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Environmental Assessment of the Alaskan Continental Shelf

Final Reports of Principal Investigators

Volume 22   **February 1984**

U.S. DEPARTMENT OF COMMERCE
National Oceanic and Atmospheric Administration
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Ocean Assessments Division

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Minerals Management Service

Outer Continental Shelf Environmental Assessment Program

ENVIRONMENTAL ASSESSMENT

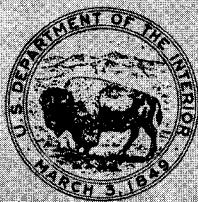OF THE

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FINAL REPORTS OF PRINCIPAL INVESTIGATORS

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JUNEAU, ALASKA

Environmental Assessment of the Alaskan Continental Shelf

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C O N T E N T S

Final Report

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

Volume II - Appendices

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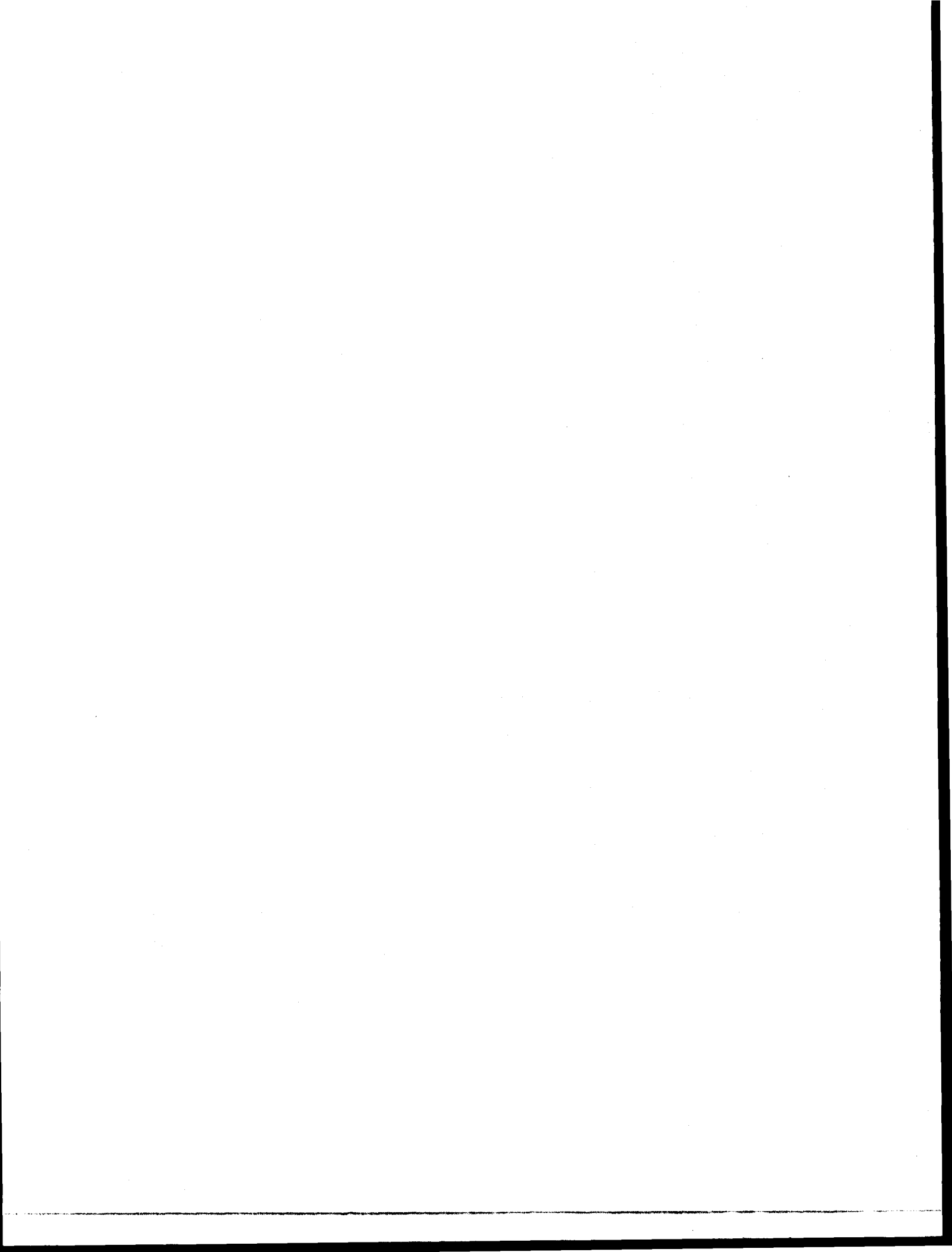
VOLUME II

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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.

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.

APPENDIX A

CODE LISTING FOR OPEN-OCEAN
OIL-WEATHERING CALCULATIONS

```
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,MTC,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,KB,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),T10(30),HVAP1(30),HVAPZ(30)
00250          2,VOLL(6,30),VOL(30),MOLES(30),MTCA(30),VIS(30),VISK(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 ANAME(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 ITEML/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.,59.5,55.4,50.8
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 DISPENSION 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='DSED:CUTVP2.OUT')
01100          OPEN(UNIT=34,DIALOG='DSED:CUTVP2.PLT')
01110          OPEN(UNIT=35,DIALOG='DSED: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(I2)
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              ITEM=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(I),I=1,5)
01620      140     FORMAT(10A5)
01630              TYPE 150
01640      150     FORMAT(1X,'ENTER AN IDENTIFICATION NUMBER FOR
01650      1 THIS CRUDE ON I5')
01660              ACCEPT 160, ITEM
01670      160     FORMAT(I5)
01680              TYPE 170
01690      170     FORMAT(1X,'ENTER A SAMPLE NUMBER ON I5')
01700              ACCEPT 160, ISAMP
01710              TYPE 180
01720      180     FORMAT(1X,'ENTER THE BULK API GRAVITY')
01730              ACCEPT 230, APIB
01740              TYPE 190
01750      190     FORMAT(/,1X,'YOU MUST ENTER THE TRUE BOILING POINT
01760      1 CUT DATA STARTING',/,1X,'WITH THE MOST VOLATILE CUT
01770      2 AND GOING TO THE BOTTOM OF THE BARREL',/)
01780      C
01790      C         CALCULATE THE BULK DENSITY OF THE CRUDE AT 60/60.
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
01940      1 FOR CUT',I3)
01950              ACCEPT 230, TB(I)
01960      230     FORMAT(F10.0)
01970              TYPE 240, I
01980      240     FORMAT(1X,'ENTER API GRAVITY FOR CUT',I3)
```

```
01990              ACCEPT 230, API(I)
02000              TYPE 250, I
02010     250      FORMAT(1X,'ENTER VOLUME PER CENT FOR CUT',I3)
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,I2,5X,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 I2')
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 ',I2
02510         1,' IS LESS THAN CUT ',I2,/,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
```

```
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             MW(NCUTS)=600.
02700             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             NV=1
02760             NC1=NCUTS
02770             DO 550 I=1,NCUTS
02780             APIN=API(I)
02790             SPGR(I)=141.5/(API(I)+131.5)
02800             SPGR(I)=0.983*SPGR(I)
02810             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             IF(TBN.LT.850.) GO TO 490
02890             NV=2
02900             NC1=NCUTS-1
02910    490      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             VISK(I)=10.**VIS1
02970             VLOGK(I)=ALOG(VISK(I))
02980             GO TO (500,550), NV
02990    C
03000    C        STORE THE CUT INFORMATION FOR A NON-RESIDUUM CUT.
03010    C
03020    500      NS(I)=NSN
03030             A(I)=AN
03040             B(I)=BN
03050             MW(I)=MW1
03060             TC(I)=TC1
03070             TC(I)=TC(I)+459.
03080             VC(I)=VC1
03090             PC(I)=PC1
03100             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             NC(I)=0
03160             YTEN=ALOG10(0.01315/PC(I))
03170             X=(TB(I)+459.)/TC(I)
03180    510      EX=EXP(-20.*(X-B(I))**2)
03190             Y=-A(I)*(1.-X)/X-EX
03200             YOBJ=Y-YTEN
03210             VP(I)=PC(I)*10.**Y
03220             TEST=ABS(VP(I)-0.01315)
03230             IF(TEST.LT.0.001315) GO TO 540
03240             NC(I)=NC(I)+1
03250             IF(NC(I).GT.20) GO TO 520
03260             DY=A(I)/(X*X)+40.*(X-B(I))*EX
03270             B1=YOBJ-DY*X
03280             X=-B1/DY
03290             GO TO 510
03300    C
```

```
03310    C          UNSUCCESSFUL EXIT FROM NEWTON-RAPHSON
03320    C
03330    520  TYPE 530, I,X,Y
03340    530  FORMAT(1X,'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 WATSONS METHOD FOR THE
03440    C          VAPOR PRESSURE BELOW 10 MMHG.  SEE GAMSON 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 (IOU,560) (ANAME(I),I=1,5)
03570    560  FORMAT(1H1,'SUMMARY OF TBP CUTS CHARACTERIZATION FOR: '
03580        1,5A5)
03590         WRITE (IOU,570)
03600    570  FORMAT(/,1X,'CODE VERSION IS CUTVP2 OF FEBRUARY 83')
03610         WRITE (IOU,580) ITEM,ISAMP
03620    580  FORMAT(1X,'ITEM ',I5,', SAMPLE ',I5)
03630         WRITE (IOU,590)
03640    590  FORMAT(/,8X,'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 (IOU,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),VISK(I),NC(I),NS(I)
03700    600  FORMAT(1X,I2,12(1X,1PE9.2),2(1X,I2))
03710    610  CONTINUE
03720         WRITE (IOU,620) APIB
03730    620  FORMAT(//,1X,'BULK API GRAVITY = ',F5.1)
03740         WRITE (IOU,630)
03750    630  FORMAT(//,1X,'TB = NORMAL BOILING TEMPERATURE, DEG F')
03760         WRITE (IOU,640)
03770    640  FORMAT(1X,'API = API GRAVITY')
03780         WRITE (IOU,650)
03790    650  FORMAT(1X,'VOL = VOLUME PER CENT OF TOTAL CRUDE')
03800         WRITE (IOU,660)
03810    660  FORMAT(1X,'MW = MOLECULAR WEIGHT')
03820         WRITE (IOU,670)
03830    670  FORMAT(1X,'TC = CRITICAL TEMPERATURE, DEG RANKINE')
03840         WRITE (IOU,680)
03850    680  FORMAT(1X,'PC = CRITICAL PRESSURE, ATMOSPHERES')
03860         WRITE (IOU,690)
03870    690  FORMAT(1X,'VC = CRITICAL VOLUME, CC/MOLE')
03880         WRITE (IOU,700)
03890    700  FORMAT(1X,'A AND B ARE PARAMETERS IN THE VAPOR PRESSURE
03900        1 EQUATION')
03910         WRITE (IOU,710)
03920    710  FORMAT(1X,'T10 IS THE TEMPERATURE IN DEG R WHERE THE VAPOR
03930        1 PRESSURE IS 10 MM HG')
03940         WRITE (IOU,720)
03950    720  FORMAT(1X,'VIS IS THE KINEMATIC VISCOSITY IN CENTISTOKES
03960        1 AT 122 DEG F')
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03970              WRITE (IOU,730)
03980      730     FORMAT(1X,'NC = ERROR CODE, SHOULD BE LESS THAN 20')
03990              WRITE (IOU,740)
04000      740     FORMAT(1X,'NS = ERROR CODE, SHOULD BE EQUAL TO 1')
04010              WRITE (IOU,750) NCUTS
04020      750     FORMAT(1X,'IGNORE THE ERROR CODES FOR COMPONENT NUMBER ',I2
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 2I5
04110      C               2.   THE CRUDE NAME ON 5A5
04120      C               3.   NCUTS ON I5
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                    KMTC, MASS TRANSFER COEFFICIENT CODE (FLOATED).
04220      C                    ALL ON 10(1X,1PE10.3).
04230      C               6.   NUMBER OF CUTS+1 ON I5
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(I5)
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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04630   C
04640   C          WHERE P1 = PRESSURE AT TR1, P2 = PRESSURE AT TR2. HVAPZ IS
04650   C          THE HEAT OF VAPORIZATION AT ABSOLUTE ZERO,
04660   C          R = 1.987 BTU/(LBMOLE, DEG R),
04670   C          TC = CRITICAL TEMPERATURE AND INTEGRAL = VAPORIZATION
04680   C          INTEGRAL BETWEEN TR1 AND TR2.
04690   C
04700              WRITE (IOU,820)
04710   820        FORMAT(1H1,'CRUDE OIL CHARACTERIZATION AND PSEUDOCOMPONENT
04720          1 EVAPORATION MODEL')
04730              WRITE (IOU,830) (ANAME(I),I=1,5)
04740   830        FORMAT(1X,'IDENTIFICATION: ',5A5,/)
04750              WRITE (IOU,580) ITEM,ISAMP
04760              WRITE (IOU,840) XPRINT
04770   840        FORMAT(1X,'VAPOR PRESSURE IN ATMOSPHERES AT ',1PE10.3,' DEG F')
04780              WRITE (IOU,850)
04790   850        FORMAT(/,12X,'VP',/)
04800              DO 900 I=1,NC1
04810              X=XSAVE
04820              IF(X.LT.T10(I)) GO TO 860
04830              X=X/TC(I)
04840              EX=EXP(-20.*(X-B(I))**2)
04850              Y=-A(I)*(1.-X)/X-EX
04860              VP(I)=PC(I)*10.**Y
04870              GO TO 880
04880   860        TR1=X/TC(I)
04890   C
04900   C          DO INTEGRAL BY SIMPSONS RULE WITH 21 POINTS
04910   C
04920              TR2=T10(I)/TC(I)
04930              DH=(TR2-TR1)/20.
04940              RESULT=YI(TR1)
04950              TR=TR1
04960              DO 870 K=1,10
04970              TR=TR+DH
04980              RESULT=RESULT+4.*YI(TR)
04990              TR=TR+DH
05000              RESULT=RESULT+2.*YI(TR)
05010   870        CONTINUE
05020              TR=TR+DH
05030              RESULT=RESULT+4.*YI(TR)
05040              TR=TR+DH
05050              RESULT=DH*(RESULT+YI(TR))/3.
05060              P1=-4.33-HVAPZ(I)*RESULT/(1.987*TC(I))
05070              VP(I)=EXP(P1)
05080   880        WRITE (IOU,890) I,VP(I)
05090   890        FORMAT(1X,I2,5X,1PE10.3)
05100   900        CONTINUE
05110              TYPE 910
05120   910        FORMAT(1X,'THE TBP CUTS HAVE BEEN CHARACTERIZED')
05130              TYPE 920
05140   920        FORMAT(1X,'DO YOU WANT TO WEATHER THIS CRUDE?')
05150              MWSCTH=1
05160              ACCEPT 340, ANS
05170              IF(ANS.EQ.'Y') GO TO 930
05180   C
05190   C          GO CALCULATE THE MEAN MOLECULAR WEIGHT OF THE CRUDE
05200   C          BEFORE EXITING. MWSCTH IS THE ROUTING SWITCH TO
05210   C          WEATHER THE CRUDE OR STOP.
05220   C
05230              MWSCTH=2
05240              BBL=1000.
05250              GO TO 1210
05260   C
05270   C          THIS ENDS THE CRUDE CHARACTERIZATION. BEGIN THE OIL-
05280   C          WEATHERING INPUT.
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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           1FICIENT')
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, KMTC
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.*SPGR(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 (IOU,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), KMTC
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, UMTC
07150          WRITE (IOU,1350) UMTC
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          UMTC=UMTC/TEMP/100.
07230          DO 1360 I=1,NC1
07240          MTC(I)=UMTC
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 1380
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 (IOU,1400) KMTC
07440    1400  FORMAT(1H1,'OVER-ALL MASS-TRANSFER COEFFICIENTS BY INPUT
07450         1 CODE',I2)
07460          WRITE (IOU,1410) KH
07470    1410  FORMAT(/,1X,'OVER-ALL MASS-TRANSFER COEFFICIENT FOR CUMENE = '
07480         1,1PE10.3,'  M/HR',/)
07490          WRITE (IOU,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 (IOU,1430) I,MTCA(I),MTC(I)
07650    1430  FORMAT(2X,I3,2(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, DATAMW
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   SPGRB=141.5/(APIB+131.5)
08350         MASS=0.1582*BBL*SPGRB
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 (IOU,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 (IOU,1650) VISMIX,XPRINT,EXPT
08810    1650   FORMAT(/,1X,'KINEMATIC VISCOSITY OF THE BULK CRUDE FROM THE
08820          1 CUTS = ',1PE8.1,' AT T = ',0PF5.1,' 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 INFOMATION 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 (IOU,1750) 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 (IOU,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          DISPENSIONS/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 (IOU,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 (IOU,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=',I3)
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,I2,5(1X,1PE9.2),1X,I3)
10150   1950   CONTINUE
10160          WRITE (ITY,1960) C1,C2P,C4
10170   1960   FORMAT(/,1X,'MOUSSE CONSTANTS: MOONEY=',1PE9.2
10180          1,', MAX H20=',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, SPGR=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 BRKG4(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-06,1.536E-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          API2=API*API
11020          TB2=TB*TB
11030          CROSS=API*TB
11040          I=1
11050          IF(API.GT.35.) I=2
11060          VIS1=V(I,1)+V(I,2)*TB+V(I,3)*API+V(I,4)*CROSS+V(I,5)*TB2
11070         1+V(I,6)*API2
11080          GO TO (10,30), NV
11090    10    I=1
11100          IF(TB.GT.500.) I=2
11110          MW1=C(I,1)+C(I,2)*TB+C(I,3)*API+C(I,4)*CROSS+C(I,5)*TB2
11120         1+C(I,6)*API2
11130          TC1=T(I,1)+T(I,2)*TB+T(I,3)*API+T(I,4)*CROSS+T(I,5)*TB2
11140         1+T(I,6)*API2
11150          TCK=(TC1+459.)/1.8
11160    C
11170    C        CALCULATE THE VISCOSITY OF THE CUT.
11180    C
11190          I=1
11200          IF(API.GT.35.) I=2
11210          VIS1=V(I,1)+V(I,2)*TB+V(I,3)*API+V(I,4)*CROSS+V(I,5)*TB2
11220         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 5, 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.  ITYP IS A HEADER PRINT SWITCH FOR THE
11880    C        80-COLUMN FILE.
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11890   C
11900          INT=1
11910          ITYP=1
11920          LINE=0
11930          NEQ1=NEQ+1
11940          NEQ2=NEQ+2
11950          NEQ3=NEQ+3
11960          NS=1
11970          IN=1
11980          IKEEP=1
11990          GONE(1)=1.
12000          DISPER=0.
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     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 (IOU,20)
12410   20     FORMAT(/,1X,'COUNT THE CUTS IN THE FOLLOWING OUTPUT FROM LEFT
12420         1 TO RIGHT',/)
12430          WRITE (IOU,30)
12440   30     FORMAT(1X,'THE INITIAL GRAM MOLES IN THE SLICK ARE:')
12450          WRITE (IOU,40) (Y(I),I=1,NEQ)
12460   40     FORMAT(11(1X,1PE10.3))
12470          WRITE (IOU,50)
12480   50     FORMAT(/,1X,'THE INITIAL MASSES (GRAMS) IN THE SLICK ARE
12490         1:')
12500          WRITE (IOU,40) (YMSAVE(I),I=1,NEQ)
12510          WRITE (IOU,60) TSAVE
12520   60     FORMAT(1X,'THE TOTAL MASS FROM THESE CUTS IS '
12530         1,1PE10.3,' GRAMS')
12540          WRITE (IOU,70)
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12550    70      FORMAT(/)
12560    C
12570    C          CALCULATE DY/DX AND SET THE STEP SIZE TO APPROXIMATE
12580    C          A 5% CHANGE IN THE MOST RAPIDLY CHANGING Y.  WHEN THIS
12590    C          Y DECREASES BY A FACTOR OF 20, RESET THE STEP SIZE
12600    C          ACCORDING TO THE NEXT Y.
12610    C          SOME Y'S WILL CHANGE SO FAST THAT THEY WILL BE GONE
12620    C          IN A FEW MINUTES.  THESE ARE DELETED BEFORE INTEGRATION
12630    C          STARTS AND NOTED ON THE PRINTED RESULTS.
12640    C
12650    C          INITIALIZE OR INCREMENT NFAST.
12660    C
12670    80      NFAST=NFAST+1
12680    90      CALL FXYZ(X,Y,K1,NEQ)
12690    C
12700    C          THE TIME UNIT IS HOUR.
12710    C          SET THE STEP SIZE TO H=0.05*Y/(DY/DX).
12720    C
12730            H=0.05*Y(NFAST)/K1(NFAST)
12740            YOLD=Y(NFAST)
12750            H=ABS(H)
12760            H2=H/2.
12770            GO TO (100,170), IN
12780    C
12790    C          IF THERE IS A RAPIDLY MOVING COMPONENT AT THE BEGINNING
12800    C          ITS STEP SIZE WILL BE VERY SMALL, DO NOT LET THE
12810    C          STEP SIZE BE LESS THAN 0.05 HOUR.
12820    C
12830    100     IF(H.GT.0.05) GO TO 130
12840    C
12850    C          Y(NFAST) CHANGES TOO FAST TO CALCULATE, DELETE IT AND MOVE
12860    C          EVERYBODY ONE SPACE TO THE LEFT.
12870    C
12880    C          WHEN YOU MOVE THE AREA BE SURE TO SUBTRACT THE CONTRIBUTION
12890    C          OF THE CUT JUST DELETED.
12900    C
12910            ISTART=1
12920            NFAST=1
12930            NDEL=NDEL+1
12940    C
12950    C          DECREASE THE NUMBER OF COMPONENTS BY 1
12960    C
12970            NEQ=NEQ-1
12980            NEQ1=NEQ+1
12990            NEQ2=NEQ+2
13000            NEQ3=NEQ+3
13010            NEQ4=NEQ+4
13020            AD=Y(1)/RHO(1)/Z
13030            DO 110 I=1,NEQ
13040    C
13050    C          SHIFT THE ARRAYS.
13060    C
13070            I1=I+1
13080            Y(I)=Y(I1)
13090            VP(I)=VP(I1)
13100            MTC(I)=MTC(I1)
13110            YSAVE(I)=YSAVE(I1)
13120            VLOG(I)=VLOG(I1)
13130            RHO(I)=RHO(I1)
13140            MWU(I)=MWU(I1)
13150            YMSAVE(I)=YMSAVE(I1)
13160    110     CONTINUE
13170    C
13180    C          BE SURE AND DO THE LAST THREE POSITIONS WHEN SHIFTING
13190    C
13200            Y(NEQ1)=Y(NEQ2)-AD
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13210          Y(NEQ2)=Y(NEQ3)
13220          Y(NEQ3)=Y(NEQ4)
13230          WRITE (IOU,120) NDEL
13240    120   FORMAT(1X,'CUT ',I2,' GOES AWAY IN MINUTES, THEREFORE IT WAS
13250         1 DELETED AND THE CUTS RENUMBERED',/)
13260          WRITE (ITY,120) NDEL
13270          GO TO 90
13280    130   IN=2
13290          GO TO (140,160) ITYP
13300    140   ITYP=2
13310          WRITE (ITY,150)
13320    150   FORMAT(/,1X,'TIME',2X,'BBL',3X,'SPGR',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 (IOU,180) H,NFAST
13460    180   FORMAT(/,2X,'STEP SIZE OF ',1PE10.3,' IS BASED ON CUT ',I3,/)
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          YM1(I)=YM(I)
13630          TMASS=TMASS+YM(I)
13640          YM(I)=YM(I)/YMSAVE(I)
13650    200   CONTINUE
13660          YM1(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 (IOU,220) X,LINE
13760    220   FORMAT(2X,'TIME = ',1PE8.1,' HOURS, MASS FRACTION OF EACH
13770         1 CUT REMAINING:',65X,I3)
13780          WRITE (IOU,230) (YM(I),I=1,NEQ)
13790    230   FORMAT(14(1X,1PE8.1))
13800          CHECK=TMASS+Y(NEQ2)+Y(NEQ3)
13810          WRITE (IOU,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 (IPU,250) NEQ1
13860    250   FORMAT(I5)
```

```
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=',1PE8.1,', AREA=',1PE8.1,' M**2. THICKNESS='
14060         2,1PE8.1,' 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=FRACTS*FB
14410          WRITE (IOU,300) W,VISCP,DISPER
14420   300    FORMAT(2X,'WEIGHT FRACTION WATER IN OIL = ',1PE8.1,', VIS
14430         1COSITY = ',1PE8.1,' CENTISTOKES, DISPERSION TERM = '
14440         2,1PE8.1,' 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)
```

```
14530          WRITE (IOU,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 (ITY,360) IX,TBBL,CSPGR,Y(NEQ1),ZP,IW,WDISP
14710          1,ERATE,WAREA,ICUT,JCUT
14720     360  FORMAT(1X,I3,1PE8.1,0PF5.2,2(1PE8.1),1X,I3
14730          1,3(1PE8.1),I2,I3)
14740          WRITE (IOU,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
```

```
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 (IOU,450)
15290    450      FORMAT(/,1X,'THE SLICK (MOLES) HAS DECREASED TO 10%
15300           1 OR LESS, THEREFORE THE CALCULATION WAS STOPPED.')
15310             WRITE (ITY,460)
15320    460      FORMAT(/,1X,'SLICK DECREASED TO 10% MASS **STOP**')
15330             GO TO 510
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), KMTC
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 (IOU,520) NDEL
15720    520      FORMAT(/,1X,'THE CUT NUMBERING BEGINS WITH',I3,' BASED ON
15730           1 THE ORIGINAL CUT NUMBERS',/)
15740             LINE=LINE+1
15750             WRITE (IOU,530) X,LINE
15760    530      FORMAT(1X,'THE FINAL MASS FRACTIONS FOR THE SLICK AT '
15770           1,1PE8.1,' HOURS ARE:',65X,I3)
15780             TYPE 540, LINE
15790    540      FORMAT(1X,'NUMBER OF LINES WRITTEN TO CUTVP2.PLT = ',I4)
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)
```

```
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(/,1X,'**************************************
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),VLOC(30),RHO(30),MW(30)
16050         1,SPGR(30),FRACTS,STEN,KB,DISPER,Z,TERM2,SPREAD,KMTC
16060          COMMON /TALE/ 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    30    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-COALESCING 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          IF(C2.GT.0.) GO TO 10
16830     C
16840     C       NO MOUSSE FOR THIS OIL, SET TERMS AND RETURN.
16850     C
16860          W=0.
16870          VTERM=1.
16880          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          IF(WINDS.EQ.WSAVE.AND.C4.EQ.C4SAVE) GO TO 20
16950          WSAVE=WINDS
16960          C4SAVE=C4
16970          U2=WINDS*WINDS
16980          C3=C4*U2
16990   20     EX=C3*TIME
17000          IF(EX.GT.20.) GO TO 80
17010          TEST=EXP(-EX)
17020     C
17030     C       BRACKET THE TIME WITH TWO VALUES OF W.
17040     C
17050          W=0.
17060          WMAX=1./C2
17070          WSTEP=WMAX/10.
17080   30     W=W+WSTEP
17090          TRY=WFUNC(W)
17100          IF(TRY.LT.TEST) GO TO 40
17110          IF(W.LT.WMAX) GO TO 30
17120          IERR=2
17130          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

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:

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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)·(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 $\exp(K_4F)$ 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:

$$(1 - K_2W) \exp\left[\frac{-2.5W}{1-K_1W}\right] \equiv \exp\left[-K_3t\right]$$

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

$$\mu = \mu_o \exp \left[\frac{-2.5W}{1-K1W} \right]$$

where μ_o 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 dispensions 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).

% Distilled	T, °F	API Gravity
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°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 Atmos-
pheric Boiling Points (see text) (Coleman, et al, 1978).

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

Alaska
North Slope

GENERAL CHARACTERISTICS

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

DISTILLATION, BUREAU OF MINES ROUTINE METHOD

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

Fraction No.	Cut temp. °F	Percent	Sum percent	Sp. gr. 60/60° F	° API 60° F	C.I.	Refractive index, n, at 20° C	Specific dispersion	S.U. visc. 100° F	Cloud test, °F
1	122									
2	167	2.1	2.1	0.693	72.7	—	1.38591	127.9		
3	212	2.6	4.7	.723	64.2	23	1.40312	139.0		
4	257	3.5	8.2	.752	56.7	27	1.41922	141.9		
5	302	3.6	11.8	.773	51.6	30	1.43082	147.0		
6	347	3.7	15.5	.790	47.6	31	1.43922	149.6		
7	392	3.5	19.0	.801	45.2	30	1.44626	152.1		
8	437	4.3	23.3	.818	41.5	33	1.45528	154.7		
9	482	4.8	28.1	.836	37.8	36	1.46565	157.0		
10	527	5.0	33.1	.851	34.8	38	1.47467	160.5		

Stage 2—Distillation continued at 40 mm Hg

11	392	2.8	35.9	0.873	30.6	45	1.48218	161.5	40	10
12	437	6.5	42.4	.881	29.1	45	1.48650	168.6	45	30
13	482	6.8	49.2	.897	26.2	49	1.49477	169.4	58	50
14	537	6.0	55.2	.910	24.0	52			93	70
15	573	7.4	62.6	.919	22.5	53			176	90
Residuum		36.3	98.9	.990	11.4					

Carbon residue, Conradson. Residuum 11.6 percent; crude 4.7 percent.

Residuum:
Sulfur, percent, —
Nitrogen, percent, —

APPROXIMATE SUMMARY

	Percent	Sp. gr.	° API	Viscosity
Light gasoline	4.7	0.710	67.9	
Total gasoline and naphtha	19.0	0.762	54.2	
Kerosine distillate	4.3	.818	41.5	
Gas oil	18.4	.860	33.1	
Nonviscous lubricating distillate	11.0	.887-.911	28.0-23.9	50-100
Medium lubricating distillate	8.1	.911-.922	23.9-22.0	100-200
Viscous lubricating distillate	1.8	.922-.924	22.0-21.6	Above 200
Residuum	36.3	.990	11.4	
Distillation 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
Repetto, Lower Pliocene
  and Puente, Miocene

California
Los Angeles County

GENERAL CHARACTERISTICS

Gravity, specific. 0.938   Gravity, ° API.....19.4.........   Pour point, ° F. below 5...........
Sulfur, percent, 1.59   Color, brownish black
Viscosity, Saybolt Universal at 100° F, 470 sec; 130° F, 229 sec.   Nitrogen, percent, 0.597

DISTILLATION, BUREAU OF MINES ROUTINE METHOD

Stage 1—Distillation at atmospheric pressure, 738 mm Hg

First drop 118 ° F

Fraction No.	Cut temp ° F	Percent	Sum percent	Sp gr 60/60° F	° API 60° F	C. I	Refractive index n₀ at 20° C	Specific dispersion	S U visc 100° F	Cloud test ° F
1....	122						....	....		
2....	167									
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....	302	2.4	7.1	.767	53.0	27	1.42308	127.1		
6....	347	2.5	9.6	.788	48.1	30	1.43480	128.8		
7....	392	2.8	12.4	.810	43.2	34	1.44651	133.3		
8....	437	3.6	16.0	.831	38.8	39	1.45771	148.6		
9....	482	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 40 mm Hg

11....	392	4.7	30.4	0.894	26.8	55	1.48843	155.3	42	below 5
12....	437	6.3	36.7	.907	24.5	57	1.49898	163.8	56	do.
13....	482	4.1	40.8	.920	22.3	60	*		87	do.
14....	527	5.5	46.3	.932	20.3	62	*		172	do.
15....	572									
Residuum....		53.3	99.6	1.008	8.9					

Carbon residue, Conradson, Residuum 9.6 percent; crude 4.9 percent.

Residuum:
Sulfur, percent, ..
Nitrogen, percent, 1.043

APPROXIMATE SUMMARY

	Percent	Sp gr	° API	Viscosity
Light gasoline	2.3	0.707	68.6	
Total gasoline and naphtha	12.4	0.765	53.4	
Kerosine distillate	–			
Gas oil	18.8	.863	32.5	
Non-viscous lubricating distillate	8.3	.901-.922	25.5-22.0	50-100
Medium lubricating distillate	5.6	.922-.936	22.0-19.7	100-200
Viscous lubricating distillate	1.2	.936-.939	19.7-19.2	Above 200
Residuum	53.3	1.008	8.9	
Distillation 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).

Cut	Cut temp, °F	Vol %	API Gravity
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 CUTVF2.FOR
LINK:   Loading
[LNKXCT CUTVF2 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
5
ENTER THE NAME OF THE CRUDE
GASOLINE CUT
ENTER AN IDENTIFICATION NUMBER FOR THIS CRUDE ON I5
11111
ENTER A SAMPLE NUMBER ON I5
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-tranfer 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 con-stants. At this point all input information has been supplied and the calcula-tion 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 discus-sion. 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)

$$(1 - K_2W) \exp \left[\frac{-2.5W}{1-K_1W} \right] \equiv \exp \left[-K_3t \right]$$

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

$$K_3 = 0.001 \ (WIND \ SPEED)^2$$

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 (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

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TABLE   11.   Illustrations of <u>Three</u> Input Options for the Mass Tranfer
            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

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

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 dispension 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 remaning 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

B-33

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 <u>at his terminal</u>. 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 B.

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 CUTVP2 OF FEBRUARY 83
ITEM   9, SAMPLE 71011

	TB	API	SPGR	VOL	MW	TC	PC	VC	A	B	T10	VIS	NC	NS
1	1.67E+02	7.27E+01	6.81E-01	2.12E+00	8.92E+01	9.31E+02	3.83E+01	3.88E+02	3.23E+00	1.98E-01	4.60E+02	4.14E-01	3	1
2	2.12E+02	6.42E+01	7.11E-01	2.63E+00	1.02E+02	9.85E+02	3.65E+01	4.37E+02	3.31E+00	2.11E-01	4.96E+02	4.92E-01	3	1
3	2.57E+02	5.67E+01	7.39E-01	3.54E+00	1.14E+02	1.04E+03	3.51E+01	4.86E+02	3.39E+00	2.23E-01	5.31E+02	6.01E-01	3	1
4	3.02E+02	5.16E+01	7.60E-01	3.64E+00	1.28E+02	1.09E+03	3.36E+01	5.41E+02	3.49E+00	2.34E-01	5.68E+02	7.47E-01	3	1
5	3.47E+02	4.76E+01	7.77E-01	3.74E+00	1.43E+02	1.14E+03	3.22E+01	6.01E+02	3.61E+00	2.45E-01	6.04E+02	9.43E-01	3	1
6	3.92E+03	4.52E+01	7.87E-01	3.54E+00	1.61E+02	1.18E+03	3.06E+01	6.71E+02	3.77E+00	2.55E-01	6.42E+02	1.20E+00	3	1
7	4.37E+02	4.15E+01	8.04E-01	4.35E+00	1.78E+02	1.23E+03	2.94E+01	7.40E+02	3.91E+00	2.64E-01	6.80E+02	1.56E+00	3	1
8	4.82E+02	3.78E+01	8.22E-01	4.85E+00	1.96E+02	1.27E+03	2.83E+01	8.11E+02	4.06E+00	2.72E-01	7.18E+02	2.05E+00	3	1
9	5.27E+02	3.48E+01	8.36E-01	5.06E+00	2.12E+02	1.32E+03	2.76E+01	8.77E+02	4.18E+00	2.79E-01	7.55E+02	2.00E+00	3	1
10	5.00E+02	3.06E+01	8.58E-01	2.83E+00	2.36E+02	1.37E+03	2.65E+01	9.71E+02	4.37E+00	2.87E-01	8.01E+02	3.04E+00	3	1
11	6.38E+02	2.91E+01	8.66E-01	6.57E+00	2.72E+02	1.42E+03	2.49E+01	1.11E+03	4.68E+00	2.97E-01	8.53E+02	5.26E+00	3	1
12	6.85E+02	2.62E+01	8.82E-01	6.88E+00	2.99E+02	1.46E+03	2.40E+01	1.22E+03	4.89E+00	3.03E-01	8.95E+02	9.26E+00	3	1
13	7.38E+02	2.40E+01	8.94E-01	6.07E+00	3.35E+02	1.51E+03	2.29E+01	1.36E+03	5.20E+00	3.10E-01	9.44E+02	1.88E+01	3	1
14	7.90E+02	2.25E+01	9.03E-01	7.48E+00	3.76E+02	1.55E+03	2.18E+01	1.52E+03	5.58E+00	3.17E-01	9.94E+02	4.05E+01	3	1
15	8.50E+02	1.14E+01	9.73E-01	3.67E+01	6.00E+02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.81E+02	0	0

BULK API GRAVITY = 27.0

TB = NORMAL BOILING TEMPERATURE, DEG F
API = API GRAVITY
VOL = VOLUME PER CENT OF TOTAL CRUDE
MW = MOLECULAR WEIGHT
TC = CRITICAL TEMPERATURE, DEG RANKINE
PC = CRITICAL PRESSURE, ATMOSPHERES
VC = 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
VIS IS THE KINEMATIC VISCOSITY IN CENTISTOKES AT 122 DEG F
NC = ERROR CODE, SHOULD BE LESS THAN 20
NS = ERROR CODE, SHOULD BE EQUAL TO 1
IGNORE THE ERROR CODES FOR COMPONENT NUMBER 15 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 = 1.926E+01 M/HR

CUT	M/HR	GM-MOLES/(HR)(ATM)(M**2)
1	2.062E+01	9.212E+02
2	2.031E+01	9.074E+02
3	2.007E+01	8.964E+02
4	1.984E+01	8.864E+02
5	1.965E+01	8.776E+02
6	1.946E+01	8.695E+02
7	1.932E+01	8.630E+02
8	1.919E+01	8.574E+02
9	1.910E+01	8.531E+02
10	1.898E+01	8.479E+02
11	1.885E+01	8.418E+02
12	1.876E+01	8.382E+02
13	1.868E+01	8.342E+02
14	1.859E+01	8.306E+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 = 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 = 1.05E+01, VSLEAD = 5.50E+02 CP

MOUSSE CONSTANTS: MOONEY= 6.20E-01, MAX H20= 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 = 1.08E-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:
2.565E+04 2.911E+04 3.633E+04 3.423E+04 3.213E+04 2.743E+04 3.108E+04 3.219E+04 3.148E+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:
2.288E+06 2.956E+06 4.138E+06 4.375E+06 4.596E+06 4.407E+06 5.530E+06 6.308E+06 6.690E+06 3.843E+06 9.005E+06
9.594E+06 8.585E+06 1.069E+07 5.652E+07
THE TOTAL MASS FROM THESE CUTS IS 1.395E+08 GRAMS

STEP SIZE OF 9.191E-02 IS BASED ON CUT   1

TIME = 0.0E+00 HOURS, MASS FRACTION OF EACH CUT REMAINING: 2
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 1.0E+00 1.0E+00 1.0E+00
1.0E+00
MASS REMAINING = 1.395E+08, MASS DISPERSED = 0.000E+00, MASS EVAPORATED = 0.000E+00, SUM = 1.395E+08
FRACTION (BASED ON MASS) REMAINING IN THE SLICK: 1.0E+00, AREA= 7.9E+03 M**2, THICKNESS= 2.0E+00 CM, MOLE WT=273.9
WEIGHT FRACTION WATER IN OIL = 6.9E-05, VISCOSITY = 5.5E+02 CENTISTOKES, DISPERSION TERM = 4.4E-04 WEIGHT FRACTION/HR
MASS/AREA= 1.8E+04 GMS/M*M, SPGR= 8.8E-01, TOTAL VOLUME= 1.0E+03 BBL, DISPERSION= 7.7E+00 GMS/M*M/HR, EVAP RATE= 0.0E+00 GMS/M*M/HR

TIME = 1.0E+00 HOURS, MASS FRACTION OF EACH CUT REMAINING: 3
2.2E-01 6.6E-01 8.1E-01 9.3E-01 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 = 1.362E+08, MASS DISPERSED = 6.123E+04, MASS EVAPORATED = 3.299E+06, SUM = 1.395E+08
FRACTION (BASED ON MASS) REMAINING IN THE SLICK= 9.8E-01, AREA= 3.1E+04 M**2, THICKNESS= 5.0E-01 CM, MOLE WT=286.7
WEIGHT FRACTION WATER IN OIL = 2.5E-02, VISCOSITY = 7.6E+02 CENTISTOKES, DISPERSION TERM = 1.5E-03 WEIGHT FRACTION/HR
MASS/AREA= 4.4E+03 GMS/M*M, SPGR= 8.8E-01, TOTAL VOLUME= 9.7E+02 BBL, DISPERSION= 6.6E+00 GMS/M*M/HR, EVAP RATE= 9.9E+01 GMS/M*M/HR

TIME = 2.0E+00 HOURS, MASS FRACTION OF EACH CUT REMAINING: 4
1.6E-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 1.0E+00 1.0E+00 1.0E+00 1.0E+00
1.0E+00
MASS REMAINING = 1.337E+08, MASS DISPERSED = 2.675E+05, MASS EVAPORATED = 5.585E+06, SUM = 1.395E+08
FRACTION (BASED ON MASS) REMAINING IN THE SLICK= 9.6E-01, AREA= 4.3E+04 M**2, THICKNESS= 3.5E-01 CM, MOLE WT=295.6
WEIGHT FRACTION WATER IN OIL = 5.0E-02, VISCOSITY = 9.7E+02 CENTISTOKES, DISPERSION TERM = 1.9E-03 WEIGHT FRACTION/HR
MASS/AREA= 3.1E+03 GMS/M*M, SPGR= 8.9E-01, TOTAL VOLUME= 9.5E+02 BBL, DISPERSION= 5.9E+00 GMS/M*M/HR, EVAP RATE= 4.2E+01 GMS/M*M/HR

STEP SIZE OF 5.591E-02 IS BASED ON CUT   2

TIME = 3.0E+00 HOURS, MASS FRACTION OF EACH CUT REMAINING: 5
5.1E-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 1.0E+00 1.0E+00 1.0E+00 1.0E+00
1.0E+00
MASS REMAINING = 1.319E+08, MASS DISPERSED = 5.228E+05, MASS EVAPORATED = 7.094E+06, SUM = 1.395E+08
FRACTION (BASED ON MASS) REMAINING IN THE SLICK= 9.5E-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= 2.5E+03 GMS/M*M, SPGR= 8.9E-01, TOTAL VOLUME= 9.3E+02 BBL, DISPERSION= 5.3E+00 GMS/M*M/HR, EVAP RATE= 2.5E+01 GMS/M*M/HR

STEP SIZE OF 4.679E-02 IS BASED ON CUT   2

TIME = .4.1E+00 HOURS, MASS FRACTION OF EACH CUT REMAINING: 6
7.5E-06 3.5E-02 4.5E-01 8.4E-01 9.6E-01 9.9E-01 9.9E-01 9.9E-01 9.9E-01 9.9E-01 9.9E-01 9.9E-01 9.9E-01 9.9E-01
9.9E-01
MASS REMAINING = 1.305E+08, MASS DISPERSED = 8.083E+05, MASS EVAPORATED = 8.237E+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=305.8
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*M, SPGR= 8.9E-01, TOTAL VOLUME= 9.2E+02 BBL, DISPERSION= 4.9E+00 GMS/M*M/HR, EVAP RATE= 1.6E+01 GMS/M*M/HR

STEP SIZE OF 4.020E-02 IS BASED ON CUT   2

TIME = 5.1E+00 HOURS, MASS FRACTION OF EACH CUT REMAINING: 7
6.8E-08 9.4E-03 3.3E-01 7.8E-01 9.5E-01 9.8E-01 9.9E-01 9.9E-01 9.9E-01 9.9E-01 9.9E-01 9.9E-01 9.9E-01 9.9E-01
9.9E-01
MASS REMAINING = 1.293E+08, MASS DISPERSED = 1.101E+06, MASS EVAPORATED = 9.126E+06, SUM = 1.395E+08
FRACTION (BASED ON MASS) REMAINING IN THE SLICK= 9.3E-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*M, SPGR= 8.9E-01, TOTAL VOLUME= 9.1E+02 BBL, DISPERSION= 4.5E+00 GMS/M*M/HR, EVAP RATE= 1.2E+01 GMS/M*M/HR

STEP SIZE OF 3.578E-02 IS BASED ON CUT   2

TIME = 6.1E+00 HOURS, MASS FRACTION OF EACH CUT REMAINING: 8
3.8E-10 2.1E-03 2.3E-01 7.2E-01 9.3E-01 9.8E-01 9.9E-01 9.9E-01 9.9E-01 9.9E-01 9.9E-01 9.9E-01 9.9E-01 9.9E-01
9.9E-01
MASS REMAINING = 1.283E+08, MASS DISPERSED = 1.401E+06, MASS EVAPORATED = 9.871E+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*M, SPGR= 8.9E-01, TOTAL VOLUME= 9.0E+02 BBL, DISPERSION= 4.2E+00 GMS/M*M/HR, EVAP RATE= 9.5E+00 GMS/M*M/HR

TIME = 7.1E+00 HOURS, MASS FRACTION OF EACH CUT REMAINING: 9
0.0E+00 4.3E-04 1.6E-01 6.7E-01 9.1E-01 9.7E-01 9.8E-01 9.9E-01 9.9E-01 9.9E-01 9.9E-01 9.9E-01 9.9E-01 9.9E-01
9.9E-01

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

54

TIME = 8.2E+01 HOURS, MASS FRACTION OF EACH CUT REMAINING:
0.0E+00 0.0E+00 0.0E+00 2.7E-08 2.9E-02 4.9E-01 8.1E-01 8.7E-01 8.9E-01 8.9E-01 8.9E-01 8.9E-01 8.9E-01 8.9E-01
8.9E-01
MASS REMAINING = 1.053E+08, MASS DISPERSED = 1.401E+07, MASS EVAPORATED = 2.018E+07, SUM = 1.395E+08
FRACTION (BASED ON MASS) REMAINING IN THE SLICK= 7.5E-01, AREA= 2.4E+05 M**2, THICKNESS= 4.9E-02 CM, MOLE WT=351.9
WEIGHT FRACTION WATER IN OIL = 7.0E-01, VISCOSITY = 2.2E+05 CENTISTOKES, DISPERSION TERM = 8.9E-04 WEIGHT FRACTION/HR
MASS/AREA= 4.5E+02 GMS/M*M, SPGR= 9.1E-01, TOTAL VOLUME= 7.3E+02 BBL, DISPERSION= 4.0E-01 GMS/M*M/HR, EVAP RATE= 1.8E-01 GMS/M*M/HR

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

55

TIME = 9.2E+01 HOURS, MASS FRACTION OF EACH CUT REMAINING:
0.0E+00 0.0E+00 0.0E+00 9.1E-10 1.5E-02 4.4E-01 7.8E-01 8.6E-01 8.8E-01 8.8E-01 8.8E-01 8.8E-01 8.8E-01 8.8E-01
8.8E-01
MASS REMAINING = 1.040E+08, MASS DISPERSED = 1.494E+07, MASS EVAPORATED = 2.058E+07, SUM = 1.395E+08
FRACTION (BASED ON MASS) REMAINING IN THE SLICK= 7.5E-01, AREA= 2.5E+05 M**2, THICKNESS= 4.6E-02 CM, MOLE WT=353.5
WEIGHT FRACTION WATER IN OIL = 7.0E-01, VISCOSITY = 2.6E+05 CENTISTOKES, DISPERSION TERM = 8.8E-04 WEIGHT FRACTION/HR
MASS/AREA= 4.2E+02 GMS/M*M, SPGR= 9.1E-01, TOTAL VOLUME= 7.2E+02 BBL, DISPERSION= 3.7E-01 GMS/M*M/HR, EVAP RATE= 1.5E-01 GMS/M*M/HR

THE CUT NUMBERING BEGINS WITH 1 BASED ON THE ORIGINAL CUT NUMBERS

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THE FINAL MASS FRACTIONS FOR THE SLICK AT 1.0E+02 HOURS ARE:
0.000E+00 0.000E+00 0.000E+00 0.000E+00 8.129E-03 3.894E-01 7.661E-01 8.562E-01 8.702E-01 8.723E-01 8.725E-01
8.725E-01 8.725E-01 8.725E-01 8.725E-01
FRACTION (BASED ON MASS) REMAINING IN THE SLICK= 7.4E-01, AREA= 2.6E+05 M**2, THICKNESS= 4.4E-02 CM, MOLE WT=353.5
MASS REMAINING = 1.029E+08, MASS DISPERSED = 1.571E+07, MASS EVAPORATED = 2.089E+07, SUM = 1.395E+08

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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	GM-MOLES/(HR)(ATM)(M**2)
1	2.062E+01	8.716E+02
2	2.031E+01	8.585E+02
3	2.007E+01	8.481E+02
4	1.984E+01	8.386E+02
5	1.965E+01	8.303E+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	1.898E+01	8.022E+02
11	1.885E+01	7.965E+02
12	1.876E+01	7.930E+02
13	1.868E+01	7.893E+02
14	1.859E+01	7.858E+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: VIS25C = 3.50E+01, ANDRADE = 9.00E+03, FRACT WEATHERED = 1.05E+01, VSLEAD = 9.30E+01 CP

MOUSSE CONSTANTS: MOONEY= 6.20E-01, MAX H20= 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 = 1.08E-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:
2.565E+04 2.911E+04 3.633E+04 3.423E+04 3.213E+04 2.743E+04 3.108E+04 3.219E+04 3.148E+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: 1
2.288E+06 2.956E+06 4.138E+06 4.375E+06 4.596E+06 4.407E+06 5.530E+06 6.308E+06 6.690E+06 3.843E+06 9.005E+06
9.594E+06 8.585E+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: 2
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 1.0E+00 1.0E+00 1.0E+00
MASS REMAINING = 1.372E+08, MASS DISPERSED = 0.000E+00, MASS EVAPORATED = 0.000E+00, SUM = 1.372E+08
FRACTION (BASED ON MASS) REMAINING IN THE SLICK= 9.8E-01, AREA= 7.8E+03 M**2, THICKNESS= 2.0E+00 CM, MOLE WT=283.7
WEIGHT FRACTION WATER IN OIL = 6.9E-05, VISCOSITY = 1.1E+02 CENTISTOKES, DISPERSION TERM = 9.8E-04 WEIGHT FRACTION/HR
MASS AREA= 1.8E+04 GMS/M*M, SPGR= 8.8E-01, TOTAL VOLUME= 9.8E+02 BBL, DISPERSION= 1.7E+01 GMS/M*M/HR, EVAP RATE= 0.0E+00 GMS/M*M HR

TIME = 1.0E+00 HOURS. MASS FRACTION OF EACH CUT REMAINING:
3.3E-01 7.3E-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 1.0E+00 1.0E+00 1.0E+00

TABLE 15.b (Continued)   Output from Oil-Weathering Calculations, Prudhoe Bay Crude Oil,
Final Time Step at 60°F (Note Renumbering of cuts).

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MASS REMAINING =  9.346E+07, MASS DISPERSED =  2.191E+07, MASS EVAPORATED =  2.187E+07, SUM =  1.372E+08
FRACTION (BASED ON MASS) REMAINING IN THE SLICK= 6.7E-01, AREA= 2.2E+05 M**2, THICKNESS= 4.6E-02 CM, MOLE WT=367.6
WEIGHT FRACTION WATER IN OIL =  7.0E-01, VISCOSITY =  1.4E+05 CENTISTOKES, DISPERSION TERM =  1.2E-03 WEIGHT FRACTION/HR
MASS/AREA= 4.2E+02 GMS/M*M, SPGR= 9.1E-01, TOTAL VOLUME= 6.4E+02 BBL, DISPERSION= 5.0E-01 GMS/M*M/HR, EVAP RATE= 2.2E-01 GMS/M*M/HR


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

TIME =  9.2E+01 HOURS, MASS FRACTION OF EACH CUT REMAINING:                                                   52
 0.0E+00  0.0E+00  0.0E+00  3.8E-08  2.9E-02  4.4E-01  7.3E-01  8.0E-01  8.1E-01  8.1E-01  8.1E-01  8.1E-01  8.1E-01  8.1E-01
MASS REMAINING =  9.190E+07, MASS DISPERSED =  2.301E+07, MASS EVAPORATED =  2.233E+07, SUM =  1.372E+08
FRACTION (BASED ON MASS) REMAINING IN THE SLICK= 6.6E-01, AREA= 2.3E+05 M**2, THICKNESS= 4.3E-02 CM, MOLE WT=369.5
WEIGHT FRACTION WATER IN OIL =  7.0E-01, VISCOSITY =  1.8E+05 CENTISTOKES, DISPERSION TERM =  1.1E-03 WEIGHT FRACTION/HR
MASS/AREA= 3.9E+02 GMS/M*M, SPGR= 9.1E-01, TOTAL VOLUME= 6.3E+02 BBL, DISPERSION= 4.5E-01 GMS/M*M/HR, EVAP RATE= 1.8E-01 GMS/M*M/HR


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


THE CUT NUMBERING BEGINS WITH  2 BASED ON THE ORIGINAL CUT NUMBERS

THE FINAL MASS FRACTIONS FOR THE SLICK AT  1.0E+02 HOURS ARE:                                                 53
 0.000E+00  0.000E+00  0.000E+00  2.582E-09  1.699E-02  3.930E-01  7.105E-01  7.850E-01  7.989E-01  8.003E-01  8.004E-01
 8.004E-01  8.004E-01  8.004E-01
FRACTION (BASED ON MASS) REMAINING IN THE SLICK= 6.5E-01, AREA= 2.4E+05 M**2, THICKNESS= 4.1E-02 CM, MOLE WT=369.5
MASS REMAINING =  9.060E+07, MASS DISPERSED =  2.394E+07, MASS EVAPORATED =  2.269E+07, SUM =  1.372E+08

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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 H20= 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

TIME	BBL	SPGR	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	4.52E+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 H20= 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]
 Logged-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>

REFERENCES

API, 1965, 108 Technical Data Book - Petroleum Refining, American Petroleum Institute, Washington, D.C.

ASTM, 1977, Method D2892-73: Standard Test Method for Distillation of Crude Petroleum (15-Theoretical Plate Column, American Society for Testing and Materials, Philadelphia, PA.

Coleman, H. J., E. M. Shelton, D. T. Nichols and C. J. Thompson, 1978, Analyses of 800 Crude Oils from United States Oil Fields, BETC/RI-78/14, Bartlesville Energy Technology Center, Department of Energy, Bartlesville, Oklahoma.

Edmister, W.C., and K.K. Okamoto, 1959, Applied Hydrocarbon Thermodynamics - Part 13: Equilibrium Flash Vaporizations Correlations for Petroleum Fractions, Petroleum Refiner, vol. 38, no. 8, pp. 117-129.

Garratt, J.R., 1977, Review of Drag Coefficients over Oceans and Continents, Monthly Weather Review, vol. 105, pp. 915-929.

Gold, P. I., and G. Olge, 1969, Estimating Thermophysical Properties of Liquids, Park 10-Viscosity, Chemical Engineering, July 14.

Hougen, O. A., K. M. Watson, and R. A. Ragatz, 1965, Chemical Process Principles, Part 1 - Material and Energy Balances, 2nd edition, John Wiley & Sons, Inc.

Liss, P. S., and P. G. Slater, 1974, Flux of Gases Across the Air-Sea Interface, Nature, vol. 247, pp. 181-184.

Mackay, D., I. Buist, R. Mascarenhas, and S. Paterson, 1980, Oil Spill Processes and Models, Research and Development Division, Environmental Emergency Branch, Environmental Impact Control Directorate, Environmental Protective Service, Environment Canada, Ottawa, Ontario, K1A 1C8.

Mackay, D., and R. S. Matsugu, 1973, Evaporation Rates of Liquid Hydrocarbon. Spills on Land and Water, the Canadian Journal of Chemical Engineering, vol. 51, pp. 434-439.

Mooney, M., 1955, The Viscosity of a Concentrated Suspension of Spherical Particles, Journal of Colloid Science, vol. 10, pp. 162-170.

O&GJ, 1973, Evaluations of World's Important Crudes, The Oil and Gas Journal, Petroleum Publishing Co, Tulsa, Oklahoma.

Payne, J. R., B. E. Kirstein, G. D. McNabb, Jr., J. L. Lambach C. de Oliveira, R. E. Jordon, W. Hom, 1983. Multivariate Analysis of Petroleum Hydrocarbon Weathering in the Subarctic Marine Environment. Proceeding of the 1983 Oil Spill Conference American Petroleum, Institute; Washington, D.C., pp. 423-434.

Perry, R. H., and C. H. Chilton, 1973, Chemical Engineer's Handbook, 5th edition, McGraw-Hill.

Reid, R. C., J. M. Pransintz, and T. K. Sherwood, 1977, The Properties of Gases and Liquids, 3rd edition, McGraw-Hill.

Tabeau, P.A. (US Coast Guard R&D Center), D. Mackay, W. R. Shin, W. Stiver, K. Hossain, D. McCurdy, and S. Paterson, Oil Weathering Under Artic Conditions, Department of Chemical Engineering and Applied Sciences, University of Toronto, Toronto, Ontario, Canada M55 1A4.

Treybal, R.E., 1955, Mass Transfer, McGraw-Hill.

Van Winkle, M., 1967, Distillation, McGraw-Hill.

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 **0**, type a C, skip a space and type the network address of your computer, followed by a carriage return.

Example:

    0C_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)	594-6644
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:

@	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⟩@⟨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.

* 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%602	MESA	254-0244	<PHOENIX>	(B/V)	254-0244
AZ%602	PHOENIX	254-0244		(B/V)	254-0244
AZ%602	SCOTTSDALE	254-0244	<PHOENIX>	(B/V)	254-0244
AZ%602	TEMPE	254-0244	<PHOENIX>	(B/V)	254-0244
AZ 602	TUCSON	745-1666		(B/V)	745-1666
CA 213	ALHAMBRA	507-0909	<GLENDALE>	(B/V)	507-0909
CA 714	ANAHEIM	558-6061	<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	558-6061	<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

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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    558-6061 <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       558-6061 <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           558-6061                        (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
                                                           (B/V) 741-4000
CO#303 BOULDER             773-8500 <DENVER>               (B/V) 694-2710
                                                           (B/V) 741-4000
CO%303 COLORADO SPRINGS    634-5676                        (B/V) 635-5361
CO#303 DENVER              773-8500                        (B/V) 694-2710
                                                           (B/V) 741-4000
CO#303 LAKEWOOD            773-8500 <DENVER>               (B/V) 694-2710
                                                           (B/V) 741-4000
CT 203 DANBURY             794-9075                        (B/V) 794-9075
CT 203 GREENWICH           348-0787 <STAMFORD>             (B/V) 348-0787
CT 203 HARTFORD            522-0344                        (B/V) 247-9479
CT%203 MILFORD             624-5954 <NEW HAVEN>            (B/V) 624-5954
CT%203 NEW HAVEN           624-5954                        (B/V) 624-5954
CT%203 STAMFORD            348-0787                        (B/V) 348-0787
CT 203 WEST HARTFORD       522-0344 <HARTFORD>             (B/V) 247-9479
DC%202 WASHINGTON          429-7896                        (B/V) 429-7800
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DE 302 WILMINGTON          454-7710                        (B/V)  454-7710
FL 813 CLEARWATER          323-4026 <ST. PETE>             (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        833-6691
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        364-0911                        (B/V)  364-0911
IA 402 COUNCIL BLUFFS      341-7733 <OMAHA, NE>            (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 <CHICAGO>              (B/V)  938-0600
IL 217 CHAMPAIGN           384-6428 <URBANA>               (B/V)  384-6428
IL 312 CHICAGO             938-0500                        (B/V)  938-0600
IL 312 CICERO              938-0500 <CHICAGO>              (B/V)  938-0600
IL 314 EAST ST LOUIS       421-4990 <ST LOUIS, MO>         (B/V)  421-4990
IL 312 OAK PARK            938-0500 <CHICAGO>              (B/V)  938-0600
IL 309 PEORIA              637-8570                        (B/V)  637-8570
IL 312 SKOKIE              938-0500 <CHICAGO>              (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 <SOUTH BEND>           (B/V)  233-7104
IN 219 OSCEOLA             233-7104 <SOUTH BEND>           (B/V)  233-7104
IN 219 SOUTH BEND          233-7104                        (B/V)  233-7104
KS 816 KANSAS CITY         221-9900 <KANSAS CITY, MO>      (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           266-6886
MD 301 BALTIMORE           962-5010                        (B/V)  727-6060
MD%202 BETHESDA            429-7896 <WASH., D.C.>          (B/V)  429-7800
MD 301 DUNDALK             962-5010 <BALTIMORE>            (B/V)  727-6060
MD%202 ROCKVILLE           429-7896 <WASH., D.C.>          (B/V)  429-7800
MD%202 SILVER SPRING       429-7896 <WASH., D.C.>          (B/V)  429-7800
MD 301 TOWSON              962-5010 <BALTIMORE>            (B/V)  727-6060
MA 617 ARLINGTON           338-1400 <BOSTON>               (B/V)  338-7495
MA 617 BOSTON              338-1400                        (B/V)  338-7495
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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 816 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
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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) 549-8135
NC 919 RESEARCH TRI.PARK    549-8311                           (B/V) 549-8135
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 614 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 605 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
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TX%915 ABILENE            676-8545                           (B/V) 676-8545
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 <SAN ANTONIO>             (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 <WASHINGTON, D.C.>        (B/V) 429-7800
VA%202 ANNANDALE          429-7896 <WASHINGTON, D.C.>        (B/V) 429-7800
VA 804 CHESAPEAKE         625-1186 <NORFOLK>                 (B/V) 625-1186
VA%202 FAIRFAX            429-7896 <WASHINGTON, D.C.>        (B/V) 429-7800
VA%202 FALLS CHURCH       429-7896 <WASHINGTON, D.C.>        (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 <NORFOLK>                 (B/V) 625-1186
VA 804 RICHMOND           788-9902                           (B/V) 788-9902
VA%202 SPRINGFIELD        429-7896 <WASHINGTON, D.C.>        (B/V) 429-7800
VA%202 VIENNA             429-7896 <WASHINGTON, D.C.>        (B/V) 429-7800
VA 804 VIRGINIA BEACH     625-1186 <NORFOLK>                 (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 <SEATTLE>                 (B/V) 625-9612
WA 206 LONGVIEW           577-5835
WA 206 SEATTLE            447-9012                           (B/V) 625-9612
WA%509 SPOKANE            455-4071                           (B/V) 455-4071
WA%206 TACOMA             627-1791                           (B/V) 627-1791
WA 509 WENATCHEE          662-1901                           (B/V) 662-1901
WI 608 MADISON            251-5904                           (B/V) 257-5010
WI 414 MILWAUKEE          271-2560                           (B/V) 271-3914
WV 304 CHARLESTON         345-6471                           (B/V) 345-6471
WY%307 CHEYENNE           638-4421                           (B/V) 638-4421
IN-WATS 800              424-9494                           (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 <u>yes</u> 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 cm^2/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
[LNKXCT 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 SLAB IN CONTACT WITH A DIFFUSION SLAB
EDDY DIFFUSIVITY = 1.850D+02 CM*CM/SEC, OIL SLICK THICKNESS = 1.00 CM, OCEAN DEPTH = 5.0 METERS
OIL/WATER SPECIES PARTITION COEFFICIENT = 2.500D+03 UNITLESS, OIL-WATER OVER-ALL MASS TRANSFER COEFFICIENT = 1.000D+00 CM/HR
INITIAL SPECIES OIL-PHASE CONCENTRATION = 5.000D-03 GM/CC, NUMBER OF TERMS IN THE SERIES = 100, NUMBER OF INTERVAL HALVINGS = 30
SIZE OF LEAD EXPONENTIAL TO APPROXIMATE STEADY STATE = 1.00D-02

DIMENSIONLESS CONCENTRATIONS AT VARIOUS TIMES AND DEPTHS FOLLOW

METERS	HOURS 8.82D-01	HOURS 2.07D+00	HOURS 4.86D+00	HOURS 1.14D+01	HOURS 2.68D+01	HOURS 6.30D+01	HOURS 1.48D+02	HOURS 3.48D+02	HOURS 8.17D+02	HOURS 1.92D+03
0.0	2.01D-03	4.38D-03	9.92D-03	2.28D-02	5.22D-02	1.17D-01	2.49D-01	4.72D-01	7.16D-01	8.25D-01
0.5	1.94D-03	4.31D-03	9.85D-03	2.27D-02	5.21D-02	1.17D-01	2.49D-01	4.72D-01	7.16D-01	8.25D-01
1.0	1.80D-03	4.25D-03	9.79D-03	2.27D-02	5.21D-02	1.17D-01	2.49D-01	4.72D-01	7.16D-01	8.25D-01
1.5	1.82D-03	4.19D-03	9.73D-03	2.26D-02	5.20D-02	1.17D-01	2.49D-01	4.72D-01	7.16D-01	8.25D-01
2.0	1.78D-03	4.14D-03	9.68D-03	2.26D-02	5.20D-02	1.17D-01	2.49D-01	4.72D-01	7.16D-01	8.25D-01
2.5	1.73D-03	4.10D-03	9.64D-03	2.25D-02	5.20D-02	1.17D-01	2.49D-01	4.72D-01	7.16D-01	8.25D-01
3.0	1.70D-03	4.07D-03	9.61D-03	2.25D-02	5.19D-02	1.17D-01	2.49D-01	4.72D-01	7.16D-01	8.25D-01
3.5	1.67D-03	4.04D-03	9.58D-03	2.25D-02	5.19D-02	1.17D-01	2.49D-01	4.72D-01	7.16D-01	8.25D-01
4.0	1.66D-03	4.03D-03	9.57D-03	2.24D-02	5.19D-02	1.17D-01	2.49D-01	4.72D-01	7.16D-01	8.25D-01
4.5	1.64D-03	4.01D-03	9.55D-03	2.24D-02	5.19D-02	1.17D-01	2.49D-01	4.72D-01	7.16D-01	8.25D-01
5.0	1.64D-03	4.01D-03	9.55D-03	2.24D-02	5.19D-02	1.17D-01	2.49D-01	4.72D-01	7.16D-01	8.25D-01
OIL CONC.	1.00D+00	9.99D-01	9.98D-01	9.95D-01	9.90D-01	9.77D-01	9.50D-01	9.06D-01	8.57D-01	8.35D-01
AVERAGE WATER CONC.	1.78D-03	4.15D-03	9.69D-03	2.26D-02	5.20D-02	1.17D-01	2.49D-01	4.72D-01	7.16D-01	8.25D-01

ACTUAL CONCENTRATIONS IN PPM AT VARIOUS TIMES AND DEPTHS

METERS	HOURS 8.82D-01	HOURS 2.07D+00	HOURS 4.86D+00	HOURS 1.14D+01	HOURS 2.68D+01	HOURS 6.30D+01	HOURS 1.48D+02	HOURS 3.48D+02	HOURS 8.17D+02	HOURS 1.92D+03
0.0	4.03D-03	8.77D-03	1.98D-02	4.56D-02	1.04D-01	2.34D-01	4.99D-01	9.44D-01	1.43D+00	1.65D+00
0.5	3.89D-03	8.63D-03	1.97D-02	4.54D-02	1.04D-01	2.34D-01	4.99D-01	9.43D-01	1.43D+00	1.65D+00
1.0	3.76D-03	8.50D-03	1.96D-02	4.53D-02	1.04D-01	2.34D-01	4.99D-01	9.43D-01	1.43D+00	1.65D+00
1.5	3.65D-03	8.39D-03	1.95D-02	4.52D-02	1.04D-01	2.34D-01	4.99D-01	9.43D-01	1.43D+00	1.65D+00
2.0	3.55D-03	8.29D-03	1.94D-02	4.51D-02	1.04D-01	2.34D-01	4.98D-01	9.43D-01	1.43D+00	1.65D+00
2.5	3.47D-03	8.21D-03	1.93D-02	4.50D-02	1.04D-01	2.34D-01	4.98D-01	9.43D-01	1.43D+00	1.65D+00
3.0	3.40D-03	8.14D-03	1.92D-02	4.50D-02	1.04D-01	2.34D-01	4.98D-01	9.43D-01	1.43D+00	1.65D+00
3.5	3.35D-03	8.09D-03	1.92D-02	4.49D-02	1.04D-01	2.34D-01	4.98D-01	9.43D-01	1.43D+00	1.65D+00
4.0	3.31D-03	8.05D-03	1.91D-02	4.49D-02	1.04D-01	2.34D-01	4.98D-01	9.43D-01	1.43D+00	1.65D+00
4.5	3.29D-03	8.03D-03	1.91D-02	4.48D-02	1.04D-01	2.34D-01	4.98D-01	9.43D-01	1.43D+00	1.65D+00
5.0	3.28D-03	8.02D-03	1.91D-02	4.48D-02	1.04D-01	2.34D-01	4.98D-01	9.43D-01	1.43D+00	1.65D+00
OIL CONC.	5.00D+03	5.00D+03	4.99D+03	4.98D+03	4.95D+03	4.88D+03	4.75D+03	4.53D+03	4.28D+03	4.17D+03
AVERAGE WATER CONC.	3.56D-03	8.30D-03	1.94D-02	4.51D-02	1.04D-01	2.34D-01	4.98D-01	9.43D-01	1.43D+00	1.65D+00

THE MASSES THAT FOLLOW ARE IN GRAMS/CM*CM, THE FLUX IS IN GRAMS/CM*CM/SEC

	HOURS 8.82D-01	HOURS 2.07D+00	HOURS 4.86D+00	HOURS 1.14D+01	HOURS 2.68D+01	HOURS 6.30D+01	HOURS 1.48D+02	HOURS 3.48D+02	HOURS 8.17D+02	HOURS 1.92D+03
MASS IN OIL	5.00D-03	5.00D-03	4.99D-03	4.98D-03	4.95D-03	4.88D-03	4.75D-03	4.53D-03	4.28D-03	4.17D-03
MASS IN WATER	1.78D-06	4.15D-06	9.69D-06	2.26D-05	5.20D-05	1.17D-04	2.49D-04	4.72D-04	7.16D-04	8.25D-04
MASS FLUX AT SURFACE	5.54D-10	5.53D-10	5.49D-10	5.40D-10	5.21D-10	4.77D-10	3.89D-10	2.41D-10	7.82D-11	5.56D-12

TABLE 3: EXAMPLE OF CALCULATED WATER COLUMN CONCENTRATIONS FOR OVER-ALL MASS TRANSFER COEFFICIENT = 10 cm/hr

WELL-STIRRED OIL SLAB IN CONTACT WITH A DIFFUSION SLAB
EDDY DIFFUSIVITY = 1.850D+02 CM*CM/SEC, OIL SLICK THICKNESS = 1.00 CM, OCEAN DEPTH = 5.0 METERS
OIL/WATER SPECIES PARTITION COEFFICIENT = 2.500D+03 UNITLESS, OIL-WATER OVER-ALL MASS TRANSFER COEFFICIENT = 1.000D+01 CM/HR
INITIAL SPECIES OIL-PHASE CONCENTRATION = 5.000D-03 CM/CC, NUMBER OF TERMS IN THE SERIES = 100, NUMBER OF INTERVAL HALVINGS = 30
SIZE OF LEAD EXPONENTIAL TO APPROXIMATE STEADY STATE = 1.00D-02

DIMENSIONLESS CONCENTRATIONS AT VARIOUS TIMES AND DEPTHS FOLLOW

METERS	HOURS 7.01D-01	HOURS 1.31D+00	HOURS 2.44D+00	HOURS 4.55D+00	HOURS 8.50D+00	HOURS 1.59D+01	HOURS 2.96D+01	HOURS 5.52D+01	HOURS 1.03D+02	HOURS 1.92D+02
0.0	1.63D-02	2.81D-02	4.96D-02	8.83D-02	1.55D-01	2.65D-01	4.24D-01	6.12D-01	7.63D-01	8.25D-01
0.5	1.56D-02	2.74D-02	4.90D-02	8.77D-02	1.55D-01	2.64D-01	4.24D-01	6.12D-01	7.63D-01	8.25D-01
1.0	1.50D-02	2.68D-02	4.84D-02	8.71D-02	1.54D-01	2.64D-01	4.24D-01	6.12D-01	7.63D-01	8.25D-01
1.5	1.44D-02	2.63D-02	4.78D-02	8.66D-02	1.54D-01	2.64D-01	4.23D-01	6.11D-01	7.63D-01	8.25D-01
2.0	1.40D-02	2.58D-02	4.74D-02	8.62D-02	1.53D-01	2.63D-01	4.23D-01	6.11D-01	7.63D-01	8.25D-01
2.5	1.36D-02	2.54D-02	4.70D-02	8.58D-02	1.53D-01	2.63D-01	4.23D-01	6.11D-01	7.63D-01	8.25D-01
3.0	1.32D-02	2.51D-02	4.67D-02	8.55D-02	1.53D-01	2.63D-01	4.23D-01	6.11D-01	7.63D-01	8.25D-01
3.5	1.30D-02	2.48D-02	4.64D-02	8.53D-02	1.53D-01	2.63D-01	4.23D-01	6.11D-01	7.63D-01	8.25D-01
4.0	1.28D-02	2.46D-02	4.63D-02	8.51D-02	1.53D-01	2.63D-01	4.22D-01	6.11D-01	7.63D-01	8.25D-01
4.5	1.27D-02	2.45D-02	4.61D-02	8.50D-02	1.52D-01	2.62D-01	4.22D-01	6.11D-01	7.63D-01	8.25D-01
5.0	1.26D-02	2.45D-02	4.61D-02	8.49D-02	1.52D-01	2.62D-01	4.22D-01	6.11D-01	7.63D-01	8.25D-01

OIL CONC.	9.97D-01	9.95D-01	9.91D-01	9.83D-01	9.69D-01	9.47D-01	9.15D-01	8.78D-01	8.47D-01	8.35D-01

AVERAGE WATER CONC.	1.39D-02	2.57D-02	4.73D-02	8.61D-02	1.53D-01	2.63D-01	4.23D-01	6.11D-01	7.63D-01	8.25D-01

ACTUAL CONCENTRATIONS IN PPM AT VARIOUS TIMES AND DEPTHS

METERS	HOURS 7.01D-01	HOURS 1.31D+00	HOURS 2.44D+00	HOURS 4.55D+00	HOURS 8.50D+00	HOURS 1.59D+01	HOURS 2.96D+01	HOURS 5.52D+01	HOURS 1.03D+02	HOURS 1.92D+02
0.0	3.26D-02	5.62D-02	9.93D-02	1.77D-01	3.11D-01	5.30D-01	8.49D-01	1.22D+00	1.53D+00	1.65D+00
0.5	3.12D-02	5.48D-02	9.79D-02	1.75D-01	3.10D-01	5.29D-01	8.48D-01	1.22D+00	1.53D+00	1.65D+00
1.0	3.00D-02	5.36D-02	9.67D-02	1.74D-01	3.09D-01	5.28D-01	8.47D-01	1.22D+00	1.53D+00	1.65D+00
1.5	2.89D-02	5.25D-02	9.57D-02	1.73D-01	3.08D-01	5.27D-01	8.47D-01	1.22D+00	1.53D+00	1.65D+00
2.0	2.79D-02	5.16D-02	9.48D-02	1.72D-01	3.07D-01	5.27D-01	8.46D-01	1.22D+00	1.53D+00	1.65D+00
2.5	2.71D-02	5.08D-02	9.40D-02	1.72D-01	3.06D-01	5.26D-01	8.46D-01	1.22D+00	1.53D+00	1.65D+00
3.0	2.65D-02	5.01D-02	9.33D-02	1.71D-01	3.06D-01	5.26D-01	8.45D-01	1.22D+00	1.53D+00	1.65D+00
3.5	2.59D-02	4.96D-02	9.29D-02	1.71D-01	3.05D-01	5.25D-01	8.45D-01	1.22D+00	1.53D+00	1.65D+00
4.0	2.56D-02	4.92D-02	9.25D-02	1.70D-01	3.05D-01	5.25D-01	8.45D-01	1.22D+00	1.53D+00	1.65D+00
4.5	2.53D-02	4.90D-02	9.23D-02	1.70D-01	3.05D-01	5.25D-01	8.45D-01	1.22D+00	1.53D+00	1.65D+00
5.0	2.53D-02	4.89D-02	9.22D-02	1.70D-01	3.05D-01	5.25D-01	8.45D-01	1.22D+00	1.53D+00	1.65D+00

OIL CONC.	4.99D+03	4.97D+03	4.95D+03	4.91D+03	4.85D+03	4.74D+03	4.58D+03	4.39D+03	4.24D+03	4.17D+03

AVERAGE WATER CONC.	2.78D-02	5.14D-02	9.46D-02	1.72D-01	3.07D-01	5.27D-01	8.46D-01	1.22D+00	1.53D+00	1.65D+00

THE MASSES THAT FOLLOW ARE IN GRAMS/CM*CM, THE FLUX IS IN GRAMS/CM*CM/SEC

MASS IN OIL	4.99D-03	4.97D-03	4.95D-03	4.91D-03	4.85D-03	4.74D-03	4.58D-03	4.39D-03	4.24D-03	4.17D-03

MASS IN WATER	1.39D-05	2.57D-05	4.73D-05	8.61D-05	1.53D-04	2.63D-04	4.23D-04	6.11D-04	7.63D-04	8.25D-04

MASS FLUX AT SURFACE	5.45D-09	5.37D-09	5.23D-09	4.97D-09	4.52D-09	3.79D-09	2.73D-09	1.48D-09	4.70D-10	5.54D-11

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:

$$\frac{1}{K_{water}} \simeq \frac{1}{k_{water}}$$

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.

REFERENCES

Jaeger, J. C., 1945, Conduction of Heat in a Slab in Contact with a Well-Stirred Fluid, Cambridge Philosophical Society, Proceedings, Vol. 41, pp. 43-49.

Pelto, M., 1982, Personnel Communication regarding vertical eddy diffusivities in the ocean.

Cohen, Y., D. Mackay, and W. Y. Shin, 1980, Mass Transfer Rates Between Oil Slicks and Water, the Canadian Journal of Chemical Engineering, Vol. 58, pp. 569-575.

Leo, A. C. Hanseh, and D. Elkins, 1971, Partition Coefficients and Their Uses, Chemical Reviews, Vol. 71, pp. 525-616.

Treybal, R. E., 1955, Mass Transfer Operations, McGraw-Hill, pp. 79-89.

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00010          IMPLICIT REAL*8  (A-H,O-Z)
00020          REAL*8 L,LCM,LCM2,M,KZ,KZS,KH,KPRME,MOIL,MWATER
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),MWATER(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     THIS CODE CALCULATES THE WATER-COLUMN CONCENTRATION
00140    C     OF A SPECIFIC COMPOUND DISSOLVING INTO THE WATER
00150    C     FROM AN OIL SLICK
00160    C
00170    C     OCTOBER, 1982
00180    C
00190          TYPE 10
00200    10    FORMAT(/,1X,'ENTER THE EDDY DIFFUSIVITY, CM*CM/SEC
00210         1, TRY 100')
00220          ACCEPT 20, DW
00230    20    FORMAT(F10.0)
00240          TYPE 30
00250    30    FORMAT(/,1X,'ENTER THE SLICK THICKNESS, TRY 1 CM')
00260          ACCEPT 20, DELTA
00270          TYPE 40
00280    40    FORMAT(/,1X,'ENTER THE OCEAN DEPTH, TRY 20 METERS')
00290          ACCEPT 20, L
00300          TYPE 50
00310    50    FORMAT(/,1X,'ENTER THE OIL/WATER PARTITION COEFFICIENT
00320         1, UNITLESS, TRY 1000')
00330          ACCEPT 20, M
00340          TYPE 60
00350    60    FORMAT(/,1X,'ENTER THE OIL-WATER OVER-ALL MASS-
00360         1TRANSFER COEFFICIENT, TRY 1 CM/HR')
00370          ACCEPT 20, KZ
00380          TYPE 70
00390    70    FORMAT(/,1X,'ENTER THE INITIAL OIL-PHASE CONCENTRATION
00400         1, GM/CC, TRY 0.001')
00410          ACCEPT 20, CZ
00420          TYPE 80
00430    80    FORMAT(/,1X,'ENTER THE NUMBER OF TERMS IN THE SERIES
00440         1, ON I3, TRY 100')
00450          ACCEPT 90, NTERM
00460    90    FORMAT(I3)
00470          TYPE 100
00480    100   FORMAT(/,1X,'ENTER THE NUMBER OF INTERVAL HALVINGS
00490         1 TO USE, ON I2, TRY 20')
00500          ACCEPT 90, NHALF
00510          TYPE 110
00520    110   FORMAT(/,1X,'ENTER VALUE FOR LEAD EXPONENTIAL
00530         1 FOR STEADY STATE APPROXIMATION,',/
00540         2,1X,'TRY 0.01')
00550          ACCEPT 20, ELEAD
00560    120   TYPE 130, DW
00570    130   FORMAT(/,1X,'1. EDDY DIFFUSIVITY     = ',1PD9.2,' CM*CM
00580         1/SEC')
00590          TYPE 140, DELTA
00600    140   FORMAT(1X,'2. SLICK THICKNESS      = ',F5.2,'  CM')
00610          TYPE 150, L
00620    150   FORMAT(1X,'3. OCEAN DEPTH          = ',F5.1,' METERS')
00630          TYPE 160, M
00640    160   FORMAT(1X,'4. OIL/WATER PARTITION = ',1PD9.2,' UNIT
00650         1LESS')
00660          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,' GM/CC')
00710           TYPE 190, NTERM
00720    190    FORMAT(1X,'7. NTERM = ',I3)
00730           TYPE 200, NHALF
00740    200    FORMAT(1X,'8. NHALF = ',I3)
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 (IOU,360)
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01330   360    FORMAT(1H1,5X,'WELL-STIRRED OIL SLAB
01340          1 IN CONTACT WITH A DIFFUSION SLAB')
01350          WRITE (IOU,370) DW,DELTA,L
01360   370    FORMAT(1X,'EDDY DIFFUSIVITY = ',1PD10.3
01370          1,' CM*CM/SEC, OIL SLICK THICKNESS = ',0PF5.2
01380          2,' CM, OCEAN DEPTH = ',F5.1,' METERS')
01390          WRITE (IOU,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 (IOU,390) CZ,NTERM,NHALF
01440   390    FORMAT(1X,'INITIAL SPECIES OIL-PHASE CONCENTRATION
01450          1 = ',1PD10.3,' GM/CC, NUMBER OF TERMS IN THE SERIES =
01460          2,I3,', NUMBER OF INTERVAL HALVINGS = ',I3)
01470          WRITE (IOU,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*COTANGENT(X)-(X*X-KH)/HCAP
01570   C
01580          CMSUM=0.D0
01590          P1=KPRME*HCAP*HCAP*(1.D0+KPRME)
01600          P2=HCAP*HCAP+HCAP-2.D0*KPRME*HCAP
01610          WRITE (IOU,410) P2,P1
01620   410    FORMAT(/,1X,'P = ALPHA**4 + ',1PD13.6,
01630          1'*ALPHA**2 + ',1PD13.6)
01640          KH=KPRME*HCAP
01650          WRITE (IOU,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 (IOU,430) CNORM,CNORM6
01740   430    FORMAT(/,1X,'THE NORMALIZING CONCENTRATION IS '
01750          1,1PD10.3,' GM/CC, OR ',1PD10.3,' PPM')
01760          WRITE (IOU,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=AN1*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 (IOU,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 (IOU,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 (IOU,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 (IOU,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          TSLOG=(DLOG10(DTIME))/10.D0
02310          TSCALE=LCM2/(3600.D0*DW)
02320          LTIME=0.D0
02330          DO 570 ITIME=1,10
02340          LTIME=LTIME+TSLOG
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 (IOU,580)
02710   580   FORMAT(//,5X,'DIMENSIONLESS CONCENTRATIONS AT
02720        1 VARIOUS TIMES AND DEPTHS FOLLOW')
02730         WRITE (IOU,590)
02740   590   FORMAT(/,5X,'METERS',3X,'HOURS',9(6X,'HOURS'))
02750         WRITE (IOU,600) (TIMEP(I),I=1,10)
02760   600   FORMAT(10X,10(2X,1PD9.2),/)
02770         DO 630 JX=1,11
02780         WRITE (IOU,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 (IOU,640) (COIL(I),I=1,10)
02850   640   FORMAT(/,6X,'OIL',/,5X,'CONC.',10(2X,1PD9.2))
02860         WRITE (IOU,650) (WATER(I),I=1,10)
02870   650   FORMAT(/,4X,'AVERAGE',/,5X,'WATER',/,5X,'CONC.'
02880        1,10(2X,1PD9.2))
02890         WRITE (IOU,660)
02900   660   FORMAT(//,5X,'ACTUAL CONCENTRATIONS IN PPM
02910        1 AT VARIOUS TIMES AND DEPTHS')
02920         WRITE (IOU,590)
02930         WRITE (IOU,600) (TIMEP(I),I=1,10)
02940         DO 670 JX=1,11
02950         WRITE (IOU,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)=DELTCZ*COIL(I)
03040         MWATER(I)=CNORML*WATER(I)
03050         COIL(I)=CZ6*COIL(I)
03060         WATER(I)=CNORM6*WATER(I)
03070   680   CONTINUE
03080         WRITE (IOU,640) (COIL(I),I=1,10)
03090         WRITE (IOU,650) (WATER(I),I=1,10)
03100         WRITE (IOU,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 (IOU,700) (MOIL(I),I=1,10)
03140   700   FORMAT(/,4X,'MASS IN',/,6X,'OIL',1X
03150        1,10(2X,1PD9.2))
03160         WRITE (IOU,710) (MWATER(I),I=1,10)
03170   710   FORMAT(/,4X,'MASS IN',/,5X,'WATER',10(2X,1PD9.2))
03180         WRITE (IOU,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,HCAP
03300         SINE=DSIN(X)
03310         COSINE=DCOS(X)
03320         F=X*COSINE/SINE-(X*X-KH)/HCAP
03330         RETURN
03340         END
```
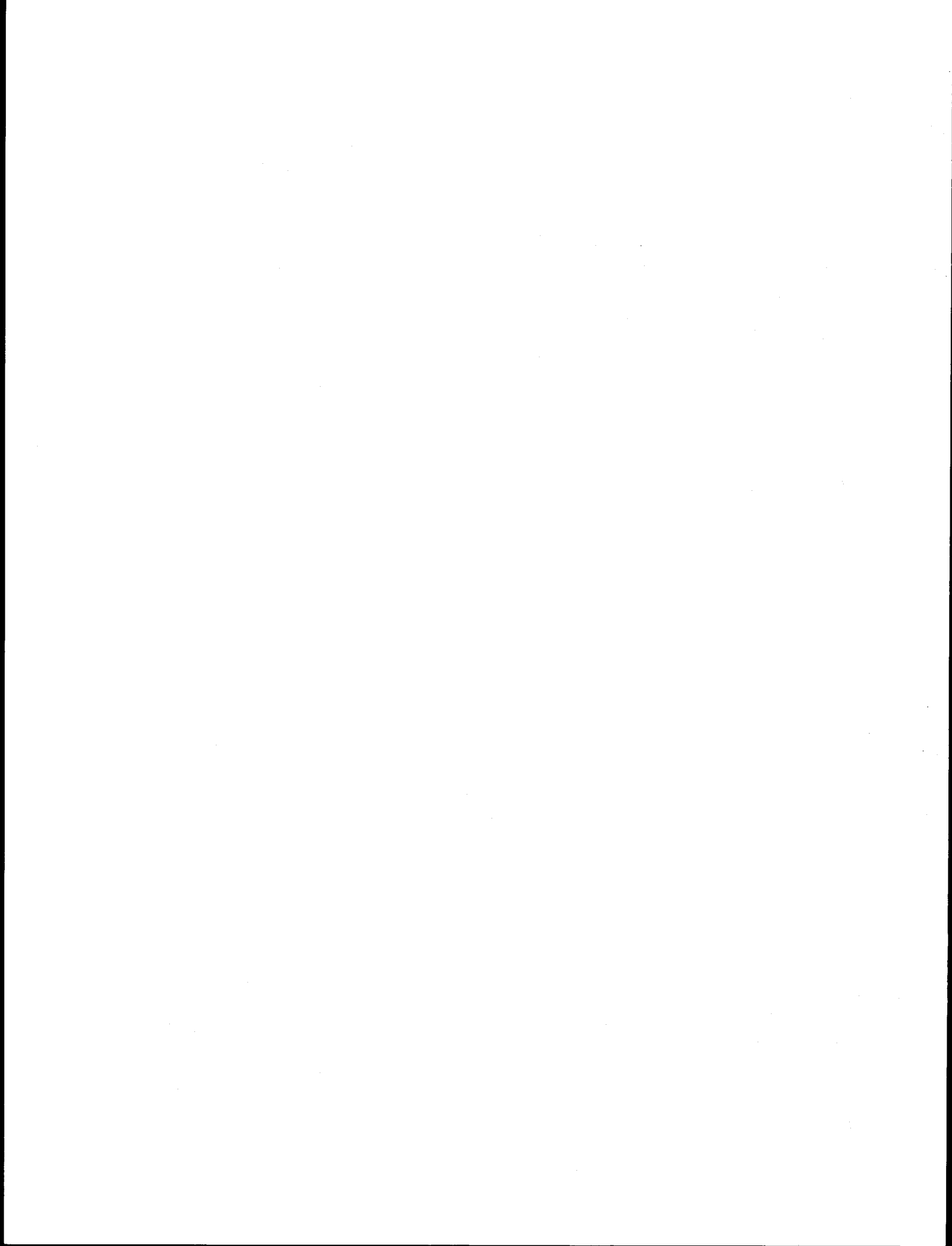
APPENDIX D

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
[LNKXCT 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*EXP(-B*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 COEFFICENTS 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 B40/3.055D-06,9.26D-06,3*0.D0/
00140          DATA ETRAP,PIE,PIE2/50.D0,3.141592654,9.869604401/
00150   C
00160   C        THIS IS A CODE TO CALCULATE THE WATER-COLUMN
00170   C        CONCENTRATION OF DISPERSED OIL WITH A FLUX BOUNDARY
00180   C        CONDITION
00190   C
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,'), GM/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,I3)
01360          TYPE 410, NEF
01370   410    FORMAT(2X,'5.   NUMBER OF EXPONENTIAL FITS = ',I2)
01380          IROW=5
01390          DO 440 I=1,NEF
01400          IROW=IROW+1
01410          TYPE 420, IROW,I,AI(I)
01420   420    FORMAT(/,1X,I2,'. 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,I2,'. 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 550
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 (IOU,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 (IOU,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 (IOU,640) KP2L
02550     640    FORMAT(/,5X,'K*PIE*PIE/L/L = ',1PD10.3
02560           1,' 1/SEC')
02570            WRITE (IOU,650) NTERM,NEF
02580     650    FORMAT(/,5X,'NUMBER OF TERMS IN THE SERIES = '
02590           1,I4,', NUMBER OF EXPONENTIAL FITS = ',I2)
02600            WRITE (IOU,660)
02610     660    FORMAT(/,5X,'THE EXPONENTIAL FIT COEFFICIENTS
02620           1 FOR THE DISPERSION RATE (RATE=A*EXP(-B*TIME)) ARE:')
02630            WRITE (IOU,670)
02640     670    FORMAT(5X,'UNITS ARE A==CM/CM*CM/SEC, B==1/SEC')
```

TABLE 2. (Continued)

```
02650          WRITE (IOU,680)
02660     680  FORMAT(/,24X,'AI(J)',15X,'BI(J)')
02670          DO 700 J=1,NEF
02680          WRITE (IOU,690) J,AI(J),BI(J)
02690     690  FORMAT(10X,I1,2(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 (IOU,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 (IOU,730)
02890     730  FORMAT(/,18X,'TIME',11X,'RATE')
02900          WRITE (IOU,740)
02910     740  FORMAT(18X,'HOUR',9X,'GM/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)*(3.6D+07)
03090          WRITE (IOU,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 (IOU,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 (IOU,800) J
03380     800  FORMAT(/,5X,'A CHECK OF THE INITIAL CONDITIONS FOR
03390         1 THE J =',I2,'    A,B INPUT SET')
03400          WRITE (IOU,810)
03410     810  FORMAT(/,15X,'DEPTH',10X,'EBL',12X,'SUM',8X
03420         1,'CONC AT T=0')
03430          WRITE (IOU,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 (IOU,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 (IOU,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 (IOU,880)
03950     880  FORMAT(/,50X,'H O U R S')
03960          WRITE (IOU,890) (TIME(IT),IT=1,10)
```

TABLE 2. (Continued)

```
03970    890    FORMAT(7X,'DEPTH',1X,10(1X,1PD9.2))
03980           WRITE (IOU,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 (IOU,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 (IOU,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 GM/(CM**4)
04570    C
04580           WRITE (IOU,980)
04590    980    FORMAT(//,5X,'THE DERIVATIVE WITH RESPECT TO X OF
04600          1 THE WATER COLUMN CONCENTRATION FOLLOWS, IN GM/(CM**4)')
04610           WRITE (IOU,880)
04620           WRITE (IOU,890) (TIME(IT),IT=1,10)
```

TABLE 2 . (Continued)

```
04630          WRITE (IOU,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 (IOU,960) XP(1),(SZERO(IT,J),IT=1,10)
04750          DO 1020 IX=1,10
04760          WRITE (IOU,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 (IOU,1040)
04930    1040  FORMAT(/,3X,'GRAMS OIL')
04940          WRITE (IOU,1050) (GRAMS(IT,J),IT=1,10)
04950    1050  FORMAT(4X,'IN WATER',1X,10(1X,1PD9.2))
04960          WRITE (IOU,1060)
04970    1060  FORMAT(3X,'PER CM*CM')
04980          WRITE (IOU,1070)
04990    1070  FORMAT(/,5X,'AVERAGE')
05000          WRITE (IOU,1080) (ACONC(IT,J),IT=1,10)
05010    1080  FORMAT(7X,'GM/CC',1X,10(1X,1PD9.2))
05020          WRITE (IOU,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 M=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 (IOU,1150) NEF
05270    1150  FORMAT(///,5X,'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 (IOU,880)
05310           WRITE (IOU,890) (TIME(IT),IT=1,10)
05320           WRITE (IOU,900)
05330           WRITE (IOU,960) XP(1),(CZERO(IT,5),IT=1,10)
05340           DO 1160 IX=1,10
05350           WRITE (IOU,960) XP(IX+1),(C(IX,IT,5),IT=1,10)
05360    1160   CONTINUE
05370           WRITE (IOU,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 (IOU,880)
05410           WRITE (IOU,890) (TIME(IT),IT=1,10)
05420           WRITE (IOU,900)
05430           WRITE (IOU,960) XP(1),(SZERO(IT,5),IT=1,10)
05440           DO 1180 IX=1,10
05450           WRITE (IOU,960) XP(IX+1),(S(IX,IT,5),IT=1,10)
05460    1180   CONTINUE
05470           WRITE (IOU,1040)
05480           WRITE (IOU,1050) (GRAMS(M,5),M=1,10)
05490           WRITE (IOU,1060)
05500           WRITE (IOU,1070)
05510           WRITE (IOU,1080) (ACONC(M,5),M=1,10)
05520           WRITE (IOU,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 <u>constant flux</u> (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 =  1.850D+02 CM*CM/SEC
2. FLUX AT THE SURFACE =  2.220D-08 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 CON-
CENTRATION 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, GM/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,' GM/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 (IOU,260)
01010      260     FORMAT(1H1,'CONCENTRATION PROFILES IN THE WATER
01020             1 COLUMN FOR DISPERSED OIL (NEUTRAL DENSITY)')
01030              WRITE (IOU,270)
01040      270     FORMAT(1X,'CALCULATED FOR A CONSTANT FLUX (
01050             1IERC SOLUTION) AT THE OCEAN SURFACE')
01060              WRITE (IOU,280) K,W
01070      280     FORMAT(/,1X,'VERTICAL EDDY DIFFUSIVITY = ',1PD9.2,
01080             1' CM*CM/SEC, DISPERSED OIL FLUX = ',1PD9.2,'
01090             2 GM/CM*CM/SEC')
01100              WRITE (IOU,290) DM,HOURS,NTERM
01110      290     FORMAT(1X,'OCEAN DEPTH = ',F5.1,' METERS, MAX
01120             1IMUM TIME = ',F5.1,' HOURS, NUMBER OF TERMS IN
01130             2 IERFC SERIES = ',I3)
01140              WRITE (IOU,300) IMAX
01150      300     FORMAT(1X,'NUMBER OF TERMS IN ERF SERIES = ',I3)
01160              WRITE (IOU,310)
01170      310     FORMAT(/,1X,'DISPERSED-OIL CONCENTRATIONS,
01180             1 GM/CC, IN THE WATER COLUMN FOR VARIOUS TIMES
01190             2 AND DEPTHS FOLLOW')
01200              WRITE (IOU,320)
01210      320     FORMAT(/,53X,'H O U R S')
01220              WRITE (IOU,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
```

E-5

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 (IOU,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 (IOU,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
```
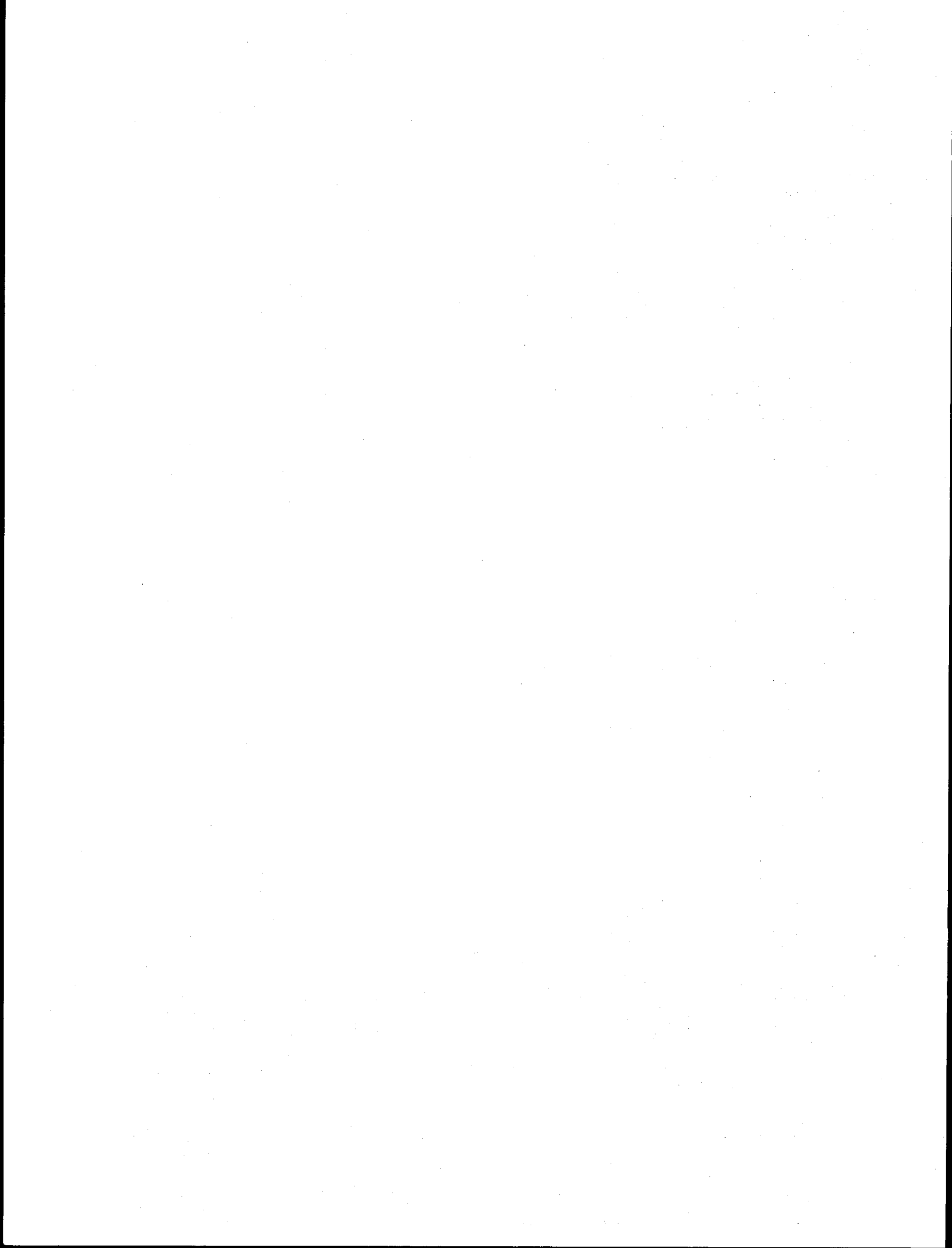
METHODS FOR MICROBIAL DEGRADATION STUDIES

^{14}C-Hydrocarbon Mineralization Assay

Three ^{14}C-labeled hydrocarbon substrates were utilized for the deter-
mination of hydrocarbon degradation potential, defined here as the percent
mineralization to $^{14}CO_2$: n(1-^{14}C) hexadecane (53.6 mCi/mmol, Amersham),
(1(4,5,8)-^{14}C) naphthalene (5 mCi/mmol, Amersham), and (1(4,5,8)-^{14} C) methyl-
naphthalene (5 mCi/mmol, Bionuclear). Working solutions were prepared with
hexane or benzene as solvents to give 0.1 μCi/μl activities, stored at 4°C,
and assayed weekly for radioactivity to insure consistency in the concentra-
tions of substrates. Seawater aliquots (50 ml) from each of the experimental
tanks and the incoming seawater were transferred to 100 ml sterile serum bot-
tles and spiked with 0.5 μCi of the ^{14}C-labeled hydrocarbons, one compound
per sample with each sample prepared in duplicate. Controls were killed with
1 μM 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 rectan-
gle of Whatman No. 1 filter paper folded into an accordian-pleated array and
wetted with 200 μl of 1N NaOH. The samples were then acidified to pH 2.0 by
injection of 0.5 ml of 1 N H$_2$SO$_4$ (through the sleeve stopper) with a hypoder-
mic syringe. After 2 hours the filter paper was transferred to a second 100
ml serum bottle containing 1 ml of 1N H$_2$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 μl of phenethylamine.

After 12-14 hours the phenethylamine wicks were transferred to a
scintillation vial containing 10 ml of Beta-Phase cocktail (West Chem Prod-
ucts) 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 μg/liter·day by the following equation.

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

where a counting efficiency of 90% was utilized, SA is the specific activity in $\mu Ci/\mu$ 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).

[3]H-Thymidine Incorporation

Thymidine (methyl-^{3}H) 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 μM $HgCl_2$) and a counting efficiency of 35%. The data were converted to nmoles/liter day of incorporation by the formula:

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

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

[3]H-Leucine and ^{3}H-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 ^{3}H-Leucine (60 Ci/mmol, New England Nuclear) were prepared by diluting an aliquot of the stock solution into distilled water. The ^{3}H-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 radio-labeled substrate. To each sample (10 ml for ^{3}H-Glucose; 15 ml for ^{3}H-Leucine) 50 μl (1.5 μCi) of radiolabeled compound was added, followed by incubation for 2 hr. in the dark at <u>in situ</u> 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:

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

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 Na$_2$B$_4$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 x 10^6/ml seawater.

References: HOBBIE 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 ^{3}H-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 gain clusters were counted by transmitted phase con rast 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 :0-12 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 chromatrography 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-Artic 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-Artic Sediments: Results of Chemical Analyses of Naturally Weathered Sediment Parts Spiked with Fresh and Artificially Weathered Cook Inlet Crude Oil".
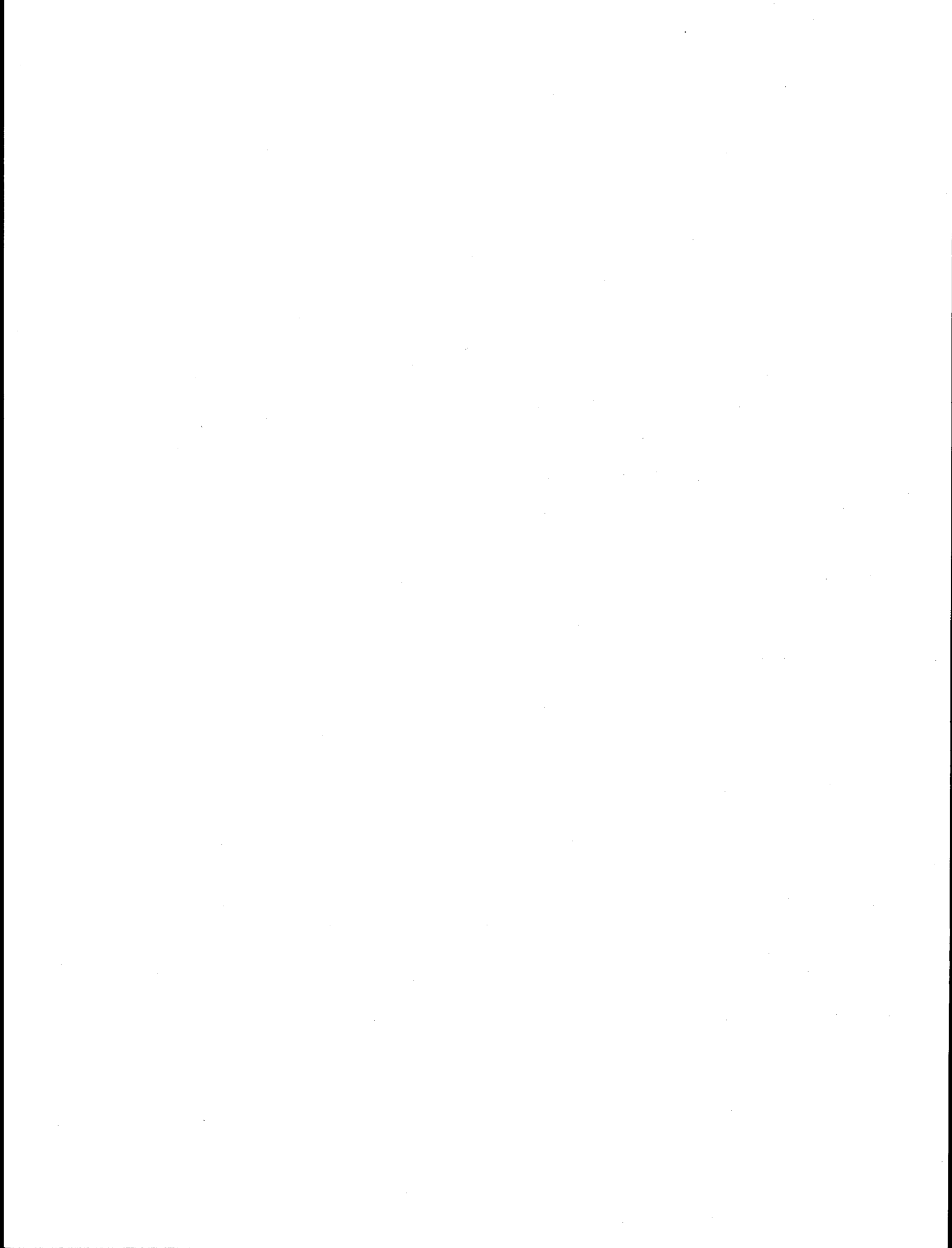
APPENDIX   G

THE X-RAY DIFFRACTION ANALYSIS OF NINE SEDIMENT SAMPLES

Report Submitted to:

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March 15, 1983

by:

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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 Poot Bay)

K-Bay Site #3 OW-3   (Kasitsna Bay)

K-Bay Site #4 OW-4   (Seldovia Bay)

K-Bay Site #5 OW-5   (Jackolof Bay)

Glacial Till OW-7   (foot of glacier)

FILTER SAMPLES:

1M (Kasitsna 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.

G-2

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. Certainity cannot be placed on the identification of these trace phaces 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, 1983.

SAMPLE: K Bay Site #1 OW-1

α-Quartz	Kaolinite	Feldspar	Calcite	Other
major	intermediate	intermediate	none	Mica - tr

SAMPLE: K Bay Site #2 OW-2

α-Quartz	Kaolinite	Feldspar	Calcite	Other
intermediate +	minor +	intermediate -	major	Mica - tr ?

SAMPLE: K Bay Site #3 OW-3

α-Quartz	Kaolinite	Feldspar	Calcite	Other
major	minor +	intermediate	none	NaCl - minor Gypsom - tr?

SAMPLE: K Bay Site #4 OW-4

α-Quartz	Kaolinite	Feldspar	Calcite	Other
major	minor +	intermediate	none	NaCl - minor

SAMPLE: K Bay Site #5   OW-5

α-Quartz	Kaolinite	Feldspar	Calcite	Other
major	intermediate-	intermediate	tr ?	NaCl-minor

SAMPLE: Glacial Till   OW-7

α-Quartz	Kaolinite	Feldspar	Calcite	Other
major	intermediate-	intermediate	none	Mica-tr

SAMPLE: Filter 1-M

α-Quartz	Kaolinite	Feldspar	Calcite	Other
major	intermediate+	minor +	none	Mica-tr ?

SAMPLE: Filter 2-M

α-Quartz	Kaolinite	Feldspar	Calcite	Other
minor +	major	minor	trace ?	Huntite?-t Mica-minor

SAMPLE: Filter 6-M

α-Quartz	Kaolinite	Feldspar	Calcite	Other
major	Intermediate	intermediate	none	Mica -tr

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

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X-ray diffraction spectrograph of sediment from Site KB-3 (Kasitsna Bay).
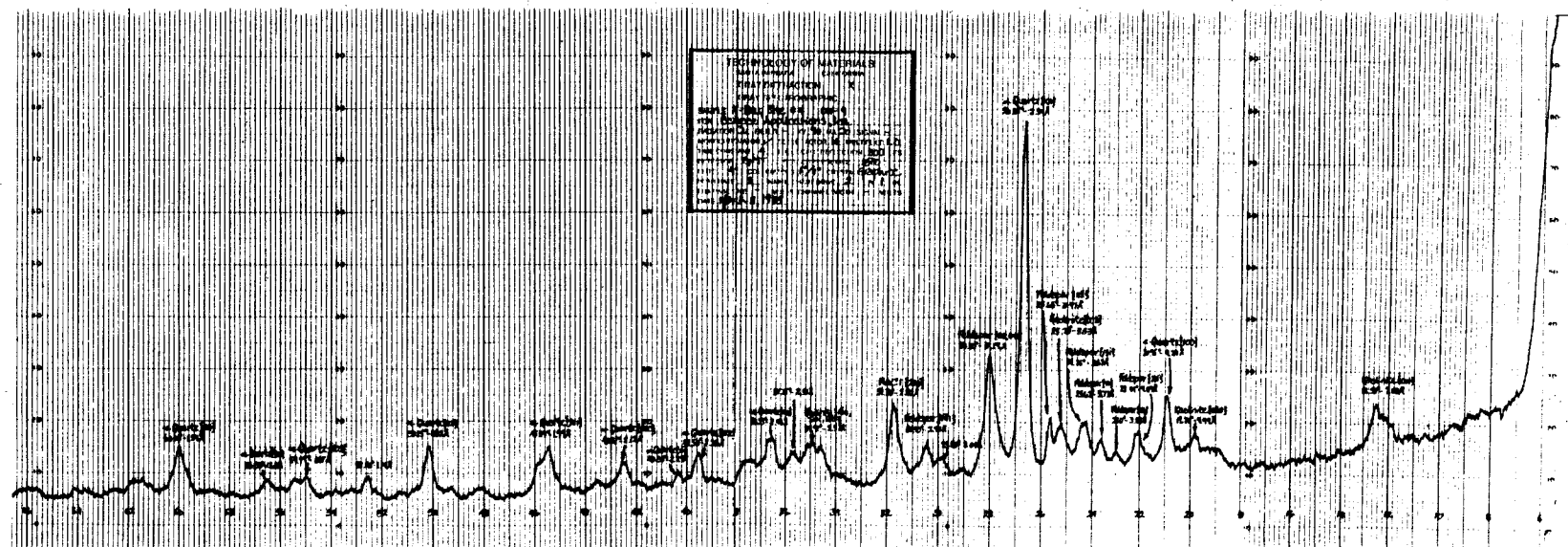
X-ray diffraction spectrograph of sediment from Site KB-4 (Seldovia Salt Marsh).
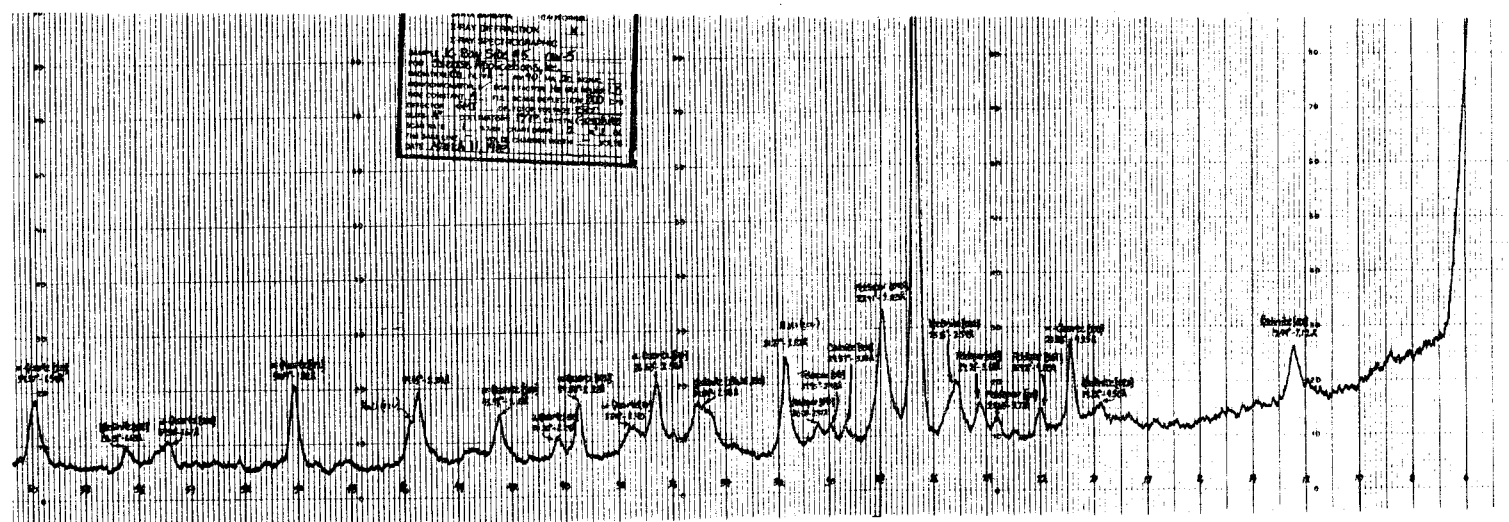
X-ray diffraction spectrograph of sediment from Site KB-5 (Jakolof Bay).

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 ARTIFICALLY WEATHERED
COOK INLET CRUDE OILS

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SPIKED WITH FRESH AND ARTIFICALLY WEATHERED
COOK INLET CRUDE OILS

Report Submitted to:

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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 pertibations to plants, organisms and the physical (areobic 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 $210^{\circ}C$ 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_3OH in CH_2Cl_2	60 ml	Polar compounds

Gas Chromatographic Analysis

All gas chrmatographic 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 casette 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° 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 μl 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.

$$\mu g \text{ compound } X/L \text{ seawater} = (A_x) \times (R.F.) \times$$

$$\left[\frac{P.I.V. + 2}{Inj.S.Vol.} \cdot \frac{Pre-C.S. \text{ Vol.}}{Post-C.S.Vol.} \cdot \frac{100}{\%NSL \text{ on } LC} \times \frac{100}{\%DW/FW} \times \frac{1}{liters} \right] \quad (1)$$

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 μg/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)

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Pre-C.S.Vol. &   = the total solvent volumes before and after an
Post-C.S. Vol.   aliquot is removed for gravimetric analysis on a
                       Cahn electrobalance

%NSL on LC   = the percent of sample non-saponifiable lipid used
                       for SiO_2 column chromatography

%DW/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.

$$\frac{\mu g \ UCM}{liter} = Area_p \times (Conf. \ F) \times \frac{S. \ Att.}{Ref. \ Att.} \times (\overline{R.F.}_{a-b}) \times [...]$$ (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 attentuation,

S. Att. and   = the GC attenuation at which the sample chromatogram
Ref. Att.   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 reten-
                        tion 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 μm 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°, and 8°C/min from 160-275°, 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 diagostic 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 com-

ponents at retention times 31.21, 35.77 and 43.08 are internal spikes

and a GC recovery standard (triisopropylbenzene, 31.21; n-decylcyclo-

hexane, 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 be-

tween nC_{20} and nC_{21}. The aromatic fraction chromatogram, B, from this
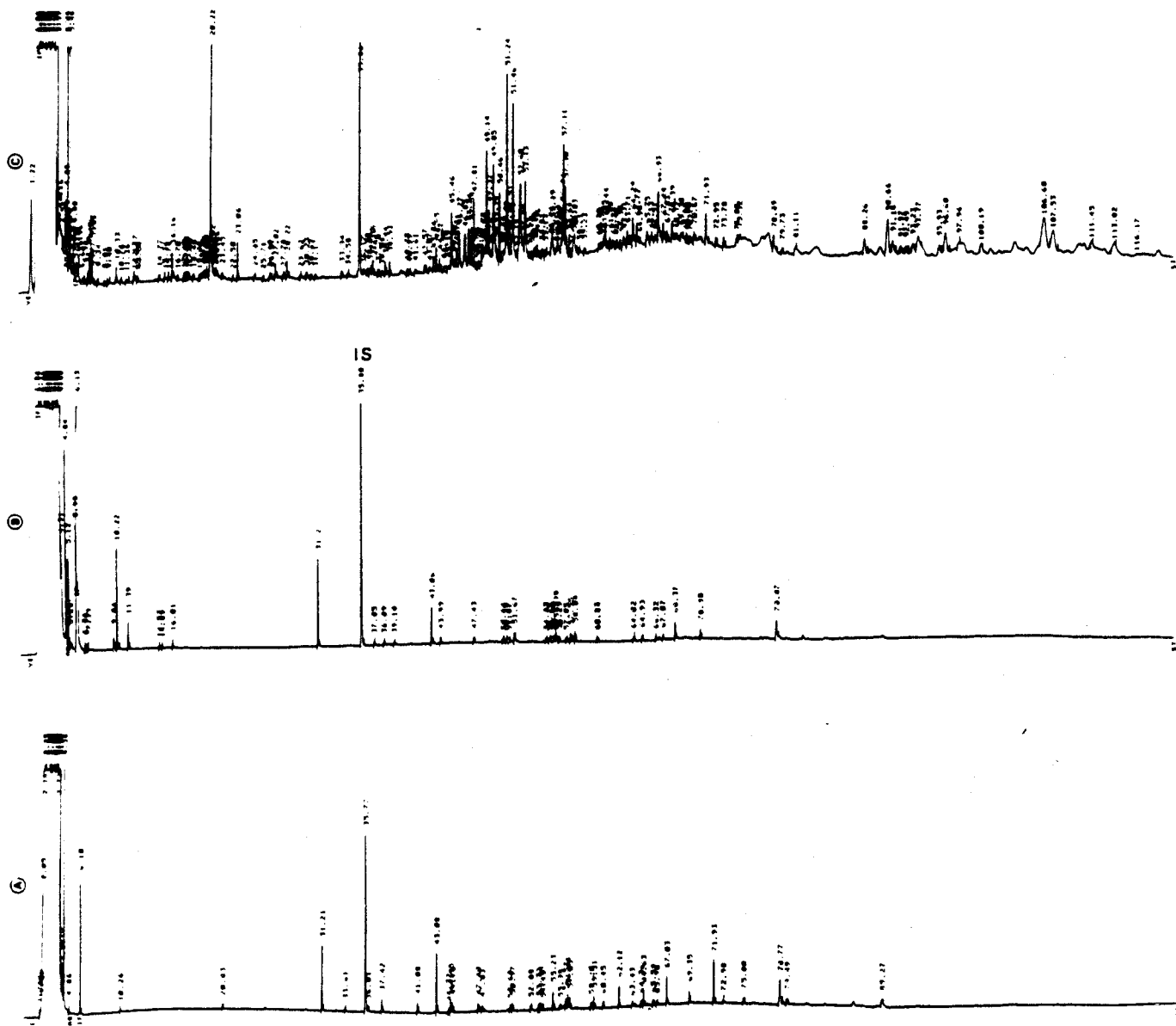
Figure 1. Flame Ionization Detector capillary gas chromatograms of: A, the aliphatic fraction; B, the aromatic fraction and C, the polar fraction extracts obtained from time zero control sediment samples from Kasitsna Bay.

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 underoing 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 I. Reduced Aliphatic Hydrocarbon Data Derived from Flame Ionization Detector Capillary GC Analyses

Sediment Sample	OSU ID No	Time In Field (years)	Total Resolved ug/g	Total UCM* ug/g	Σ n-alkanes ug/g	Σ even n-alkanes ug/g	Σ odd n-alkanes ug/g	pristane + phytane / n-alkanes	odd alk / even alk	prist / nC_{17}	phy / nC_{18}	pris / phyt	n-alk / branched
KASITSNA BAY CONTROL	1	0	5.89	0.	2.76	0.449	2.31	0.0157	5.15	0.758	0.	4--	0.883
KASITSNA BAY CONTROL	625	1	1.22	0.	0.533	0.06	0.473	0	7.86	0.	0.	0.	0.776
FRESH CRUDE SPIKE 50ppt	5	0	2840.	4090.	1460.	742.	722.	0.0749	0.973	0.681	0.343	2.63	1.06
FRESH CRUDE SPIKE 1ppt	4	0	83.3	154.	52.8	24.2	28.6	0.055	1.18	0.630	0.411	2.18	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	0.380	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	1R	2430.	1740.	1080.	560.	515.	0.0861	0.921	0.761	0.354	2.63	0.796
FRESH CRUDE SPIKE 50ppt	629	1R	2700.	3770.	1250.	645.	605.	0.0799	0.934	0.700	0.386	2.43	0.860
FRESH CRUDE SPIKE 50ppt	630	1R	2060.	3010.	950.	494.	458.	0.0832	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	0.0320	5.10	0.800	0.	3--	0.496
WEATHERED CRUDE SPIKE 50	637	1	1530.	3710.	949.	449.	499.	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.	0.243
SADIE COVE CONTROL	206	0	26.1	0.	10.7	1.37	9.33	0	6.81	0.	0.	0.	0.773
SADIE COVE OIL & STARCH	782	1	3760.	5200.	1605.	837.	768.	0.071	0.917	0.762	0.391	2.55	0.743
SADIE COVE OIL	779	1	4730.	6100.	1920.	983.	932.	0.0838	0.948	0.880	0.420	2.75	0.681
SADIE COVE OIL & CHITIN	780	1	4700.	6670.	1986.	1020.	968.	0.0630	0.951	0.626	0.345	2.14	0.732
COOK INLET CRUDE OIL													
FRESH	-	N.A.	84000	77600	33000	18300	14700	0.0703	0.804	0.673	0.331	2.41	0.648
WEATHERED	-	N.A.	38700.	54500.	24500.	11600.	12900.	0.0989	1.12	0.654	0.380	2.23	1.73

*UCM - Unresolved Complex Mixture

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

Sediment Sample	OSU ID No	Time in field (years)	Total Resolved ug/g	Total UCM* ug/g	Naphthalene (1185)**	2 Methyl-naphthalene (1295)	1 Methyl-naphthalene (1313)	Biphenyl (1381)	2,6 Dimethyl naphthalene (1404)	Fluorene (1586)	Phenanthrene (1786)	Anthracene	1 Methyl-phenanthrene	Fluoranthene	Pyrene
KASITSNA BAY CONTROL	1	0	3.08	0.	nd	nd	nd	nd	nd	nd	0.0262	nd	nd	nd	0.0392
KASITSNA BAY CONTROL	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.	94.9	16.2	65.4	32.5	56.6	nd	18.0	nd	nd
FRESH CRUDE SPIKE 1ppt	4	0	12.2	22.3	0.363	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	0.0021	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.	880.	13.3	35.2	21.0	1.17	17.9	4.27	5.98	nd	2.40	0.840	nd
FRESH CRUDE SPIKE 50ppt	630	1	300.	2020.	9.75	30.4	18.6	nd	17.5	4.44	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	0.383	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 COVE CONTROL	206	0	2.92	0	nd	nd	nd	nd	nd	nd	0.10258	nd	nd	0.02803	0.21073
SADIE COVE 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 COVE OIL	779	1	872.	2440.	32.6	75.0	43.2	nd	32.3	6.27	10.2	nd	5.71	2.04	nd
SADIE COVE OIL & CHITIN	780	1	1070.	1660.	33.8	77.8	45.7	1.80	31.0	6.24	9.99	nd	6.66	nd	nd
COOK INLET CRUDE OIL															
FRESH	-	N.A.	34700.	41600.	484.	1110.	644.	nd	540.	nd	190.	nd	nd	nd	nd
WEATHERED	-	N.A.	15400.	31400.	nd	nd	nd	nd	223.	102.	235.	nd	nd	nd	nd

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

| 1	C-2 Benzenes
2	C-3 Benzenes
3	C-4 Benzenes
4	Naphthalene
5	Methyl Naphth.
6	Dimethyl Naphth.
7	Trimethyl Naphth.
8	Phenanthrene
9	Methyl Phen.
10	Dimethyl Phen.
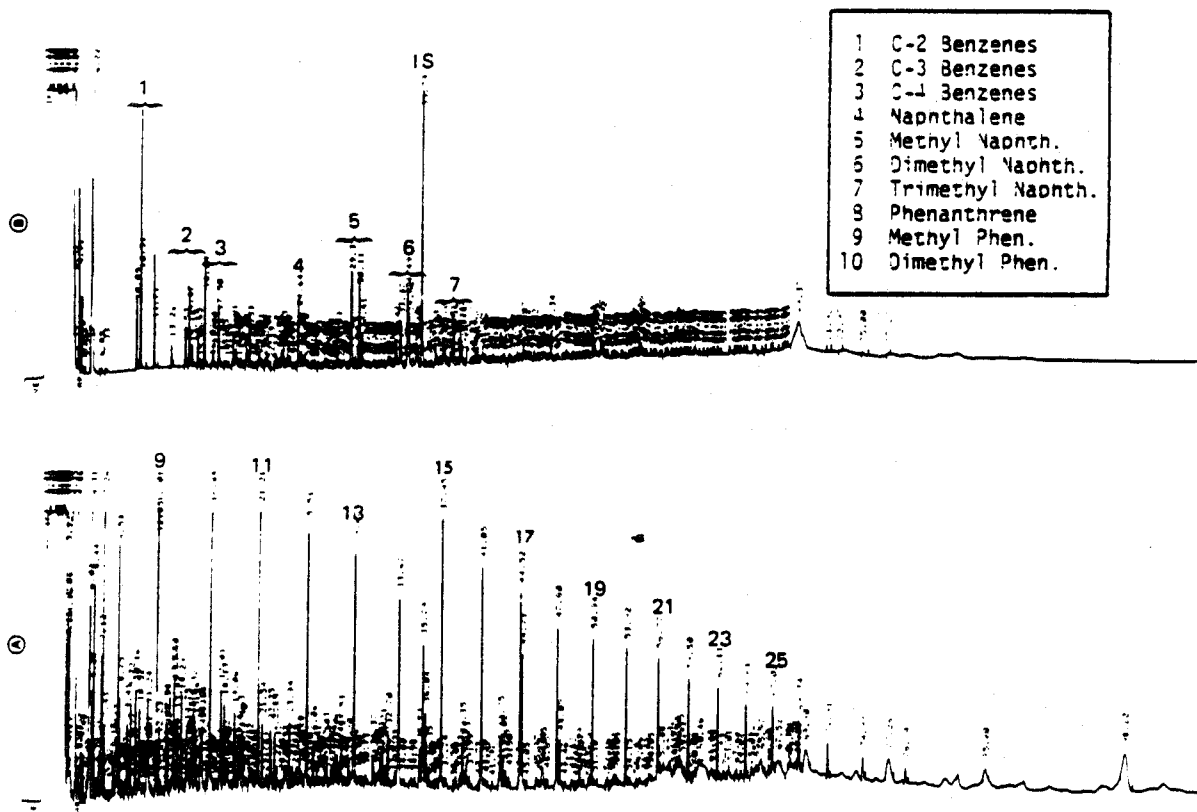
Figure 2. Flame Ionization Detector capillary gas chromatograms of: A, the aliphatic fraction, and B, the aromatic fraction extracts obtained on the fresh Cook Inlet Crude Oil used to spike the Kasitsna Bay sediment samples.
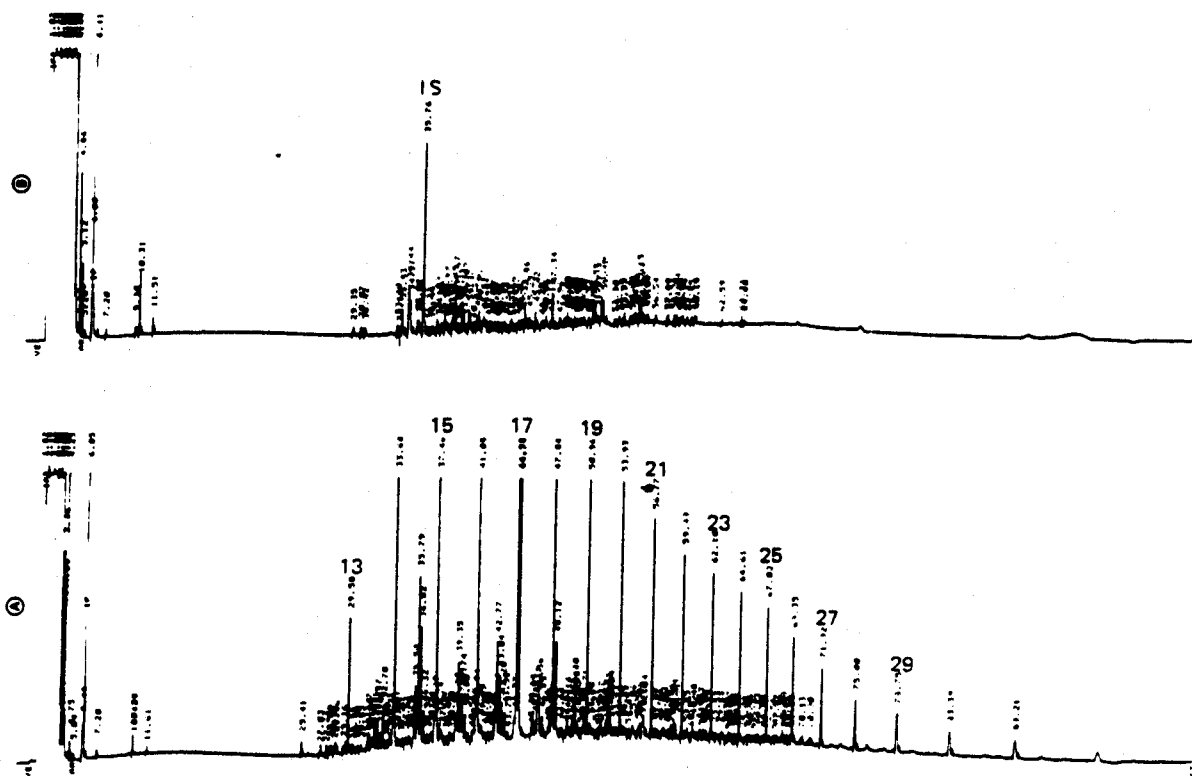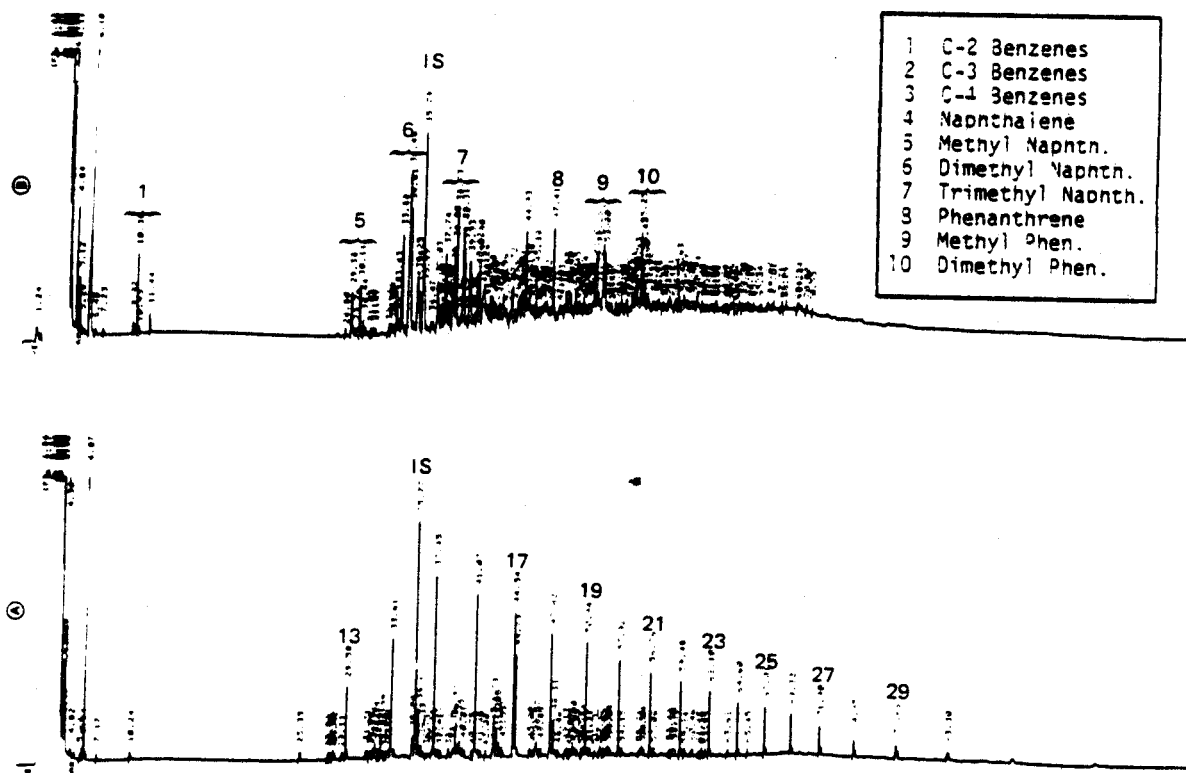
Figure 3. Flame Ionization Detector capillary gas chromatograms of: A, the aliphatic fraction, and B, the aromatic fraction extracts obtained from the Artifically Weathered Cook Inlet Crude Oil used to spike the Kasitsna Bay sediment samples.

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 napthalene (RT 24.64), 2-methylnapthalene (RT 29.38), 1-methylnapthalene (RT 30.11), 2,6-dimethylnapthalene (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 dimethylnapthalene; 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
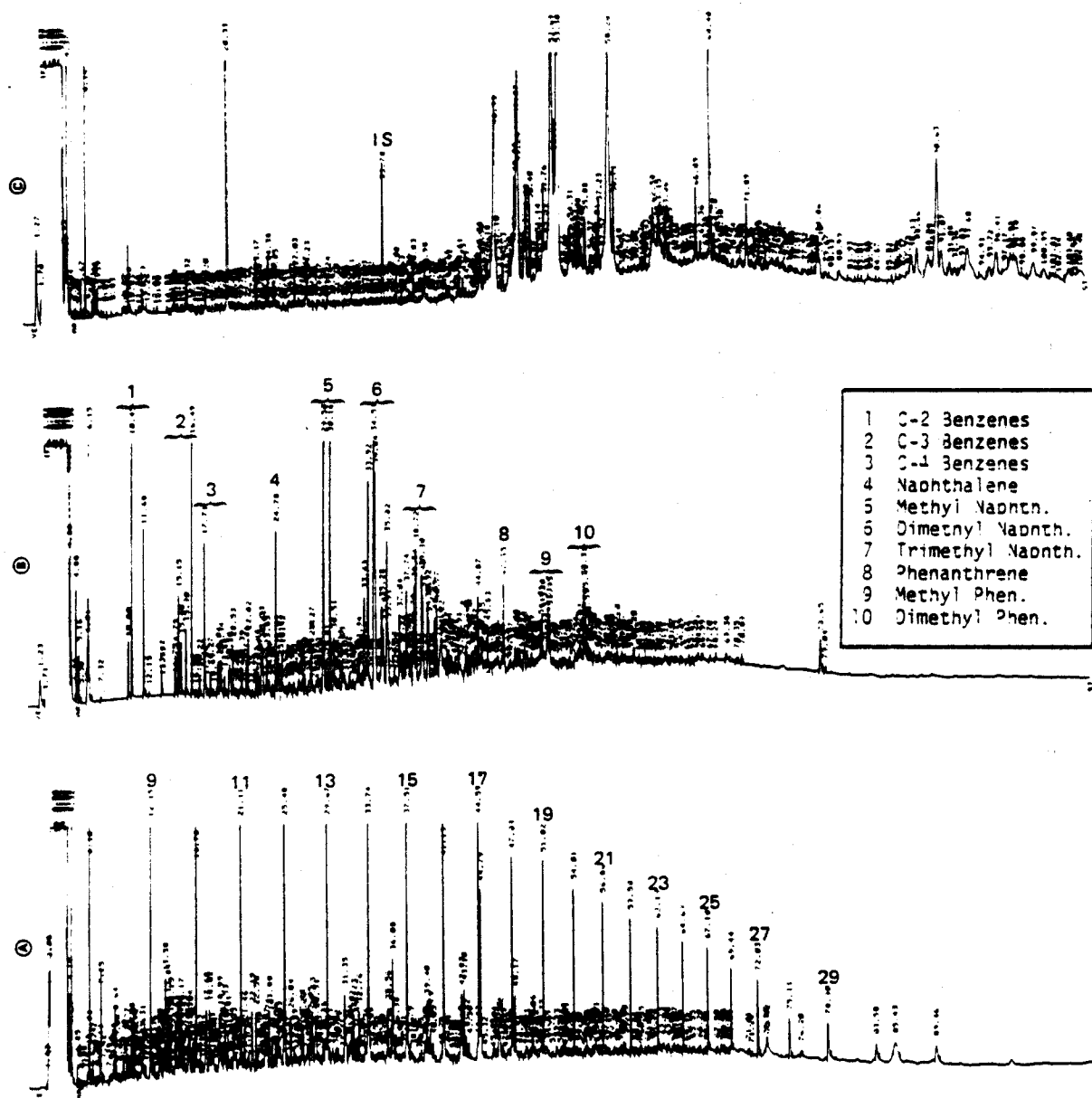
Figure 4. Flame Ionization Detector capillary gas chromatograms of: A, the aliphatic fraction, B, the aromatic fraction, and C, the polar fraction extracts obtained from time zero Kasitsna Bay sediment samples which had been spiked with fresh Cook Inlet Crude Oil at 1 ppt.

sample show many of the same aromatic compounds in the napthalene (KOVAT 1185) to pyrene (KOVAT 2124) range and the alkyl-substituted aromatic compounds at KOVAT indices 800 to1012 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-methylnapthalene at 30.11, 2,6-dimethylnapthalene 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 artifically 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 Artifically 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 sub-samples 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.
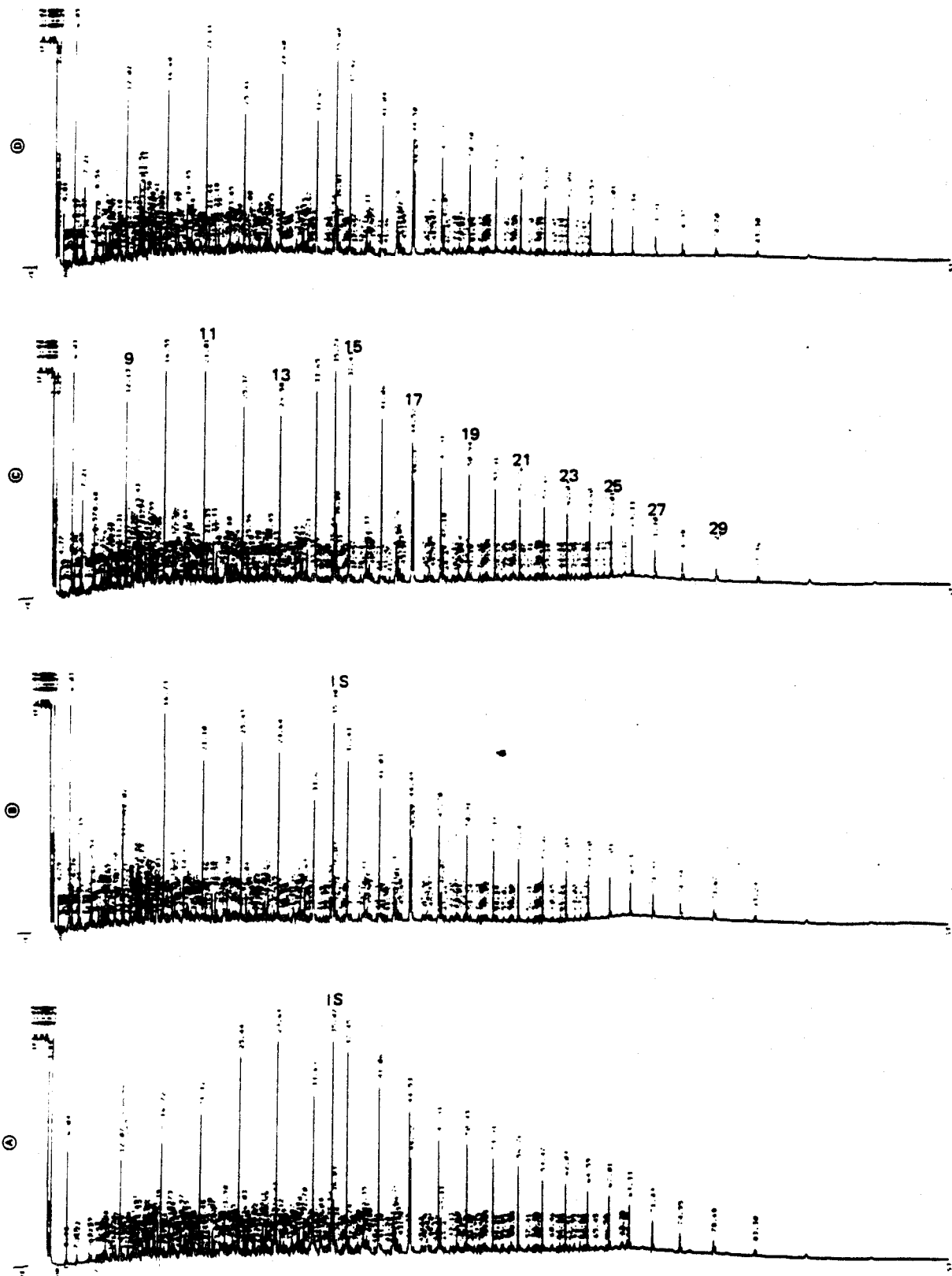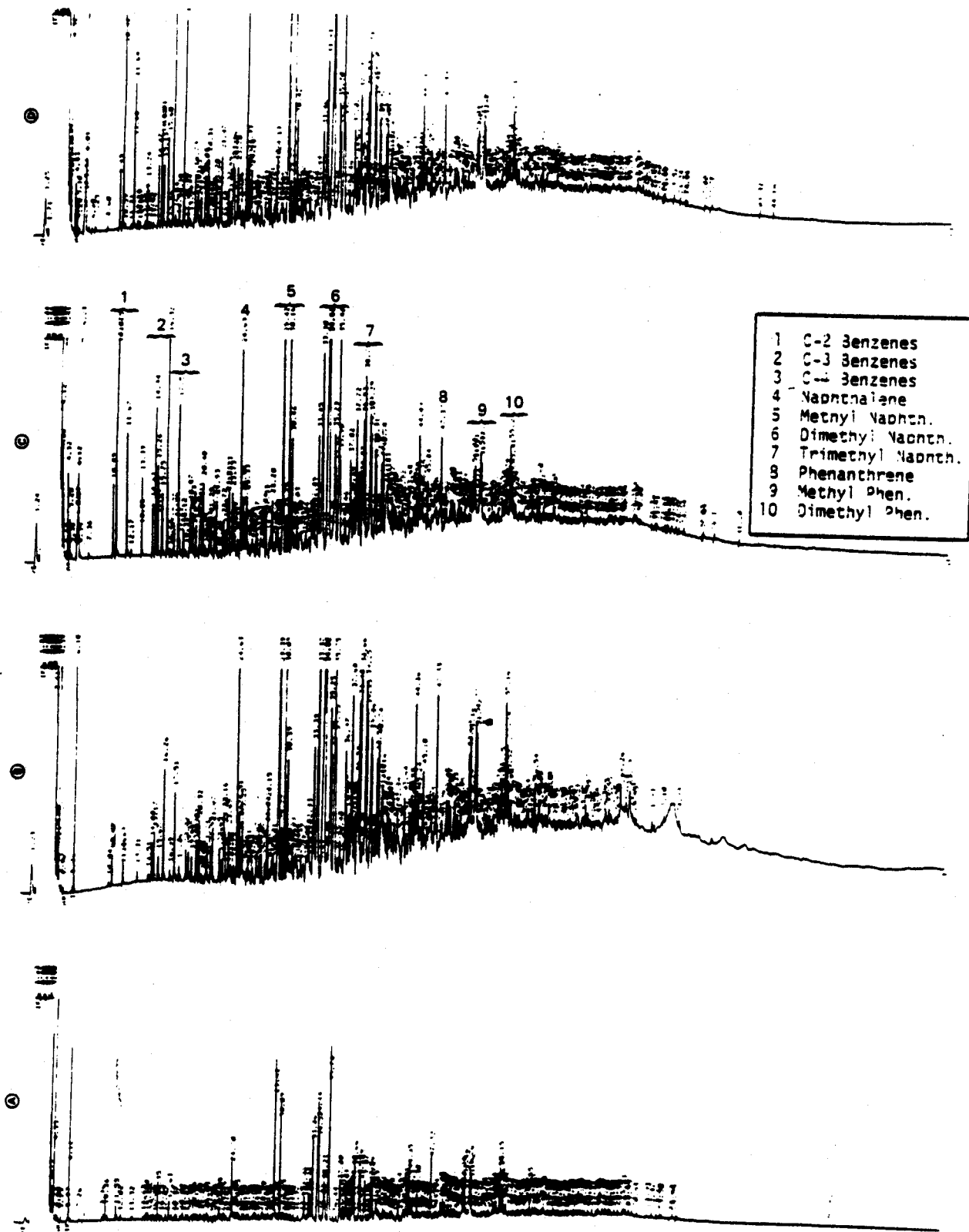
Figure 6. Flame Ionization Detector capillary gas chromatograms of: A, the aliphatic fraction of the 50 ppt fresh Cook Inlet Crude Oil spiked into the sediment at time zero, and B, C, and D, the aliphatic fractions of the triplicate samples examined after one year of natural weathering in Kasitsna Bay.
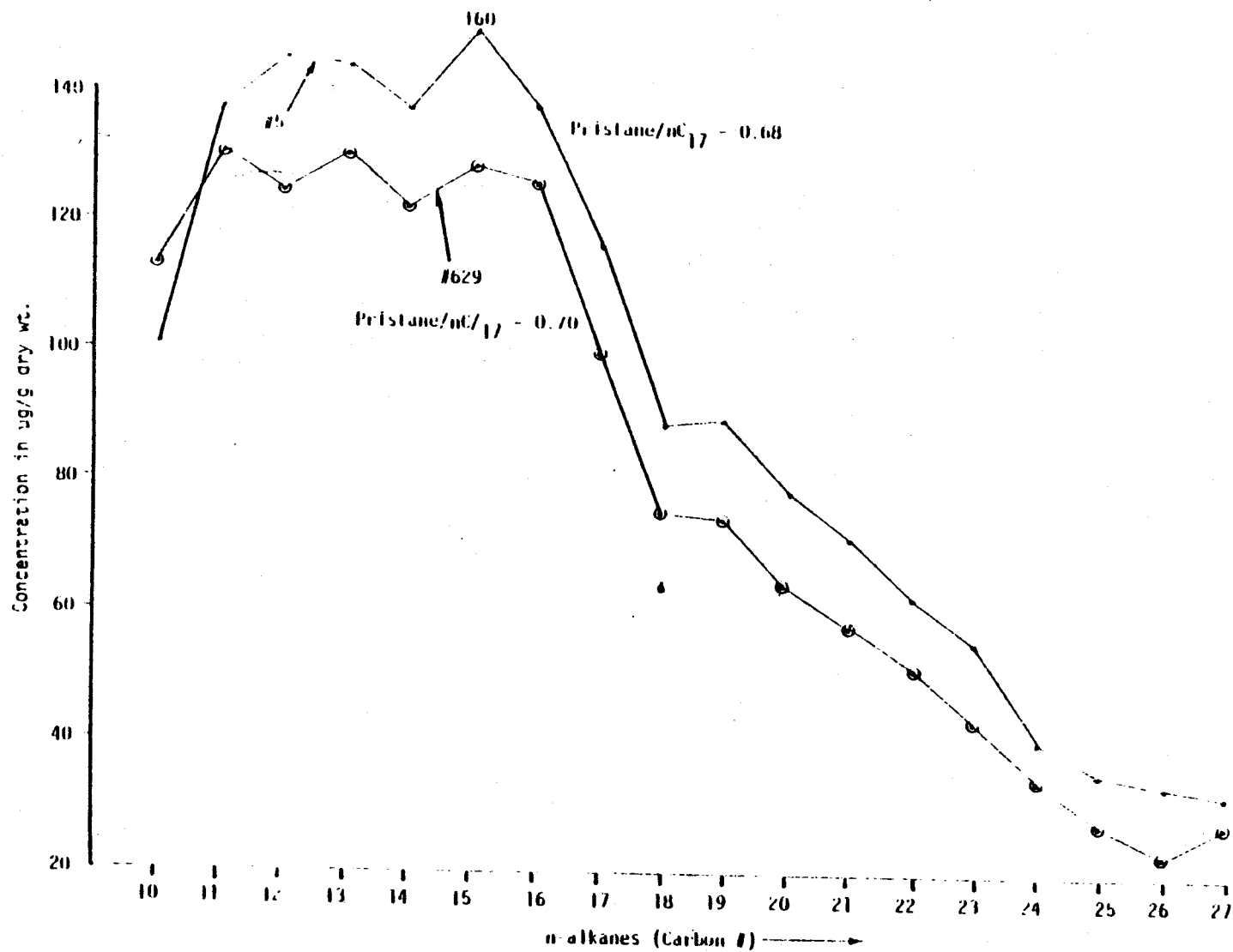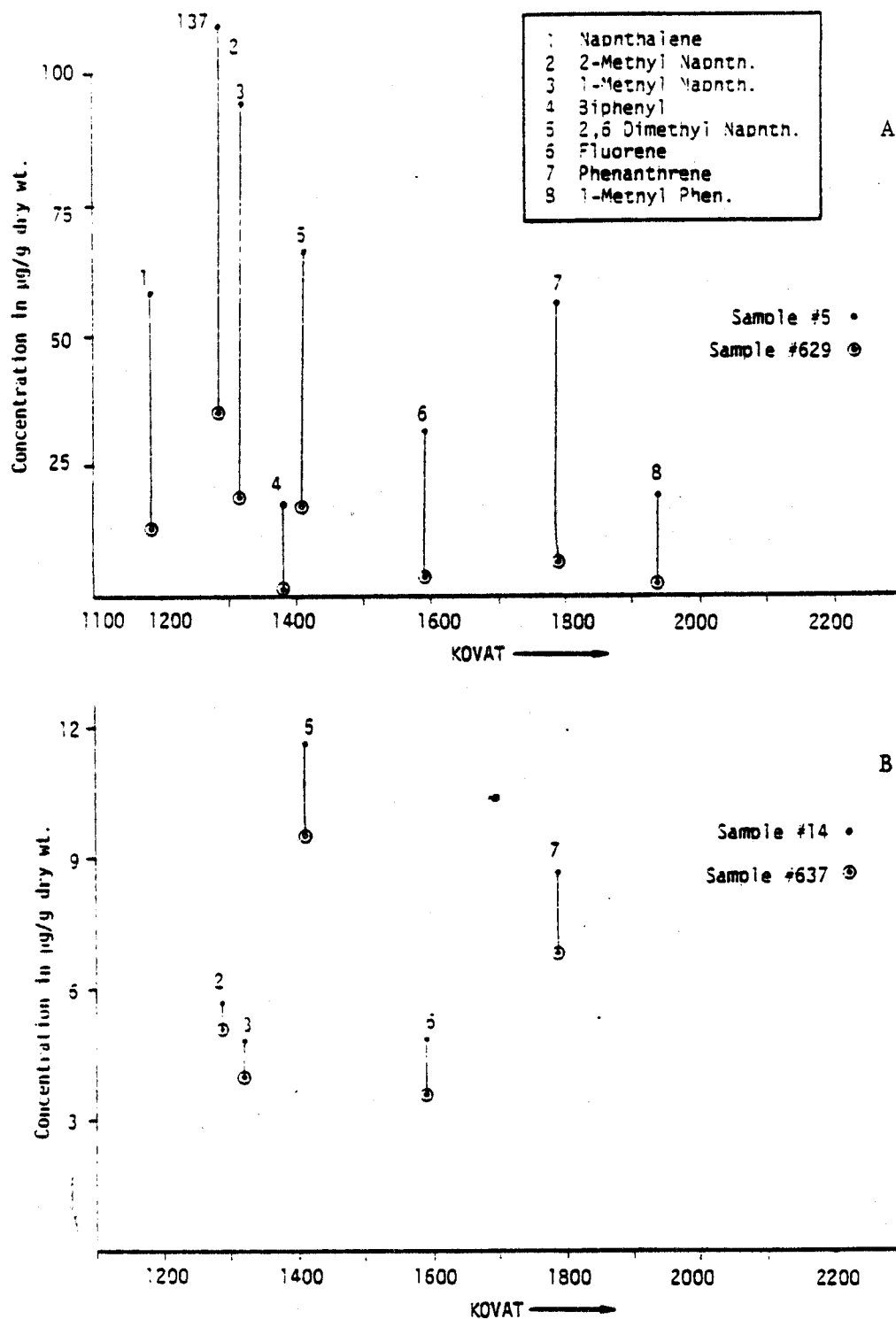
Figure 7. Concentration abundance of the n-alkanes in a sediment sample spiked with 50 parts per thousand fresh crude illustrating the time zero sample (·) and sample after one year of weathering (⊙).

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 homogeniety 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

The legend within the figure reads:

1	C-2 Benzenes
2	C-3 Benzenes
3	C-4 Benzenes
4	Naphthalene
5	Methyl Naphth.
6	Dimethyl Naphth.
7	Trimethyl Naphth.
8	Phenanthrene
9	Methyl Phen.
10	Dimethyl Phen.

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 hydro-
carbons 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 artifically 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 napthalene through 2,6-dimethylnapthalene), 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 aroma-

tics with Kovat indices ranging from 1500 to 2000. This presumably re-

flects two things: 1) the greater volatility and water solubility of the

lower molecular weight aromatic compounds, and 2) the lower relative a-

bundance of the higher molecular weight aromatics in the crude oil to be-

gin with.

Figure 9B shows the relative losses of aromatic hydrocarbons in

the artifically weathered crude oil spiked into the Kasitsna Bay sedi-

ments 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 rang-

ed between only 6 and 12 micrograms per gram dry weight of sediment when

artifically weathered crude was used to spike the sample at time zero.

These levels were not significantly reduced after one year of weather-

ing in the sediments of Kasitsna Bay: the most significant weathering

occurred while the oil was "artifically 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 s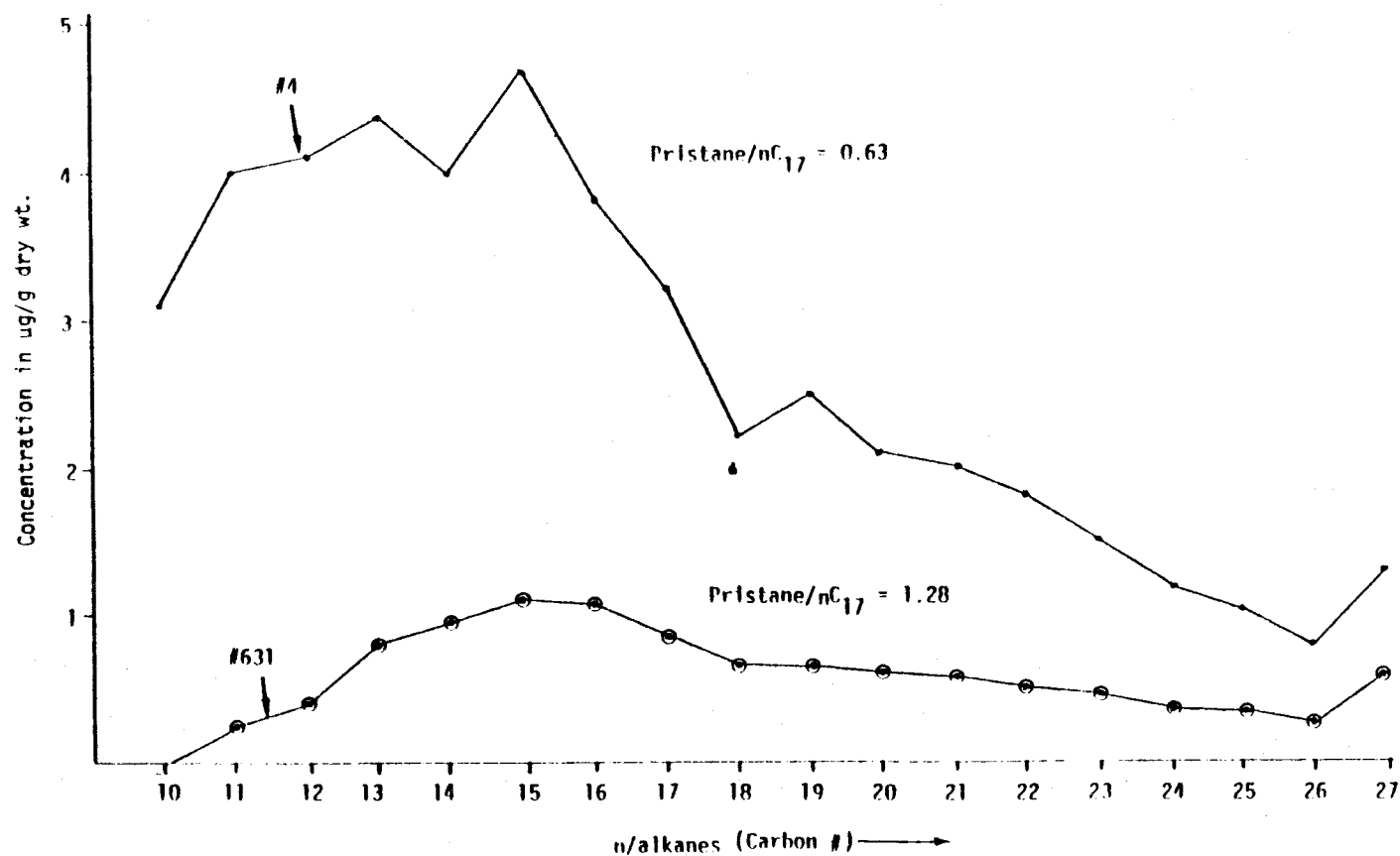piked sediment after one year of weathering in Kasitsna Bay. In comparison with Figure 4 which shows the starting 1.0 ppm spiked material, it is clear that significant weathering of the sample has occurred. This is reflected first in the significantly greater relative loss of the lower molecular weight 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
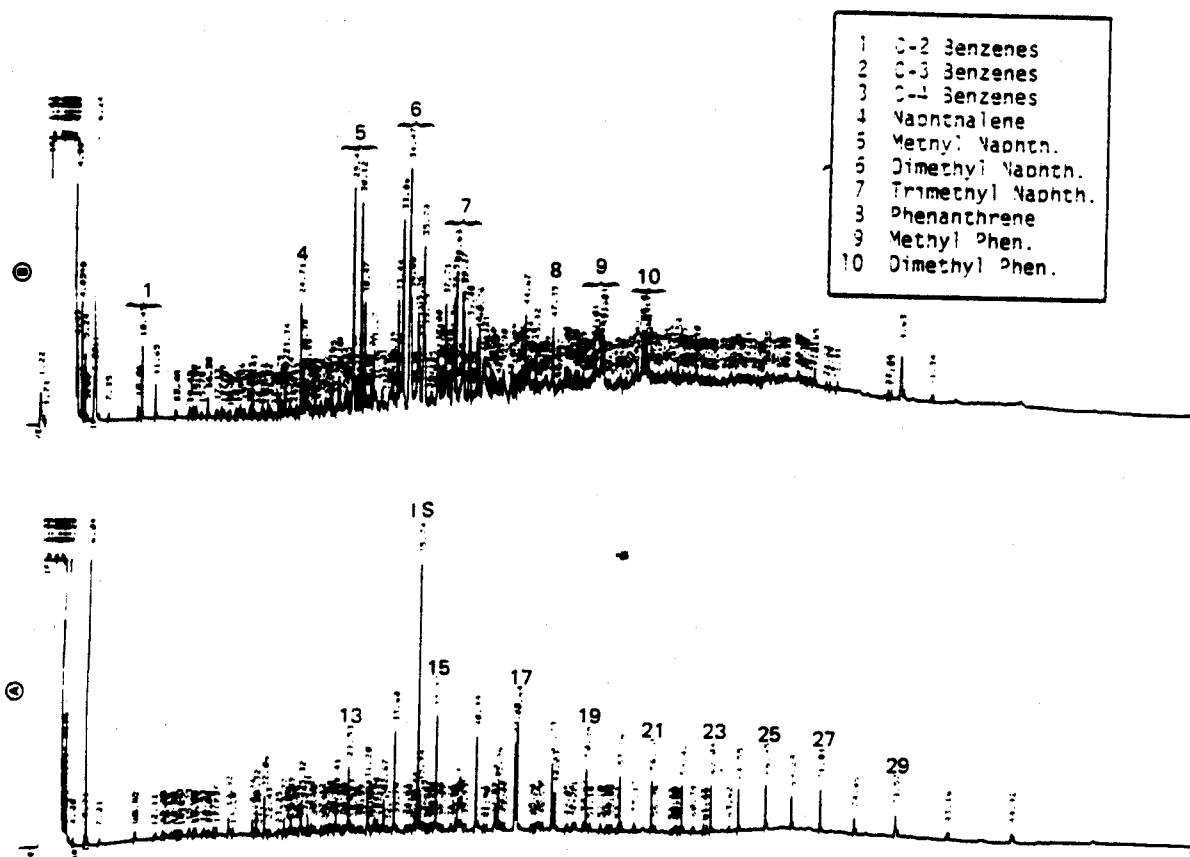
Figure 10. Flame Ionization Detector gas chromatograms of: A, the aliphatic fraction and B, the aromatic fraction extracts obtained from 1 ppt fresh Cook Inlet Crude Oil spiked sediments after one year of weathering in Kasitsna Bay.

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 µg/g dry weight during the year of exposure and the unresolved complex mixture decreased from 154 to 98 µg/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-methylnapthalene (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
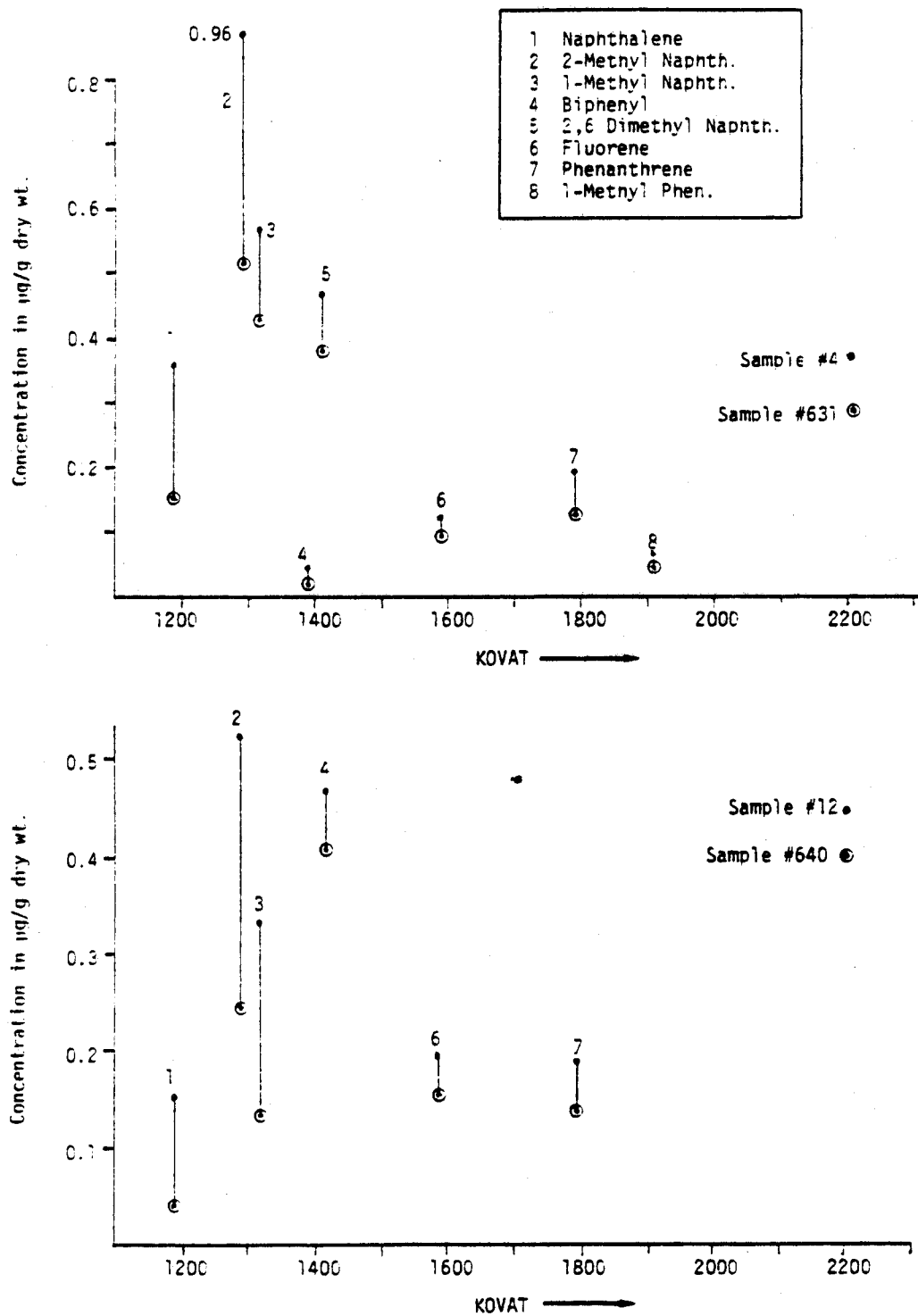
Figure 12. Concentration abundance of selected aromatic hydro-
carbons from a 1.0 part per thousand spike of fresh
crude (Top) showing the time zero sample (·) and
sample after one year of weathering (⊙). Bottom
shows a 1.0 ppt spike of artifically weathered crude
for the time zero sample (·) and sample after one
year of weathering (⊙).

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

Clearly, while biological degradation of the aliphatic hydro-
carbons (primarily n-alkane) occurred at the 1 ppt level, concommitant
degradation of the higher molecular weight polynuclear aromatics com-
pounds with molecular weights above that of methylnapthalene 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 substi-
tuted 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-methylnapthalene at reten-
tion time 29.41 (B) are present in nearly identical relative concentra-
tions. The chromatogram in 13C shows that the same compounds were also
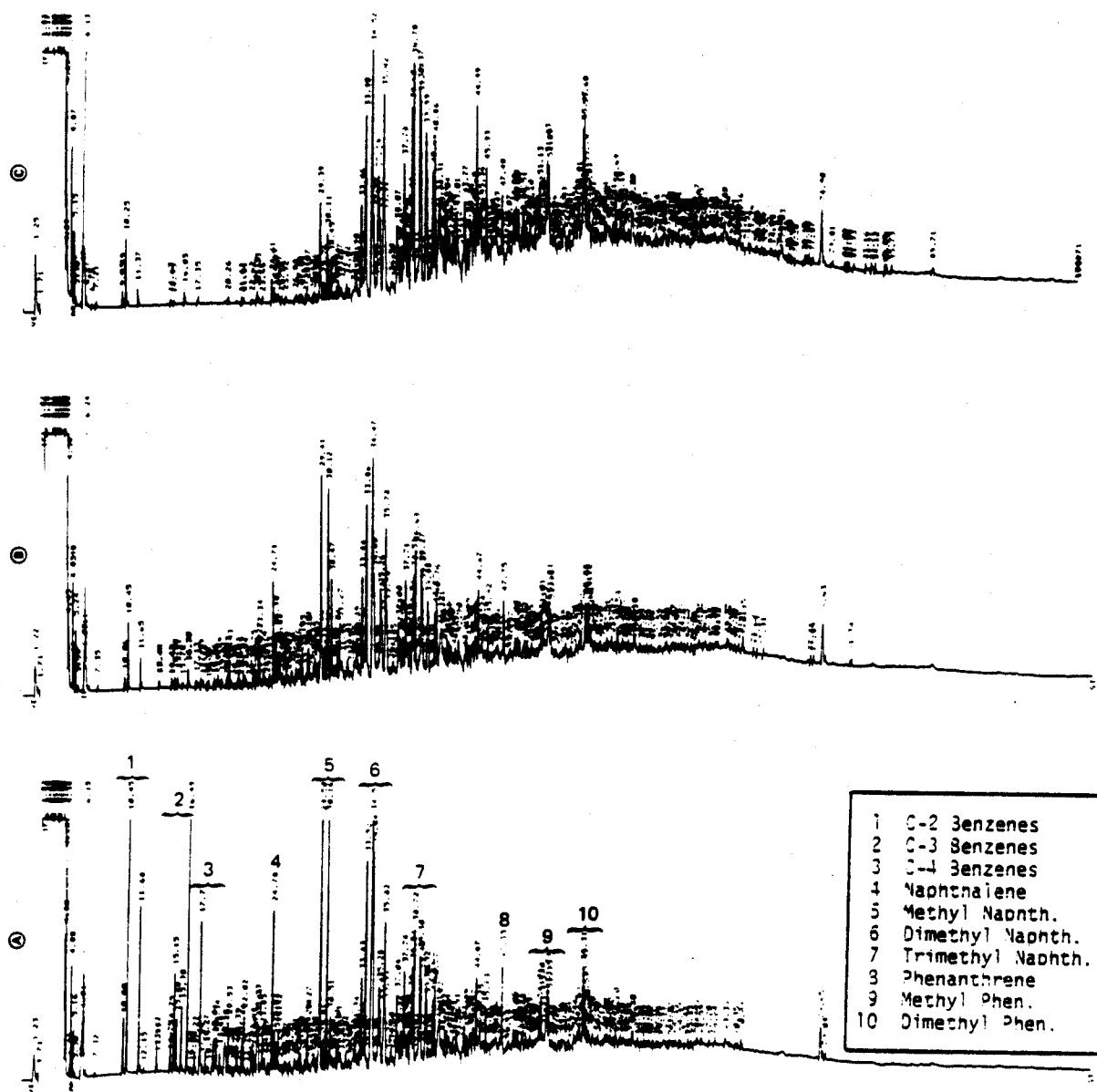
Figure 13. Flame Ionization Detector gas chromatograms of extracts of the aromatic fractions obtained from: A, the sediment spiked with 1 ppt fresh crude oil at time zero; B, the 1 ppt fresh crude sample after one year of natural weathering in Kasitsna Bay and C, the 1 ppt sediment sample spiked with artifically weathered crude oil after one year of additional weathering in Kasitsna Bay.

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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
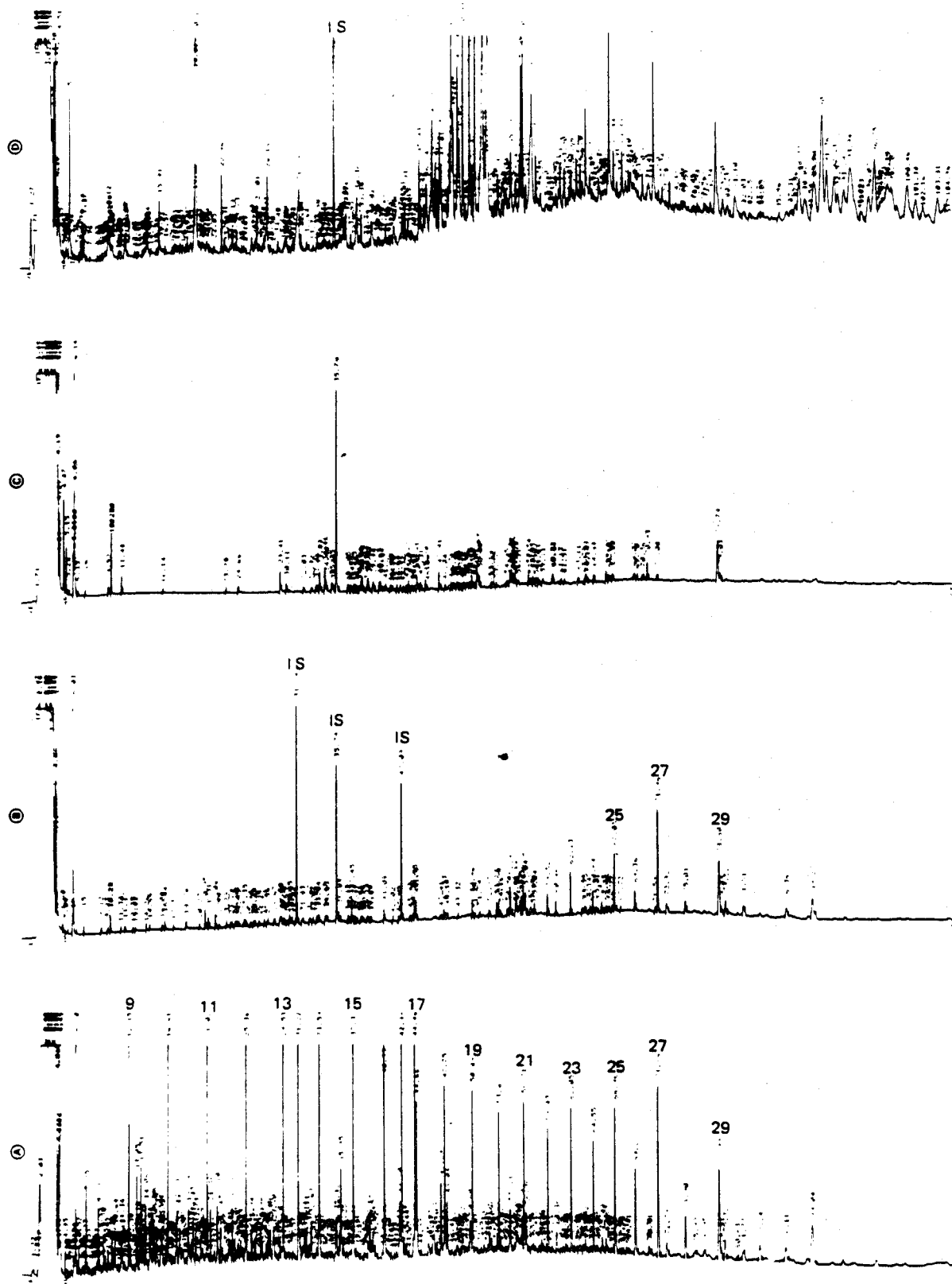
Figure 14. Flame Ionization Detector capillary gas chromatograms of: A, the aliphatic fraction of the sediment spiked with 0.1 ppt Fresh Crude Oil at time zero and B, the aliphatic fraction, C, the aromatic fraction, and D, the polar fraction extracts obtained on the 0.1 ppt Fresh Crude Oil spiked sample 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
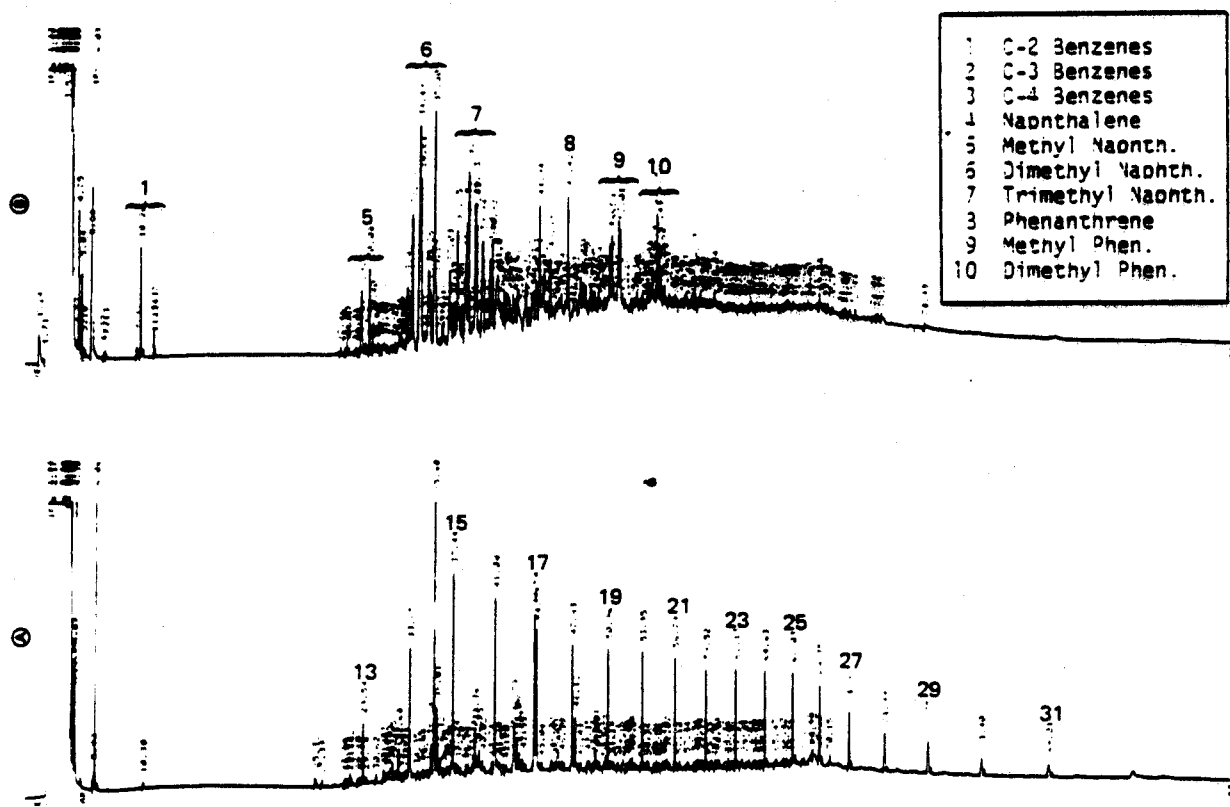
Figure 15.   Flame Ionization Detector capillary gas chromatograms of: A, the aliphatic fraction and B, the Aromatic fraction extracts obtained from the time one year Kasitsna Bay sample spiked with Artificially Weathered Cook Inlet Crude Oil at 50 ppt.
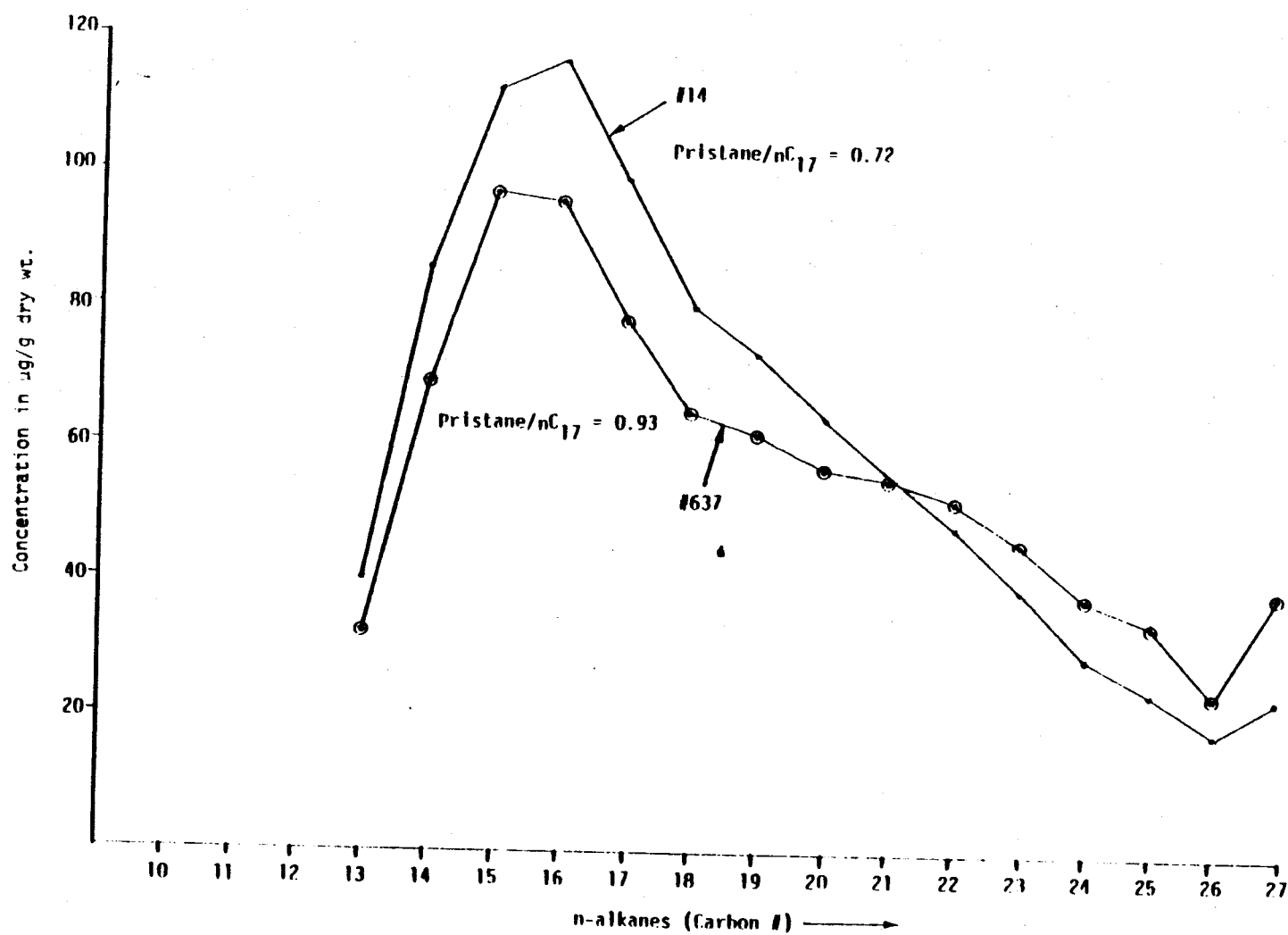
Figure 16. Concentration abundance of the n-alkanes for a sediment oil spike of 50 parts per thousand artifically weathered crude illustrating the time zero sample (·) and sample after one year of weathering (⊙).

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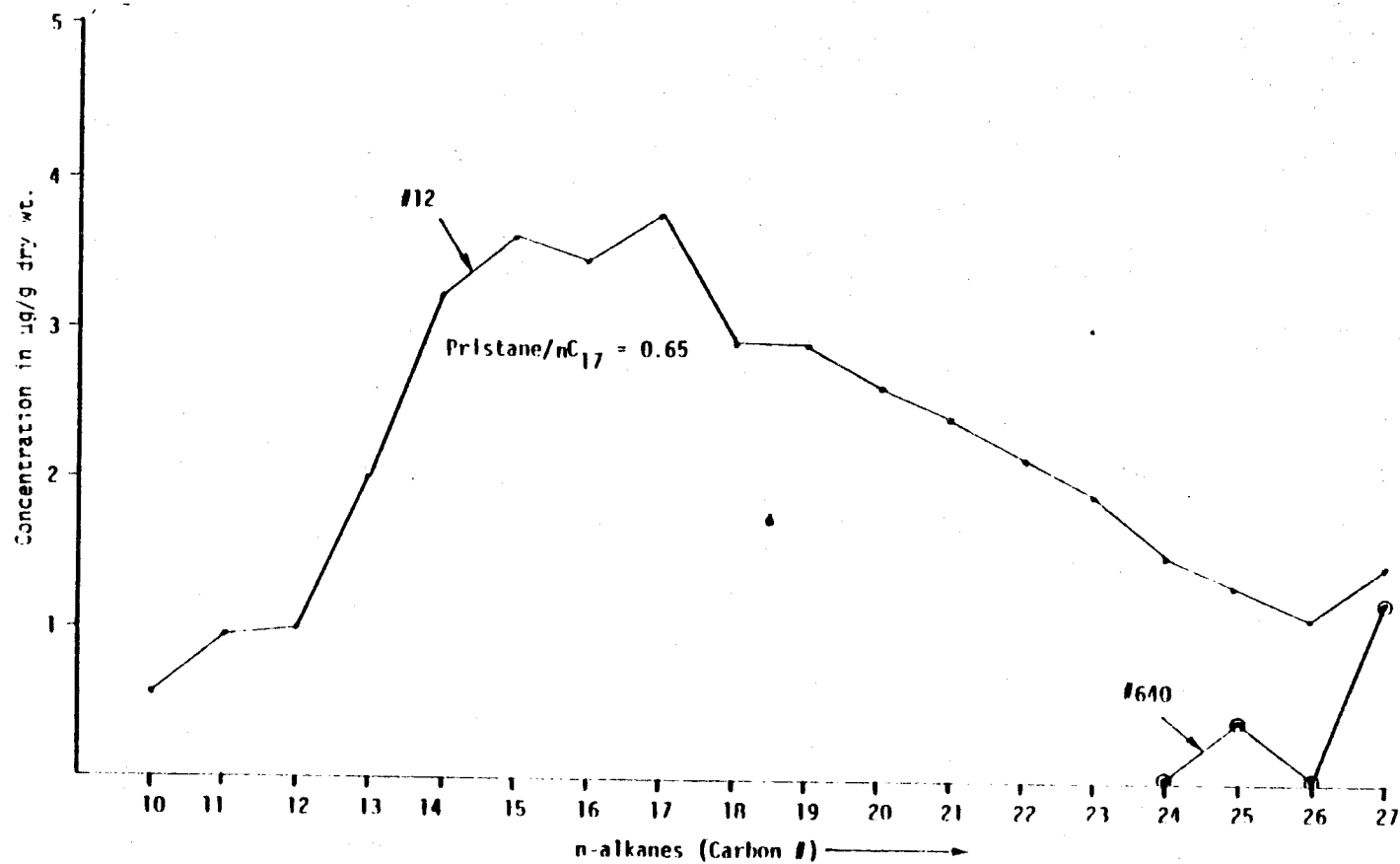
Figure 17. Concentration abundance of the n-alkanes for a sediment oil spike of 1.0 parts per thousand artifically weathered crude illustrating the time zero sample (·) and sample after one year of weathering (⊙).

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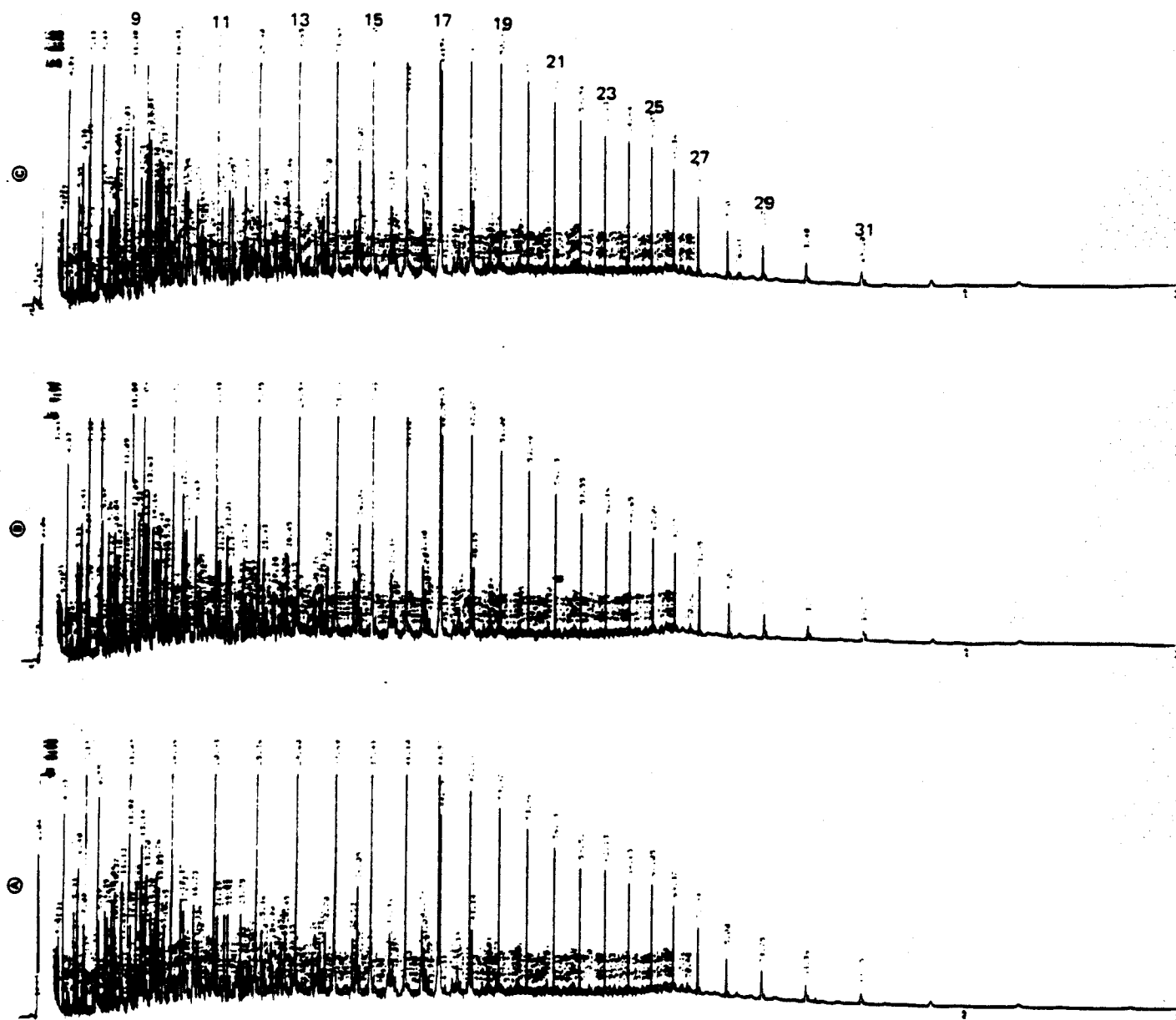
Figure 18. Flame Ionization Detector capillary gas chromatograms of
aliphatic fraction extracts obtained on: A, 50 ppt fresh Oil plus
starch, B, 50 ppt fresh Oil alone, and C, 50 ppt fresh Oil plus
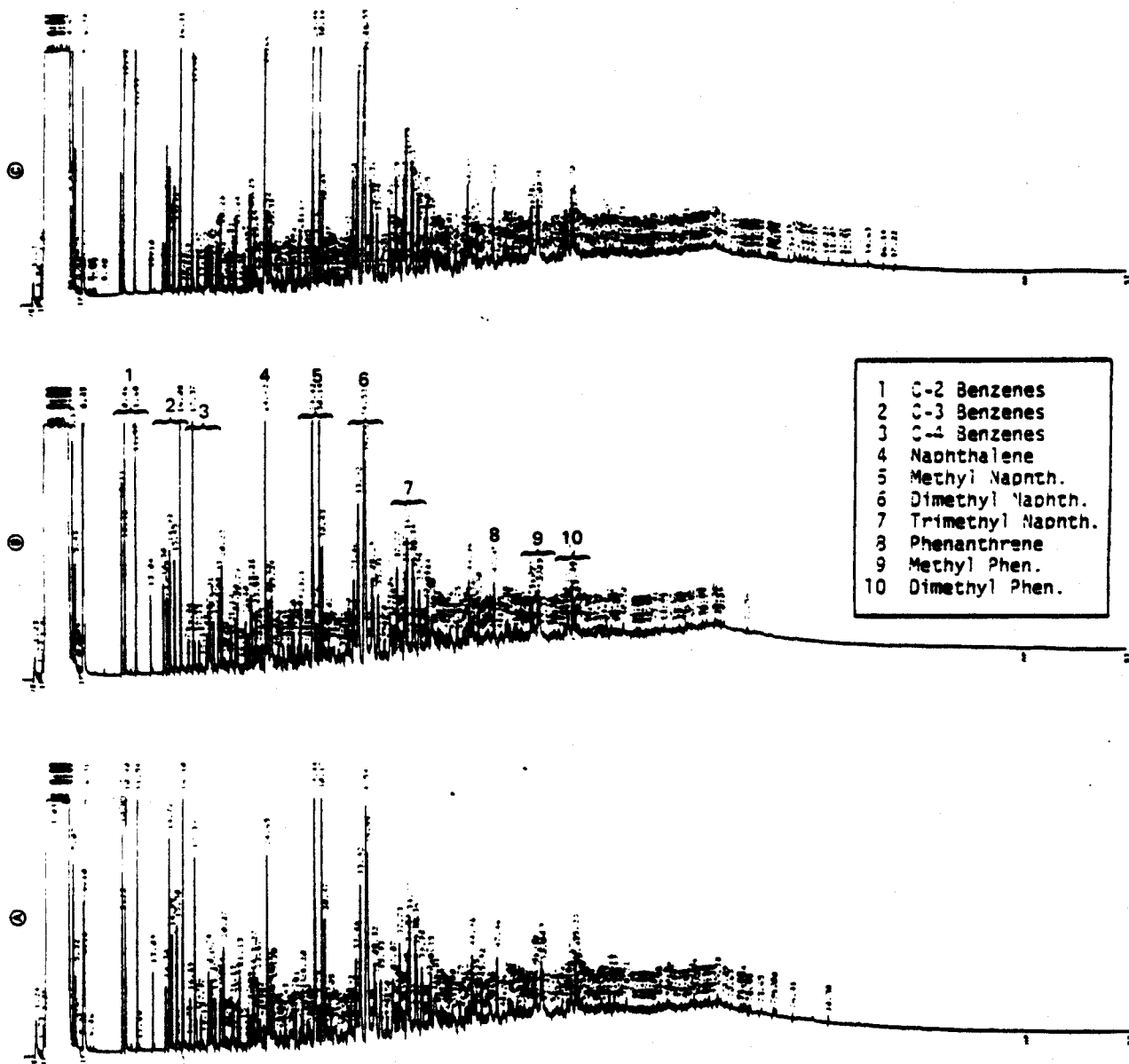Chitin after one year of natural weathering in the sediments of
Sadie Cove.

1	C-2 Benzenes
2	C-3 Benzenes
3	C-4 Benzenes
4	Naphthalene
5	Methyl Napnth.
6	Dimethyl Naphth.
7	Trimethyl Napnth.
8	Phenanthrene
9	Methyl Phen.
10	Dimethyl Phen.

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.

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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.

REFERENCES

American Institute of Biological Sciences, 1978. The Proceedings of the Conference on Assessment of Ecological Impacts of Oil Spills, Keystone, Colorado, 14-17 June 1980, 936 pgs.

Bassin, J.J., T. Ichiye. 1977. Flocculation behavior of suspended sediments and oil emulsions. Journal of Sedimentary Petrology 47(2): 671-677.

Brown, D.W., L.S. Ramos, M.Y. Uyeda, A.J. Friedman, and W.D. MacLeod, Jr. (1980): Ambient-temperature extraction of hydrocarbons from marine sediments—comparison with boiling-solvent extractions. In: Petroleum in the Marine Environment, L. Petrakis and F.T. Weiss (Eds.), Advances in Chemistry Series 185, American Chemical Society, Washington, DC, pp. 313-326.

D'Oxouville, L., M.O. Hayes, E.R. Gundlach, W.J. Sexton, and J. Michel. 1979. Occurrence of oil in offshore bottom sediments at the AMOCO CADIZ oil spill site, In: Proceedings of the 1979 Oil Spill Conference, March 19-22, Los Angeles, CA, p. 187-192.

Gearing, J.N., P.J. Gearing, T. Wade, J.G. Quinn, H. B. McCarty, J. Farrington and R.F. Lee. 1979. The rates of transport and fates of petroleum hydrocarbons in a controlled marine ecosystem and a note on analytical variability, p. 555-564. In: Proceedings of the 1979 Oil Spill Conference (Prevention, Behavior, Control, Cleanup) 19-22 March 1979, Los Angeles, Calif.

Jordon, R.E. and J.R. Payne, Fate and Weathering of Petroleum Spills in the Marine Environment: A Literature Review and Synopsis. Ann Arbor Science Publishers Inc., Ann Arbor, Michigan. 1980. 175 pp.

MacLeod, W.D., Jr. and J.R. Fisher, 1980. Intercalibration of Analytical Laboratories. Manuscript presented at the Researcher/Pierce IXTOC-I Symposium, Miami, Florida, 9-11 June, 1980. 7 pp.

Mayo, D.W., D.S. Page, J. Cooley, E. Sorenson, F. Bradley, E.S. Gilfillan, F.A. Hanson. 1978. Weathering characteristics of petroleum hydrocarbons deposited in fine clay marine sediments, Searsport, Maine, Journal of Fisheries Research Board of Canada, 35(5):552-565.

Meyers, P.A. 1976. Sediments—sources of sinks for petroleum hydrocarbons? In: Sources, Effects and Sinks of Hydrocarbons in the Aquatic Environment; Proceedings of the Symposium, American University, Washington, D.C., 9-11 August, 1976 (American Institute of Biological Sciences 1977).

Meyers, P.A. and J.G. Quinn. 1973. Association of hydrocarbons and mineral particles in saline solutions. Nature 244:23-4.

National Academy of Sciences. 1975. Petroleum in the marine environment, Washington, D.C., 107 pp.

Parker, P.L. and S. Macko. 1978. An intensive study of the heavy hydrocarbons in the suspended particulate matter of seawater, ch. 11 of South Texas Outer-Continental Shelf BLM Study.

Payne, J.R., P.J. Mankiewicz, J.R. Nemmers, R.E. Jordan, I.R. Kaplan, M.I. Venkatesan, S. Brenner, J. Bonilla, D. Meredith, B. Meyers, B. Haddad, A.L. Burlingame, A. Ensminger, G. Gould, and M.L. Moberg. 1978 a. High molecular weight petroleum hydrocarbon analytical procedures. Southern California Baseline Study, Benthic Year II. Volume III, Report 5.0. Final report submitted to the Bureau of Land Management, Department of Interior, Washington, D.C. by Science Applications, Inc.

Payne, J.R., J.R. Clayton, Jr., B.W. de Lappe, P.L. Millikin, J.S. Parkin, R.K. Okazaki, E.F. Letterman, and R.W. Risebrough. Hydrocarbons in the Water Column. Southern California Baseline Study, Vol. III, Report 3.2.3., p. 1-207. 1978 b. Final Report, submitted to the Bureau of Land Management, Washington D.C. by the University of California Bodega Marine Laboratory, Bodega Bay, California, and Science Applications, Inc., La Jolla, California.

Payne, J.R., J.E. Nemmers, R.E. Jordan, P.J. Mankiewicz, A.D. Oesterle, S. Laughon, and G. Smith. Measurement of petroleum hydrocarbon burdens in marine sediments by three commonly accepted procedures: results of a NOAA inter-laboratory calibration exercise, Fall, 1978. Submitted to Dr. John A. Calder, Staff Chemist, OCSEAP, U.S. Department of Commerce, National Oceanic and Atmospheric Administration, Environmental Research Laboratory, Boulder, CO, January 1979. pp. 1-34, plus appendix.

Payne, J.R., G.S. Smith, P.J. Mankiewicz, R.F. Shokes, N.W. Flynn, W. Moreno and J. Altamirano. Horizontal and Vertical Transport of Dissolved and Particulate-Bound Higher Molecular Weight Hydrocarbons from the IXTOC-1 Blowout. Manuscript presented at the RESEARCHER/PIERCE IXTOC-I Symposium, Miami, Florida, June 9-11, 1980. 47 pp.

Teal, J.M., C. Burns, and J. Farrington. 1978. Analysis of aromatic hydrocarbons in intertidal sediments, resulting in two spills of Number 2 Fuel Oil in Buzzard's Bay, Massachusetts. Journal of Fisheries Research Board of Canada 35(5):510-520.

Winters, J.K. 1978. Fate of petroleum derived aromatic compounds in seawater held in outdoor tanks and South Texas Outer-continental Shelf Study-BLM, ch. 12. Draft final report.

Zurcher, F. and M. Thuer. 1978. Rapid weathering processes of fuel oil in natural waters. Analysis and interpretations. Environmental Science and Tech. 12(7):838-843.

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