),BD(500,5),KP2LN(500)
00050      2,RATE(10),GRAMS(10,5),ACONC(10,5),A10(5),B10(5)
00060      3,A20(5),B20(5),A40(5),B40(5),S(10,10,5),SZERO(10,5)
00070      4,CZERO(10,5),XP(11)
00080      DATA A10/1.89D-07,2.03D-08,3*0.D0/
00090      DATA B10/1.436D-05,1.02D-06,3*0.D0/
00100      DATA A20/6.4D-08,5.1D-07,3*0.D0/
00110      DATA B20/2.03D-06,3.19D-05,3*0.D0/
00120      DATA A40/1.12D-07,4.04D-07,3*0.D0/
00130      DATA B40/3.053D-06,9.26D-06,3*0.D0/
00140      DATA ETRAP,PIE,PIE2/50.D0,3.141592654,9.869604401/
00150      C
00160      C
00170      C      THIS IS A CODE TO CALCULATE THE WATER-COLUMN
00180      C      CONCENTRATION OF DISPERSED OIL WITH A FLUX BOUNDARY
00190      C      CONDITION
00200      C      DECEMBER, 1982
00210      C
00220      OPEN(UNIT=33,DIALOG='DSKD:DSFLUX.OUT')
00230      IOU=33
00240      TYPE 10
00250      10  FORMAT(/,1X,'DO YOU WANT DETAILED INPUT INSTRUCTIONS?')
00260      ACCEPT 460,ANS
00270      IF(ANS.EQ.'N') GO TO 120
00280      TYPE 20
00290      20  FORMAT(/,1X,'THIS CODE CALCULATES THE WATER-COLUMN
00300      1  CONCENTRATION OF DISPERSED OIL.')
00310      TYPE 30
00320      30  FORMAT(1X,'YOU MUST ENTER THE FLUX AT THE SURFACE IN
00330      1  THE FORM OF A*EXP(-B*TIME).')
00340      TYPE 40
00350      40  FORMAT(1X,'YOU CAN ENTER THE FLUX AS A SUM OF THESE
00360      1  EXPONENTIALS.')
00370      TYPE 50
00380      50  FORMAT(1X,'AN EXAMPLE DERIVED FROM THE OIL-WEATHERING
00390      1  CODE FOR A')
00400      TYPE 60
00410      60  FORMAT(1X,'DISPERSION FLUX (20-KNOT WIND) FITTED WITH
00420      1  TWO EXPONENTIALS IS:')
00430      TYPE 70
00440      70  FORMAT(1X,'A(1)=6.4D-08 CM/CM*CM/SEC')
00450      TYPE 80
00460      80  FORMAT(1X,'B(1)=2.03D-06 INVERSE SECONDS')
00470      TYPE 90
00480      90  FORMAT(1X,'A(2)=5.1D-07')
00490      TYPE 100
00500      100 FORMAT(1X,'B(2)=3.19D-05')
00510      TYPE 110
00520      110 FORMAT(1X,'FOR THE NUMBER OF TERMS IN THE SERIES,
00530      1  USE 100')
00540      120 TYPE 130
00550      130 FORMAT(/,1X,'ENTER THE VERTICAL DIFFUSIVITY, CM*CM
00560      1/SEC')
00570      ACCEPT 140,K
00580      140 FORMAT(F10.0)
00590      TYPE 150
00600      150 FORMAT(/,1X,'ENTER THE OCEAN DEPTH, METERS')
00610      ACCEPT 140,DEPTH
00620      TYPE 160
00630      160 FORMAT(/,1X,'ENTER THE MAXIMUM TIME, HOURS')
00640      ACCEPT 140,HOURS
00650      TYPE 170
00660      170 FORMAT(/,1X,'ENTER THE NUMBER OF TERMS IN THE SERIES

```


TABLE 2. (Continued)

```

00670      1 ON I3')
00680      ACCEPT 180, NTERM
00690 180    FORMAT(I3)
00700      LIB=1
00710      TYPE 190
00720 190    FORMAT(/,1X,'DO YOU WANT PREVIOUSLY STORED DISPERSION
00730      1 RATE COEFFICENTS TO BE USED')
00740      TYPE 200
00750 200    FORMAT(1X,'FOR A 10-, 20-, OR 40-KNOT WIND?')
00760      ACCEPT 460, ANS
00770      IF(ANS.EQ.'N') GO TO 270
00780      NEF=2
00790      LIB=2
00800      TYPE 210
00810 210    FORMAT(/,1X,'ENTER 10, 20 OR 40 FOR THE WIND SPEED
00820      1 YOU WANT')
00830      ACCEPT 140, WIND
00840 220    IF(WIND.EQ.40.) GO TO 250
00850      IF(WIND.EQ.20.) GO TO 260
00860      IF(WIND.EQ.10.) GO TO 240
00870      TYPE 230
00880 230    FORMAT(/,1X,'YOU MUST ENTER 10, 20 OR 40, BUT
00890      1 YOU CAN ENTER 0 TO ENTER THE DATA YOURSELF')
00900      ACCEPT 140, WIND
00910      IF(WIND.EQ.0.) GO TO 270
00920      GO TO 220
00930 240    AI(1)=A10(1)
00940      BI(1)=B10(1)
00950      AI(2)=A10(2)
00960      BI(2)=B10(2)
00970      GO TO 360
00980 250    AI(1)=A40(1)
00990      BI(1)=B40(1)
01000      AI(2)=A40(2)
01010      BI(2)=B40(2)
01020      GO TO 360
01030 260    AI(1)=A20(1)
01040      BI(1)=B20(1)
01050      AI(2)=A20(2)
01060      BI(2)=B20(2)
01070      GO TO 360
01080 270    TYPE 280
01090 280    FORMAT(/,1X,'ENTER THE NUMBER OF EXPONENTIAL FITS ON I1')
01100      ACCEPT 290, NEF
01110 290    FORMAT(I1)
01120      IF(NEF.LT.5) GO TO 320
01130      TYPE 300
01140 300    FORMAT(/,1X,'THE NUMBER OF EXPONENTIAL FITS MUST
01150      1 BE 4 OR LESS.')
01160      TYPE 310
01170 310    FORMAT(1X,'AND THIS NUMBER HAS BEEN RESET TO 4')
01180      NEF=4
01190 320    DO 350 I=1,NEF
01200      TYPE 330, I
01210 330    FORMAT(/,1X,'ENTER A('',I1,''), CM/CM*CM/SEC')
01220      ACCEPT 140, AI(I)
01230      TYPE 340, I
01240 340    FORMAT(/,1X,'ENTER B('',I1,''), 1/SEC')
01250      ACCEPT 140, BI(I)
01260 350    CONTINUE
01270 360    TYPE 370, K
01280 370    FORMAT(/,2X,'1. VERTICAL K = ',1PD10.3,' CM*CM/SEC')
01290      TYPE 380, DEPTH
01300 380    FORMAT(2X,'2. OCEAN DEPTH = ',F5.1,' METERS')
01310      TYPE 390, HOURS
01320 390    FORMAT(2X,'3. MAXIMUM TIME = ',F5.0,' HOURS')

```

TABLE 2. (Continued)

```

01330      TYPE 400, NTERM
01340      400  FORMAT(2X,'4.  NUMBER OF TERMS IN THE SERIES = '
01350      1,13)
01360      TYPE 410, NEF
01370      410  FORMAT(2X,'5.  NUMBER OF EXPONENTIAL FITS = ',12)
01380      IROW=5
01390      DO 440 I=1,NEF
01400      IROW=IROW+1
01410      TYPE 420, IROW,I,AI(I)
01420      420  FORMAT(/,1X,12,'.  A('',I1,'') = ',1PD10.3,' CM
01430      1/CM*CM/SEC')
01440      IROW=IROW+1
01450      TYPE 430, IROW,I,BI(I)
01460      430  FORMAT(/,1X,12,'.  B('',I1,'') = ',1PD10.3,' 1/SEC')
01470      440  CONTINUE
01480      TYPE 450
01490      450  FORMAT(/,1X,'WANT TO CHANGE ANY?')
01500      ACCEPT 460, ANS
01510      460  FORMAT(A1)
01520      IF(ANS.EQ.'N') GO TO 530
01530      TYPE 470
01540      470  FORMAT(/,1X,'ENTER THE LINE NUMBER TO BE CHANGED')
01550      ACCEPT 290, ICHNG
01560      IF(ICHNG.GT.5) GO TO 530
01570      GO TO (480,490,500,510,520), ICHNG
01580      480  TYPE 130
01590      ACCEPT 140, K
01600      GO TO 360
01610      490  TYPE 150
01620      ACCEPT 140, DEPTH
01630      GO TO 360
01640      500  TYPE 160
01650      ACCEPT 140, HOURS
01660      GO TO 360
01670      510  TYPE 170
01680      ACCEPT 180, NTERM
01690      GO TO 360
01700      520  TYPE 280
01710      ACCEPT 290, NEF
01720      IF(NEF.LT.5) GO TO 360
01730      TYPE 300
01740      TYPE 310
01750      NEF=4
01760      GO TO 360
01770      C
01780      C      IS ICHNG EVEN OR ODD?
01790      C
01800      530  Z=DFLOAT(ICHNG)
01810      D=Z/2.D0
01820      M=D
01830      E=DFLOAT(M)
01840      TEST=DABS(E-D)
01850      IF(TEST.GT.0.1D0) GO TO 540
01860      C
01870      C      ICHNG IS EVEN, ENTER AI(J)
01880      C
01890      I=(ICHNG-4)/2
01900      TYPE 330, I
01910      ACCEPT 140, AI(I)
01920      GO TO 360
01930      540  I=(ICHNG-5)/2
01940      C
01950      C      ICHNG IS ODD, ENTER BI(J)
01960      C
01970      TYPE 340, I
01980      ACCEPT 140, BI(I)

```

TABLE 2. (Continued)

```

01990      GO TO 360
02000 550    CONTINUE
02010      GO TO (560,610) LIB
02020 560    TYPE 570
02030 570    FORMAT(/,1X,'THE WIND SPEED IS USED FOR IDENTIFICATION
02040      1 PURPOSES.')
```

```

02050 590    TYPE 580
02060 580    FORMAT(1X,'SO ENTER THE WIND SPEED IN KNOTS')
02070      ACCEPT 140, WIND
02080      TYPE 600, WIND
02090 600    FORMAT(/,1X,'YOU ENTERED ',F5.0,' KNOTS. IS THIS
02100      1 OK?')
02110      ACCEPT 460, ANS
02120      IF(ANS.EQ.'N') GO TO 590
02130      C
02140      C      CALCULATE THE CONTRIBUTION FOR THE WATER-COLUMN
02150      C      CONCENTRATION FOR EACH A.B SET
02160      C
02170      C      THE CONCENTRATION ARRAY IS SET UP SO THAT THE:
02180      C      ROW INDEX IS DEPTH
02190      C      COLUMN INDEX IS TIME
02200      C      LEVEL INDEX IS A.B SET NUMBER = J
02210      C
02220      C
02230      C      CONVERT THE TIME TO SECONDS
02240      C
02250 610    TSEC=3600.D0*HOURS
02260      TSTEP=TSEC/10.D0
02270      C
02280      C      *****
02290      C
02300      C      WARNING: THE COORDINATE FRAME FOR THIS PROBLEM IS
02310      C      REVERSED, I.E., THE OCEAN BOTTOM IS AT X=0, THE SURFACE
02320      C      IS AT X=L
02330      C
02340      C      *****
02350      C
02360      C      CONVERT THE DEPTH TO CENTIMETERS
02370      C
02380      L=100.D0*DEPTH
02390      XSTEP=L/10.D0
02400      L2=L*L
02410      KP2L=K*PIE2/L2
02420      PIEL=PIE/L
02430      C
02440      C      THE J INDEX RUNS THE A.B SET NUMBER
02450      C
02460      WRITE (100,620)
02470 620    FORMAT(1H1,4X,'CONCENTRATION OF DISPERSED OIL IN THE
02480      1 WATER COLUMN, CALCULATED BY EXPONENTIAL FITS TO A GIVEN
02490      2 DISPERSION RATE')
02500      WRITE (100,630) K,DEPTH,HOURS
02510 630    FORMAT(/,5X,'VERTICAL DIFFUSIVITY = ',1PD10.3
02520      1,' CM*CM/SEC, DEPTH = ',0PF6.0,' METERS, MAXIMUM
02530      2 TIME = ',F6.0,' HOURS')
02540      WRITE (100,640) KP2L
02550 640    FORMAT(/,5X,'K*PIE*PIE/L/L = ',1PD10.3
02560      1,' 1/SEC')
02570      WRITE (100,650) NTERM,NEF
02580 650    FORMAT(/,5X,'NUMBER OF TERMS IN THE SERIES = '
02590      1,I4,'. NUMBER OF EXPONENTIAL FITS = ',12)
02600      WRITE (100,660)
02610 660    FORMAT(/,5X,'THE EXPONENTIAL FIT COEFFICIENTS
02620      1 FOR THE DISPERSION RATE (RATE=A*EXP(-B*TIME)) ARE:')
02630      WRITE (100,670)
02640 670    FORMAT(5X,'UNITS ARE A==CM/CM*CM/SEC, B==1/SEC')
```

TABLE 2. (Continued)

```

02650      WRITE (10U,680)
02660      680  FORMAT(/,24X,'AI(J)',15X,'BI(J)')
02670      DO 700 J=1,NEF
02680      WRITE (10U,690) J,AI(J),BI(J)
02690      690  FORMAT(10X,11,2(10X,1PD10.3))
02700      700  CONTINUE
02710      C
02720      C      SET UP THE TIME STEPS FOR PRINTING
02730      C
02740      TS=HOURS/10.D0
02750      T=0.D0
02760      DO 710 IT=1,10
02770      T=T+TS
02780      TIME(IT)=T
02790      710  CONTINUE
02800      C
02810      C      WRITE OUT WHAT THE DISPERSION RATES ARE FOR THE
02820      C      A,B DATA SETS SO YOU CAN TELL IF YOU GOT
02830      C      THE CORRECT INPUT
02840      C
02850      WRITE (10U,720) WIND
02860      720  FORMAT(/,5X,'THE DISPERSION RATE FROM THE ABOVE
02870      1 A,B DATA SET FOR A WIND SPEED OF '.F5.0.' KNOTS IS:')
02880      WRITE (10U,730)
02890      730  FORMAT(/,18X,'TIME',11X,'RATE')
02900      WRITE (10U,740)
02910      740  FORMAT(18X,'HOUR',9X,'CM/M*M/HR')
02920      T=0.D0
02930      DO 770 IT=1,10
02940      T=T+TSTEP
02950      RATE (IT)=0.D0
02960      C
02970      C      NOW CALCULATE THE CONTRIBUTIONS TO THE
02980      C      CONCENTRATION PROFILE FOR EACH A,B INPUT SET
02990      C
03000      DO 750 J=1,NEF
03010      TARG=T*BI(J)
03020      IF(TARG.GT.ETRAP) GO TO 750
03030      RATE(IT)=RATE(IT)+AI(J)*DEXP(-TARG)
03040      750  CONTINUE
03050      C
03060      C      CONVERT THE RATE TO CM/M*M/HR AND PRINT IT
03070      C
03080      RATE(IT)=RATE(IT)*(3.60+07)
03090      WRITE (10U,760) TIME(IT),RATE(IT)
03100      760  FORMAT(10X,2(5X,1PD10.3))
03110      770  CONTINUE
03120      C
03130      C      BEGIN CALCULATING J CONTRIBUTIONS TO THE WATER-
03140      C      COLUMN CONCENTRATIONS OF DISPERSED OIL
03150      C
03160      DO 780 I=1,10
03170      GRAMS(I,5)=0.D0
03180      ACONC(I,5)=0.D0
03190      CZERO(I,5)=0.D0
03200      SZERO(I,5)=0.D0
03210      DO 780 J=1,10
03220      C(I,J,5)=0.D0
03230      S(I,J,5)=0.D0
03240      780  CONTINUE
03250      DO 1100 J=1,NEF
03260      C
03270      C      ABL(J) IS THE LEAD CONSTANT FOR CONCENTRATION
03280      C
03290      ABL(J)=AI(J)/(BI(J)*L)
03300      SQRTBK(J)=DSQRT(BI(J)/K)

```

TABLE 2. (Continued)

```

03310      SQRTKB(J)=DSQRT(K*BI(J))
03320      ARG=L*SQRTBK(J)
03330      WRITE (100,790) ABL(J)
03340 790    FORMAT(/,5X,'THE TIME = INFINITY WATER-COLUMN
03350      1 CONCENTRATION OF DISPERSED OIL = ',1PD10.3
03360      2,' GM/CC')
03370      WRITE (100,800) J
03380 800    FORMAT(/,5X,'A CHECK OF THE INITIAL CONDITIONS FOR
03390      1 THE J = ',12,' A,B INPUT SET')
03400      WRITE (100,810)
03410 810    FORMAT(/,15X,'DEPTH',10X,'EBL',12X,'SUM',8X
03420      1,'CONC AT T=0')
03430      WRITE (100,820)
03440 820    FORMAT(15X,'METER',8X,'COS TERM',8X,'SERIES',/)
03450      C
03460      C      SINGLE(J) IS THE LEAD EXPONENTIAL TERM NOT IN
03470      C      THE SUMMATION
03480      C
03490      C      TRAP ON SIN(ARG)=0
03500      C
03510      SINGLE(J)=AI(J)/(SQRTKB(J)*DSIN(ARG))
03520      COSL=DCOS(ARG)
03530      C
03540      C      SLEAD IS THE LEAD COEFFICIENT ON THE SUMMATION
03550      C
03560      SLEAD=2.D0*AI(J)/L
03570      DLEAD=AI(J)/(K*DSIN(ARG))
03580      C
03590      C      GENERATE THE TERMS IN THE SERIES FOR J
03600      C
03610      SIGN=1.D0
03620      DO 830 N=1,NTerm
03630      AN=DFLOAT(N)
03640      SIGN=-1.D0*SIGN
03650      KP2LN(N)=KP2L*AN*AN
03660      BD(N,J)=SIGN*SLEAD/(BI(J)-KP2LN(N))
03670 830    CONTINUE
03680      C
03690      C      CHECK THE INITIAL CONDITION
03700      C
03710      X=L
03720      DO 860 IX=1,11
03730      XARG=X*PIEL
03740      SUM=0.D0
03750      DO 840 N=1,NTerm
03760      AN=DFLOAT(N)
03770      SUM=SUM+BD(N,J)*DCOS(AN*XARG)
03780 840    CONTINUE
03790      EBL=SINGLE(J)*DCOS(SQRTBK(J)*X)
03800      CONC=ABL(J)-EBL+SUM
03810      XP(IX)=(L-X)/100.D0
03820      WRITE (100,850) XP(IX),EBL,SUM,CONC
03830 850    FORMAT(7X,4(5X,1PD10.3))
03840      X=X-XSTEP
03850 860    CONTINUE
03860      C
03870      C      NOW GENERATE SOME CONCENTRATIONS VERSES TIME
03880      C      AND DEPTH
03890      C
03900      WRITE (100,870)
03910 870    FORMAT(/,5X,'DISPERSED-OIL CONCENTRATIONS, GM/CC
03920      1. IN THE WATER COLUMN FOR VARIOUS TIMES AND DEPTHS
03930      2 FOLLOW')
03940      WRITE (100,880)
03950 880    FORMAT(/,50X,'H O U R S')
03960      WRITE (100,890) (TIME(IT),IT=1,10)

```

TABLE 2. (Continued)

```

03970 890  FORMAT(7X,'DEPTH',1X,10(1X,1PD9.2))
03980      WRITE (10U,900)
03990 900  FORMAT(7X,'METER')
04000 C
04010 C      DO THE SURFACE OF THE OCEAN FIRST
04020 C
04030      T=0.D0
04040      DO 920 IT=1,10
04050      T=T+TSTEP
04060      ARG=BI(J)*T
04070      EX=0.D0
04080      IF(ARG.LT.ETRAP) EX=DEXP(-ARG)
04090      CZERO(IT,J)=ABL(J)-SINGLE(J)*COSL*EX
04100      SIGN=1.D0
04110      DO 910 N=1,NTERM
04120      ARG=KP2LN(N)*T
04130      IF(ARG.GT.ETRAP) GO TO 920
04140      EX=DEXP(-ARG)
04150      SIGN=-1.D0*SIGN
04160      CZERO(IT,J)=CZERO(IT,J)+SIGN*BD(N,J)*EX
04170 910  CONTINUE
04180 920  CONTINUE
04190      WRITE (10U,960) XP(1),(CZERO(IT,J),IT=1,10)
04200      X=L
04210      DO 970 IX=1,10
04220      X=X-XSTEP
04230      CARG=X*PIEL
04240      XARG=SQRTBK(J)*X
04250      CTERM1=SINGLE(J)*DCOS(XARG)
04260      STERM1=DLEAD*DSIN(XARG)
04270      T=0.D0
04280      DO 950 IT=1,10
04290      T=T+TSTEP
04300      ARG=BI(J)*T
04310      EXBT=0.D0
04320      IF(ARG.LT.ETRAP) EXBT=DEXP(-ARG)
04330      EBT=EXBT*CTERM1
04340      STERM2=STERM1*EXBT
04350      SUM=ABL(J)-EBT
04360      SLOPE=0.D0
04370      DO 930 N=1,NTERM
04380      AN=DFLOAT(N)
04390      ARG=KP2LN(N)*T
04400      IF(ARG.GT.ETRAP) GO TO 940
04410      EX=DEXP(-ARG)
04420      ANCARG=AN*CARG
04430      CTERM=DCOS(ANCARG)
04440      STERM=DSIN(ANCARG)
04450      SUM=SUM+BD(N,J)*EX*CTERM
04460      SLOPE=SLOPE-BD(N,J)*EX*STERM*AN*PIEL
04470 930  CONTINUE
04480 940  C(IX,IT,J)=SUM
04490      S(IX,IT,J)=SLOPE+STERM2
04500 950  CONTINUE
04510      WRITE (10U,960) XP(IX+1),(C(IX,IT,J),IT=1,10)
04520 960  FORMAT(5X,F7.1,1X,10(1X,1PD9.2))
04530 970  CONTINUE
04540 C
04550 C      WRITE OUT THE WATER-COLUMN CONCENTRATION DERIVATIVE
04560 C      WITH RESPECT TO X. IN CM/(CM**4)
04570 C
04580      WRITE (10U,980)
04590 980  FORMAT(//,5X,'THE DERIVATIVE WITH RESPECT TO X OF
04600      1 THE WATER COLUMN CONCENTRATION FOLLOWS. IN CM/(CM**4)')
04610      WRITE (10U,880)
04620      WRITE (10U,890) (TIME(IT),IT=1,10)

```

TABLE 2 . (Continued)

```

04630      WRITE (100,900)
04640      DO 990 IT=1,10
04650      SZERO(IT,J)=0.D0
04660  990    CONTINUE
04670      T=0.D0
04680      DO 1000 IT=1,10
04690      T=T+TSTEP
04700      ARG=BI(J)*T
04710      IF(ARG.GT.ETRAP) GO TO 1010
04720      SZERO(IT,J)=AI(J)*DEXP(-ARG)/K
04730  1000   CONTINUE
04740  1010   WRITE (100,960) XP(1),(SZERO(IT,J),IT=1,10)
04750      DO 1020 IX=1,10
04760      WRITE (100,960) XP(IX+1),(S(IX,IT,J),IT=1,10)
04770  1020   CONTINUE
04780  C
04790  C      CALCULATE THE GRAMS FLUXED INTO THE WATER COLUMN
04800  C      BY INTEGRATING THE SPECIFIED FLUX
04810  C
04820      AB=AI(J)/BI(J)
04830      T=0.D0
04840      DO 1030 IT=1,10
04850      T=T+TSTEP
04860      TARG=T*BI(J)
04870      EX=0.D0
04880      IF(TARG.LT.ETRAP) EX=DEXP(-TARG)
04890      GRAMS(IT,J)=AB*(1.D0-EX)
04900      ACONC(IT,J)=GRAMS(IT,J)/L
04910  1030   CONTINUE
04920      WRITE (100,1040)
04930  1040   FORMAT(/,3X,'GRAMS OIL')
04940      WRITE (100,1050) (GRAMS(IT,J),IT=1,10)
04950  1050   FORMAT(4X,'IN WATER',1X,10(1X,1PD9.2))
04960      WRITE (100,1060)
04970  1060   FORMAT(3X,'PER CM*CM')
04980      WRITE (100,1070)
04990  1070   FORMAT(/,5X,'AVERAGE')
05000      WRITE (100,1080) (ACONC(IT,J),IT=1,10)
05010  1080   FORMAT(7X,'GM/CC',1X,10(1X,1PD9.2))
05020      WRITE (100,1090) J,J
05030  1090   FORMAT(/,5X,'*****')
05040  1      END OF CALCULATION FOR A('I1,'). B('I1,')
05050  1100   CONTINUE
05060      IF(NEF.EQ.1) GO TO 1200
05070  C
05080  C      SUM UP THE CONCENTRATION CONTRIBUTIONS FOR EACH
05090  C      SET OF EXPONENTIAL FITS TO THE DISPERSION RATES
05100  C
05110      DO 1120 I=1,10
05120      DO 1120 M=1,10
05130      DO 1110 J=1,NEF
05140      S(I,M,5)=S(I,M,5)+S(I,M,J)
05150      C(I,M,5)=C(I,M,5)+C(I,M,J)
05160  1110   CONTINUE
05170  1120   CONTINUE
05180      DO 1140 N=1,10
05190      DO 1130 J=1,NEF
05200      CZERO(M,5)=CZERO(M,5)+CZERO(M,J)
05210      SZERO(M,5)=SZERO(M,5)+SZERO(M,J)
05220      GRAMS(M,5)=GRAMS(M,5)+GRAMS(M,J)
05230      ACONC(M,5)=ACONC(M,5)+ACONC(M,J)
05240  1130   CONTINUE
05250  1140   CONTINUE
05260      WRITE (100,1150) NEF
05270  1150   FORMAT(/,3X,'CONCENTRATIONS VERSES TIME AND DEPTH
05280  1 FOR 'I1,' A,B DATA SETS (ADD UP THE PREVIOUS

```

TABLE 2. (Continued)

```

05290      2 RESULTS'))
05300      WRITE (10U,880)
05310      WRITE (10U,890) (TIME(IT),IT=1,10)
05320      WRITE (10U,900)
05330      WRITE (10U,960) XP(1),(CZERO(IT,5),IT=1,10)
05340      DO 1160 IX=1,10
05350      WRITE (10U,960) XP(IX+1),(C(IX,IT,5),IT=1,10)
05360 1160 CONTINUE
05370      WRITE (10U,1170) NEF
05380 1170 FORMAT(/,5X,'THE DERIVATIVE OF THE CONCENTRATION
05390 1 WITH RESPECT TO X FOR '.I1,' A.B DATA SETS')
05400      WRITE (10U,880)
05410      WRITE (10U,890) (TIME(IT),IT=1,10)
05420      WRITE (10U,900)
05430      WRITE (10U,960) XP(1),(SZERO(IT,5),IT=1,10)
05440      DO 1180 IX=1,10
05450      WRITE (10U,960) XP(IX+1),(S(IX,IT,5),IT=1,10)
05460 1180 CONTINUE
05470      WRITE (10U,1040)
05480      WRITE (10U,1050) (GRAMS(M,5),M=1,10)
05490      WRITE (10U,1060)
05500      WRITE (10U,1070)
05510      WRITE (10U,1080) (ACONC(M,5),M=1,10)
05520      WRITE (10U,1190) NEF
05530 1190 FORMAT(/,5X,'*****')
05540 1 END OF CALCULATION FOR ALL '.I1,' OF THE A.B SETS')
05550 1200 TYPE 1210
05560 1210 FORMAT(/,1X,'DO IT AGAIN?')
05570      ACCEPT 460, ANS
05580      IF(ANS.EQ.'Y') GO TO 360
05590      END

```


APPENDIX E

CODE LISTING FOR DISPERSED-OIL CONCENTRATION
PROFILES WITH A CONSTANT FLUX

The computer code listing and user's instructions in this Appendix are for the calculation of dispersed-oil concentrations in the water column for a constant flux (Section 4.9). The user's instructions presented in the following example prompt the user for specific input.

TABLE 1. User Input Instructions to Calculate Dispersed-oil
Profiles with a Constant Flux

.EX CFLUX.FOR
FORTRAN: CFLUX
MAIN.
ERFC1
LINK: Loading
[LNKXCT CFLUX execution]

ENTER THE VERTICAL EDDY DIFFUSIVITY, CM*CM/SEC
185.

ENTER THE CONSTANT FLUX AT THE SURFACE, GM/CM*CM/SEC
2.22E-08

ENTER THE OCEAN DEPTH, METERS
50.

ENTER THE MAXIMUM TIME, HOURS
12.5

ENTER THE NUMBER OF TERMS IN THE IERFC SERIES
99

ENTER THE NUMBER OF TERMS IN THE ERF SERIES
99

1. VERTICAL DIFFUSIVITY = 1.8500×10^2 CM*CM/SEC
2. FLUX AT THE SURFACE = 2.2200×10^{-8} GM/CM*CM/SEC
3. OCEAN DEPTH = 50.0 METERS
4. MAXIMUM TIME = 12.5 HOURS
5. NUMBER OF TERMS IN IERFC SERIES = 99
6. NUMBER OF TERMS IN ERF SERIES = 99

WANT TO CHANGE ANY?
NO

DO IT AGAIN?
N

CPU time 3.13 Elapsed time 1:00.40

TABLE 2. COMPUTER CODE LISTING FOR CALCULATING DISPERSED-OIL CONCENTRATION PROFILE IN WATER COLUMN FOR A CONSTANT FLUX SOURCE.

```

00010      IMPLICIT REAL*8 (A-H,O-Z)
00020      REAL*8 K,L
00030      COMMON /EXTRA/ ERF,ETRAP,IMAX
00040      DIMENSION SUM(10),D(11),DP(11),T(10),TP(10)
00050      1,TIME4(10),TIMEK(10)
00060      DATA ETRAP/70.D0/
00070      OPEN(UNIT=32,DIALOG='DSKD:CFLUX.OUT')
00080
00090      C      THIS IS A CODE TO CALCULATE THE WATER-COLUMN
00100      C      CONCENTRATION OF DISPERSED OIL WITH A CONSTANT-
00110      C      FLUX BOUNDARY CONDITION.
00120      C
00130      C      MAY, 1983
00140      C
00150      IOU=32
00160      TYPE 10
00170      10  FORMAT(/,1X,'ENTER THE VERTICAL EDDY DIFFUSIVITY
00180      1, CM*CM/SEC')
00190      ACCEPT 20, K
00200      20  FORMAT(F10.0)
00210      TYPE 30
00220      30  FORMAT(/,1X,'ENTER THE CONSTANT FLUX AT THE
00230      1 SURFACE, CM/CM*CM/SEC')
00240      ACCEPT 20, W
00250      TYPE 40
00260      40  FORMAT(/,1X,'ENTER THE OCEAN DEPTH, METERS')
00270      ACCEPT 20, DM
00280      TYPE 50
00290      50  FORMAT(/,1X,'ENTER THE MAXIMUM TIME, HOURS')
00300      ACCEPT 20, HOURS
00310      TYPE 60
00320      60  FORMAT(/,1X,'ENTER THE NUMBER OF TERMS IN THE IERFC
00330      1 SERIES')
00340      ACCEPT 70, NTERM
00350      70  FORMAT(I2)
00360      TYPE 80
00370      80  FORMAT(/,1X,'ENTER THE NUMBER OF TERMS IN THE ERF
00380      1 SERIES')
00390      ACCEPT 70, IMAX
00400      C
00410      C      ECHO CHECK
00420      C
00430      90  LINE=1
00440      TYPE 100, LINE,K
00450      100  FORMAT(/,1X,I1,'. VERTICAL DIFFUSIVITY = '
00460      1,1PD10.3,' CM*CM/SEC')
00470      LINE=LINE+1
00480      TYPE 110, LINE,W
00490      110  FORMAT(1X,I1,'. FLUX AT THE SURFACE = ',1PD10.3
00500      1,' CM/CM*CM/SEC')
00510      LINE=LINE+1
00520      TYPE 120, LINE,DM
00530      120  FORMAT(1X,I1,'. OCEAN DEPTH = ',F5.1,' METERS')
00540      LINE=LINE+1
00550      TYPE 130, LINE,HOURS
00560      130  FORMAT(1X,I1,'. MAXIMUM TIME = ',F5.1,' HOURS')
00570      LINE=LINE+1
00580      TYPE 140, LINE,NTERM
00590      140  FORMAT(1X,I1,'. NUMBER OF TERMS IN IERFC SERIES = ',I2)
00600      LINE=LINE+1
00610      TYPE 150, LINE,IMAX
00620      150  FORMAT(1X,I1,'. NUMBER OF TERMS IN ERF SERIES = ',I2)
00630      TYPE 160
00640      160  FORMAT(/,1X,'WANT TO CHANGE ANY?')
00650      ACCEPT 170, ANS
00660      170  FORMAT(A1)

```

TABLE 2. (Continued)

```

00670      IF(ANS.EQ.'N') GO TO 250
00680      TYPE 180
00690 180    FORMAT(/,1X,'ENTER LINE NUMBER TO BE CHANGED')
00700      ACCEPT 70, LINE
00710      GO TO (190,200,210,220,230,240) LINE
00720 190    TYPE 10
00730      ACCEPT 20, K
00740      GO TO 90
00750 200    TYPE 40
00760      ACCEPT 20, W
00770      GO TO 90
00780 210    TYPE 50
00790      ACCEPT 20, DM
00800      GO TO 90
00810 220    TYPE 50
00820      ACCEPT 20, HOURS
00830      GO TO 90
00840 230    TYPE 60
00850      ACCEPT 70, NTERM
00860      GO TO 90
00870 240    TYPE 80
00880      ACCEPT 70, IMAX
00890      GO TO 90
00900      C
00910      C      CALCULATE THE CONCENTRATION PROFILES.
00920      C
00930 250    TSEC=HOURS*3600.D0
00940      TS1=TSEC/10.D0
00950      TS2=HOURS/10.D0
00960      DCM=100.D0*DM
00970      L=DCM
00980      DS1=DCM/10.D0
00990      DS2=DM/10.D0
01000      WRITE (10U,260)
01010 260    FORMAT(1H1,'CONCENTRATION PROFILES IN THE WATER
01020      1 COLUMN FOR DISPERSED OIL (NEUTRAL DENSITY)')
01030      WRITE (10U,270)
01040 270    FORMAT(1X,'CALCULATED FOR A CONSTANT FLUX (
01050      1 IERC SOLUTION) AT THE OCEAN SURFACE')
01060      WRITE (10U,280) K,W
01070 280    FORMAT(/,1X,'VERTICAL EDDY DIFFUSIVITY = ',1PD9.2,
01080      1 ' CM*CM/SEC. DISPERSED OIL FLUX = ',1PD9.2,
01090      2 ' CM/CM*CM/SEC')
01100      WRITE (10U,290) DM,HOURS,NTERM
01110 290    FORMAT(1X,'OCEAN DEPTH = ',F5.1,' METERS, MAX
01120      1 INUM TIME = ',F5.1,' HOURS, NUMBER OF TERMS IN
01130      2 IERFC SERIES = ',I3)
01140      WRITE (10U,300) IMAX
01150 300    FORMAT(1X,'NUMBER OF TERMS IN ERF SERIES = ',I3)
01160      WRITE (10U,310)
01170 310    FORMAT(/,1X,'DISPERSED-OIL CONCENTRATIONS,
01180      1 CM/CC, IN THE WATER COLUMN FOR VARIOUS TIMES
01190      2 AND DEPTHS FOLLOW')
01200      WRITE (10U,320)
01210 320    FORMAT(/,53X,'H O U R S')
01220      WRITE (10U,330)
01230 330    FORMAT(5X,'DEPTH')
01240      C
01250      C      SET UP THE DEPTHS.
01260      C
01270      DO 340 I=1,11
01280      A=I-1
01290      D(I)=A*DS1
01300      DP(I)=A*DS2
01310 340    CONTINUE
01320      C

```

TABLE 2. (Continued)

```

01330 C      SET UP THE TIMES.
01340 C
01350      DO 350 I=1,10
01360      A=I
01370      T(I)=A*TS1
01380      TIME4(I)=W*2.D0*DSQRT(T(I)/K)
01390      TIMEK(I)=2.D0*DSQRT(K*T(I))
01400      TP(I)=A*TS2
01410 350 CONTINUE
01420      WRITE (10U,360) (TP(I),I=1,10)
01430 360 FORMAT(5X,'METER',2X,10(2X,1PD9.2),/)
01440 C
01450 C      CALCULATE THE CONCENTRATION PROFILES.
01460 C
01470      DO 400 I=1,11
01480      A=I-1
01490      X=DCM-A*DS1
01500      DO 380 J=1,10
01510      SUM(J)=0.D0
01520      DO 370 N=1,NTERM
01530      A=2*(N-1)+1
01540      AL=A*L
01550      ARG1=(AL-X)/TIMEK(J)
01560      ARG2=(AL+X)/TIMEK(J)
01570      E1=ERFC1(ARG1)
01580      E2=ERFC1(ARG2)
01590      SUM(J)=SUM(J)+E1+E2
01600 370 CONTINUE
01610      SUM(J)=TIME4(J)*SUM(J)
01620 380 CONTINUE
01630      WRITE (10U,390) DP(I),(SUM(J),J=1,10)
01640 390 FORMAT(5X,F5.1,2X,10(2X,1PD9.2))
01650 400 CONTINUE
01660      TYPE 410
01670 410 FORMAT(/,1X,'DO IT AGAIN?')
01680      ACCEPT 170,ANS
01690      IF(ANS.EQ.'Y') GO TO 90
01700      END
01710      DOUBLE PRECISION FUNCTION ERFC1(X)
01720      IMPLICIT REAL*8 (A-H,O-Z)
01730      COMMON /EXTRA/ ERF,ETRAP,IMAX
01740      DIMENSION A(100)
01750 C
01760 C      CALCULATE THE FIRST REPEATED INTEGRAL OF THE ERROR
01770 C      FUNCTION ACCORDING TO EQN(11), PAGE 484, IN
01780 C      CARSLAW AND JAEGER, 1967.
01790 C
01800 C      IERFC(X)=(EXP(-X*X))/SQRT(PIE)-X*ERFC(X)
01810 C
01820 C      MAY 13, 1983
01830 C      CALCULATE ERF(X) ACCORDING TO EQN (7.1.6) PAGE 297 IN NBS
01840 C      MATH HANDBOOK BY ABRAMOWITZ AND STEGUN.
01850 C      SYMMETRY IS ERF(-X) = -ERF(X). IF X.GT.3 THEN ERF = 1.
01860 C      20 TERMS IN THE SERIES APPEARS TO BE QUITE SUFFICIENT.
01870 C      THIS ROUTINE RETURNS ERF(X) AND DOES NOT DESTROY X OR THE
01880 C      SIGN OF X.
01890 C
01900 C      MAY 12, 1981
01910 C
01920      DATA PISQRT,IN/1.7724538509D0,1/
01930      GO TO (10,30), IN
01940 10 IN=2
01950      A(1)=1.0D0
01960      DO 20 I=1,IMAX
01970      A(I+1)=2.0D0*A(I)/(2.0D0*DFLOAT(I)+1.0D0)
01980 20 CONTINUE

```


TABLE 2. (Continued)

```

01990      30      SIGN=1.D0
02000      IF(X.GT.0.D0) GO TO 40
02010      X=DABS(X)
02020      SIGN=-1.D0
02030      40      IF(X.GT.3.D0) GO TO 70
02040      ERF=A(1)*X
02050      DO 50 I=1,IMAX
02060      IPOW=2*I+1
02070      TEMP=A(I+1)*X**IPOW
02080      IF(TEMP.LT.1.0D-10) GO TO 60
02090      50      ERF=ERF+TEMP
02100      60      ERF=2.0D0*DEXP(-X*X)*ERF/PISQRT
02110      GO TO 80
02120      70      ERF=1.D0
02130      X=SIGN*X
02140      80      ERF=SIGN*ERF
02150      C
02160      C      NOW CALCULATE IERFC(X)
02170      C
02180      XARG=X*X
02190      EX=0.D0
02200      IF(XARG.LT.ETRAP) EX=DEXP(-XARG)
02210      ERFC1=EX/PISQRT-X*(1.D0-ERF)
02220      RETURN
02230      END

```

APPENDIX F

METHODS FOR MICROBIAL DEGRADATION STUDIES

^{14}C -Hydrocarbon Mineralization Assay

Three ^{14}C -labeled hydrocarbon substrates were utilized for the determination of hydrocarbon degradation potential, defined here as the percent mineralization to $^{14}\text{CO}_2$: $n(1\text{-}^{14}\text{C})$ hexadecane (53.6 mCi/mmol, Amersham), $(1(4,5,8)\text{-}^{14}\text{C})$ naphthalene (5 mCi/mmol, Amersham), and $(1(4,5,8)\text{-}^{14}\text{C})$ methyl-naphthalene (5 mCi/mmol, Bionuclear). Working solutions were prepared with hexane or benzene as solvents to give $0.1\ \mu\text{Ci}/\mu\text{l}$ activities, stored at 4°C , and assayed weekly for radioactivity to insure consistency in the concentrations of substrates. Seawater aliquots (50 ml) from each of the experimental tanks and the incoming seawater were transferred to 100 ml sterile serum bottles and spiked with $0.5\ \mu\text{Ci}$ of the ^{14}C -labeled hydrocarbons, one compound per sample with each sample prepared in duplicate. Controls were killed with $1\ \mu\text{M}\ \text{HgCl}_2$ prior to spiking with the labeled compound.

The spiked seawater samples were capped with sleeve stoppers and incubated in the dark for 24 hours at in situ temperatures in a seawater bath. After the incubation period the stoppers were replaced with identical stoppers fitted with a polypropylene "center well" containing a 25-mm by 30-mm rectangle of Whatman No. 1 filter paper folded into an accordion-pleated array and wetted with $200\ \mu\text{l}$ of $1\text{N}\ \text{NaOH}$. The samples were then acidified to pH 2.0 by injection of $0.5\ \text{ml}$ of $1\ \text{N}\ \text{H}_2\text{SO}_4$ (through the sleeve stopper) with a hypodermic syringe. After 2 hours the filter paper was transferred to a second 100 ml serum bottle containing $1\ \text{ml}$ of $1\text{N}\ \text{H}_2\text{SO}_4$ which was quickly capped with a sleeve stopper fitted with a center well (as before) and a wick which had been wetted with $200\ \mu\text{l}$ of phenethylamine.

After 12-14 hours the phenethylamine wicks were transferred to a scintillation vial containing $10\ \text{ml}$ of Beta-Phase cocktail (West Chem Products) and assayed for radioactivity on a Beckman LS100C scintillation counter.

The resulting counts for duplicates were averaged and corrected for the control counts prior to further data treatment. The data (in counts per minute) were converted to $\mu\text{g/liter}\cdot\text{day}$ by the following equation.

$$\mu\text{g/l}\cdot\text{day} = (\text{cpm}) \left(\frac{1 \text{ dpm}}{0.9 \text{ cpm}} \right) \left(\frac{1 \mu\text{Ci}}{2.22 \times 10^6 \text{ dpm}} \right) (\text{S.A.}^{-1}) (\text{m.w.}) \left(\frac{1000 \text{ ml}}{1 \text{ l}} \right) \left(\frac{1}{50 \text{ ml}} \right) \left(\frac{1}{\text{day}} \right)$$

where a counting efficiency of 90% was utilized, SA is the specific activity in $\mu\text{Ci}/\mu\text{mole}$, and M.W. is the molecular weight of the particular labeled substrate.

References: WATSON et al. (1971); CAPARELLO and LA ROCK (1975); WALKER and COLWELL (1976); HODSON et al. (1977).

³H-Thymidine Incorporation

Thymidine (methyl-³H) solutions were stored as supplied (20 Ci/mmol, New England Nuclear) in 70% aqueous ethanol for maximum stability. Working solutions were prepared by evaporating to dryness the appropriate volume under a stream of dry filtered air and reconstituting with distilled water. These solutions were stored at 4°C and checked weekly for radioactivity.

Duplicate seawater aliquots (10 ml) from each experimental aquarium and the incoming seawater were spiked with 5nM of labeled thymidine and incubated in the dark at in situ temperatures for 1 hour. Incubation uptake was terminated by filtration through a 25-mm dia. type HA membrane (0.45 μm nominal pore size, Millipore Corp.). After filtration the vacuum was stopped and 10 ml of ice-cold (< 5°C) filtered (sterile) seawater was added to cool the filter. This was filtered through and the vacuum was stopped prior to addition of 15 ml ice-cold (< 5°C) 5% trichloroacetic acid (TCA) to extract the soluble thymidine pools from the cells. Temperature control is critical during the extraction as a temperature rise above 10°C for TCA will hydrolyse DNA and allow incorporated label to solubilize and pass through the filter. After

3 min. the vacuum was started and the filter was rinsed twice with ~5 ml ice-cold 5%, TCA, and then placed in a scintillation vial. Ethyl acetate (1 ml) was added to dissolve the filter; 10 ml of Beta-Phase cocktail was added and the radioactivity was assayed by liquid scintillation spectrometry.

The resulting counts for duplicates were averaged and corrected for poisoned controls ($1 \mu\text{M HgCl}_2$) and a counting efficiency of 35%. The data were converted to nmoles/liter day of incorporation by the formula:

$$\text{n moles/l} \cdot \text{day} = (\text{cpm}) \left(\frac{1 \text{ dpm}}{0.35 \text{ cpm}} \right) \left(\frac{1 \text{ Ci}}{2.22 \times 10^{12} \text{ dpm}} \right) \left(\frac{1 \text{ m mol}}{20 \text{ Ci}} \right) \left(\frac{10^6 \text{ n mol}}{\text{m mol}} \right) \left(\frac{24 \text{ hr}}{\text{day}} \right) \left(\frac{1}{0.015 \text{ l}} \right) \left(\frac{1}{1 \text{ hr}} \right)$$

References: FUHRMAN and AZAM (1980); FUHRMAN et al. (1980); FUHRMAN and AZAM (in press, 1981)

^3H -Leucine and ^3H -Glucose Uptake

The procedure for both substrates was identical except for the amino acid leucine, in that a larger sample was prepared such that an aliquot could be saved and preserved for the autoradiography procedure (details in this section).

Working solutions of ^3H -Leucine (60 Ci/mmol, New England Nuclear) were prepared by diluting an aliquot of the stock solution into distilled water. The ^3H -Glucose solutions (30 Ci/mmol, New England Nuclear) were prepared by evaporating an aliquot under a stream of dry, filtered air followed by reconstitution in distilled water. All solutions were stored at 4°C and assayed weekly for radioactivity to check stability.

Each experimental aquarium and the incoming seawater was sampled in duplicate and controls were killed with 1 M HgCl_2 prior to addition of radiolabeled substrate. To each sample (10 ml for ^3H -Glucose; 15 ml for ^3H -Leucine) 50 μl (1.5 μCi) of radiolabeled compound was added, followed by incubation for 2 hr. in the dark at in situ temperature.

The incubation was terminated by sample filtration through a HA membrane (0.45 μm nominal pore size, Millipore Corp.), followed by several washes with filter-sterilized seawater to remove any nonincorporated label. After filtration, each filter was placed in a scintillation vial, and 1 ml Ethyl acetate added to dissolve the membrane. After approximately 10 min., 10 ml of Beta-Phase cocktail was added and the sample assayed for radioactivity by liquid scintillation spectrometry. Duplicates were averaged and corrected for control blanks, and the resulting counts were converted to uptake in nmoles/liter day with the formula:

$$\text{n moles/l-day} = (\text{cpm}) \left(\frac{1 \text{ dpm}}{0.35 \text{ cpm}} \right) \left(\frac{1 \text{ Ci}}{2.22 \times 10^{12} \text{ dpm}} \right) (\text{S.A.}^{-1}) \left(\frac{10^6 \text{ n mol}}{\text{m mol}} \right) \left(\frac{24 \text{ hr}}{\text{day}} \right) \left(\frac{1}{2 \text{ hr}} \right) \left(\frac{1}{0.015 \text{ l}} \right)$$

where a counting efficiency of 35% was utilized and S.A. is the specific activity (in Ci/mmol) for the labeled substrate.

References: AZAM and HOLM-HANSEN (1973); FUHRMAN et al. (1980).

Epifluorescence Enumeration

Seawater samples (10-15 ml) from each experimental aquarium and the incoming seawater were immediately preserved with 4% filter-sterilized formalin (buffered with $\text{Na}_2\text{B}_4\text{O}_7$), and the cellular DNA was stained to fluoresce with Acridine orange (0.01%, 2 min.) prior to filtration. The Nucleopore polycarbonate filters were stained prior to use with Irgalan black (to eliminate autofluorescence) and a type AA (0.8 μm , Millipore) membrane was

used as a back filter to distribute the vacuum evenly. After filtration, the filter was mounted on a microscope slide with a cover slip affixed with paraffin oil. Blanks were prepared in a similar fashion except that filter-sterilized seawater (GS, 0.2 μm , Millipore Corp.) was preserved and stained.

The slides were examined by epifluorescence microscopy and counted in a random fashion by grids. All counts for each grid were averaged (10 grids per slide) for duplicate slides and the data converted to cells $\times 10^6/\text{ml}$ seawater.

References: HOBBIÉ et al. (1977); FUHRMAN and AZAM (1980).

Autoradiography Assay

The micro-autoradiographic technique provides for simultaneous examination by phase contrast microscopy of bacterial cells stained with acridine orange and labeled with developed silver grains. The method of preparation provides for orientation of bacteria between the photographic emulsion and the microscope objective to prevent visual interference by the silver grains.

The 5 ml aliquots from the ^3H -leucine uptake assays (preserved with 4% formalin) were stained with sterile-filtered 0.01% acridine orange for 1 min., followed by filtration through a 0.2 μm pore size nucleospore membrane (25 mm dia.). A type AA filter (0.8 μm , Millipore) was used as a back filter for even vacuum distribution. The filter was rinsed with sterile, filtered, distilled water, and kept damp for subsequent transfer of cells onto the surface of a mounted gelatin-coated coverslip. (Details of the gelatin-coated coverslip preparation are presented elsewhere - see References below).

Resulting autoradiograms were prepared in total darkness with Kodak NTB2 Nuclear track emulsion coating, dried, and exposed at 4°C. After the appropriate exposure time, the autoradiograms were developed, fixed and further prepared as detailed elsewhere (see References below). Bacteria were

counted by epifluorescence microscopy and silver grain clusters were counted by transmitted phase contrast microscopy.

References: MEYER-REIL (1978); FUHRMAN and AZAM (in press, 1981).

METHODS FOR HYDROCARBON ANALYSES AND PHOTOCHEMICAL/MICROBIAL OXIDATION PRODUCT CHARACTERIZATION

Volatile Hydrocarbon Analyses

Volatile hydrocarbons are sampled from the air above the slick in the evaporation/dissolution chamber (or the flow-through outdoor tanks in Alaska) by vacuum-pumping measured volumes of air through 1/8 in. ID x 12 in. long stainless tubes packed with Tenax® GC polymer. For each sample, two tubes are connected in series with Swagelok fittings, and prior to and immediately after sampling, all tubes are sealed with Swagelok endcaps and plugs. Sampling is achieved by use of a Gast Mfg. Corp. vacuum pump attached to the Tenax® traps via flow regulators and flexible Teflon tubing. Air velocities above the slick in the evaporation/dissolution chamber are measured with a Kurz air velocity meter 4m above the oil/seawater interface.

Before each sample is obtained, the Tenax® trap's flow velocity is checked with a bubble flow meter. Approximately 60 second samples are generally obtained at flow rates ranging from 20 to 30 ml/min; thus, sample volumes ranged from 20-30 ml.

Water samples for analysis of dissolved lower-molecular-weight aliphatic and aromatic hydrocarbons are taken in Pierce septum-capped vials for subsequent purge and trap analysis by GC/MS techniques similar to those developed by Bellar and Lichtenberg (1974) and others.

Following collection, the water samples are refrigerated (no preservatives are added), and they are maintained at 3°C until analysis. Capped stainless-steel Tenax® traps are stored at ambient temperature until analysis.

The Tenax® air samples are analyzed by heat desorption followed by Flame Ionization Detector (FID) gas chromatography on a Hewlett Packard 57330A

instrument or gas chromatography/mass spectrometry (GC/MS) using a Finnigan 4021 quadrupole instrument. The heat desorption is accomplished by installing the Tenax® traps in a Tekmar liquid sample concentrator (LSC-2) interfaced to the injection port system of either the FID GC or GC/MS (PAYNE et al., 1980b).

At the time of desorption (5 min. at 180°C at 20 ml/min He flow) the gas chromatographic column (packed 6 ft. x 22 mm I.D. SP-1000) and oven are cryogenically cooled to 30°C. Following desorption, the oven is programmed rapidly (30°C/min) to 100°C and then from 100°C to 200°C at 10°C/min. The final temperature of 200°C is held for the duration of the chromatographic run. A GC column flow rate of 20 ml/min He is also used and the injector temperature is held at 200°C.

The effluent from the gas chromatograph is then analyzed by FID on the HP-GC or it is passed through a glass jet separator for enrichment and then directly into the ion source of the GC/MS (operated in the electron impact-mode at 300°C). Spectra are acquired by operating the ion source at 70eV from 35 to 300 amu in 1.95 sec. A hold time of 0.05 sec is used to allow the electronics to stabilize before the next scan. The ion source is tuned for maximum sensitivity with perfluorotributylamine and the ion fragments at m/e 69 and m/e 219 are calibrated to give a 2.5:1 ratio; the electron multiplier is operated at 1600V with the preamplifier gain at 10^{-7} amps/volt. GC/MS data acquisition is initiated at the moment of desorption. Typically, 900-1000 scans are acquired for each data file.

The water samples stored in Pierce vials are allowed to come to room temperature and 5-ml aliquots are withdrawn and injected into the purge device of the LSC-2. Before purging in mass spectrometry operations, 100 ng each of three internal standards, dichlorobutane (m/e 55), bromochloromethane (m/e 130), and bromochloropropane (m/e 77) are added. This allows correction of recovered values for matrix effects and corrects for differences in ionization potential, lens voltage, etc., among runs. Instrumental conditions are identical to those described for Tenax® column analysis.

Before analyses with either instrument, response factors are determined for 10-12 target aliphatic and aromatic compounds of interest by spiking several known mixed standards into salt water blanks which are then analyzed as samples (PAYNE et al., 1980b).

Higher Molecular Weight Petroleum Hydrocarbon Analyses

Water sediment and oil/mousse samples are analyzed by procedures which basically involve: 1) extraction, 2) fractionation into aliphatic, aromatic and polar constituents by liquid/solid (SiO_2) column chromatography and analysis by FID capillary gas chromatography and capillary gas chromatography/mass spectrometry. Specific details with regard to these analytical procedures (including instrument calibrations, sensitivity, data reduction, etc.) are presented in Appendix H to this report (Methods Section, page 4 of "Chemical Weathering of Petroleum Hydrocarbons in Sub-Arctic Sediments: Results of Chemical Analyses of Naturally Weathered Sediment Plots Spiked with Fresh and Artificially Weathered Cook Inlet Crude Oil").

Water samples from the flow-through seawater systems are collected in 20-liter carboys and pH was adjusted to 2.0. Three hundred-fifty ml of methylene chloride is then added to each carboy (approximately 200 ml of methylene chloride goes into solution on the first addition) and the mixture is stirred vigorously for 3 minutes. The methylene chloride is removed by pressurizing the carboys with N_2 and forcing the methylene chloride through a stainless steel syphon tube into a separatory funnel. This procedure is repeated two more times. The methylene chloride extract is concentrated to 100 ml in K-D concentrators and then passed through sodium sulfate to remove the residual water. The anhydrous methylene chloride extract is then concentrated to 2 ml and solvent-exchanged to hexane. The concentrate is then fractionated on silica gel using the three fraction schemes described in Appendix H, page 4 of "Chemical Weathering of Petroleum Hydrocarbons in Sub-Arctic Sediments: Results of Chemical Analyses of Naturally Weathered Sediment Parts Spiked with Fresh and Artificially Weathered Cook Inlet Crude Oil".

APPENDIX G

THE X-RAY DIFFRACTION ANALYSIS OF NINE SEDIMENT SAMPLES

Report Submitted to:

James R. Payne
Science Applications, Inc.
La Jolla, CA 92037

March 15, 1983

by:

Technology of Materials
Santa Barbara, CA 93103

INTRODUCTION

Nine sediment samples were received in the laboratory for X-ray diffraction analysis. Of particular interest was the characterization of possible clay types and other mineral identification. The following report represents the results of the studies and is submitted respectfully.

SAMPLES

Samples were received with the following identifications:

BULK SAMPLES:

K-Bay Site #1 OW-1 (Grewingk Glacier Spit)
K-Bay Site #2 OW-2 (China Pool Bay)
K-Bay Site #3 OW-3 (Kasituna Bay)
K-Bay Site #4 OW-4 (Seldovia Bay)
K-Bay Site #5 OW-5 (Jackabul Bay)
Glacial Till OW-7 (Foot of Glacier)

FILTER SAMPLES:

1M (Kasituna Bay SPM)
2M (Seldovia Bay SPM)
6M (Glacial till SPM)

SAMPLE PREPARATION AND STUDY METHODS

Aliquotes of each sample were first very lightly ground to break up agglomerates. Care was taken to not break down the larger particals.

By using a combination of washing, seiving and centrifugation, the fraction faalling below 50 microns was separated for the studies. After drying, the powders were packed into standard sample holders and run in a Philips Electronics X-ray diffractometer equipped with a crystal monochrometer. The operating conditions are marked on the enclosed X-ray diffraction charts. The filter samples were studied without further treatment by placing the filters across the openings of a sample holder.

In order to further identify the clay fractions, several other techniques were utilized on the bulk specimens where there was a sufficient quantity of fine material. Using gravometric separation of a clay suspension in water, the heavy fraction was allowed to settle out and the light suspension was then decanted and concentrated by centrifugation. This light fraction was reslurried and allowed to settle on a microscope slide, forming an oriented mount with the clay platelets tending to lie flat causing a stronger diffraction of the clay (001) reflections. This mount was also run in the diffractometer.

A portion of this fine (less than 3 micron) fraction was also studied using long exposure Debye-Scherrer powder camera methods. Specific tests for montmorillonite were also performed on a portion of the clay which was heat treated to 350 degrees C to remove the absorbed water. Portions of this heat treated clay were then subjected to ethylene

glycol treatment. A separate portion was modified by strontium ion exchange using strontium chloride. Both of these methods sharpen the (001) diffraction peaks and shift them to a different d-spacing value by interlayer expansion.

All three samples were found to contain measurable amounts of carbonate minerals. The samples were therefore refined by leaching out these carbonates using dilute hydrochloric acid. These treated samples were neutralized, dried, and reweighed, then rerun in the X-ray diffractometer.

DISCUSSION

The x-ray diffraction charts enclosed are marked with the interplanar spacing measurements (d-spacings) in angstrom units and with the corresponding Miller Index (hkl) of the crystallographic planes causing each reflection. Phase identification was made by comparison with standard data in the JCPDS/ASTM diffraction files.

All of the samples show quartz and feldspar to be the major constituents, however some differences were encountered. Although spectrochemical data was not obtained for the feldspar mineral, the X-ray pattern is quite similar to that of Laboradorite, which is an anorthite-albite rich feldspar mineral.

Sample OW-2B shows a high calcite concentration (probably in the range of 30-40 percent), while the other samples have little or none.

Traces of mica are found in many of the samples and a possible trace of gypsum (calcium sulfate dihydrate) may be in OW-3. Certainty cannot be placed on the identification of these trace phases due to lack of confirming reflections.

A summary of the diffraction data is presented in chart form on a separate page. Rough quantitative approximations have been given as follows:

Major.....	over 50%
Intermediate +.....	40-50%
Intermediate.....	20-40%
Intermediate -.....	10-20%..
Minor +.....	5-10%
Minor.....	2-5%
Trace.....	less than 2%

The tests for expanding clays were negative. Sensitivity for this clay type is variable depending upon the degree of crystallinity.

However it can be said to be present to less than 10%.

SUMMARY OF MINERAL CONTENT

March 11, 198:

SAMPLE: K Bay Site #1 OW-1

<u>α-Quartz</u>	<u>Kaolinite</u>	<u>Feldspar</u>	<u>Calcite</u>	<u>Other</u>
major	intermediate	intermediate	none	Mica - tr

SAMPLE: K Bay Site #2 OW-2

<u>α-Quartz</u>	<u>Kaolinite</u>	<u>Feldspar</u>	<u>Calcite</u>	<u>Other</u>
intermediate + minor +		intermediate - major		Mica - tr ?

SAMPLE: K Bay Site #3 OW-3

<u>α-Quartz</u>	<u>Kaolinite</u>	<u>Feldspar</u>	<u>Calcite</u>	<u>Other</u>
major	minor +	intermediate	none	NaCl - minor Gypsum - tr

SAMPLE: K Bay Site #4 OW-4

<u>α-Quartz</u>	<u>Kaolinite</u>	<u>Feldspar</u>	<u>Calcite</u>	<u>Other</u>
major	minor +	intermediate	none	NaCl - minor

SUMMARY OF MINERAL CONTENT (cont.)

March 11, 1983

SAMPLE: K Bay Site #5 OW-5

<u>α-Quartz</u>	<u>Kaolinite</u>	<u>Feldspar</u>	<u>Calcite</u>	<u>Other</u>
major	intermediate-	intermediate	tr?	NaCl-minor

SAMPLE: Glacial Till OW-7

<u>α-Quartz</u>	<u>Kaolinite</u>	<u>Feldspar</u>	<u>Calcite</u>	<u>Other</u>
major	intermediate-	intermediate	none	Mica-tr

SAMPLE: Filter 1-M

<u>α-Quartz</u>	<u>Kaolinite</u>	<u>Feldspar</u>	<u>Calcite</u>	<u>Other</u>
major	intermediate +	minor +	none	Mica-tr?

SAMPLE: Filter 2-M

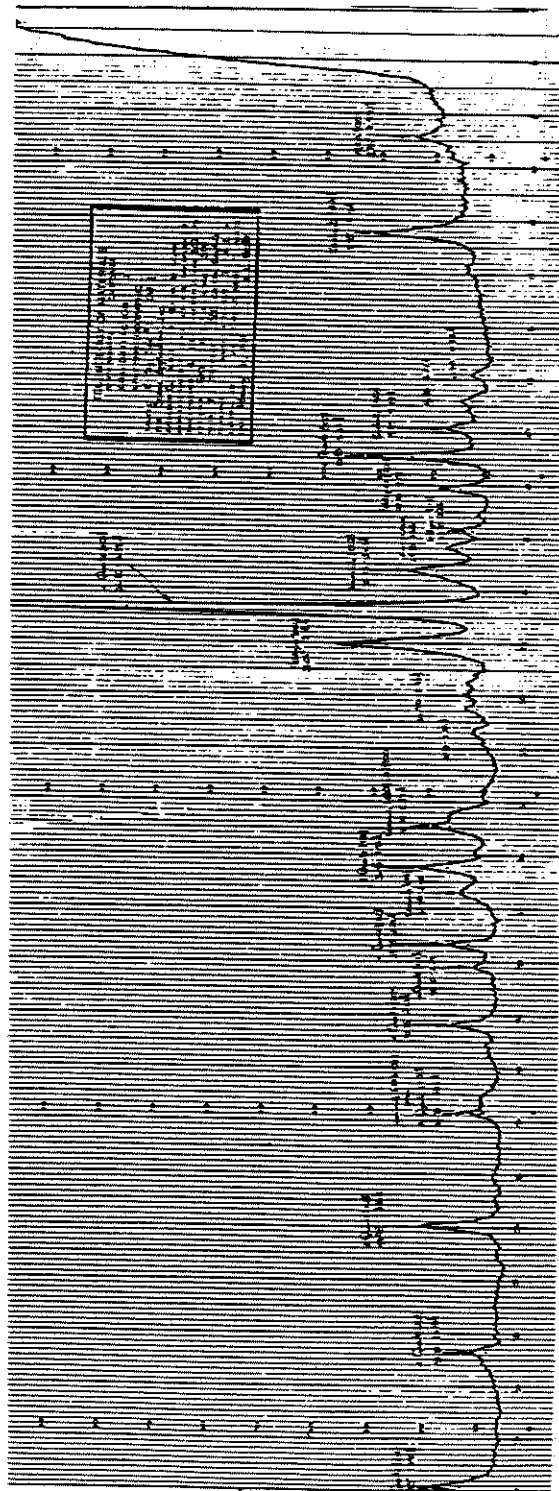
<u>α-Quartz</u>	<u>Kaolinite</u>	<u>Feldspar</u>	<u>Calcite</u>	<u>Other</u>
minor +	major	minor	trace?	Huntite? -t Mica-minor

SUMMARY OF MINERAL CONTENT (cont.)

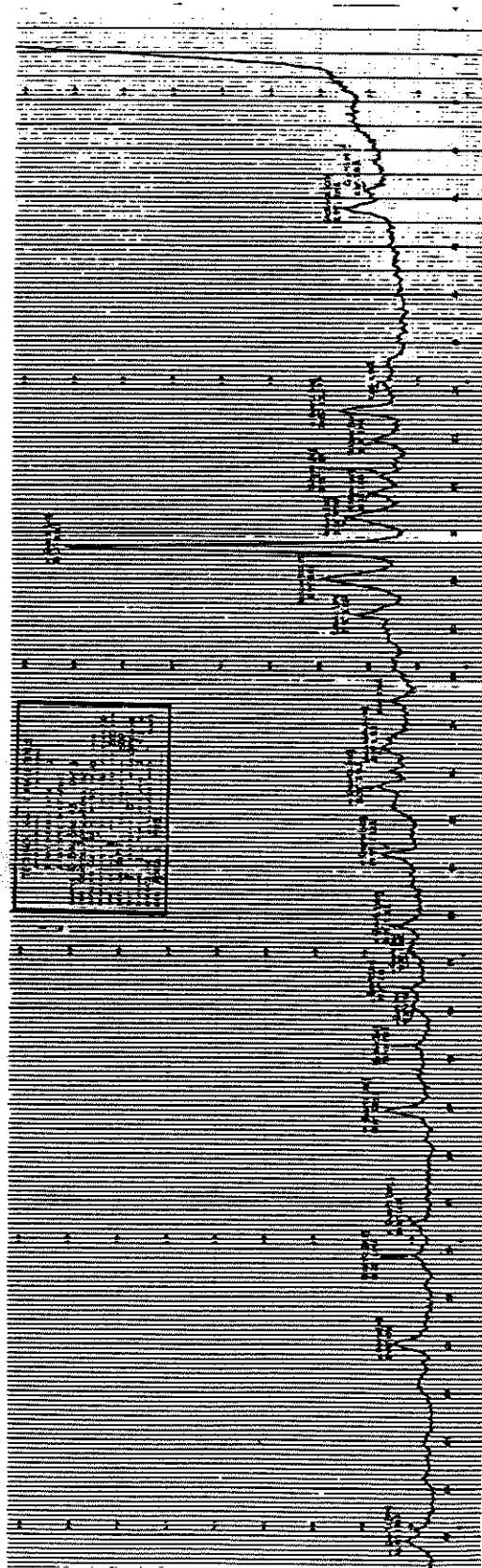
March 11, 1983.

SAMPLE: Filter G-M

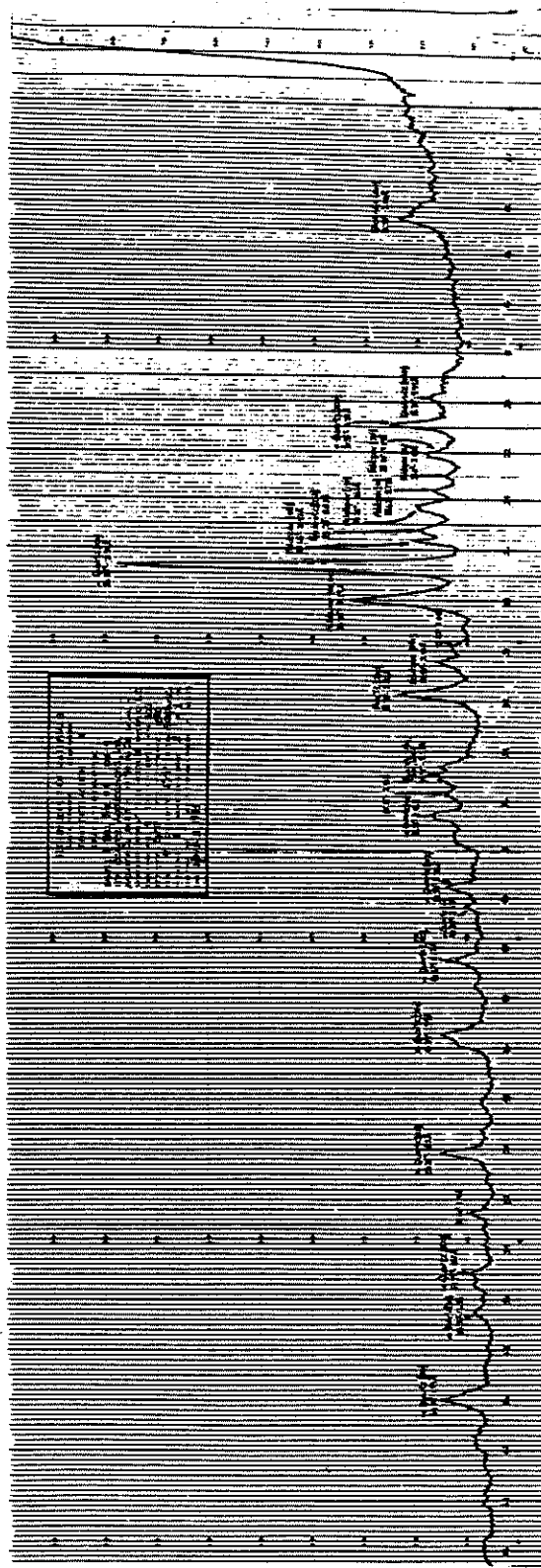
<u>α-Quartz</u>	<u>Kaolinite</u>	<u>Feldspar</u>	<u>Calcite</u>	<u>Other</u>
major	intermediate	intermediate	none	Mica-tr



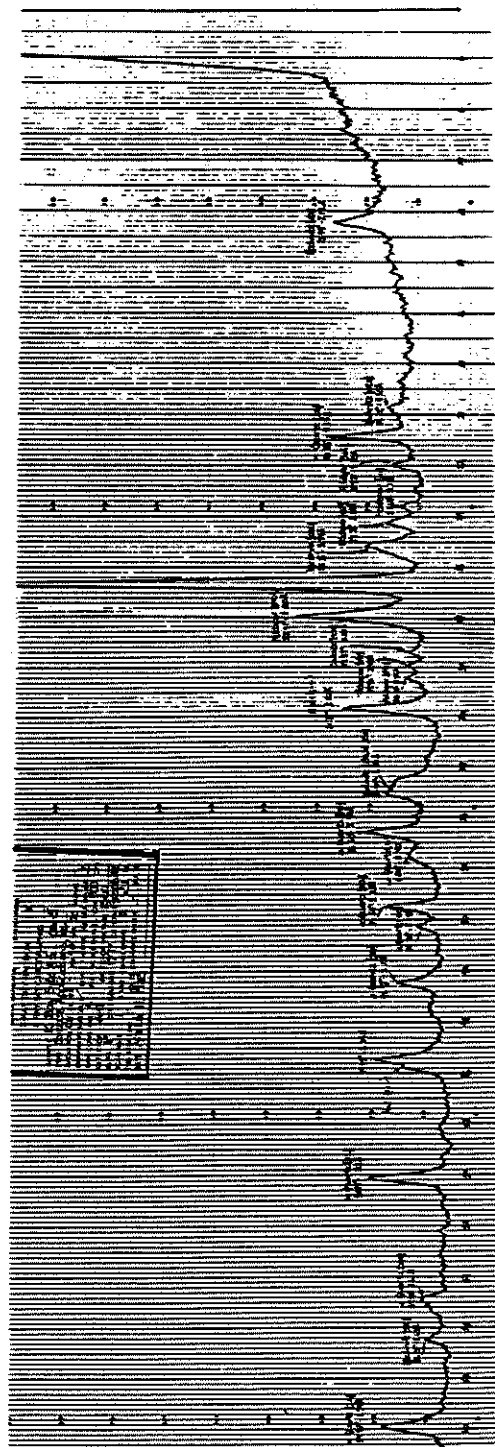
X-ray diffraction spectrograph of sediment from Site KB-1 (Grewingk Glacier Spit).



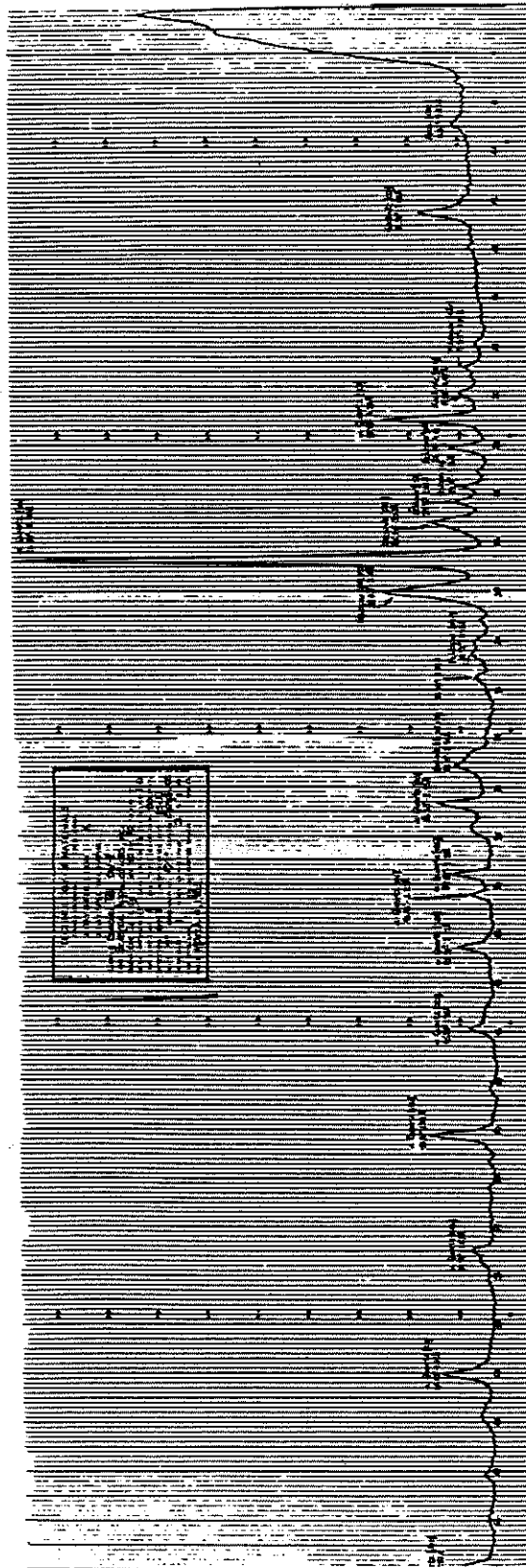
X-ray diffraction spectrograph of sediment from Site KB-3 (Kasitsna Bay).



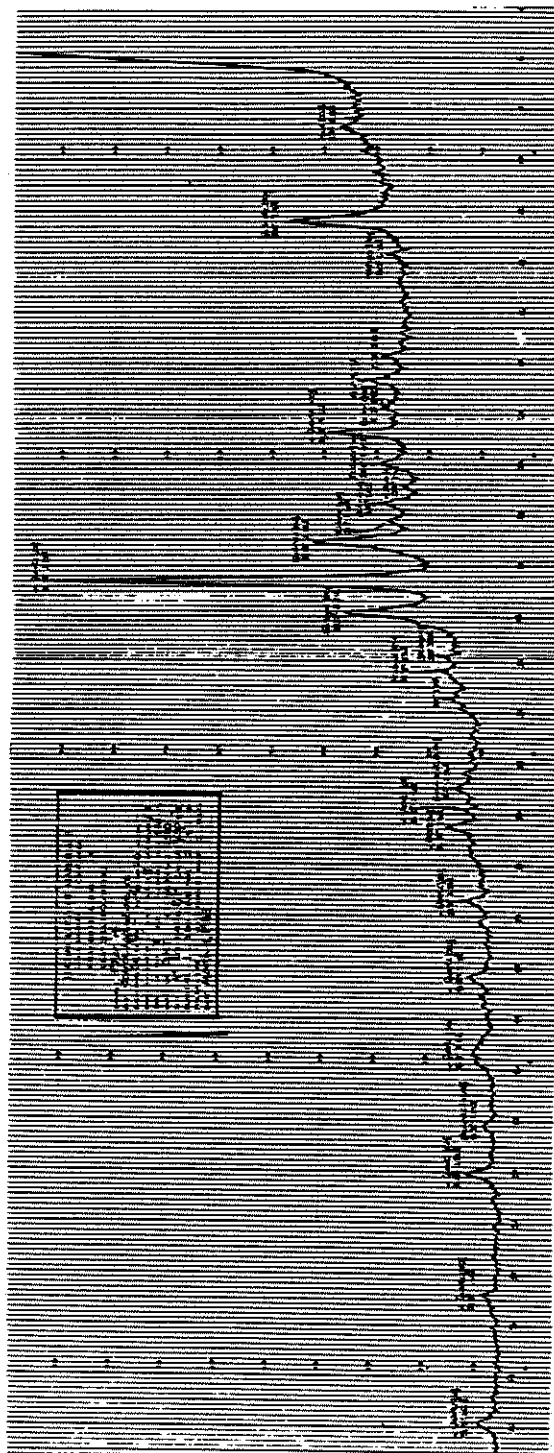
X-ray diffraction spectrograph of sediment from Site KB-4 (Seldovia Salt Marsh).



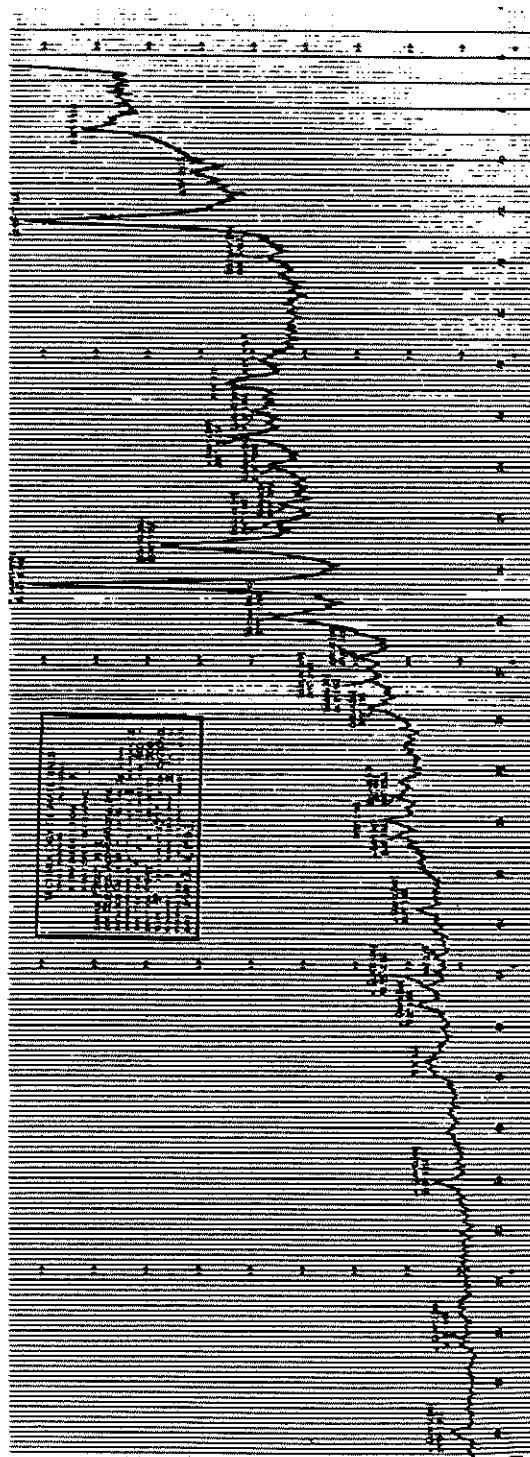
X-ray diffraction spectrograph of sediment from Site KB-5 (Jakolof Bay).



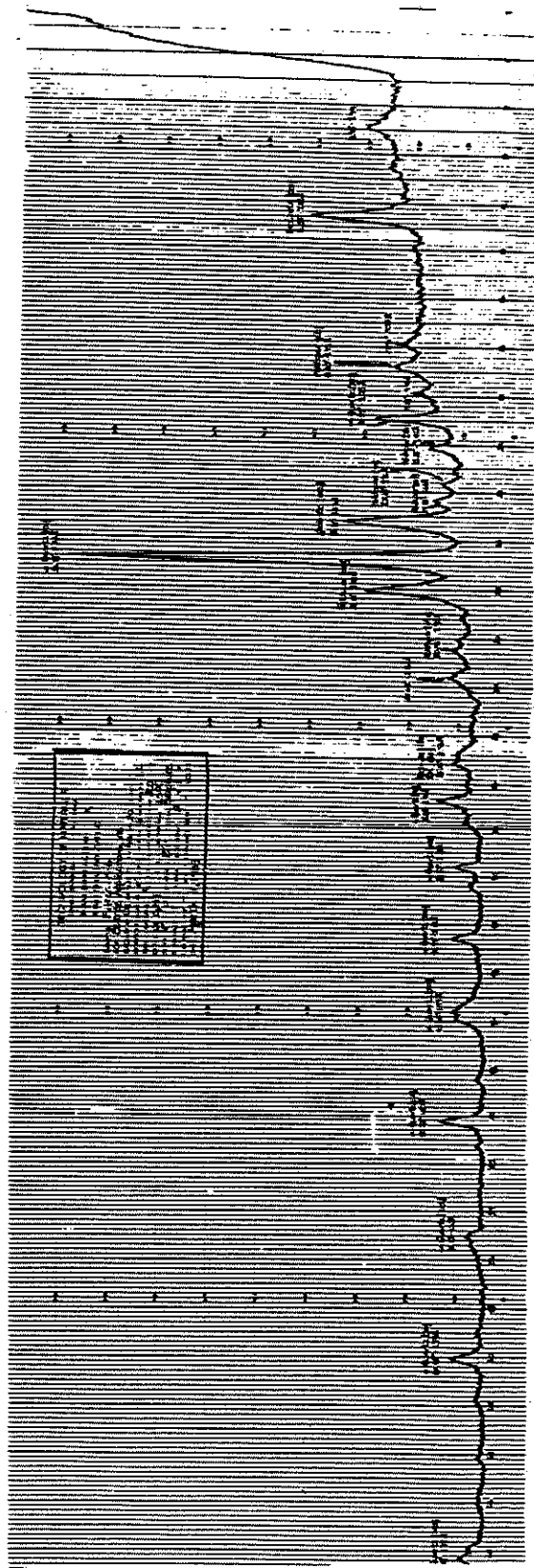
X-ray diffraction spectrograph of sediment collected from the base of Grewingk Glacier.



X-ray diffraction spectrograph of Kasitsna Bay SPM from Wave Tank #1.



X-ray diffraction spectrograph of Seldovia Salt Marsh SPM from Wave Tank # 2.



X-ray diffraction spectrograph of Glacial Till SPM from Wave Tank # 4.

APPENDIX H

CHEMICAL WEATHERING OF PETROLEUM HYDROCARBONS
IN SUB-ARCTIC SEDIMENTS: RESULTS OF CHEMICAL
ANALYSES OF NATURALLY WEATHERED SEDIMENT PLOTS
SPIKED WITH FRESH AND ARTIFICIALLY WEATHERED
COOK INLET CRUDE OILS

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APPENDIX H

CHEMICAL WEATHERING OF PETROLEUM HYDROCARBONS
IN SUB-ARCTIC SEDIMENTS: RESULTS OF CHEMICAL
ANALYSES OF NATURALLY WEATHERED SEDIMENT PLOTS
SPIKED WITH FRESH AND ARTIFICIALLY WEATHERED
COOK INLET CRUDE OILS

Report Submitted to:

Dr. Robert Griffith
Department of Microbiology
Oregon State University
Corvallis, Oregon

by:

James R. Payne, Gary S. Smith, James L. Lambach
and Paul J. Mankiewicz

Division of Environmental
Chemistry and Geochemistry
Science Applications, Inc.
476 Prospect Street
La Jolla, California 92038

December, 1980

OBJECTIVES

The primary goal of this program was to examine the biological and chemical impact of fresh and weathered crude oil after its incorporation into sub-arctic sedimentary regimes. The experiments that were used in this program were designed by Dr. Robert Griffith and his colleagues at Oregon State University to study one-year time series changes in biological productivity, recruitment and recolonization as a function of the chemical composition of the oil within the sedimentary study plots.

In an effort to assist Dr. Griffith in this program, the Environmental Chemistry and Geochemistry Division of Science Applications, Inc. (SAI) undertook detailed chemical analyses of the sediment samples used in these experiments. Specifically, hydrocarbon profiles (concentrations) were determined in control and experimental sedimentary plots which had been spiked with three different levels of fresh and artificially weathered Cook Inlet Crude Oil. These sediments were examined: first, after the initial spiking, and second, after one year of natural weathering in the sedimentary regime at Kasitsna Bay, Alaska. Additional studies were also undertaken in Sadie Cove, Alaska, where oiled sediments were spiked with Chiton and starch before deployment into the field, to determine if biotic weathering processes were controlled by limited nutrient concentrations.

Results of the hydrocarbon analyses from these experiments are presented in this section.

IMPLICATIONS FOR OFF-SHORE OIL AND GAS DEVELOPMENT

Many investigators have long suspected that spilled oil on the water surface or in the water column does not constitute as great an environmental threat as oil which has been incorporated into sedimentary regimes. Ironically, in the case of most major oil spills and laboratory studies, the sediments have been found to be the ultimate repository or sink for the bulk of the higher molecular weight components in the released oil (Jordan and Payne, 1980, D'Oxouville et al., 1979; Meyers, 1978; Mayo et al., 1978; Gearing et al., 1979; Winters 1978; Meyers and Quinn 1973; Zurcher and Thuer 1978; Bassin and Ichiye 1977). Once incorporated into the sediments, many of the unweathered toxic components of oil are retained unaltered for extended periods (Teal et al., 1978; Mayo et al., 1978) causing a variety of long term perturbations to plants, organisms and the physical (anaerobic vs. an aerobic) nature of the sediment itself. If contaminant concentrations reach high enough levels, the biological productivity of an entire area may be completely destroyed immediately after the spill impact, and residual toxic levels may prevent recolonization of native species for a number of years (American Institute of Biological Sciences, 1978). This is a significant problem in areas of high productivity or in sedimentary regimes critical to the survival of juvenile species. Alternately, competing species with different degrees of tolerance to oil could opportunistically recolonize an area, thus further altering the biological balance at the spill site for years.

In these experiments, we attempted to determine the levels or concentrations of oil in sub-Arctic sediments that could cause limited recovery or long term damage to an area. We also sought to determine concentrations and conditions under which specific compounds in the complex hydrocarbon mixture are selectively removed due to biotic and abiotic processes after incorporation of oil into the sediments. The results of these studies indicate that spiked levels of oil approaching 50 parts per thousand (ppt) (total oil wt/wt) cause extensive and significant long term damage to sub-Arctic sediments, and that little or no significant additional weathering (removal of toxic components) occurs at least up to one year following initial exposure. This was observed when both fresh and artificially weathered crude oils were spiked into the sedimentary matrix at the 50 ppt level. Similar trends were observed at the 1 ppt level, but some evidence of selective lower molecular weight hydrocarbon degradation after one year was found. The experimental results also suggest that at levels of oil approaching 50 ppt, the biotic utilization of specific hydrocarbon components is not inhibited by limited nutrient levels but rather by the toxicity of the oil itself.

A recommendation which can be drawn from these results is that in oil spill prevention, mitigation, and clean-up efforts, every attempt should be made to prevent oil from reaching sub-Arctic sediments particularly in low energy nearshore subtidal regimes where high biological productivity is observed.

METHODS

Techniques for artificially weathering Cook Inlet Crude Oil and subsequent spiking, homogenization, and deployment of sediment into the experimental trays for in situ weathering are described elsewhere. Subsamples of the spiked and control sediments from the experimental trays were frozen at the initiation of the experiment and again after one year in the field. All frozen sediment samples were shipped on ice to SAI's Trace Environmental Chemistry Laboratory in one lot on 17 October 1980, where they were subsequently stored at -4°C until analyses were begun.

Extraction

Each sediment sample was extracted using a shaker-table procedure which is similar to that described by Payne et al. (1978) and Brown et al. (1980) and which has been shown to yield comparable results to Soxhlet extraction (MacLeod and Fischer, 1980; and Payne et al., 1979). Briefly, the thawed sediment was placed in tared 500 ml Teflon jars and a wet weight was determined. Approximately 50 ml of methanol was added to the sediment for water removal, and the jars were sealed and agitated on a shaker table for 15 minutes. The jars were then centrifuged at 3000 rpm for 20 minutes at room temperature and the supernatant was decanted off and saved, and the drying procedure was repeated. After the second drying step, 150 ml of methylene chloride (CH_2Cl_2) and methanol (65:35 v/v) were added to the jars and agitation

was continued for 12 hours. The samples were centrifuged, the supernatant saved, and the procedure was repeated with the agitation occurring for a period of 6 hours. The methanol-water washes and the methanol-methylene chloride extracts were combined in a separatory funnel and back extracted with 400-500 ml of saturated sodium chloride in distilled water which had been previously extracted with hexane. The lower layer (CH_2Cl_2) was removed and the water phase was back extracted with three additional 100 ml aliquots of CH_2Cl_2 . The combined CH_2Cl_2 extracts were concentrated to approximately 100 ml using a Kuderna-Danish (K-D) apparatus, and dried by passage through a column of sodium sulfate followed by additional elution with CH_2Cl_2 . The dried extract was concentrated to about 10 ml using a K-D apparatus and solvent exchanged (3x) into hexane, followed by solvent reduction to 1-2 ml in preparation for column chromatography.

Liquid Column Chromatography

To fractionate the sediment extracts, a three-part fractionation scheme was employed to separate the aliphatic, aromatic, and polar compounds (Payne, et al., 1980). A 10 mm I.D. x 23 cm long column with a 16 ml pore volume was packed with 1.5 cm of activated copper at the base of the column (to remove elemental sulfur), followed by a hexane slurry of 60/200-mesh silica gel that had been cleaned with CH_2Cl_2 and activated at 210°C for 24 hours. The elution scheme was as follows:

Fraction/Solvent	Amount	Compound Class
1. Hexane	30 ml	Aliphatic hydrocarbons
2. Hexane: Benzene 50:50	45 ml	Aromatic hydrocarbons
3. 50% CH ₃ OH in CH ₂ Cl ₂	60 ml	Polar compounds

Gas Chromatographic Analysis

All gas chromatographic results were obtained on a Hewlett-Packard 5840A gas chromatograph equipped with an 18835A glass capillary inlet system and flame ionization detector. The microprocessor-based instrument was interfaced to a Texas Instruments Silent 700 ASR data terminal equipped with cassette tape drive, allowing permanent storage of calibration data, retention times, and peak areas required for the data reduction system.

A 30-meter J&W Scientific Co. SE-54 wall-coated open tubular fused silica capillary column was utilized for the desired chromatographic separations. Temperature programming used with this column included:

Initial Temperature	50°C for 5 minutes
Program Rate	3.5°C/min
Final Temperature	275°C for 60 minutes

The injection port and detector were maintained at 280° and 350°C, respectively. All injections were made in the splitless mode of operation with an injection port backflush 1 minute into the run.

Constant injection volumes of 1.0 μ l were analyzed automatically using a Hewlett-Packard model 7671A Automatic Liquid Sampler, increasing precision substantially relative to manual injection.

Gas Chromatogram Data Reduction

Hydrocarbon concentrations for individual resolved peaks in each gas chromatogram were calculated on a DEC-10 System Computer using the formula given in equation 1. This particular example is of the program used for seawater analysis. Operator-controlled modification of the DEC-10 program allows similar data reduction on sediments, tissues, or individual oil (mousse) samples.

$$\mu\text{g compound X/L seawater} = (A_x) \times (R.F.) \times \left[\frac{P.I.V. + 2}{\text{Inj.S.Vol.}} \times \frac{\text{Pre-C.S. Vol.}}{\text{Post-C.S.Vol.}} \times \frac{100}{\% \text{NSL on LC}} \times \frac{100}{\% \text{DW/FW}} \times \frac{1}{\text{liters}} \right] \quad (1)$$

where:

- A_x = the area of peak X as integrated by the gas chromatograph (in arbitrary GC area units)
- R.F. = the response factor (in units of $\mu\text{g/GC area unit}$)
- P.I.V. + 1 = the post-injection volume (in μl) from which a 1- μl aliquot had been removed for analysis by GC (measured by syringe immediately following sample injection)
- Inj.S.Vol. = the volume of sample injected into the GC (always 1.0 μl as measured by an HP Automatic Liquid Sampler)

- Pre-C.S.Vol. & Post-C.S. Vol. = the total solvent volumes before and after an aliquot is removed for gravimetric analysis on a Cahn electrobalance
- ZNSL on LC = the percent of sample non-saponifiable lipid used for SiO_2 column chromatography
- ZDW/FW = the percent dry weight of wet weight in the sediment tissue, or oil sample being analyzed
- liters = liters of seawater initially extracted (or grams wet weight of oil or sediment).

During analysis of the extracts, the 5840A gas chromatograph was recalibrated after every 8 to 10 injections, and individual response factors were calculated for all detected even and odd n-alkanes between nC_8 and nC_{32} . Concentrations of other components (e.g., branched and cyclic) that eluted between the major n-alkanes were calculated by linear interpolation of the adjacent n-alkane response factors and the unknown compound peak's KOVAT index. By incorporating the post-injection volume (PIV) into the calculation, the amount of hydrocarbons measured in the injected sample were converted to the total hydrocarbon concentration in the sample.

Unresolved complex mixtures (UCM's) were measured in triplicate by planimetry; the planimeter area was converted to the gas chromatograph's standard area units at a given attenuation and then quantitated using the average response factors of all the n-alkanes occurring within the range of the UCM, as shown in equation 2.

$$\frac{\mu\text{g UCM}}{\text{liter}} = \text{Area}_p \times (\text{Conv. F}) \times \frac{\text{S. Att.}}{\text{Ref. Att.}} \times (\overline{\text{R.F.}}_{a-b}) \times [\dots] \quad (2)$$

where:

- Area = UCM area in arbitrary planimeter units,
- Conv. F. = a factor for converting arbitrary planimeter units to GC area units at a specific GC attenuation,
- S. Att. and Ref. Att. = the GC attenuation at which the sample chromatogram was run and the reference attenuation to determine the conversion factor (Conv. F.), respectively,
- R.F._{a-b} = the mean response factor for all sequential n-alkanes (with carbon numbers a to b) whose retention times fall within the retention time window of the UCM, and
- [...] = the same parameters enclosed in brackets in equation 1.

Confirmation of KOVAT index assignment to n-alkanes was done by computer correlation with n-alkane standard retention times and direct data-reduction-operator input.

Assignment of a KOVAT index to each branched or cyclic compound eluting between the n-alkanes was done by interpolation using the unknown compound and adjacent n-alkane retention times. Assignment of KOVAT indices to peaks in the aromatic fraction was made by direct correlation of unknown peaks with retention times from the n-alkane and aromatic standard runs completed prior to sample injection (Payne, et al., 1978b).

Capillary Gas Chromatography Mass Spectrometry

Selected extractable organic compounds previously analyzed by fused silica capillary column-FID GC were also subjected to fused silica capillary gas chromatography/mass spectrometry (GC/MS). A 30-meter J&W Scientific Co. SE-54 capillary column (0.25-mm I.D. with a film thickness of 25 μ m) was used to achieve chromatographic separation in a Finnigan 4021 quadrupole mass spectrometer. The capillary system was operated in the splitless (Grob-type) mode. The static time upon injection was 0.8 min, after which time the injection port was backflushed with the split and septum sweep flows at a combined rate of 35 ml/min. Linear velocity was set at 35 cm/sec, which gave a flow rate of 1.18 ml/min. The GC was programmed to remain isothermal at 30°C for 1.5 min following injection, elevated at 4°C/min from 30 to 160°C, and 8°C/min from 160-275°C, after which the oven was held isothermally at 275°C for approximately 20 minutes.

The flexible fused silica column was routed directly into the ion source of the mass spectrometer, which was operated in the electron impact mode at 70eV with the lens potentials optimized for maximum ion transmission. The quadrupole offset and offset programs were adjusted to yield a fragmentation ratio for perfluorotributylamine m/e 69-to-219 of 4:1. This tuning yields quadrupole electron impact spectra that are comparable to magnetic sector electron impact spectra, thereby allowing optimal matches in the computer search routines used in the INCOS data system that scans the quadrupole rods from 35-475 amu in

0.95 sec. A hold time of 0.05 sec between scans allows the electronics to stabilize prior to the next scan. The mass spectrometer was tuned at the beginning of each day using perfluorotributylamine. A calibration was accomplished with a routine diagnostic fit of 2% mass accuracy. Prior to analysis of samples, standard mixtures of n-alkanes, pristane, phytane, and mixed aromatic hydrocarbons were injected.

RESULTS AND DISCUSSION

Time Zero Samples

Figure 1 presents the FID capillary gas chromatograms obtained on the control sediment samples taken from Kasitsna Bay at the beginning of the spiked sediment experiments. The most characteristic feature in the aliphatic fraction chromatogram, A, is the predominance of odd numbered n-alkanes in the molecular weight range of nC_{21} to nC_{29} , (RT 56.53; 62.12; 67.03; 71.93; 78.77) reflecting biogenic input. The sample also contains very low levels of nC_{17} and pristane (RT 44.55; 44.75) and nC_{18} and phytane (RT 47.40; 47.83). The three major components at retention times 31.21, 35.77 and 43.08 are internal spikes and a GC recovery standard (triisopropylbenzene, 31.21; n-decylcyclohexane, 43.08; and hexamethylbenzene, 35.77, respectively). There is no apparent evidence of any petroleum contamination and there appears to be a small cluster of branched and unsaturated biogenic hydrocarbons between nC_{20} and nC_{21} . The aromatic fraction chromatogram, B, from this

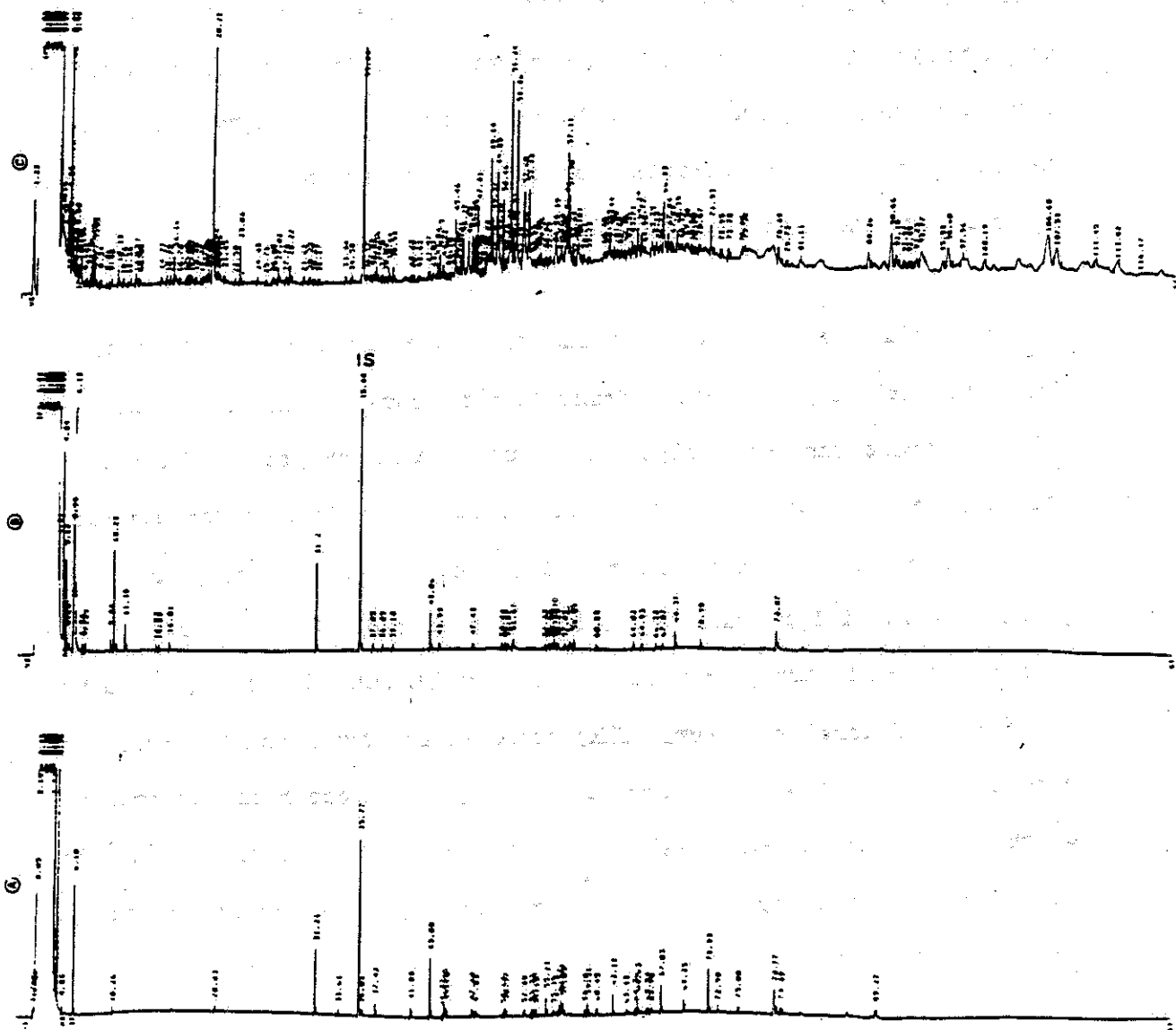


Figure 1. Flame Ionization Detector capillary gas chromatograms of: A, the aliphatic fraction; B, the aromatic fraction and C, the polar fractions obtained from time zero control sediment samples from Kasitsna Bay.

sample shows very little contamination of any kind, with only sub-nanogram per gram-dry-weight components present. The polar fraction chromatogram, C, does show evidence of several polar materials which are currently undergoing analysis by GC/MS. From GC/MS analyses of similar sediment samples, the identities of these peaks are suspected to be long chain fatty acid esters of biogenic origin.

Tables 1 and 2 present the reduced quantitative data obtained from the capillary FID gas chromatographic runs of these and all the other sediment samples analyzed as part of this program. The data in Tables 1 and 2 illustrate several interesting quantitative aspects which should be considered when interpreting the results. First, the background levels of hydrocarbons in the control samples from Kasitsna Bay at times zero and one year were both extremely low. In neither case was an Unresolved Complex Mixture (UCM) present, and the highest hydrocarbon concentration in these two samples was only six micrograms per gram dry weight. The odd to even n-alkane ratios for these samples (1 and 625) were high, ranging from 5.2 to 7.9, reflecting predominance of the odd n-alkanes of biogenic origin.

Figures 2 and 3 present gas chromatograms of the hexane and benzene fractions from the fresh Cook Inlet crude oil and the artificially weathered Cook Inlet crude oil used to spike the sediment samples, respectively. Figure 2A clearly shows a high degree of complexity in the lower molecular weight range from nC_8 through nC_{12} ,

Table 1. Reduced Aliphatic Hydrocarbon Data Derived from Flame Ionization Detector Capillary GC Analyses

Sediment Sample	OSI ID No	Time In Field (years)	Total Resolved ug/g	Total ICH* ug/g	F. n-alkanes ug/g	F. even n-alkanes ug/g	F. odd n-alkanes ug/g	pristane n-alkanes	phytane n-alkanes	old alk even alk	prist n-17	phy n-18	prist: n-alk phyl branched
VASTICHA BAY CONTROL	1	0	5.89	0	2.76	0.449	2.31	0.0157		5.15	0.758	0	4-- 0.083
VASTICHA BAY CONTROL	625	1	1.22	0	0.533	0.06	0.473	0		7.06	0	0	0.776
FRESH CRUDE SPIKE 50ppt	5	0	2840	4090	1460	742	722	0.0749		0.973	0.681	0.343	2.61 1.06
FRESH CRUDE SPIKE 1ppt	4	0	83.3	154	52.6	24.2	28.6	0.085		1.18	0.630	0.411	2.10 0.690
FRESH CRUDE SPIKE 0.1ppt	3	0	11.3	12.8	5.03	2.11	2.92	0.596		1.39	0.601	0.300	2.40 0.803
WEATHERED CRUDE SPIKE 50	14	0	1530	3020	945	460	485	0.104		1.06	0.721	0.326	2.75 1.62
WEATHERED CRUDE SPIKE 1	12	0	62.2	136	40.3	19.3	21.0	0.0871		1.09	0.645	0.371	2.27 1.84
FRESH CRUDE SPIKE 50ppt	628	18	2430	1740	1000	560	515	0.0861		0.921	0.761	0.354	2.63 0.796
FRESH CRUDE SPIKE 50ppt	629	18	2700	3770	1250	645	605	0.0799		0.934	0.700	0.306	2.43 0.860
FRESH CRUDE SPIKE 50ppt	630	18	2060	3030	950	494	458	0.0812		0.927	0.708	0.357	2.41 0.862
FRESH CRUDE SPIKE 1ppt	631	1	21.3	98.1	10.9	4.89	6.04	0.144		1.24	1.28	0.709	2.40 1.06
FRESH CRUDE SPIKE 0.1ppt	634	1	3.29	13.1	1.09	0.179	0.912	0.0120		5.10	0.800	0	3-- 0.496
WEATHERED CRUDE SPIKE 50	637	1	1530	3710	949	449	490	0.109		1.11	0.926	0.463	2.40 1.64
WEATHERED CRUDE SPIKE 1	640	1	14.3	319	2.81	0	2.81	0		2--	0	0	0.243
SADIE COVE CONTROL	206	0	26.1	0	10.7	1.37	9.33	0		6.81	0	0	0.773
SADIE COVE OIL & STARCH	782	1	3760	5200	1605	817	768	0.071		0.917	0.762	0.391	2.55 0.741
SADIE COVE OIL	779	1	4730	6100	1920	983	932	0.0810		0.948	0.880	0.420	2.75 0.681
SADIE COVE OIL & CHITIN	780	1	4700	6670	1906	1020	968	0.0610		0.951	0.626	0.345	2.14 0.732
COOK INLET CRUDE OIL													
FRESH		N.A.	84000	27600	31000	18300	14700	0.0703		0.804	0.673	0.311	2.41 0.648
WEATHERED		N.A.	38700	54500	24500	11600	12900	0.0989		1.17	0.654	0.300	2.23 1.73

*ICH = Unresolved Complex Mixture

Table 2. Reduced Aromatic Hydrocarbon Data Derived from Flame Ionization Detector
Capillary GC Analyses.

Sediment Sample	USC ID No	Time in Field (years)	Total Resolved ug/g	Total DCA ug/g	Naphthalene (1185)**	2 Methyl- naphthalene (1295)	1 Methyl- naphthalene (1313)	Biphenyl (1381)	2,6 Dimethyl naphthalene (1405)	Fluorene (1586)	Phenanthrene (1706)	Anthracene	1 Methyl- phenanthrene	Fluoranthene	Pyrene
KASITSHA BAY COREBOX	1	0	3.08	0.	nd	nd	nd	nd	nd	nd	0.0262	nd	nd	nd	0.0392
KASITSHA BAY COREBOX	625	1	1.212	0.	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd
FRESH CRUDE SPIKE 50ppt	5	0	1460.	1740.	58.0	137.	91.9	16.2	65.4	32.5	56.6	nd	18.0	nd	nd
FRESH CRUDE SPIKE 1ppt	4	0	12.2	22.3	0.163	0.960	0.570	0.0418	0.469	0.120	0.190	nd	0.0658	nd	nd
FRESH CRUDE SPIKE 0.1ppt	3	0	0.0289	0.0259	0.00025	0.00064	0.00037	nd	0.0032	nd	0.00032	nd	nd	0.00012	0.00012
WEATHERED CRUDE SPIKE 50	14	0	210.	824.	nd	5.59	4.77	nd	11.7	4.88	8.65	nd	nd	1.47	nd
WEATHERED CRUDE SPIKE 1	12	0	10.7	40.62	0.152	0.513	0.334	nd	0.467	0.150	0.255	nd	nd	nd	0.0376
FRESH CRUDE SPIKE 50ppt	628	1	469.	1235.	15.3	39.6	23.7	1.48	19.2	4.84	6.7	nd	2.48	1.00	nd
FRESH CRUDE SPIKE 50ppt	629	1	428.	800.	13.3	35.2	21.0	1.17	17.9	4.27	5.98	nd	2.40	0.810	nd
FRESH CRUDE SPIKE 50ppt	630	1	300.	2020.	9.75	30.4	18.6	nd	17.5	4.46	7.15	nd	2.95	nd	nd
FRESH CRUDE SPIKE 1ppt	631	1	9.33	29.7	0.163	0.517	0.433	0.0311	0.303	0.107	0.129	nd	0.0621	nd	nd
FRESH CRUDE SPIKE 0.1ppt	634	1	2.23	3.98	nd	0.0257	nd	nd	0.0321	nd	0.0307	nd	nd	nd	0.0185
WEATHERED CRUDE SPIKE 50	637	1	288.	901.	nd	5.19	4.07	nd	9.58	3.71	6.80	nd	nd	nd	nd
WEATHERED CRUDE SPIKE 1	640	1	12.28	51.84	0.0429	0.243	0.134	0.0234	0.420	0.195	0.137	nd	0.116	0.032	0.0297
SADIE COAL COREBOX	206	0	2.92	0	nd	nd	nd	nd	nd	nd	0.10258	nd	nd	0.02803	0.21073
SADIE COAL OIL & STARCH	782	1	781.	2010.	22.2	51.0	29.5	1.21	22.2	4.50	8.37	nd	2.64	nd	nd
SADIE COAL OIL	779	1	872.	2440.	32.6	75.0	41.2	nd	32.3	6.27	10.2	nd	5.71	2.04	nd
SADIE COAL OIL & CUTLIM	780	1	1070.	1650.	33.8	77.8	45.7	1.80	31.0	6.24	9.99	nd	6.66	nd	nd
CRUDE FUEL CRUDE OIL															
FRESH		M.A.	34700.	41600.	484.	1110.	644.	nd	540.	nd	190.	nd	nd	nd	nd
WEATHERED		M.A.	15400.	31400.	nd	nd	nd	nd	223.	102.	235.	nd	nd	nd	nd

* Unresolved complex mixture.
** Retention indices in parentheses.
nd = not detected.

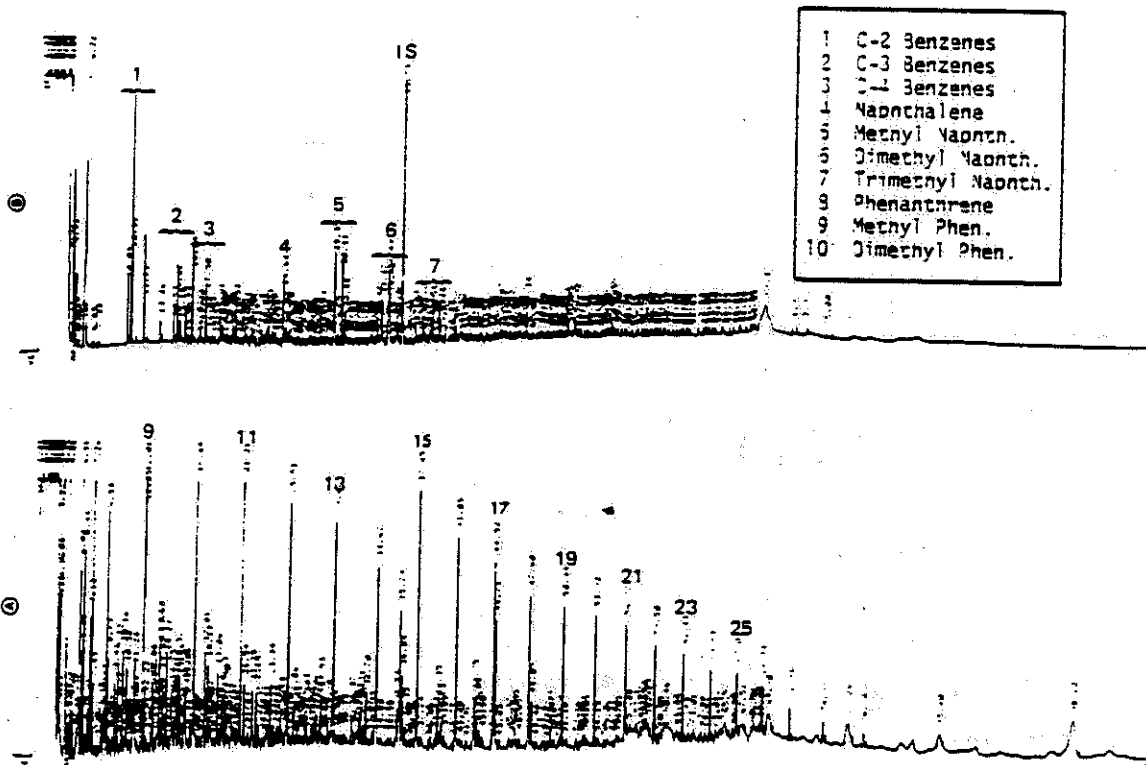


Figure 2. Flame Ionization Detector capillary gas chromatograms of: A, the aliphatic fraction, and B, the aromatic fraction extracts obtained on the fresh Cook Inlet Crude Oil used to spike the Kasitsna Bay sediment samples.

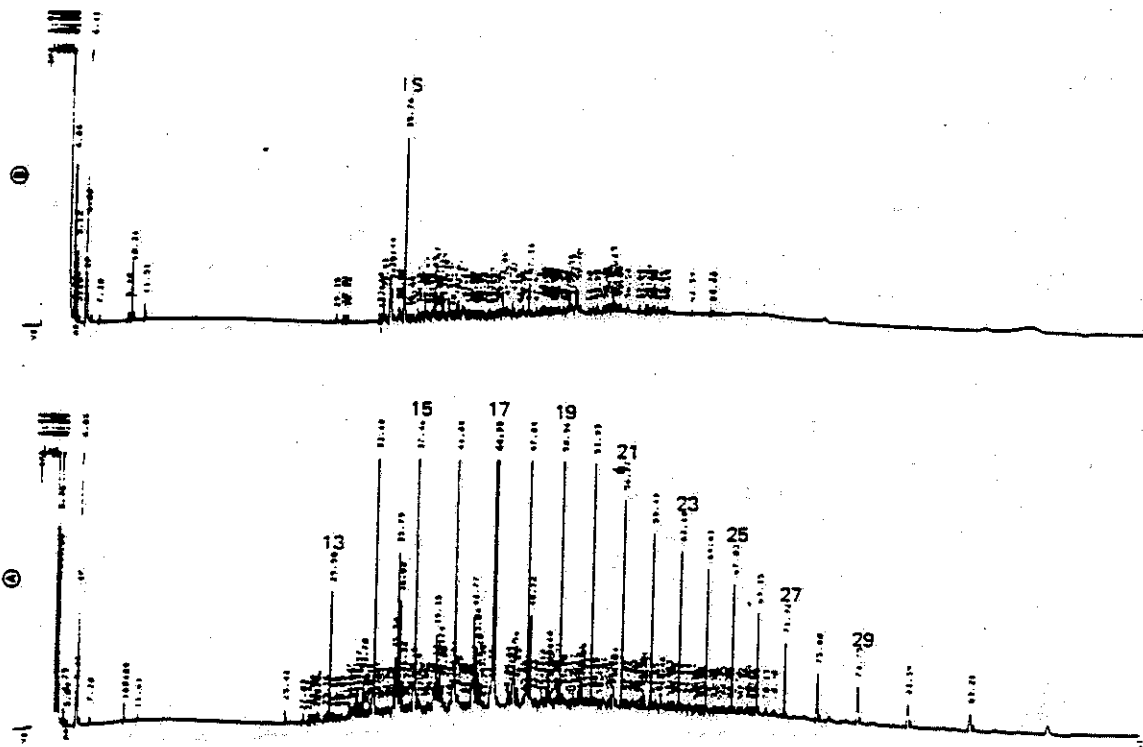


Figure 3. Flame Ionization Detector capillary gas chromatograms of: A. the aliphatic fraction, and B, the aromatic fraction extracts obtained from the Artificially Weathered Cook Inlet Crude Oil used to spike the Kasitsna Bay sediment samples.

although the aliphatic fraction is characterized in general, by n-alkanes from nC_8 through nC_{32} . The aromatic fraction shows a number of lower molecular weight aromatic compounds in the range of KOVAT index 800 to KOVAT index 1500 (RT 10.09 to 35.79). These compounds were identified by GC/MS as alkyl substituted benzenes such as xylenes, ethylbenzene, trimethylbenzene and propylbenzenes. The large peak at RT 35.79 is the GC internal standard hexamethylbenzene. Also in this sample are peaks identified as naphthalene (RT 24.64), 2-methylnaphthalene (RT 29.38), 1-methylnaphthalene (RT 30.11), 2,6-dimethylnaphthalene (RT 33.87), and several low level alkyl substituted phenanthrenes, as shown by the data in Table 2.

Figure 3 shows the gas chromatograms of artificially weathered crude oil used to spike the sediment samples. Clearly the aliphatic fraction, Figure 3A, shows loss of the lower molecular weight n-alkanes below nC_{13} ; however, the higher molecular weight materials are present at approximately the same ratios as in the starting crude oil. This is illustrated by the consistency in the pristane/phytane, pristane/ nC_{17} , and phytane/ nC_{18} ratios for the fresh and weathered crude oils, as shown by the data in Table 1. The aromatic fraction of the artificially weathered crude shows nearly complete diminution of the lower molecular weight hydrocarbons below dimethylnaphthalene; however, there still are several higher molecular weight polynuclears present. These are primarily phenanthrene at RT 47.34 (KOVAT 1790), 1-methylphenanthrene at RT 51.97 (KOVAT 1933), and fluoranthene at RT 55.45 (KOVAT 2070). Higher

molecular weight compounds such as benz(a)anthracene, benzo(e)pyrene, benzo(a)pyrene and perylene are not apparently present in either the starting or weathered Cook Inlet crude oil to an appreciable degree.

Figure 4 shows the gas chromatograms of the aliphatic, aromatic and polar fractions obtained on the Kasitsna Bay time zero sample spiked with fresh crude oil at 1.0 ppt. The chromatograms obtained on the sediments spiked at 50 ppt were essentially identical in appearance to those in Figure 4, and thus the heavier spiked sample's chromatograms are not shown here. Further, the concentrations of crude oil in the 50 ppt samples were at such a high level that only approximately 2% of the extractable materials could be effectively applied to the liquid chromatography columns for separation into aliphatic, aromatic and polar fractions. This allowed accurate quantitation of the materials but did not figuratively show the presence of the lower molecular weight compounds to the same degree as the lower level spiked samples where the entire sample could be fractionated and analyzed without prior dilution.

With regard to the chromatograms in Figure 4, the aliphatic fraction, A, is nearly identical to the aliphatic fraction of the starting fresh Cook Inlet Crude oil shown in Figure 2. This is reflected qualitatively in the chromatograms presented in the figures and also quantitatively by the pristane/phytane, pristane/ nC_{17} and phytane/ nC_{18} ratio data presented in Table 1. The suite of nC_{20} - nC_{21} branched/unsaturated compounds in the background control sample are completely masked in the spiked sediment samples. The aromatic fractions of the spiked

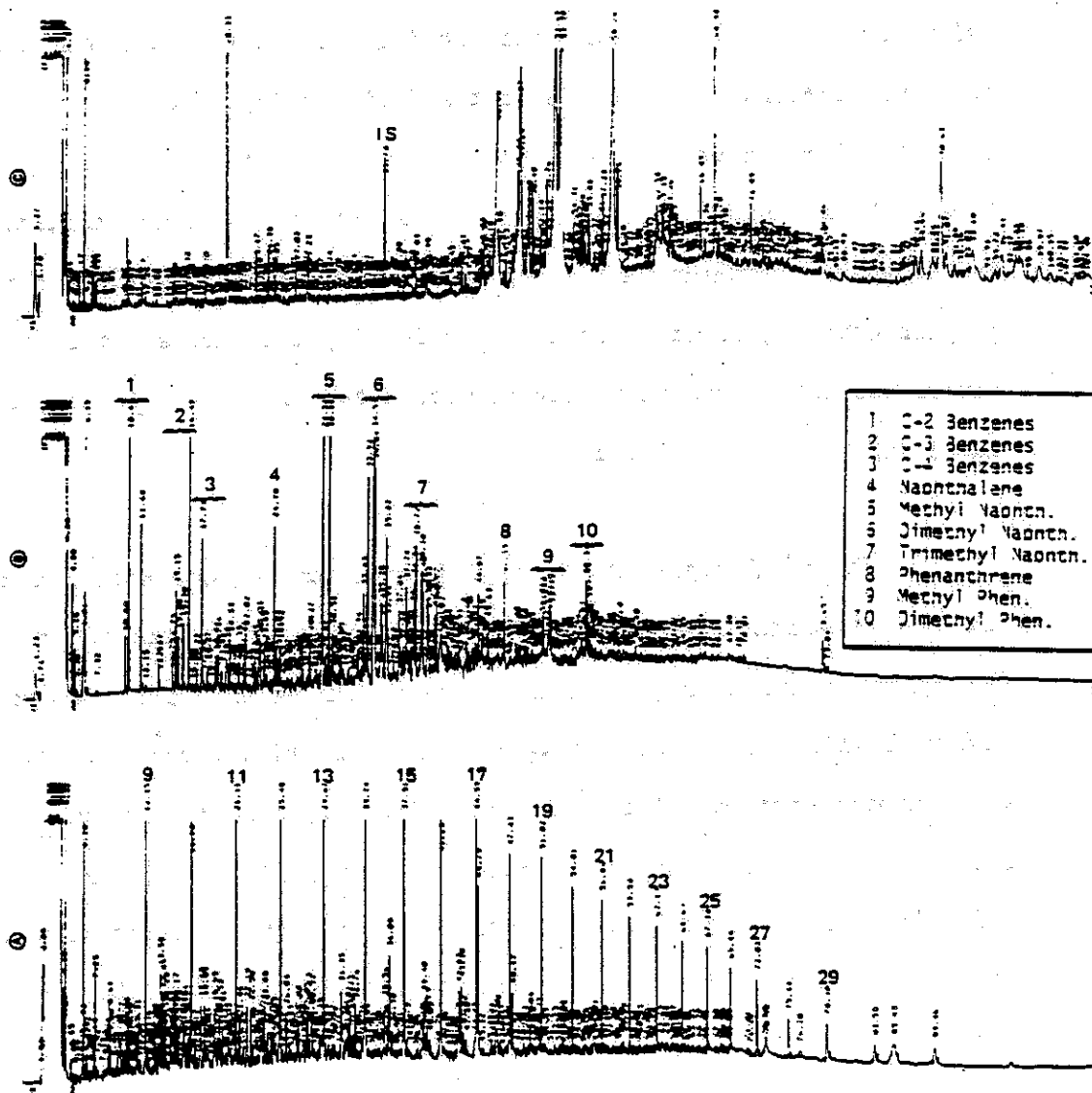


Figure 4. Flame Ionization Detector capillary gas chromatograms of: A, the aliphatic fraction, B, the aromatic fraction, and C, the polar fraction extracts obtained from time zero Kasitsna Bay sediment samples which had been spiked with fresh Cook Inlet Crude Oil at 1 ppt.

sample show many of the same aromatic compounds in the naphthalene (KOVAT 1185) to pyrene (KOVAT 2124) range and the alkyl-substituted aromatic compounds at KOVAT indices 800 to 1012 as in the starting crude oil. The polar fraction of the fresh spiked sediment at time zero shows many of the same biogenic compounds as in the Kasitsna Bay control sediment. This is particularly true of the compounds between retention times 46.99 and 68.40. These compounds are present at a greater apparent concentration in the spiked sediment sample; however, examination of reduced chromatographic data output shows that this primarily reflects a smaller final sample extract volume resulting in more material being loaded on the fused silica capillary column.

Figure 5 presents the capillary chromatograms obtained on the time zero sediment samples spiked with artificially weathered crude oil. The chromatograms are qualitatively very similar to those shown in Figure 3 which presented the weathered Cook Inlet crude used to spike the sediment samples. Aliphatics are virtually absent below nC_{13} as are aromatic compounds with KOVAT indices below 1300. A number of higher molecular weight polynuclear aromatic compounds can be identified in the weathered crude, and these are 2-methylnaphthalene at 29.38, 1-methylnaphthalene at 30.11, 2,6-dimethylnaphthalene at 33.88, fluorene at 40.61, phenanthrene at 47.41, 1-methylphenanthrene at 51.85 and fluoranthene at 55.45. There appear to be no polynuclear aromatic hydrocarbons with molecular weights greater than chrysene in the time zero artificially weathered sediment sample.

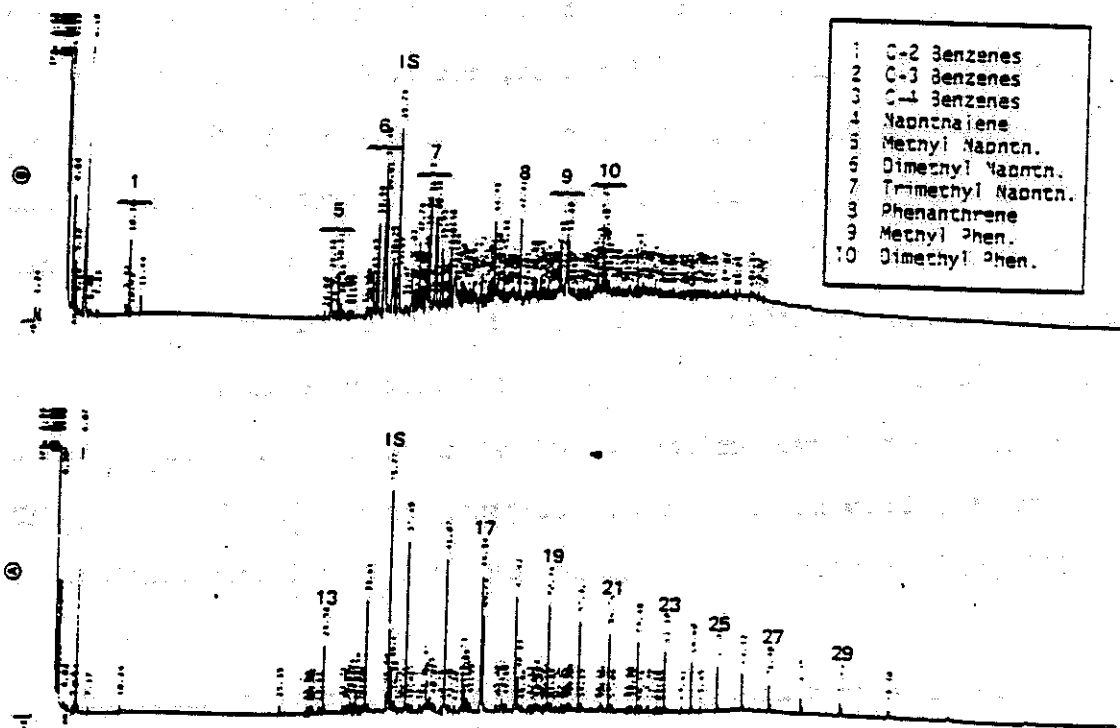


Figure 5. Flame Ionization Detector capillary gas chromatograms of: A, the aliphatic fraction and B, the aromatic fraction extracts obtained from time zero Kasitsna Bay sediment samples spiked with Artificially Weathered Cook Inlet Crude Oil at 50 ppt.

Time One Year Samples

Each sediment sample was spiked and placed in a sediment tray; the sediment samples were deployed at various depths in Kasitsna Bay and Sadie Cove. After one year of exposure the trays were retrieved and subsamples of the sediments were collected. Figure 6 shows the chromatograms obtained on the aliphatic fraction of A, the 50 ppt fresh crude oil spiked into the sediment at time zero, and B, C, and D, the triplicate samples examined after one year of natural weathering. Several features are significant in this figure. The first and most obvious feature is the lack of any appreciable weathering of the oil at this high level of concentration. This is reflected in the qualitative appearance of the chromatograms and in the data presented in Table 1. Specifically, the lower molecular weight n-alkanes from nC_8 through nC_{12} , and the branched and cyclic compounds occurring between KOVAT index 900 and 1000 appear to be nearly identical in all four samples.

Figure 7 graphically presents the concentration abundance of the n-alkanes in the 50 ppt spiked sediment sample at time zero and again after one year of weathering in Kasitsna Bay. Note that in addition to the concentrations of the time zero and one year samples being very similar, the overall trends showing decreases in the higher molecular weight compounds are nearly identical for both samples, illustrating the lack of any appreciable selective weathering.

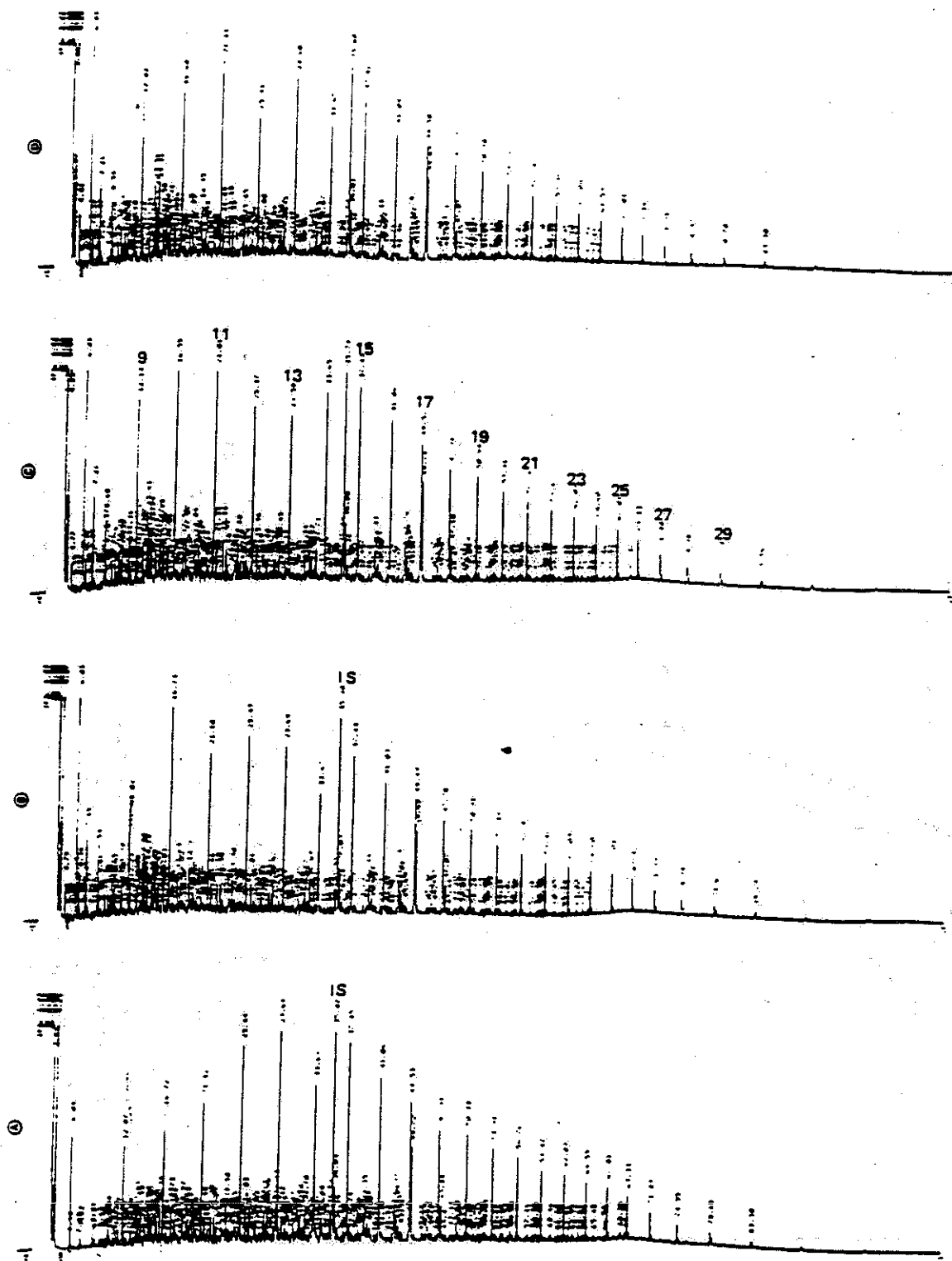


Figure 6. Flame Ionization Detector capillary gas chromatograms of: A, the aliphatic fraction of the 50 ppt fresh Cook Inlet Crude Oil spiked into the sediment at time zero, and B, C, and D, the aliphatic fractions of the triplicate samples examined after one year of natural weathering in Kasitsna Bay.

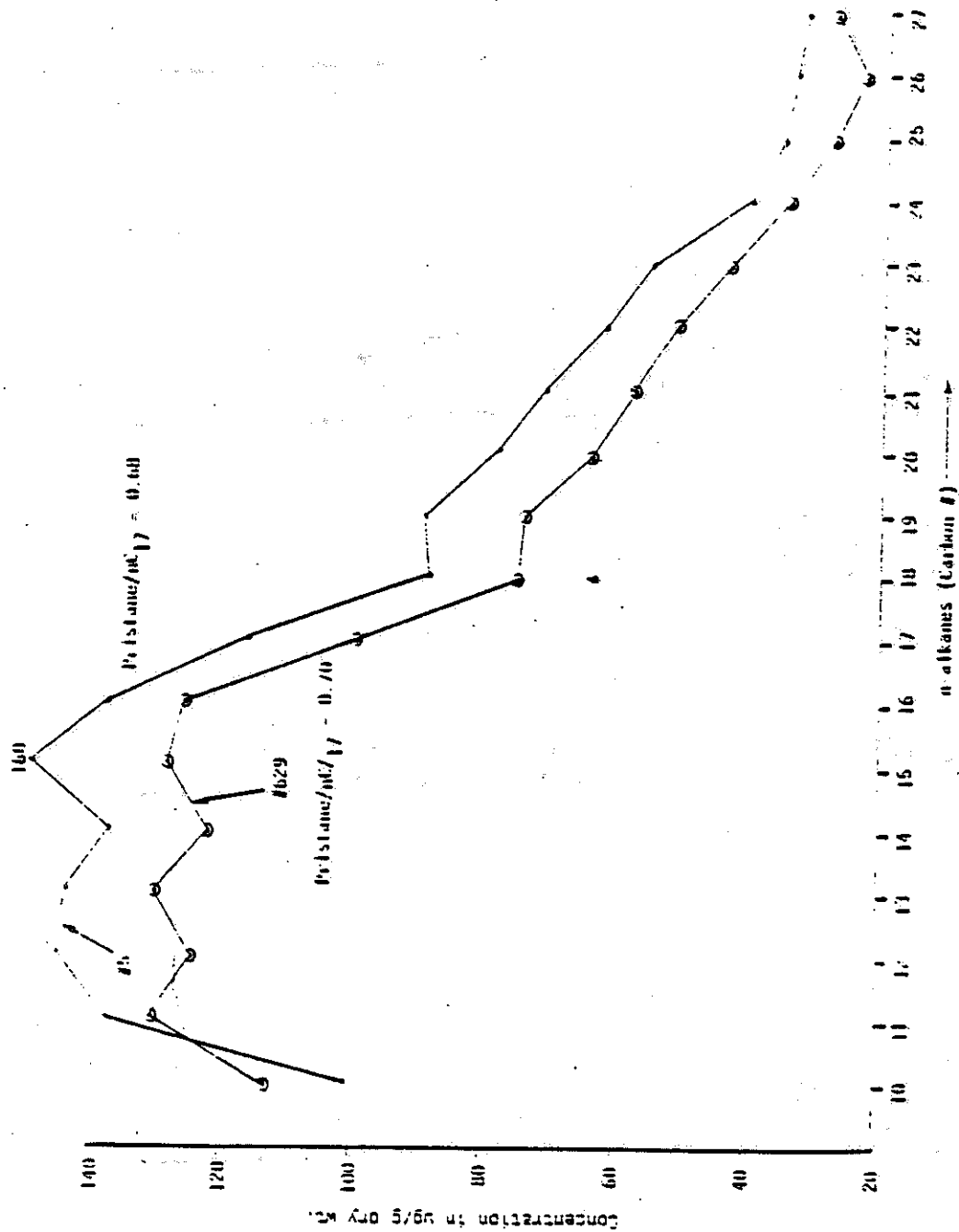


Figure 7. Concentration abundance of the n-alkanes in a sediment sample spiked with 50 parts per thousand fresh crude illustrating the time zero sample (·) and sample after one year of weathering (⊙).

The similarity of the pristane/ nC_{17} and phytane/ nC_{18} ratios, as observed qualitatively in Figure 6 and Table 1, also illustrates the lack of any appreciable biotic or abiotic weathering in these samples. The chromatographic profiles are essentially superimposable, reflecting the homogeneity of the initial spiked sediment, the replicability of the weathering process in the field and the precision of the analytical method. Individual values for these three fractions are presented in Table 1, and the agreement of such features as the total n-alkanes, sum of the odd n-alkanes, even n-alkanes, pristane/phytane ratios, etc., is worthy of consideration.

Figure 8 presents the gas chromatograms of the aromatic fractions obtained on the 50 ppt fresh Cook Inlet-spiked sediment at time zero (A) and the replicate fractions (B, C and D) obtained from analyses of the triplicate sediment samples after one year of natural weathering. As in Figure 6, there does not appear to be any selective weathering of the individual components present; however, examination of the reduced data in Table 2 and Figure 9 shows that some decreases in aromatic hydrocarbon concentrations did occur after 1 year. The apparent lower levels of material in chromatogram A (Figure 8) only reflect a larger final sample extract volume from which an aliquot was removed for analysis by GC. Figure 9A presents a graphical representation of the concentrations of eight selected aromatic compounds in the fresh 50 ppt

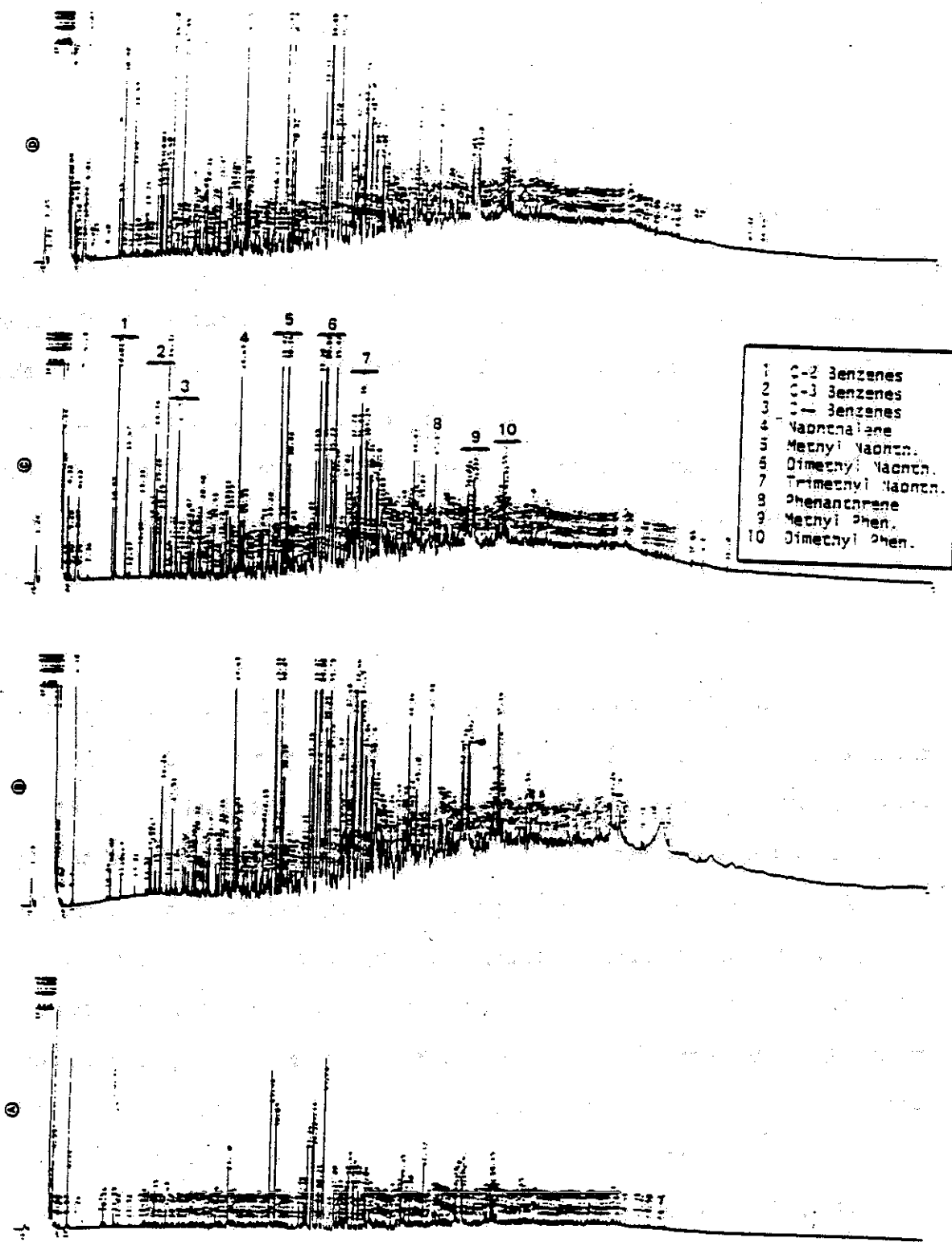


Figure 8. Flame Ionization Detector gas chromatograms of: A, the aromatic fraction of the 50 ppt fresh Cook Inlet Crude Oil spiked into the sediment at time zero and B, C, and D, the aromatic fractions of the triplicate samples examined after one year of natural weathering in Kasitsna Bay.

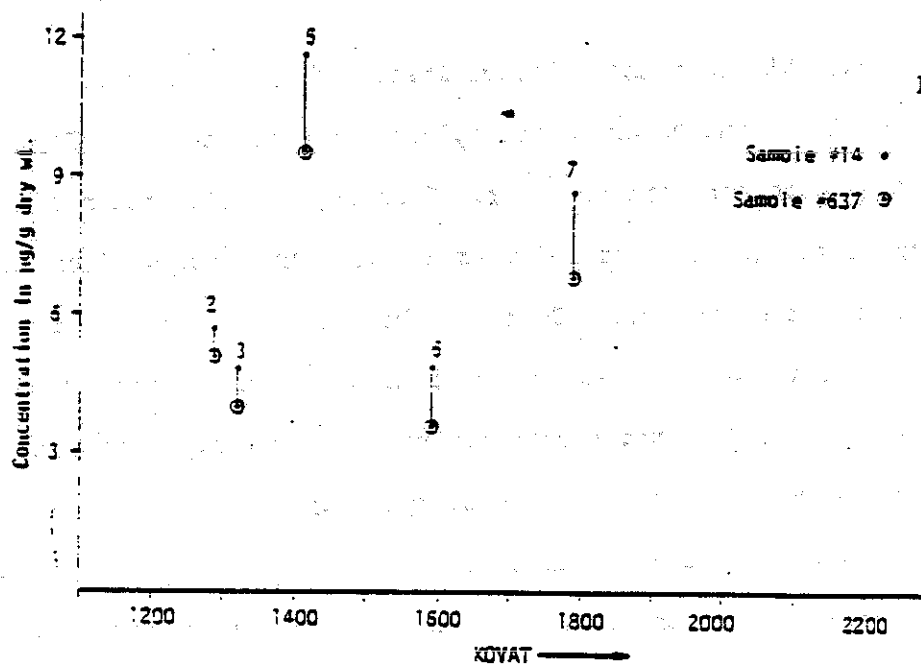
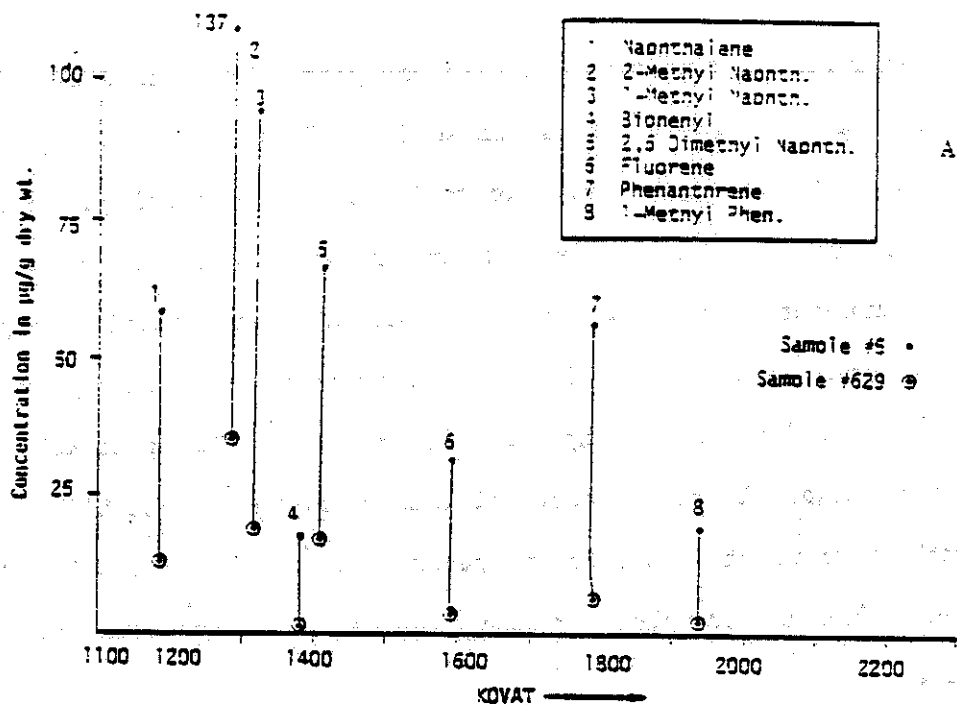


Figure 9. Concentration abundance of selected aromatic hydrocarbons from a 50 parts per thousand spike of fresh crude (Top) showing the time zero sample (•) and sample after one year of weathering (⊙), and bottom, a 50 ppt spike of artificially weathered crude at time zero (•) and after one year of weathering (⊙).

spiked sediments at time zero and time one year. While time zero levels of individual aromatic compounds ranged from 50 to 137 micrograms per gram dry weight (for naphthalene through 2,6-dimethylnaphthalene), after one year these compounds were present at concentrations ranging from 15 to 40 micrograms per gram dry weight. The decreases in aromatic compounds from Kovat indices 1100 to 1500 were greater than the decreases in aromatics with Kovat indices ranging from 1500 to 2000. This presumably reflects two things: 1) the greater volatility and water solubility of the lower molecular weight aromatic compounds, and 2) the lower relative abundance of the higher molecular weight aromatics in the crude oil to begin with.

Figure 9B shows the relative losses of aromatic hydrocarbons in the artificially weathered crude oil spiked into the Kasitsna Bay sediments at time zero and time one year. This figure illustrates that much smaller relative changes occurred over the one year period after the oil was spiked into the sediment. That is, the starting concentrations of aromatic compounds such as 2-methylnaphthalene through phenanthrene ranged between only 6 and 12 micrograms per gram dry weight of sediment when artificially weathered crude was used to spike the sample at time zero. These levels were not significantly reduced after one year of weathering in the sediments of Kasitsna Bay: the most significant weathering occurred while the oil was "artificially weathered" on the surface of a

salt water aquarium before the oil was spiked into the sediment. Nevertheless, once these compounds are introduced into the sediments, they are not as rapidly removed as they would be from simple dissolution in the starting oil itself.

Figure 10 presents the gas chromatograms of the aliphatic and aromatic fractions obtained on the 1 ppt fresh-crude oil spiked sediment after one year of weathering in Kasitsna Bay. In comparison with Figure 4 which shows the starting 1.0 ppm spiked material, it is clear that significant weathering of the sample has occurred. This is reflected first in the significantly greater relative loss of the lower molecular weight alkanes below nC_{13} , presumably due to a combination of biological and abiotic (dissolution) processes. Evidence of biochemical degradation is shown in examining the pristane/ nC_{17} and phytane/ nC_{18} levels in the aliphatic fraction in Figure 10 compared to the aliphatic fraction in Figure 4, and by examining the numerical values for these ratios in Table 1. Clearly the straight chain alkanes have been preferentially removed relative to the branched chain isoprenoids. The overall levels of other aliphatic hydrocarbons are also significantly reduced as illustrated qualitatively in Figure 10 and by the data in Table 1. Figure 11 graphically presents the concentration abundance of n-alkanes in the 1.0 ppt fresh crude oil sediment spike at time zero and after one year of natural weathering. Clearly all of the lower molecular weight alkanes below nC_{18} are reduced by a factor of from 2 to 5 and the higher molecular weight n-alkanes are reduced by at least a factor of 2 compared to the sample taken at time zero. For the 1 ppt sample the total

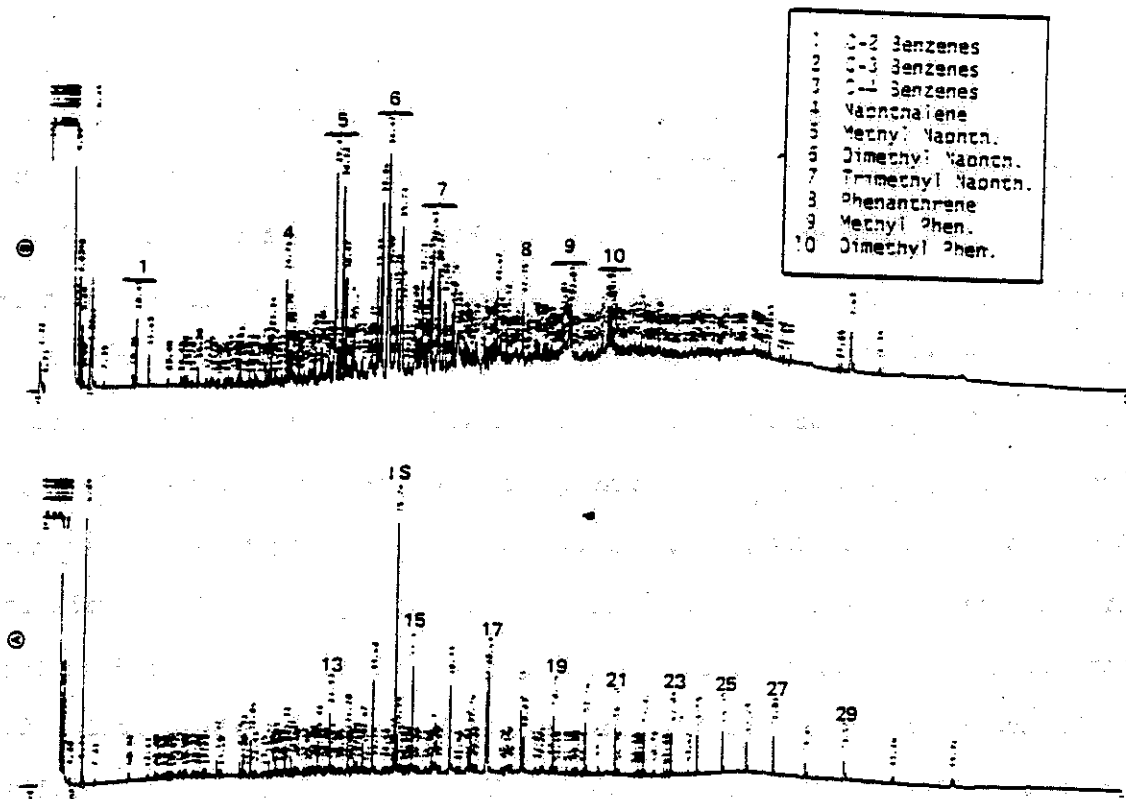


Figure 10. Flame Ionization Detector gas chromatograms of: A. the aliphatic fraction and B, the aromatic fraction extracts obtained from 1 ppt fresh Cook Inlet Crude Oil spiked sediments after one year of weathering in Kasitsna Bay.

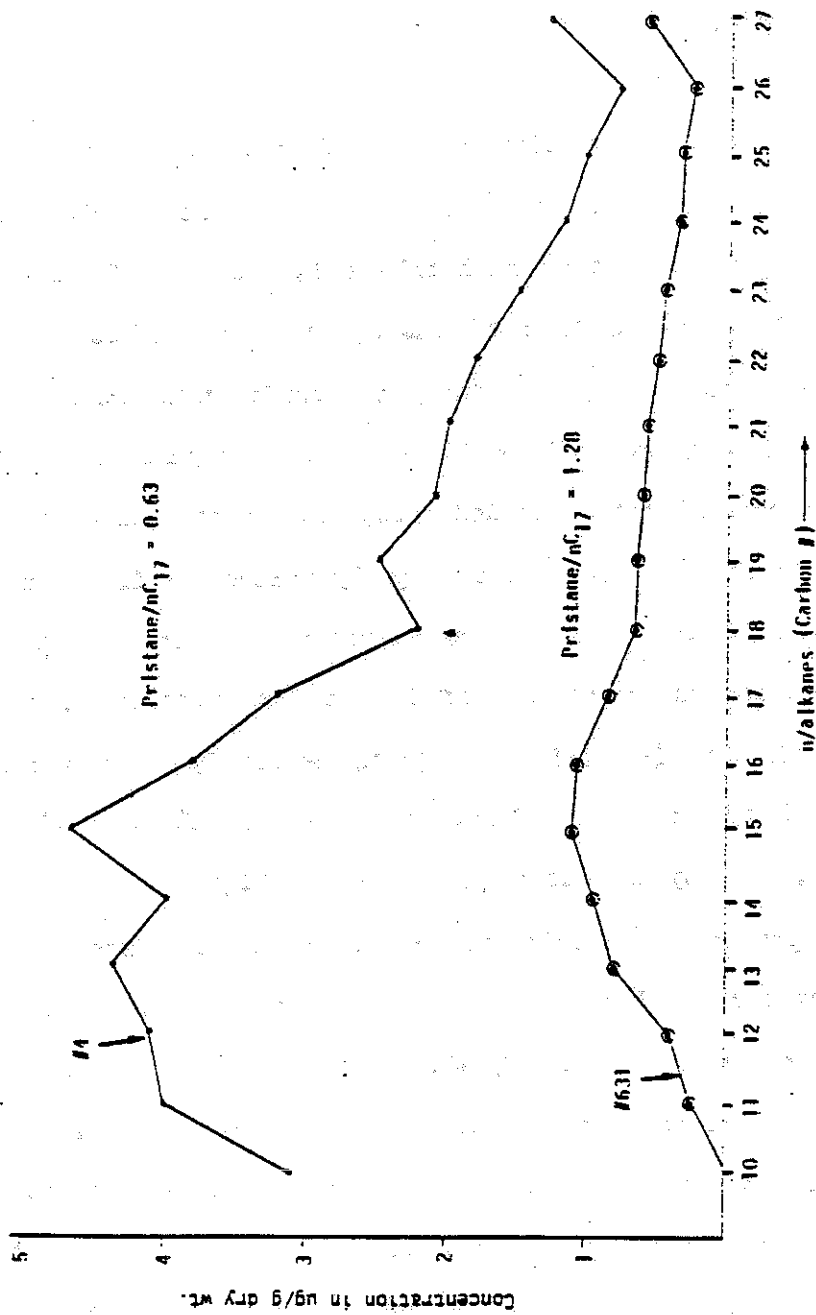


Figure 11. Concentration abundance of the n-alkanes for a sediment oil spike of 1.0 part per thousand fresh crude illustrating the time zero sample (•) and sample after one year of weathering (⊙).

resolved hydrocarbons decreased from 83 to 21 $\mu\text{g/g}$ dry weight during the year of exposure and the unresolved complex mixture decreased from 154 to 98 $\mu\text{g/g}$ dry weight.

The aromatic fraction data in Figure 10B show somewhat less degradation compared to the aliphatic fraction. Compounds with molecular weights less than naphthalene (KOVAT < 1185) are obviously removed due to a combination of biological and abiotic factors (dissolution and evaporation); however, compounds with molecular weights greater than 1-methylnaphthalene (KOVAT > 1315) appear to be present in relatively identical concentrations compared to the starting materials. That is, while overall levels are slightly reduced as illustrated by the data in Table 2, the relative concentrations of the individual polynuclear aromatics are very similar in the time zero and time one year samples. This is also reflected quite obviously by the qualitative appearance of the aromatic fractions shown in Figures 4B and 10B, respectively, and by the data presented in Figure 12A. Figure 12A graphically presents the relative concentration abundance of selected aromatic hydrocarbons from the 1 ppt spike of fresh crude oil at time zero and after one year. Clearly while the relative range of concentrations of all of the compounds in the time zero and one year samples are lower compared to the 50 ppt sample shown in Figure 9A, the overall concentrations of the time zero and naturally weathered 1 ppt samples are still relatively similar. This is particularly true of the higher molecular weight compounds, bi-phenyl, fluorene, phenanthrene and

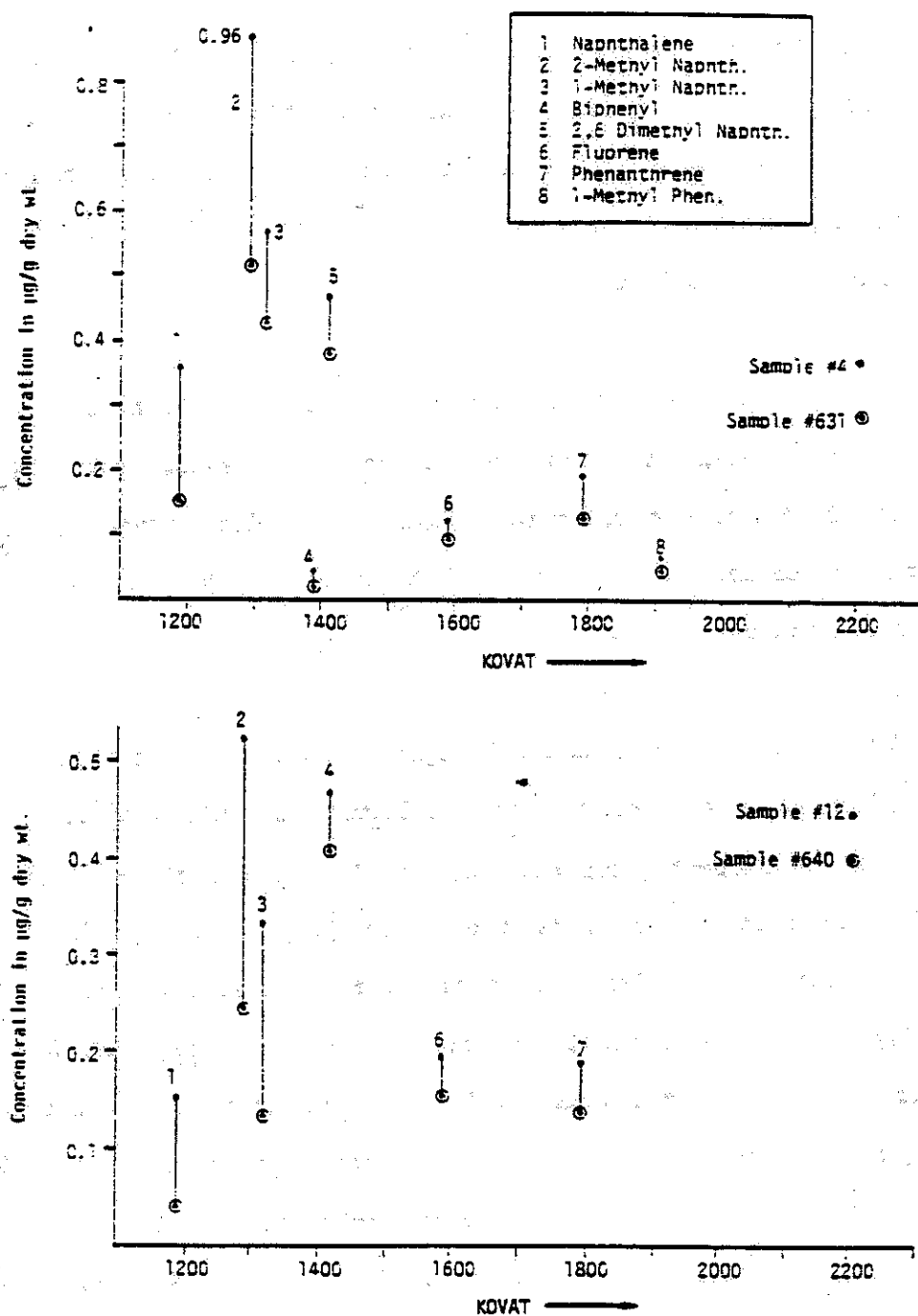


Figure 12. Concentration abundance of selected aromatic hydrocarbons from a 1.0 part per thousand spike of fresh crude (Top) showing the time zero sample (•) and sample after one year of weathering (⊙). Bottom shows a 1.0 ppt spike of artificially weathered crude for the time zero sample (•) and sample after one year of weathering (⊙).

1-methylphenanthrene. As in Figure 9A and B, the relative concentrations of artificially weathered aromatic compounds from the 1.0 ppt sample shown in 12B show that concentrations are in the same range in the artificially weathered sample as in the fresh sample after it had been weathered for a full year.

Clearly, while biological degradation of the aliphatic hydrocarbons (primarily n-alkane) occurred at the 1 ppt level, concomitant degradation of the higher molecular weight polynuclear aromatics compounds with molecular weights above that of methyl-naphthalene did not occur at a significant level.

This lack of degradation of higher molecular weight PNA's at the 1.0 ppt level is also illustrated in Figure 13, which presents the aromatic fraction chromatograms of: A) the 1 part per thousand fresh crude spiked into the sediment at time zero; B) the aromatic fraction obtained from the 1 ppt sediment after one year of in situ weathering in Kasitsna Bay; and C) the aromatic fraction of the 1 ppt sediment spiked with artificially weathered crude oil after one year of additional weathering in Kasitsna Bay. Clearly, examination of chromatograms 13A and B shows that some loss of the lower molecular weight alkyl substituted benzenes at retention times 10.45, 11.68, 15.15, 15.90, 16.49 and 17.71 has occurred due to either evaporation or dissolution. Compounds with molecular weights greater than that of 1-methyl-naphthalene at retention time 29.41 (B) are present in nearly identical relative concentrations. The chromatogram in 13C shows that the same compounds were also

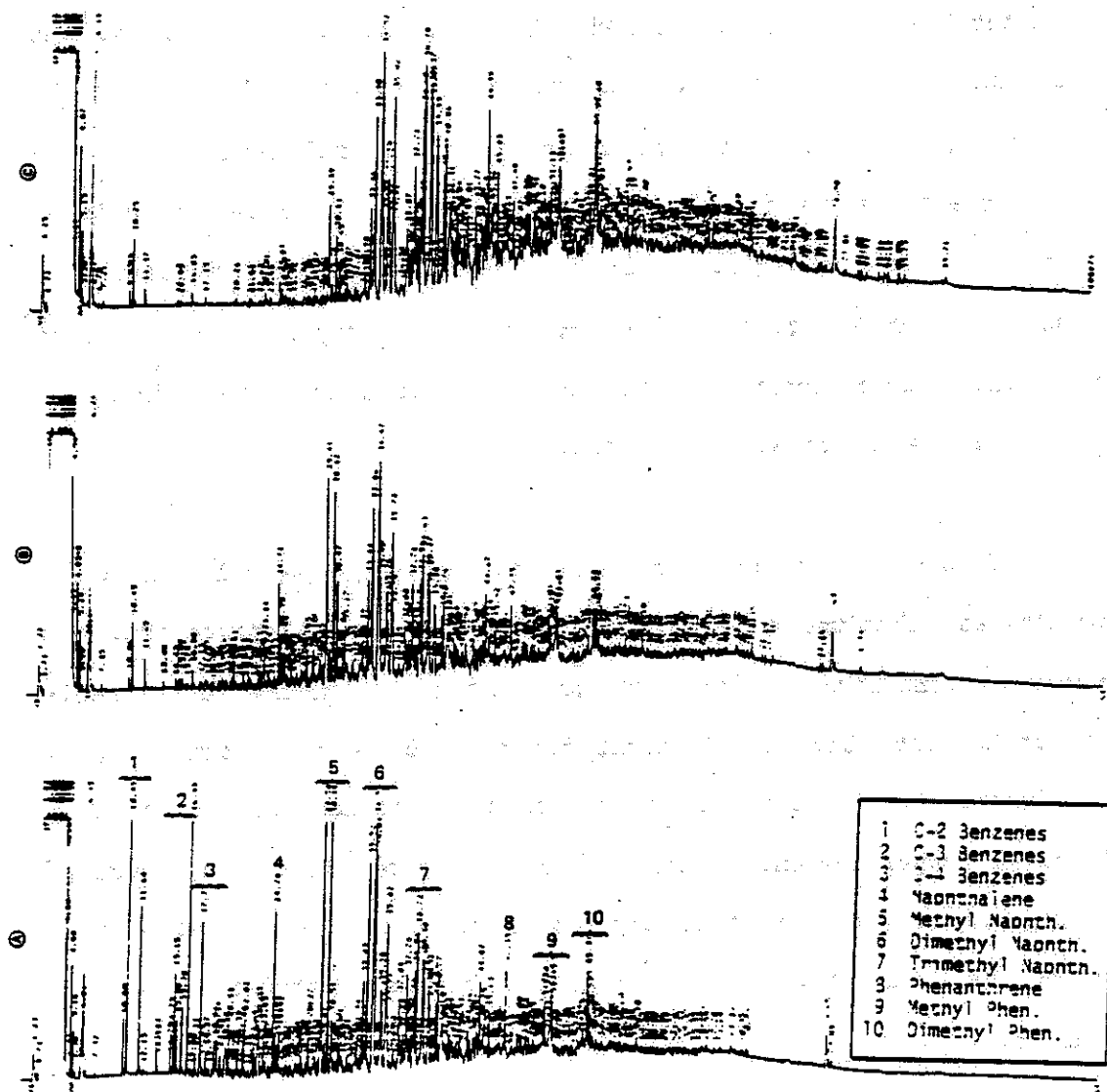


Figure 13. Flame Ionization Detector gas chromatograms of extracts of the aromatic fractions obtained from: A, the sediment spiked with 1 ppt fresh crude oil at time zero; B, the 1 ppt fresh crude sample after one year of natural weathering in Kasitsna Bay and C, the 1 ppt sediment sample spiked with artificially weathered crude oil after one year of additional weathering in Kasitsna Bay.

present in the "artificially weathered" oil which was spiked into the sediment after an additional year of natural weathering. This suggests that although many lower molecular weight aromatic compounds are removed from natural weathering of spilled oil while the oil is still at the surface, once the less water soluble and volatile higher molecular weight PNA's are incorporated into the sediment, additional degradative processes are extremely slow. Thus, while the relatively non-toxic aliphatic hydrocarbons are significantly degraded by biological processes in the sediments at 1 ppt, the more toxic aromatic compounds appear to be longer lived when introduced to the sediment from either fresh or weathered crude oil at similar levels.

Figure 14 presents the aliphatic, aromatic and polar fraction chromatograms obtained on the 0.1 ppt fresh crude oil spiked into the sediment at time zero (a) and after one year of weathering in the sediments of Kasitsna Bay (b, aliphatic fraction; c, aromatic fraction; d, polar fraction). Clearly, almost all of the n-alkanes in the starting oil are no longer present in the sediment after one year of weathering. In fact, the only compounds of any significance in the aliphatic fraction of the fully weathered sediment are higher molecular weight odd n-alkanes, nC_{23} , nC_{25} , nC_{27} , and nC_{29} . These same compounds are also predominant in the fresh crude sample shown in Figure 14A. That is, instead of seeing a regular decrease in higher molecular weight n-alkanes from nC_{22} through nC_{32} , the odd carbons at 23, 25 and 27 from biogenic input are clearly present. These are the only compounds which

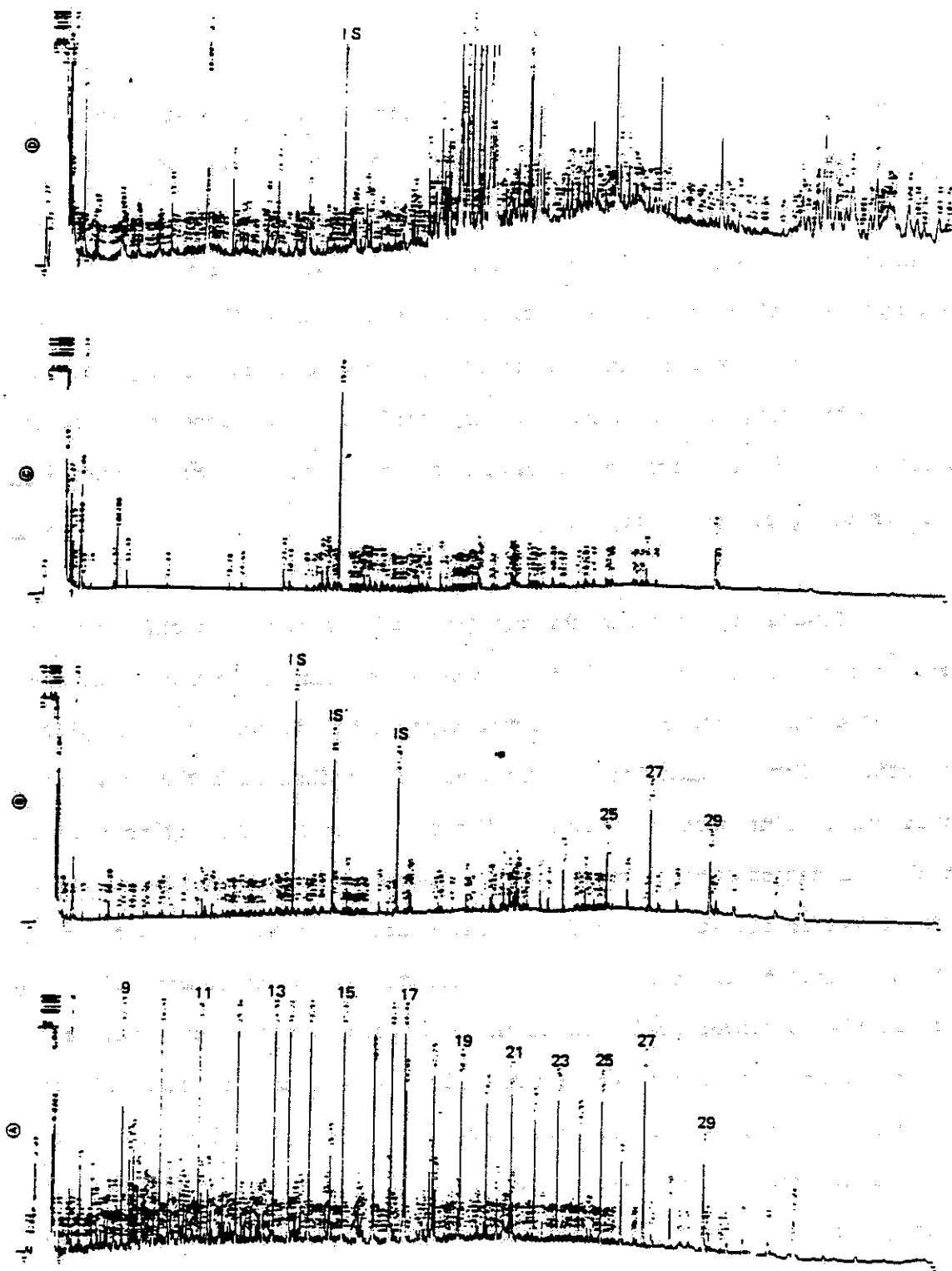


Figure 14. Flame Ionization Detector capillary gas chromatograms of: A, the aliphatic fraction of the sediment spiked with 0.1 ppt Fresh Crude Oil at time zero and B, the aliphatic fraction, C, the aromatic fraction, and D, the polar fraction extracts obtained on the 0.1 ppt Fresh Crude Oil spiked sample after one year of Natural Weathering in Kasitsna Bay.

remain in the sediment after one year, although there is some evidence that several unsaturated compounds between KOVAT indices 1900 and 2200 are present in Figure 14B. The aromatic fraction 14C shows only extremely low levels of residual materials with some evidence of pyrene perhaps remaining in the sediment at retention time 78.70. This compound was not detected in the starting crude oil to an appreciable degree, however, so its presence may reflect input from some other source. GC/MS characterization of the compounds in the polar fraction, 14D, is being completed at this time.

Figure 15 shows the chromatograms of the aliphatic and aromatic fractions of the 50 ppt artificially weathered crude oil spiked into the sediment after one year of additional degradation in the sediment plots in Kasitsna Bay. Comparison of the sediments spiked with the weathered crude oil at time zero, as shown in Figure 5, shows little or no change in the oil composition after one year of additional weathering. This is perhaps better illustrated in Figure 16, which presents the concentration abundance of the n-alkanes in the sediment spike at 50 ppt of the artificially weathered crude oil in the time zero sample and after one year of additional natural weathering. The data illustrate that all compounds below the level of nC_{14} are drastically reduced in both the starting material and the residual oil isolated after one year of natural weathering; however, the higher molecular weight compounds are not significantly altered. The corresponding data for the aromatic fraction of the 50 ppt spike of artificially weathered crude are shown in Figure 9B. These

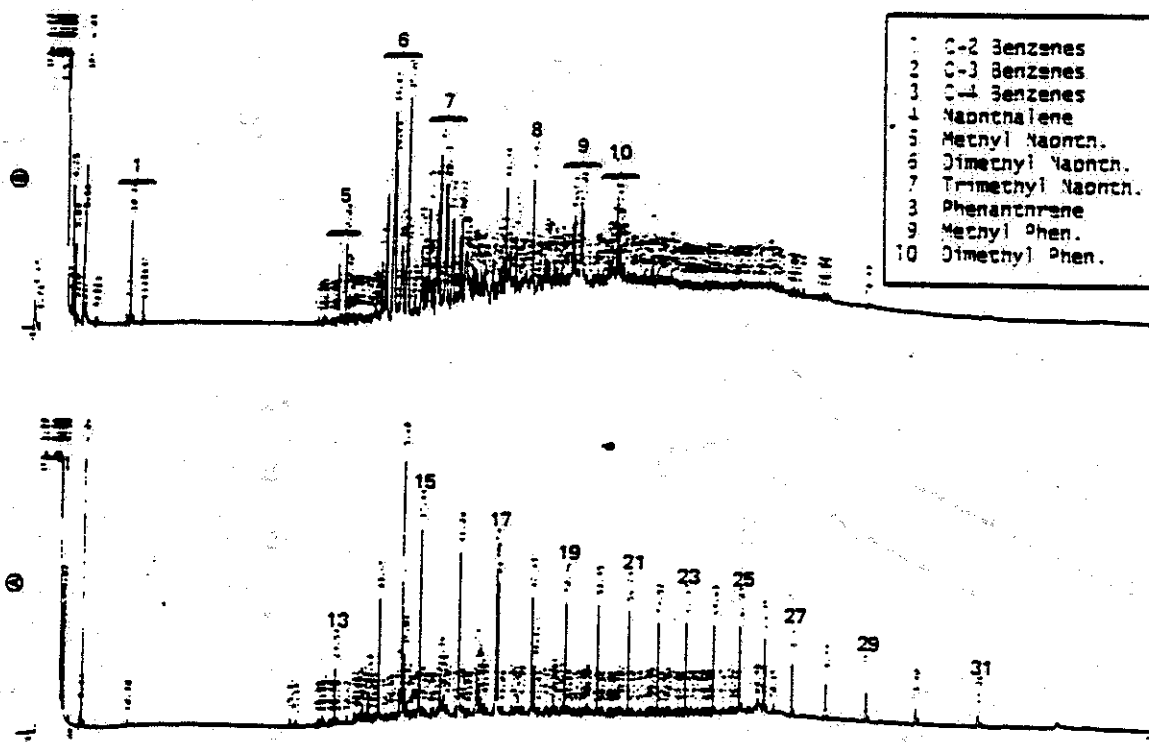


Figure 15. Flame Ionization Detector capillary gas chromatograms of: A, the aliphatic fraction and B, the Aromatic fraction extracts obtained from the time one year Kasitsna Bay sample spiked with Artificially Weathered Cook Inlet Crude Oil at 50 ppt.

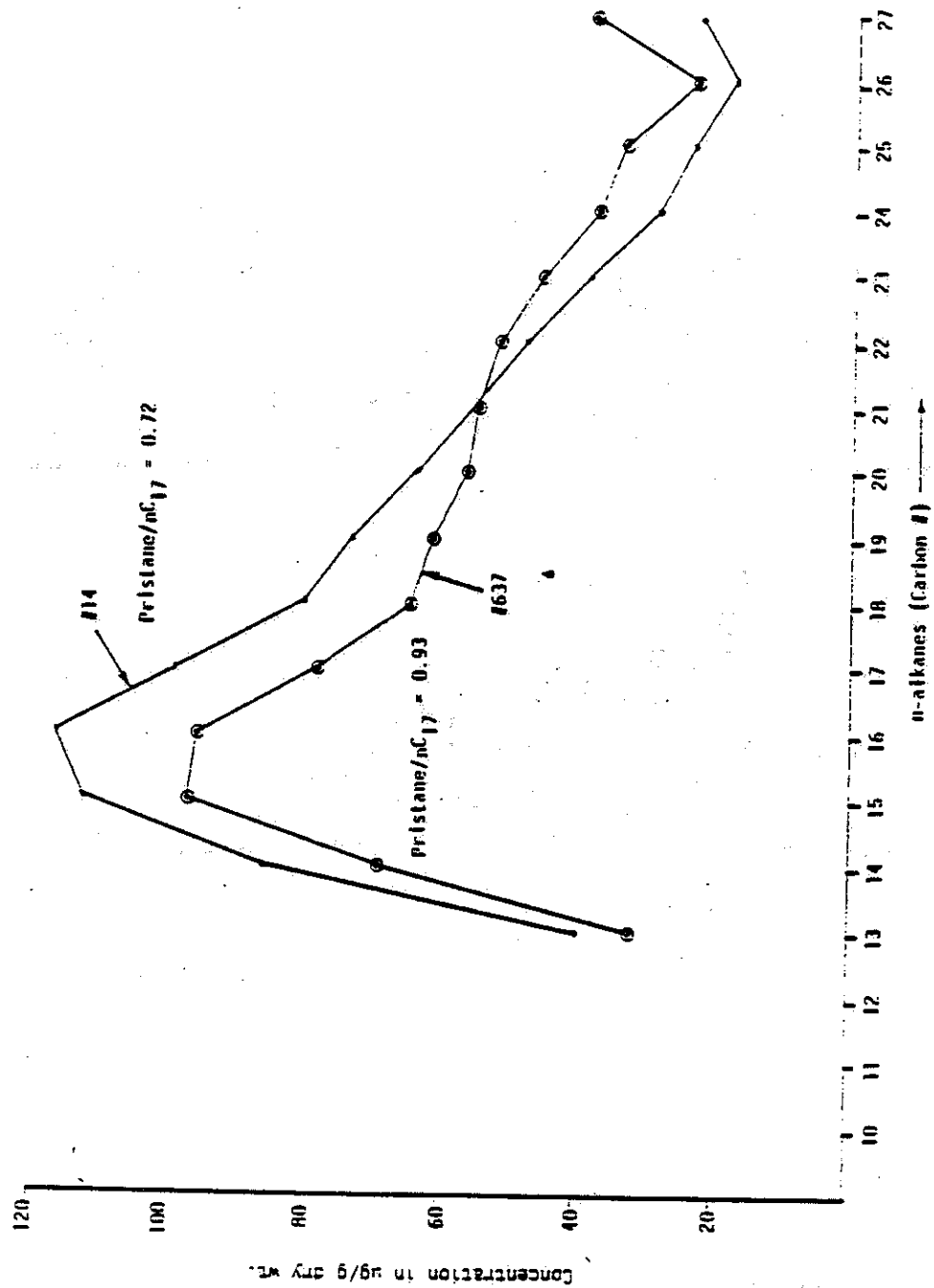


Figure 16. Concentration abundance of the n-alkanes for a sediment oil spike of 50 parts per thousand artificially weathered crude illustrating the time zero sample (•) and sample after one year of weathering (⊙).

show that while the overall concentrations of the lower molecular weight mono and di-cyclic aromatic compounds were reduced in the weathered crude oil compared to the fresh crude oil, once the artificially weathered oil reached the sediment, further degradation and loss of the aromatic compounds did not occur.

When 1.0 ppt weathered crude oil was spiked into the sediments, much greater degradation and loss of the lower molecular weight n-alkanes occurred as illustrated by the data in Figure 17. In Figure 17 the loss of lower molecular weight aliphatic compounds can clearly be observed in the artificially weathered oil as it was spiked into the sediments. The sample collected after one year of weathering at Kasistna Bay contained essentially no aliphatic hydrocarbons below nC_{24} . This was very similar to the case when 1.0 ppt fresh crude oil was spiked into the sediments and similar decreases in the aliphatic fraction were observed. The data in Figure 12B, however, show that the relative concentrations of aromatics in the 1.0 ppt weathered crude did not decrease significantly over the year period after the oil was introduced into the sediment. Quite clearly from these results, after fresh or weathered oil is incorporated into the sub-Arctic sedimentary regime at concentrations greater than 1.0 ppt, only limited additional degradation of the aromatic fraction occurs, at least in periods up to one year.

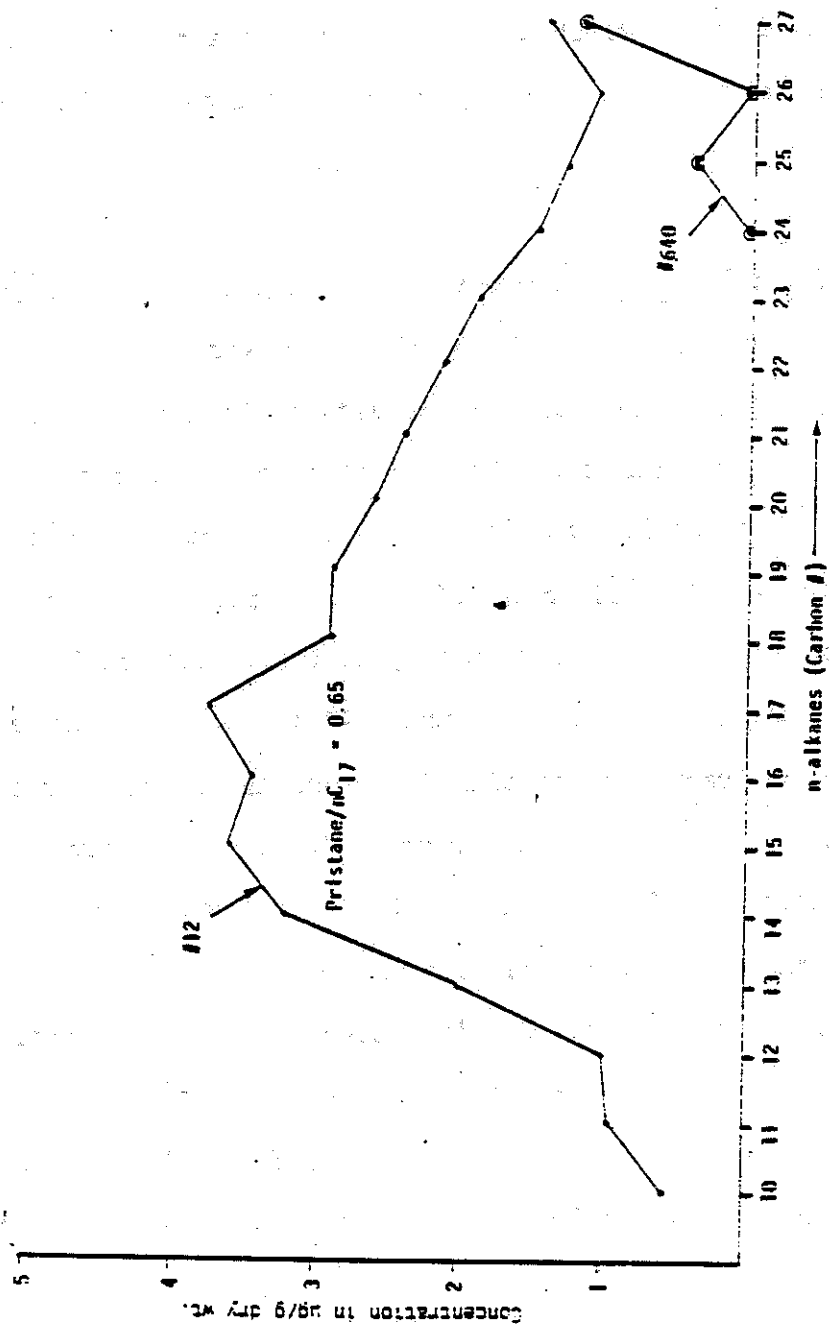


Figure 17. Concentration abundance of the n-alkanes for a sediment oil spike of 1.0 parts per thousand artificially weathered crude illustrating the time zero sample (·) and sample after one year of weathering (⊙).

Sadie Cove Oil/Nutrient Soiked Experiments

Figure 18 presents the aliphatic fraction chromatograms obtained on a) the 50 ppt oil plus starch b) 50 ppt oil alone and c) 50 ppt oil plus Chiton samples from Sadie Cove. The three chromatograms are essentially identical showing that little or no degradation of the oil occurred at the 50 ppt level. This is also reflected quantitatively by comparing the numbers in Table 1 for samples No.s 782, 779 and 780. These data suggest that the total resolved hydrocarbons and unresolved complex mixtures are essentially identical in the three samples. Other similarities include the odd/even hydrocarbon ratios, the ratio of the sum of pristane plus phytane to the total n-alkanes, and the pristane/ nC_{17} and phytane/ nC_{18} ratios. Essentially, these data suggest that at the 50 ppt level degradation is not nutrient limited. Figure 19 presents the aromatic fraction chromatograms obtained on the same three Sadie Cove sediment samples: a) oil plus starch, b) oil alone and c) oil plus Chiton. As the data in Table 2 illustrate, the aromatic compounds which were identified appear to be essentially the same in all three samples, although there may be some decrease in the levels of aromatic compounds in the oil and starch sample (a). Replicate analyses would be required to determine if the subtle difference in overall aromatic compound levels is statistically significant. Alternatively, it may be prudent to examine 1.0 ppt oil spikes in the presence and absence of nutrients to determine if enhanced aromatic hydrocarbon degradation can be induced to lower overall hydrocarbon levels where the inherent toxicity may be reduced.

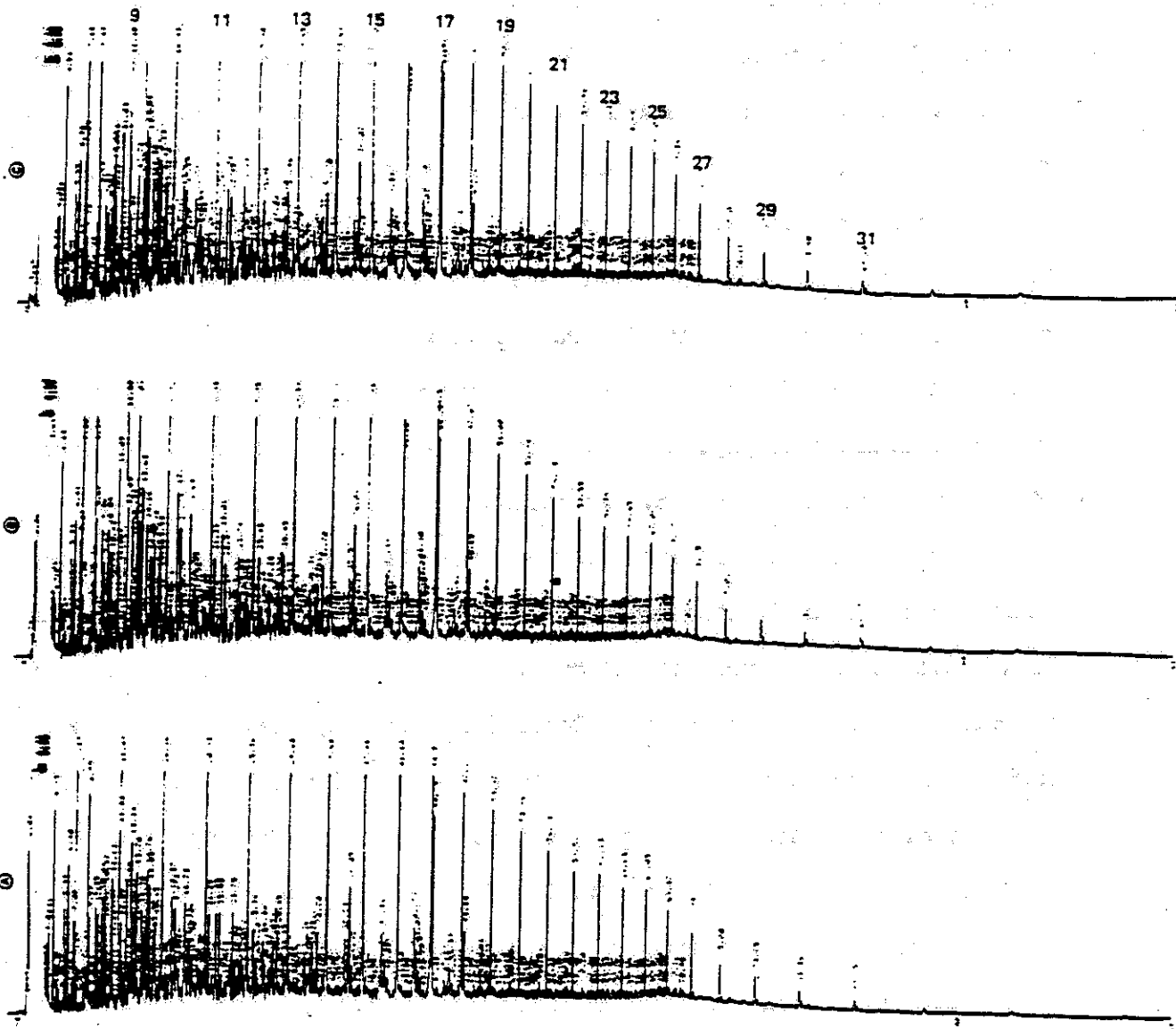


Figure 18. Flame Ionization Detector capillary gas chromatograms of aliphatic fraction extracts obtained on: A, 50 ppt fresh Oil plus starch. B, 50 ppt fresh Oil alone, and C, 50 ppt fresh Oil plus Chitin after one year of natural weathering in the sediments of Sadie Cove.

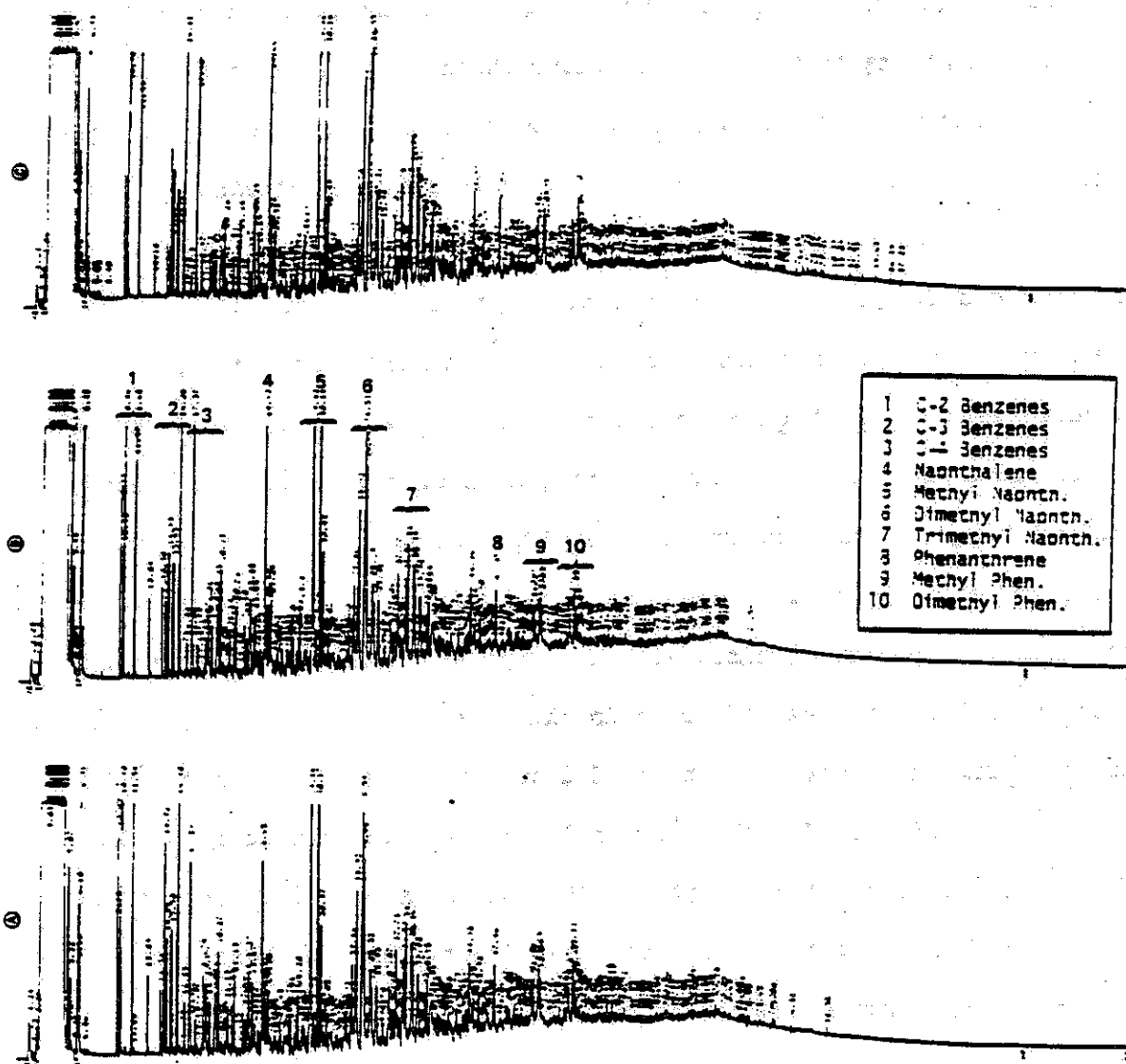


Figure 19. Flame Ionization Detector capillary gas chromatograms of aromatic fraction extracts obtained on: A, 50 ppt fresh Oil plus starch, B, 50 ppt Oil alone, and C, 50 ppt fresh Oil plus Chitin after one year of natural weathering in the sediments of Sadie Cove.

SUMMARY

The results presented here support the conclusion that in a major oil spill event in the sub-Arctic marine environment, the most significant weathering of the oil will occur at the air/sea interface or in the water column before the oil is incorporated into the sedimentary regime. This is particularly true in fine-grain sediment matrices in low-energy environments. Once levels of fresh and weathered Cook Inlet Crude oil reached concentrations in excess of 1 ppt in the sediment plots examined in the study, very little additional weathering or loss of higher molecular weight aromatic hydrocarbons occurred. At spiked levels of 50 ppt with both fresh and weathered crude oil, nearly complete inhibition of microbiological utilization or selective removal of aliphatic hydrocarbons was also observed, especially for those sediments spiked with fresh crude. Recovery of biological activity and selective utilization of aliphatic hydrocarbons did occur in the samples spiked with fresh and weathered crude at 1 ppt, and in the 0.1 ppt spiked samples, there was little or no evidence of either aliphatic or aromatic petroleum hydrocarbon contamination after one year. At that time, the 0.1 ppt spiked samples appeared to contain only the same biogenic hydrocarbons observed in the non-spiked control sediment samples from Kasitsna Bay.

In the study plots which were spiked with 50 ppt oil plus added nutrients (starch and Chitin), there was no evidence of any enhanced biotic recovery or selective hydrocarbon utilization with either fresh or weathered crude oil. This suggests inhibition of biological processes

from the high levels of toxic aromatic compounds in the oil itself rather than inhibition from limited nutrient concentrations. To more accurately address the role of added nutrients in oil degradation, detailed analyses should be completed on lower spiked oil concentrations in the presence and absence of nutrients. Also, experiments to assess the role of dissolved oxygen, grain-size, the energy (tidal and wave) input to the sedimentary environment, total organic carbon content and other factors such as total bio-mass, could be considered in future studies.

From the results obtained on the fresh and weathered crude oils and the sediment samples examined in this program, it appears that the maximum amount of weathering and removal (dissolution and evaporation) of toxic components can be achieved if spill clean up and treatment efforts are designed to prolong the time that the oil remains on the water surface or suspended in the water column. This may suggest limited use of dispersants or detergents in certain spill situations, particularly if damage to coastal zones is not imminent. Containment and recovery of the residual higher molecular weight materials should take precedence over other strategies such as chemical dispersal which may result in higher sub-tidal sediment loadings.

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