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
National Ocean Service
Office of Oceanography and Marine Services
Ocean Assessments Division

U.S. DEPARTMENT OF THE INTERIOR
Minerals Management Service

Outer Continental Shelf Environmental Assessment Program

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OF THE
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Juneau, Alaska

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

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[“Multivariate Analysis of Petroleum Weathering in the Marine Environment - Sub Arctic. Volume I - Technical Results,” is contained in Volume 21 of OCSEAP Final Reports.]

Contract No. NA80RAC00018
Research Unit No. 597

Final Report

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

Volume II - Appendices

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January 18, 1984

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 detraction 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

```
C           ***** CUTVP2.FOR *****
C
C           THIS IS THE OPEN-OCEAN OIL-WEATHERING CODE AND
C           THE OIL PHASE IS CONSIDERED WELL-STIRRED ALL THE
C           TIME.
C
C           THIS VERSION OF THE OIL-WEATHERING CODE DIFFERS
C           FROM CUTVP1 IN THE VISCOSITY CALCULATION.
C
C           JANUARY, 1983
C
C           GET YOUR OUTPUT FROM CUTVP2.OUT/FILE:FORTRAN
C           THE PLOT FILE IS CUTVP2.PLT
C           THE TYPE FILE IS CUTVP2.TYP
C
       REAL*4 MW, MW1,KH,MTCA,MTC,MASS ,MOLES,KOIL,KAIR ,KA,KB
      1,MK3,MK4,MK3L ,MK4L
       COMMON /COIL./ MW1,TC1,VC1,PC1,CNUM1,VIS1
       COMMON /SPILL/ MTC(30),VP(30 ),VLOG(30 ),RHO(30),MW(30)
      1 ,SPGR(30),FRACTS ,STEN,KB,DISPER ,Z,TERM2,SPREAD ,KMTC
       COMMON /PCODE/ VSLEAD, MK4,IOU,IPU, ITY
       COMMON /MOOSE/ WINDS,C1 ,C2,C3,C4
       DIMENSION TB(30 ),API(30),A(30) ,B(30),TBL(6,30) ,APIL(6,30)
      1 ,TC(30),PC(30) ,CNUM(30) ,T10(30),HVAP1 (30) ,HVAPZ(30)
      2. VOLL( 6,30),VOL(30) ,MOLES(30),MTCA(30),V IS(30),VISK(30)
      3, VLOCK(30 ),HLAW(30) ,VC(30),APIBL(6 ),NC(30 )
      4,NCTS(6) ,NS(30) ,ITEML(6) ,ISAMPL(6)
       DIMENSION ANAME( 5),ANAMEL( 6,5),C 1L(6) ,C2L(6),C4L(6)
      1,STENL( 6),VISZL(6 ),MK3L(6) ,MK4L(6)
       DATA (ANAMEL(1,J),J=1,5)/'PRUDH ','OE BA','Y, AL', 'ASKA '
      1,'       '/
       DATA (ANAMEL(2,J),J=1,5)/'COOK ', ' INLET'.'. ALA', 'SKA '
      1,'       '/
       DATA (ANAMEL(3,J),J=1,5)/'WILMI ', 'NCTON' .', CAL','IFORN'
      1, "IA   '/
       DATA (ANAMEL(4,J),J=1,5)/'MURBA ','N, AB','U DHA','BI '
      1.'      '/
       DATA (ANAMEL(5,J),J=1,5)/'LAKE ',"CHICO', "T, LO','UISIA'
      1, 'NA   '/
       DATA (ANAMEL(6,J),J=1,5)/'LIGHT' ,' DIES', 'EL CU','T '.
      1'       '/
       DATA APIBL/27 . ..35.4.19.4,40.5.54.7,38. 9/
       DATA  ITEML/9,7,94,99999,221   , 1 /
       DATA ISAMPL/71011 ,72025,71052,99999,54062 ,2/
       DATA NCTS/15,16,13,16,16,1 1/
C
C          FOR CRUDE OIL THE RESIDUUM CUT IS ASSIGNED A NORMAL
C          BOILING POINT OF 850.
C
       DATA (TBL(1,J),J=1,30)/167 .,212. ,257.,302.,347. ,392.
      1,437.,482. ,527.,580.,638.,685.,738. ,790.,850.,15*0./
       DATA (TBL(2,J),J=1,20)/122 . ,167.,212.,257.,302 .,347.
      1,392 .,437.,482., 527.,580.,638.,685 .,738.,790.,850.
      2,4',.0./
       DATA (TBL(3,J),J=1,20)/212 . ,257.,302.,347.,392 .,437.
      1,482.,527 . ,580.,638.,685..738. ,850.,7*0./
       DATA (TBL(4,J),J=1,20)/122 . ,167.,212.,257.,302. ,347.
      1,392.,437.,482.,527.,580.,638.,685.,738.,790 ..850.
      2,4*0./
       DATA (TBL(5,J),J=1,20)/122 ., 167. ,2]2. ,257.,302. ,347.
      1,392.,437.,482.,527.,580.,638.,685.,738.,790.,850.
      2,4*0./
       DATA (TBL(6,J),J=1,11)/313 .,342. ,366. ,395. ,415 .,438. ,461.
      1,479.,501 .,518.,538./
       DATA (APIL(1,J),J=1,30)/72 .7.64 .2.56.7,51.6.47. 6,43.2
      1,41 .5,37.8,34.8,30. 6,29.1,26.2,24. ,22.5 ,11.4,15*0./
```

```
      DATA (APIL(2,J),J=1,20)/89.2 ,77.2 ,65..59.5.55.4,50.8
     1,46.5,43..39.6,37.,32 .8,31.3,28.7 .26.6.25 .,11.6,4*0./
      DATA (APIL(3,J),J=1.20)/68. 6.58.7 .53.,48.1.43.2 ,38.8
     1 ,35.4,32.3.26.8,24.5 22--3,20.3.8.9.7*0./
      DATA (APIL(4.J).J=1.20)/96.7 .86.2.70. 6.62.3,55.7,51 .6
     1,48. 5,45. 6,43.,40.,35 .8.34 . ,30. .28.4,26.6. 16.7,4*0./
      DATA (APIL(5,J),J=1,20)/92 .4.81 ..68.9.62.1,57.2 .52.5
     1 .48.8.45.2,41.7,38.2 .34 .4,33.2,30.6.28.9 .26.1,18.1,4*0./
      DATA (APIL(6,J),J=1,11)/49. 6,47.3.46.,44..38.6,38.8.37.2
     1,35.4,33.9.33.1,32 .2/
      DATA (VOLL( 1,J),J=1,30)/2 . 1.2.6.3.5.3.6.3.7.3 .5.4.3.4.8
     1,5..2.8,6. 5,6.8,6.0,7.4 .36.3.15*0./
      DATA (VOLL(2,J),J=1,20)/2.4 ,2 .5.5.9,6.1,5.1,5.2,4 .9
     1 ,5.1,5.2.5 . ,3.3.5.2,7.,4.2.4.2 ,25.6,4*0./
      DATA (VOLL(3,J),J=1,20)/2 .3,2.4 .2.4,2.5,2.[3,3 .6,4.4
     1,5.3,4.7,6.3.4.1.5. 5,53.3,7*0./
      DATA (VOLL(4,J ),J=1,20)/1.7 ,2.9,4 .9,6. ,6.8,6.5,5 .7
     1,5.6.6 . ,4.9,5.7,5.6,6.5,6 .,5.6,19.3,4*0./
      DATA (VOLL(5,J),J=1,20)/7 .3,8.2, 9.7.11 ..(). 1.0 .3.7.2
     1 ,7.2.7 .4,6.9,3.5,3. ,1 .6,1.4,1.9.2..4*0./
      DATA (VOLL(6,J),J=1,11)/4 .78,9 .57.9.09.9.57,9 .57,9.57
     1,9.57,9.57,9.57,9.57 ,9.57/
C
C        C1L, C2L. AND C4L ARE THE MOUSSE FORMATION CONSTANTS.
C        C1L IS THE VISCOSITY CONSTANT.
C        C2L IS THE INVERSE OF THEMAXIMUM WATER IN OIL WEIGHT
C        FRACTION.  C4L IS THE WATER INCORPORATION RATE.
C
      DATA C1L/0.62,0.62,0.63,0 .64,0.65,0.65/
      DATA C2L/1.42,3.33,1.43,5 .,-1.,-1./
      DATA C4L/0 .001,0.001,0.01,0 .001.0.,0./
C
C        FOR THE DISPERSION PROCESS, KA IS THE CONSTANT IN THE
C        SEA SURFACE I)] SPENS I ON EQUAT I ON .  KB I S THE CONST ANT I N
C        THE DROPLET FRACTION EQUATION.  STENL(6) 1S THE l,1RRAR%
C        OIL-WATER SURFACE TENSION IN DYNES/CM.
C
      DATA KA,KB,STENL/0.108,50 . .30..30..30..30.,30 ..30./
      DATA VISZL/35.,35.,195.,15 .,13.5,11.5/
      DATA MK3L/9000.,9000. ,9000.,9000.,9000. ,3000./
      DATA MK4L/10.5,7.4,15.3,10 .5,2.,2./
      YI(X)=((1.-X)**0.38)/(X*X )
      OPEN(UNIT=32,DIALOG= 'DSKD:CUTVP2 .OUT' )
      OPEN(UNIT=34,DIALOG= 'DSKD:CUTVP2 .PLT' )
      OPEN(UNIT=35 ,DIALOG='DSKD :CUTVP2.TYP ' )
      I OU=32
      I PU=34
      ITY=35
C
C        FILL IN SOME LIBRARY IDENTIFICATIONS.
C
10    TYPE 20
20    FORMAT(1X,'ENTER THE NUMBER OF TBP CUTS TO BE CHARACTERIZED
     1 ON 12')
      TYPE 30
30    FORMAT(1X,'IF YOU HAVE NO INPUT DATA JUST ENTER 99' )
      TYPE  4 0
40    FORMAT(1X,'A 99 ENTRY WILL USE A LIBRARY EXAMPLE' )
      ICODE=1
      ACCEPT 50, NCUTS
50    FORNAT(I2)
      LSWTCH=NCUTS
C
C        LSWTCH=99 IS USED TO INDICATE THAT A LIBRARY CRUDE WAS
C        CHOSEN .
C
```

```
      IF(NCUTS. NE. 99) CO TO 120
C
C       USING A LIBRARY CRUDE.
C
      TYPE 60
 60   FORMAT(1X,'CHOOSE A CRUDE ACCORDING TO:')
      DO 80 I=1,6
      TYPE 7'0,  I, (ANAMEL( I,J),J=1 ,5)
 70   FORMAT(1X, 11,' = ',5A5)
 80   CONTINUE
      ACCEPT 90. IC
 90   FORMAT(I1)
      APIB=APIBL(IC)
      ITEM=ITEML(I C)
      ISAMP= ISAMPL(IC)
      NCUTS=NCTS(I C)
      ICODE=2
      DO 100 J=1,5
      ANAME(J)=ANAMEL( IC,J)
 100  CONTINUE
      TYPE 110,  (ANAME(J),J=1 .5)
 110  FORMAT(/, 1X,'YOU CHOSE: '.5A5)
      GO TO 200
C
C       USER IS ENTERING THE CRUDE DATA.
C
 120  TYPE 130
 130  FORMAT( 1X, 'ENTER THE NAME OF THE CRUDE')
      ACCEPT 140, (ANAME(I) ,I=1,5)
 140  FORMAT( 10A5)
      TYPE 150
 150  FORMAT( 1X,'ENTER AN IDENTIFICATION NUMBER FOR
     I THIS CRUDE ON 15')
      ACCEPT 160, ITEM
 160  FORMAT( 15)
      TYPE 170
 170  FORMAT( 1 X , "ENTER A SAMPLE NUMBER ON 15')
      ACCEPT 160, ISAMP
      TYPE 180
 180  FORMAT( Ix. 'ENTER THE BULK API GRAVITY")
      ACCEPT 230, APIB
      TYPE 190
 190  FORMAT(/,1X, 'YOU MUST ENTER THE TRUE BOILING POINT
     1 CUT DATA STARTING',/,1X, 'WITH THE MOST VOLATILE CUT
     2 AND GOING TO THE BOTTOM OF THE BARREL',/)
C
C       CALCULATE THE BULK DENSITY OF THE CRUDE AT 60/60.
C
 200  DCRUDE=141.5/(APIB+131 .5)
      DCRUDE=0 .983*DCRUDE
C
C       TRANSFER CRUDE INPUT DATA TO THE VARIABLES USED IN
C       THE CALCULATIONS.
C
      DO 270 I=1,NCUTS
      GO TO (210,260), ICODE
 210  TYPE 220, I
C
C       ENTER THE CRUDE CUT DATA.
C
 220  FORMAT( IX, 'ENTER THE BOILING POINT AT 1 ATM IN DEG F
     1 FOR CUT' ,I3)
      ACCEPT 230, TB(I)
 230  FORMAT(F10.0)
      TYPE 240, I
 240  FORMAT(1X,'ENTER API GRAVITY FOR CUT' ,13)
```

```
      ACCEPT 230. API(1)
      TYPE 250, I
250   FORMAT(1X, 'ENTER VOLUME PER CENT FOR CUT' ,13)
      ACCEPT 230, VOL(I)
      CO TO 270
C
C       TRANSFER CRUDE CUT INPUT DATA FROM THE LIBRARY.
C
260   TB(I)=TBL(IC,I)
      API (I)=APIL(IC, I)
      VOL(I)=VOLL(IC, 1)
270   CONTINUE
C
C       DISPLAY THE CUTS BACK TO THE USER.
C
280   TYPE 290
290   FORMAT(/,1X,'CUT',5X,'TB',10X,'API',8X,'VOL')
      DO 310 I=1,NCUTS
      TYPE 300, I,TB(I),API(I),VOL(I)
300   FORMAT( 1X,I2,5X,F5.1 ,7X ,F4.1,6X,F5.1)
310   CONTINUE
      TYPE 320
320   FORMAT(1X,'DO YOU WANT TO CHANGE ANY?")
330   ACCEPT 340, ANS
340   FORNAT(A1)
      IF(ANS.EQ. 'N') GO TO 420
C
C       ALLOW THE INPUT To BE CHANGED.
C
      TYPE 350
350   FORMAT(1X,'ENTER THE CUT NUMBER TO BE CHANGED ON 12')
      ACCEPT 50, N
      TYPE 360
360   FORMAT( 1X, ' ENTER 1 TO CHANGE TB, 2 FOR API , 3 FOR VOL%')
      ACCEPT 370, IC
370   FORMAT(I1 )
      TYPE 380
380   FORMAT( 1X,'ENTER THE CHANCED DATA")
      GO TO (390,400,410), IC
390   ACCEPT 230, TB(N)
      GO TO 280
400   ACCEPT 230, API (N)
      GO TO 280
410   ACCEPT 230, VOL(N)
      GO TO 280
420   DO 430 I=2,NCUTS
      IM1=I-1
      IF(TB(I ).LT.TB(IM1)) CO TO 440
430   CONTINUE
      GO TO 460
440   TYPE 450, I,IM1
450   FORMAT(/,1X,'THE BOILING POINT OF CUT ",12
     1.'  IS LESS THAN CUT ',12,/,1X,'AND THIS ORDER IS NOT
     2 ACCEPTABLE, SO START OVER' ,/)
      GO TO 10
C
C       ALWAYS RENORMALIZE THE INPUT VOLUMES TO 100%.
C
460   VTOTAL=0.
      DO 470 I=1,NCUTS
      VTOTAL=VTOTAL+VOL (I)
470   CONTINUE
      DO 480 I=1,NCUTS
      VOL(I)=100. *VOL(I)/VTOTAL
480   CONT I NUE
C
```

```
C        NOW CHARACTERIZE ALL THE CUTS.  IF THE LAST CUT IS
C        RESIDUUM DO NOT CHARACTERIZE IT BUT USE A VAPOR
C        PRESSURE OF 0. AND A MOLECULAR WEIGHT OF 600.
C
      MW(NCUTS)=600.
      VP(NCUTS)=0 .
C
C        NV=1 MEANS NO RESIDUUM CUT PRESENT.
C        NV=2 MEANS A RESIDUUM IS PRESENT.
C
      NV=1
      NC1=NCUTS
      DO 550 I=1,NCUTS
      APIN=API(I)
      SPGR(I)=141.5/(API(I)+131.5)
      SPGR(I)=0.983*SPGR(I)
      TBN=TB(I)
C
C        THE RESIDUUM CUT IS IDENTIFIED BY A NORMAL BOILING
C        POINT OF 850.  LOOP AROUND THE NV=2 SWITCH IF A
C        RESIDUUM IS PRESENT.  NC1 IS THE NUMBER OF PSEUDO COMPONENTS
C        WITH FINITE VAPOR PRESSURES.
C
      IF(TBN.LT.850.) GO TO 490
      NV=2
      NC1=NCUTS-1
490   CALL CHAR(APIN,TBN,AN,BN,NSN,NV)
C
C        THE CHARACTERIZATION SUBROUTINE RETURNS THE LOG10 OF THE
C        KINEMATIC VISCOSITY (CENTISTOKES) AT 122 DEG F.
C
      VISK(I)=10.**VIS1
      VLOGK(I)=ALOG(VISK(I))
      GO TO (500,550), NV
C
C        STORE THE CUT INFORMATION FOR A NON-RESIDUUM CUT.
C
500   NS(I)=NSN
      A(I)=AN
      B(I)=BN
      MW(I)=MW1
      TC(I)=TC1
      TC(I)=TC(I)+459.
      VC(I)=VC1
      PC(I)=PC1
      CNUM(I)=CNUM1
C
C        FIND THE TEMPERATURE AT WHICH THE VAPOR PRESSURE IS 10 MMHG
C        BY USING NEWTON-RAPHSON WITH TB AS THE FIRST GUESS.
C
      NC(I)=0
      YTEN=ALOG10(0.01315/PC(I))
      X=(TB(I)+459.)/TC(I)
510   EX=EXP(-20.*(X-B(I))**2)
      Y=-A(I)*(1.-X)/X-EX
      YOBJ=Y-YTEN
      VP(I)=PC(I)*10.**Y
      TEST=ABS(VP(I)-0.01315)
      IF(TEST.LT.0.001315) GO TO 540
      NC(I)=NC(I)+1
      IF(NC(I).GT.20) GO TO 520
      DY=A(I)/(X*X)+40.*(X-B(I))*EX
      BI=YOBJ-DY*X
      X=-BI/DY
      GO TO 510
C
```

```
C        UNSUCCESSFUL EXIT FROM NEWTON-RAPHSON
C
520   TYPE 530, I,X,Y
530   FORMAT(1X,'T10 FAILURE FOR',I4,' AT T =  ,1PE10.3,' WHERE
     1 LOG10(P) =  ,1PE10.3)
      GO TO 2130
C
C        SUCCESSFUL EXIT FROM NEWTON-RAPHSON
C
540   T10(   =X*TC I
C
C        CALCULATE THE HEAT OF VAPORIZATION AT 10 MMHG WITH THE
C        CLAPEYRON EQUATION AND USE WATSONS METHOD FOR THE
C        VAPOR PRESSURE BELOW 10 MMHG.  SEE GAMSON AND WATSON
C        1944, NATIONAL PETROLEUM NEWS  R-258 TO R-264.
C
      TR2=T10(I)/TC(
      EX=92.12*(TR2-B(I))*EXP(-20.*(TR2-B(I))**2)
      HVAP=1.987*T10(I)*T10(I)*(2.303*A(I)/(TR2*TR2 +EX)/TC( )
      HVAP1(I)=HVAP/MW(I)
      HVAPZ(I)=HVAP/(1.-TR2)**0.38
550   CONTINUE
C
C        END OF TRUE-BOILING-POINT CUTS CHARACTERIZATION
C
      WRITE (IOU,560) (ANAME(I),I=1,5)
560   FORMAT(1H1,'SUMMARY OF TBP CUTS CHARACTERIZATION FOR: '
     1,5A5)
      WRITE (IOU,570)
570   FORMAT(/,1X,'CODE VERSION IS CUTVP2 OF FEBRUARY 83
      WRITE (IOU,580) ITEM,ISAMP
580   FORMAT(1X,'ITEM ',I5,', SAMPLE ',I5)
      WRITE (IOU,590)
590   FORMAT(/,8X,'TB',7X,'API',6X,'SPGR',7X,'VOL',8X,'MW',8X
     1,'TC',8X,'PC',8X,'VC',8X,'A',9X,'B',8X,'T10',7X,'VIS'
     2,4X,'NC NS')
      DO 610 I=1,NCUTS
      WRITE (IOU,600) I,TB(I),API(I),SPGR(I),VOL(I),MW(I),TC(I)
     1,PC(I),VC(I),A(I),B(I),T10(I),VISK(I),NC(I),NS(I)
600   FORMAT(1X,I2,12(1X,1PE9.2),2(1X,I2))
610   CONTINUE
      WRITE (IOU,620) APIB
620   FORMAT(//,1X,'BULK API GRAVITY = ',F5.1)
      WRITE (IOU,630)
630   FORMAT(//,1X,'TB = NORMAL BOILING TEMPERATURE, DEG F'
      WRITE (IOU,640)
640   FORMAT(1X,'API = API GRAVITY')
      WRITE (IOU,650)
650   FORMAT(1X,'VOL = VOLUME PER CENT OF TOTAL CRUDE'
      WRITE (IOU,660)
660   FORMAT(1X,'MW = MOLECULAR WEIGHT')
      WRITE (IOU,670)
670   FORMAT(1X,'TC = CRITICAL TEMPERATURE, DEG RANKINE')
      WRITE (IOU,680)
680   FORMAT(1X,'PC = CRITICAL PRESSURE, ATMOSPHERES')
      WRITE (IOU,690)
690   FORMAT(1X,'VC = CRITICAL VOLUME, CC/MOLE')
      WRITE (IOU,700)
700   FORMAT(1X,'A AND B ARE PARAMETERS IN THE VAPOR PRESSURE
     1 EQUATION')
      WRITE (IOU,710)
710   FORMAT(1X,'T10 IS THE TEMPERATURE IN DEG R WHERE THE VAPOR
     1 PRESSURE IS 10 MM HG')
      WRITE (IOU,720)
720   FORMAT(1X,'VIS IS THE KINEMATIC VISCOSITY IN CENTISTOKES
     1 AT 122 DEG F')
```

```
        WRITE (IOU,730)
  730   FORMAT(1X,'NC = ERROR CODE. SHOULD BE LESS THAN 20')
        WRITE (IOU,740)
  740   FORMAT(1X,'NS = ERROR CODE, SHOULD BE EQUAL TO 1')
        WRITE (IOU,750) NCUTS
  750   FORMAT(1X,'IGNORE THE ERROR CODES FOR COMPONENT NUMBER ',I2
       1,' IF IT IS A RESIDUUM')
  760   WRITE (IPU,770) ITEM,ISAMP
  770   FORMAT(2I5)
        WRITE (IPU,780) (ANAME(I),I=1,5)
  780   FORMAT(5A5)
  C
  C       THE CUTVP2.PLT PLOT FILE IS WRITTEN AS:
  C               1.  ITEM AND SAMPLE NUMBER ON 2I5
  C               2.  THE CRUDE NAME ON 5A5
  C               3.  NCUTS ON I5
  C               4.  BOILING POINT IN DEG F OF EACH CUT ON
  C                   10(1X,1PE10.3).
  C               5   TEMPERATURE IN DEG F OF EVAPORATION, XPRINT
  C                   WIND SPEED IN KNOTS, WINDS
  C                   KA AND KB IN THE DISPERSION EQUATION,
  C                   SURFACE TENSIONIN DYNES/CM, STEN
  C                   VOLUME OF THE SPILL IN BARRELS. BBL
  C                   C1, C2, AND C4 IN THE MOUSSE EQUATION,
  C                   KMTC, MASS TRANSFER COEFFICIENT CODE (FLOATED).
  C                   ALL ON 10(1X,1PE10.3).
  C               6.  NUMBER OF CUTS+1 ON I5
  C               7.  TIME, MASS OF CUTS, AREA ON 10(1X,1PE10.3)
  C               8.  TOTAL MASS FRACTION REMAINING IN THE OIL
  C                   SLICK FOR EACH TIME STEP PRINTED ON
  C                   10(1X,1PE10.3)
  C
  C       ITEMS 6 AND 7 ABOVE ARE WRITTEN FOR EACH TIME STEP
  C       WITH THE FIRST TIME STEP BEING ZERO.  WHEN THE
  C       VERY LAST TIME STEP IS WRITTEN THEN ITEM 8 IS WRITTEN.
  C
  C       THE NUMBER OF LINES WHITTEN ON THE CUTVP2.PLT PLOT FILE
  C       REFERS TO THE NUMBER OF 'TIMES' WRITTEN THROUGH
  C       ITEMS 6 AND 7 AROVE.
  C
        WRITE (IPU,790) NCUTS
  790   FORMAT(I5)
        WRITE (IPU,800) (TB(I), I=1,NCUTS)
  800   FORMAT( 10(1X,1PE10.3) )
        TYPE 810
  810   FORMAT(1X,'ENTER THE TEMPERATURE IN DEG F FOR
       1 THE VAPOR PRESSURE CALCULATION')
        ACCEPT 230, XSAVE
  C
  C       TK IS THE ABSOLUTE TEMPERATURE IN DEG K.
  C
        TK=(XSAVE-32.)/1.8+273.
        XPRINT=XSAVE
  C
  C       CALCULATE AN ABSOLUTE TEMPERATURE IN DEG RANKINE.
  C
        XSAVE=XSAVE+459.
  C
  C       CALCULATE THE VAPOR PRESSURE AT THE INPUT TEMPERATURE.
  C
  C       AT THIS POINT IF THE INPUT TEMPERATURE IS LESS THAN THE
  C       10-MMHG TEMPERATURE USE THE WATSON-CLAPEYRON EQUATION.
  C
  C       THE WATSON-CLAPEYRON EQUATION IS:
  C
  C       LN(P2/P1) = (HVAPZ/(R*TC))*INTEGRAL
```

```
C
C       WHERE P1 = PRESSURE AT TR1, P2 = PRESSURE AT TR2, HVAPZ IS
C       THE HEAT OF VAPORIZATION AT ABSOLUTE ZERO,
C       R = 1.987 BTU/(LBMOLE, DEG R),
C       TC = CRITICAL TEMPERATURE AND INTEGRAL = VAPORIZATION
C       INTEGRAL BETWEEN TR1 AND TR2.
C
      WRITE (IOU,820)
 820  FORMAT(1H1 . 'CRUDE OIL CHARACTERIZATION AND PSEUDOCOMPONENT
     1 EVAPORATION MODEL')
      WRITE (IOU,830) (ANAME(I ),I=1,5)
 830  FORMAT( 1X,'IDENTIFICATION : ',5A5,/)
      WRITE (IOU,580) ITEM,ISAMP
      WRITE (IOU,840) XPRINT
 840  FORMAT(1X, 'VAPOR PRESSURE IN ATMOSPHERES AT ',1PE10.3, ' DEG F')
      WRITE (IOU,850)
 850  FORMAT(/,12X,'VP',/)
      DO 900 I=1,NC1
      X=XSAVE
      IF(X.LT.TIO(I)) GO TO 860
      X=X/TC(I)
      EX=EXP( 20.*(X-B(1) ))**2 )
      Y=-A(I)*(1.-X)/X-EX
      VP(I) =PC(I)*10.**Y
      GO TO 880
 860  TR1=X/TC(I)
C
C       DO INTEGRAL BY SIMPSONS RULE WITH 21 POINTS
C
      TR2=T10(I)/TC(I)
      DH=(TR2-TR1 )/20.
      RESULT=YI(TR1 )
      TR=TR1
      DO 870 K=1,10
      TR=TR+DH
      RESULT=RESULT+4 .*YI(TR)
      TR=TR+DH
      RESULT=RESULT+2 .*YI(TR)
 870  CONTINUE
      TR=TR+DH
      RESULT=RESULT+4 .*YI(TR)
      TR=TR+DH
      RESULT=DH* (RESULT+YI(TR) )/3.
      P1=-4.33-HVAPZ( I)*RESULT/( 1 .987*TC(I))
      VP(I)=EXP(P1)
 880  WRITE (IOU,890) I,VP(I)
 890  FORMAT( 1X,I2,5X,1PE10 .3)
 900  CONTINUE
      TYPE 910
 910  FORMAT(1X,'THE TBP CUTS HAVE BEEN CHARACTERIZED')
      TYPE 920
 920  FORMAT(1X, 'DO YOU WANT TO WEATHER THIS CRUDE?' )
      MWSCTH=1
      ACCEPT 340, ANS
      IF(ANS.EQ. 'Y') GO TO 930
C
C      GO CALCULATE THE MEAN MOLECULAR WEIGHT OF THE CRUDE
C      BEFORE EXITING, MWSCTH IS THE ROUTING SWITCH TO
C      WEATHER THE CRUDE OR STOP.
C
      MWSCTH = 2
      BBL=1000.
      GO TO 1210
C
C      THIS ENDS THE CRUDE CHARACTERIZATION. BEGIN THE OIL-
C      WEATHERING INPUT.
```

```
C
930     TYPE 940
940     FORMAT(1X,'ENTER THE SPILL SIZE IN BARRELS'
        ACCEPT 230, BBL
        TYPE 950
950     FORMAT(1X,'ENTER NUMBER OF HOURS FOR OIL WEATHERING TO OCCUR')
        ACCEPT 230, X2
        IF(LSWTCH.EQ.99  GO TO 980
        TYPE  960
960     FORMAT(1X,'S NCE YOU DID NOT USE A LIBRARY CRUDE,')
        TYPE 970
970     FORMAT(1X,'YOU MUST ENTER THE FOLLOWING THREE MOUSSE
         FORMATION CONSTANTS')
        GO TO 1000
980     TYPE 990
990     FORMAT(1X,'DO YOU WANT TO ENTER MOUSSE FORMATION CONS
        TANTS?')
        ACCEPT 340, ANS
        IF(ANS.EQ.'N') GO TO 1060
C
C         TO SPECIFY NO MOUSSE, ENTER C2  = 0
C
1000    TYPE 1010
1010    FORMAT(1X,'1. ENTER THE MAXIMUM WEIGHT FRACTION WATER
         IN OIL')
        ACCEPT 230, C2
        IF(C2.GT.0.) GO TO 1030
C
C         SET C2=-1.  F A MOUSSE CANNOT BE FORMED AND LOOP OUT.
C
        C2=-1.
        TYPE 1020
1020    FORMAT(/,1X,'SINCE A 0% WATER CONTENT WAS SPECIFIED
       1, THE REMAINING TWO MOUSSE',/,1X,'CONSTANTS ARE NOT
       2 NEEDED')
        GO TO 1070
1030    C2=1./C2
        TYPE 1040
1040    FORMAT(1X,'2. ENTER THE MOUSSE-VISCOSITY CONSTANT
       1, TRY 0.65')
        ACCEPT 230, C1
        TYPE 1050
1050    FORMAT(1X,'3. ENTER THE WATER INCORPORATION RATE CONSTANT
        , TRY 0.001')
        ACCEPT 230, C4
        GO TO  070
1060    C1=C1L(IC)
        C2=C2L(IC)
        C4=C4L(IC)
1070    IF(LSWTCH.EQ.99) GO TO 1100
        TYPE 1080
1080    FORMAT(/,1X,'YOU MUST ALSO ENTER AN OIL-WATER SURFACE
       1 TENSION (DYNES/CM')
        TYPE 1090
1090    FORMAT(1X,'FOR DISPERSION, TRY 30.')
        GO TO 1130
1100    TYPE 1110
1110    FORMAT(1X,'DO YOU WANT TO ENTER AN OIL-WATER SURFACE
       1 TENSION (DYNES/CM)?')
        ACCEPT 340, ANS
        IF(ANS.EQ.'N') GO TO 1140
        TYPE 1120
1120    FORMAT(1X,'TRY 30.')
1130    ACCEPT 230, STEN
        GO TO 1150
1140    STEN=STENL( C
```

```
C
C       START THE MASS-TRANSFER COEFFICIENT SPECIFICATION.
C
 1150  TYPE 1160
 1160  FORMAT(1X,'ENTER THE MASS-TRANSFER COEFFICIENT CODE: t
      1, 2, OR 3 WHERE:')
       TYPE 1170
 1170  FORMAT(1X,'1=USER SPECIFIED OVER-ALL MASS-TRANSFER COEF
      1FICIENT')
       TYPE 1180
 1180  FORMAT(1X,'2=CORRELATION MASS-TRANSFER COEFFICIENT BY
      1 MACKAY & MATSUGU')
       TYPE 1190
 1190  FORMAT( 1X, '3=INDIVIDUAL-PHASE MASS-TRANSFER COEFFICIENTS')
       ACCEPT 370, KMTC
C
C       NOW ENTER THE WIND SPEED IN KNOTS AND CONVERT TO METER/SEC
C       AND METER/HOUR.
C
       TYPE 1200
 12(IO FORMAT(1X,'ENTER THE WIND SPEED IN KNOTS")
       ACCEPT 230, WINDS
C
C       NEVER LET THE WIND SPEED DROP BELOW 2 KNOTS.  A ZERO WIND
C       SPEED DESTROYS THE MASS-TRANSFER CALCULATION AND KILL
C       YIELD A ZERO MASS-TRANSFER COEFFICIENT.
C
       IF(WINDS.LT.2.) WINDS=2.
       WINDMS=0 .514*WINDS
       WINDMH= 1853.*WINDS
C
C       NOW CALCULATE THE INITIAL CRAM MOLES FOR EACH COMPONENT TO
C       GET THE 1NFEGRATION STARTED.
C
 1210  BM=0.159*BBL
       TMOLES=0.
       DO 1220 I=1,NCUTS
       AMASS=1582.*SPGR (I )*BBL*VOL(I )
       MOLES( I)=AMASS/MW (1 )
       TMOLES=TMOLES+MOLES (I)
C
C       RHO 1S THE DENSITY IN GM MOLES/CUBIC METER.
C
       RHO(I)=100.*MOLES(I)/(BM*VOL( I))
 1220  CONTINUE
C
C       CALCULATE THE MEAN MOLECULAR WEIGHT OF THE CRUDE
C
       WTMOLE=0.
       DO 1230 I=1,NCUTS
       WTMOLE=WTMOLE+MW( I )*MOLES(I)/TMOLES
 1230  CONTINUE
       WRITE (IOU,1240) WTMOLE
 1240  FORMAT(/,1X,'MEAN MOLECULAR WEIGHT OF THE CRUDE = ',1PE10.3)
C
C       IF MWSCTH=1 . WEATHER THE OIL.
C       IF MWSCTH=2, EXIT,
C
       CO TO (1250,2110) MWSCTH
C
C       SPECIFY SLICK SPREADING.
C
 1250  SPREAD=0.
       TYPE 1260
 1260  FORMAT(1X, 'DO YOU WANT THE SLICK TO SPREAD?')
       ACCEPT 340, ANS
```

```
           IF(ANS. EQ. 'N') GO TO 1270
           SP READ=1 .
           GO TO 1290
      C
      C      CALCULATE AN' AREA IN SAME WAY IT WILL BE CALCULATED
      C      AS THE SLICK WEATHERS.  Z=THICKNESS IN METERS.
      C
      1270 TYPE 1280
      1280 FORMAT( 1X, 'SINCE THE SLICK DOES NOT SPREAD, ENTER
          1 A STARTING THICKNESS IN CM')
           ACCEPT 230, Z
           Z=Z/100.
           GO TO 1300
      C
      C      THE SLICK ALWAYS STARTS AT 2-CM THICKNESS.
      C
      1290 Z=0.02
      1300 VOLUM=0.
           DO 1310 I=1,NCUTS
           VOLUM=VOLUM+MOLES (I)/RHO(I)
      1310 CONT I NUE
      C
      C      CALCULATE THE INITIAL AREA AND DIAMETER.
      C
           AREA=VOLUM/Z
           DIA=SQRT(AREA/0 .785)
      C
      C      THE MISS-TRANSFER COEFFICIENT CAN BE CALCULATED ACCORDING TO:
      C
      C              1.   A USER-SPECIFIED OVER-ALL MASS-TRANSFER COEFFICIENT.
      C
      C              2.   THE MASS-TRANSFER COEFFICIENT CORRELATION ACCORDING
      C                   TO MACKAY AND MATSUGU, 1973, CAN. J. CHE, V51,
      C                   P434-439.
      C
      C              3.   INDIVIDUAL OIL- AND AIR-PHASE MASS-TRANSFER COEFFI-
      C                   CIENTS BASED ON SOME REAL ENVIRONMENTAL DATA SUCH
      C                   AS THAT OF LISS AND SLATER.  SCALE THE AIR-PHASE
      C                   VALUE WITH RESPECT TO WIND SPEED ACCORDING TO
      C                   GARRATT, 1977, MONTHLY WEATHER REVIEW, V105,
      C                   P915-920.
      C
      C      TEMP IS R*T AND USED TO CHANGE THE UNITS ON THE MASS-
      C      TRANSFER COEFFICIENT.
      C
      1320 TEMP=(8.2E-05 )*TK
           GO TO (1330,1370,1450), KMTC
      C
      C      USER SPECIFIED OVER-ALL MASS-TRANSFER COEFFICIENT.
      C
      1330 TYPE 1340
      1340 FORMAT(1X,"ENTER THE OVER-ALL MASS-TRANSFER COEFFICIENT
          1, C M/HR .  THY lo')
           ACCEPT 230, UMTC
           WRITE (1oU,1350) UMTC
      1350 FORMAT( 1111 , 'OVER-ALL MASS-TRANSFER COEFFICIENT WAS USER
          1-SPECIFIED AT' ,1PE10.3,' CM/HR BY INPUT CODE 1 ')
      C
      C      CONVERT CM/HR TO GM-MOLES/(HR)(ATM)(M**2 ) SINCE VAPOR
      C      PRESSURE IS THE DRIVING FORCE FOR MASS TRANSFER.
      C
           UMTC=UMTC/TEMP/ 100.
           DO 1360 I=1,NC1
           MTC(I)=UMTC
      1360 CONTINUE
           co TO 1530
```

```
C
C        USE THE MACKAY AND MATSUGU MASS-TRANSFER COEFFICIENT.
C
 1370  TERM1=0.015*WINDMH**0.78
       IF(SPREAD .EQ .0.) GO TO 1380
       TERM2=DIA**(-0.11)
       GO TO 1390
C
C        IF THE SLICK DOES NOT SPREAD BASE THE DIAMETER DEPENDENCE
C        ON 1000 METERS AND DIVIDE THE RESULT BY 0.7
C
 1380  TERM2=0.65
C
C        KH INCLUDES THE SCHMIDT NUMBER FOR CUMENE.
C
 1390  KH=TERM1*TERM2
       WRITE (IOU,1400) KMTC
 1400  FORMAT(1H1,'OVER-ALL MASS-TRANSFER COEFFICIENTS BY INPUT
      1 CODE',I2)
       WRITE (IOU,1410) KH
 1410  FORMAT(/,1X,'OVER-ALL MASS-TRANSFER COEFFICIENT FOR CUMENE = '
      1,1PE10.3,' M/HR',/)
       WRITE (IOU,1420)
 1420  FORMAT(3X,'CUT',12X,'M/HR',7X,'GM-MOLES/(HR)(ATM)(M**2)')
       DO 1440 I=1,NC1
C
C        THE MASS-TRANSFER COEFFICIENT IS CORRECTED FOR THE
C        DIFFUSIVITY OF COMPONENT J IN AIR.  THE SQRT IS USED
C         (I.E. LISS AND SLATER).  BUT THIS 1/3 POWER COULD ALSO
C        BE USED (I.E. THE SCHMIDT NUMBER),
C
       MTCA(I)=KH*0.93*SQRT((MW(I)+29.)/MW(I))
C
C        MTC(I) IS THE OVER-ALL MASS-TRANSFER COEFFICIENT DIVIDED
C        BY R*T.  R=82.06E-06 (ATM)(M**3)/(G-MOLE)(DEG K)
C
       MTC(I)=MTCA(I)/TEMP
       WRITE (IOU,1430) I,MTCA(I),MTC(I)
 1430  FORMAT(2X,I3,2(10X,1PE10.3))
 1440  CONTINUE
       GO TO 1530
C
C        USER SPECIFIED INDIVIDUAL-PHASE MASS-TRANSFER
C        COEFFICIENTS.
C
 1450  TYPE 1460
 1460  FORMAT(1X,'ENTER THE OIL-PHASE MASS-TRANSFER COEFFICIENT
      1 IN CM/HR, TRY 10')
       ACCEPT 230, KOIL
       TYPE 1470
 1470  FORMAT(1X,'ENTER THE AIR-PHASE MASS-TRANSFER COEFFICIENT
      1 IN CM/HR, TRY 1000')
       ACCEPT 230, KAIR
       TYPE 1480
 1480  FORMAT(1X,'ENTER THE MOLECULAR WEIGHT OF THE COMPOUND
      1 FOR K-AIR ABOVE, TRY 200')
       ACCEPT 230, DATAMW
C
C        SCALE K-AIR ACCORDING TO WIND SPEED (GARRATT, 1977),
C        SO THAT AS THE WIND SPEED GOES UP THE MASS TRANSFER
C        GOES UP, I.E., THE CONDUCTANCE INCREASES.
C
       KAIR=KAIR*(1.+0.089*WINDMS)
       RKAIR=1./KAIR
C
C        CALCULATE R*T IN ATM*CM**3/GM-MOLE
```

```
c
         RT=82 . 06*TK
         HTERM= WTMOLE/ ( DCRUDE*RT)
         WRITE (IOU,1400) KMTC
c
c          WRITE THE USERS INPUT, WIND SPEED, AND HENRYS LAW
c          TERM TO THE OUTPUT.
C
         WRITE (IOU,1490) KAIR,KOIL,DATAMW
 1490    FORMAT(/,1X,'K-AIR = ',1PE10.3,', AND K-OIL = ',1PE10.3
        1,' CM/HR, BASED ON A MOLECULAR WEIGHT OF ' ,1PE10.3)
         WHITE (10U,I500) WINDMS
 1500    FORMAT(1X,*WIND SPEED = ' ,IPE10.3,' M/S')
         WRITE (IOU,1510) HTERM
 1510    FORMAT(1X,'THE HENRYS LAW CONVERSION TERM FOR OIL = '
        1,1PE10.3,' 1/ATM')
         WRITE (IOU,1420)
C
C          CLACULATE THE OVER-ALL MASS-TRANSFER COEFFICIENT BASED
C          ON GAS-PHASE CONCENTRATIONS FOR EACH CUT.
C
         DO 1520 I=1,NC1
         HLAW(I )=HTERM*VP(I )
         MTCA(I )=RKAIR+HLAW (I)/KOIL
C
C          NOW TAKE THE INVERSE TO OBTAIN CM/HR AND THEN MULTIPLY
C          BY 0.01 TO GET M/HR.
C
         MTCA(I)=0.01/MTCA(I)
C
C          CORRECT FOR MOLECULAR WEIGHT ACCORDING TO LISS & SLATER,
C          1974, NATURE, V247, P181-184.
C
         MTCA(I )=MTCA(I)*SQRT( DATAMW/MW(I ))
         MTC(I)=MTCA (I)/TEMP
C
C          AND WRITE THE OVER-ALL MASS-TRANSFER COEFFICIENT
C           IN M/HR AND MOLE/HR*ATM*M*M.
C
         WRITE (IOU,1430) I,MTCA(I),MTC(I)
 1520    CONTINUE
 1530    SPCRB=141.5/(APIB+131 .5)
         MASS=0. 1582*BBL*SPCRB
         WRITE (10U,1540) BBL,MASS
 1540    FORMAT(/,1X , 'FOR THIS SPILL OF ',1PE10.3,' BARRELS, THE
        1 MASS IS ",1PE10.3.' METRIC TONNES')
         VOLUMB=VOLUM/0 . 159
         WRITE (IOU,1550) VOLUM,VOLUMB
 1550    FORMAT(/,1X , 'VOLUME FROM SUMMING THE CUTS = '.1PE8.1 - " M**3
        1, OR ' ,1PE10.3, ' BARRELS')
         GO TO (1500,1560,1580), KMTC
 1560    WRITE (IOU,1570) WINDS,WINDMH
 1570    FORMAT (/ , 1X , 'WIND SPEED = ',1PE10.3,' KNOTS, OR ',1PE10.3
        1,' M/HR')
 1580    WRITE (10U,1590) DIA,AREA
 1590    FORMAT(/,1X , ' INITIAL SLICK DIAMETER = ',IPE10.3,' M, OR AREA
        1 = ' ,1PE10.3,' M**2')
         IF(SPREAD .GT.0.) GO TO 1610
         WRITE (10U,1600)
 1600    FORMAT(/,1X,'THIS SLICK DOES NOT SPREAD FOR THIS CALCULATION')
C
C          CALCULATE THE KINEMATIC VISCOSITY OF THE CRUDE AT 122
C          DEG F AND THE ENTERED ENVIRONMENTAL TEMPERATURE.
C          USE THE VISCOSITY MIXING RULE OF (MOLE FRACTION)*(LW),
C          SEE PACE 460 OF REID, PRAUSNITZ & SHERWOOD IN
C          THE BOOK 'THE PROPERTIES OF CASES AND LIQUIDS'
```

```
C
1610  VISMIX=0.
      DO 1620 I=1, NCUTS
      VISMIX=VISMIX+MOLES( I)*VLOGK(I)/TMOLES
1620  CONTINUE
      VISMIX=EXP(VISMIX)
      WRITE (IOU,1630) VISMIX
1630  FORMAT(/,1X, 'KINEMATIC VISCOSITY OF THE BULK CRUDE FROM
     1 THE CUTS = ',1PE8.1,' CENTISTOKES AT 122 DEG F')
      VISMIX=0.
C
C        SCALE THE VISCOSITY WITH TEMPERATURE ACCORDING TO
C        ANDRADE.
C
      EXPT=EXP(1923.*( 1./XSAVE-0.001721 ))
      DO 1640 I=1,NCUTS
      VIS(I)=VISK( I)*EXPT
      VLOG(I )=ALOG(VIS(I))
      VISMIX=VISMIX+MOLES( I )*VLOG(I)/TMOLES
1640  CONTINUE
      VISMIX=EXP(VISMIX)
      WRITE (IOU,1650) VISMIX,XPRINT,EXPT
1650  FORMAT(/,1X, 'KINEMATIC VISCOSITY OF THE BULK CRUDE FROM THE
     1 CUTS = ',1PE8.1,' AT T =',0PF5.1,' DEG F, SCALE
     2 FACTOR = ',1PE8.1)
C
C         IMPORTANT NOTE:  THE VISCOSITY PREDICTION OF THE WHOLE
C         CRUDE FROM CUT INFORMATION IS NOT GOOD AT ALL.  SO THE
C         VISCOSITY INFORMATION CALCULATED ABOVE IS NOT USED IN
C         THIS VERSION OF THE CODE, BUT IT COULD BE IF A GOOD
C         MIXING RULE IS EVER DETERMINED.
C         THEREFORE. FOR THE TIME BEING, THE VISCOSITY OF THE WHOLE
C         WEATHERED CRUDE IS CALCULATED ACCORDING TO MACKAY.
C
C         NOW LOAD THE VISCOSITY INFORMATION IN THE FORM
C         OF THREE CONSTANTS:
C               1.   THE VISCOSITY IN CP AT 25 DEG C
C               2.   THE ANDRADE-VISCOSITY-SCALING CONSTANT
C                    WITH RESPECT TO TEMPERATURE, SEE GOLD &
C                    OGLE, 1969. CHEM. ENG., JULY 14, P121-123
C               3.   THE VISCOSITY AS AN EXPONENTIAL. FUNCTION OF
C                    THE FRACTION OF OIL WEATHERED
C
      IF(LSWTCH.EQ.99) GO TO 1670
      TYPE 1660
1660  FORMAT(1X,'SINCE A LIBRARY CRUDE WAS NOT USED
     1,',/,1X,'ENTER THE FOLLOWING THREE VISCOSITY CONSTANTS')
      GO TO 1690
1670  TYPE 1680
1680  FORMAT(1X,'DO YOU WANT TO ENTER VISCOSITY CONSTANTS?')
      ACCEPT 340, ANS
      IF(ANS.EQ.'N') GO TO 1730
1690  TYPE 1700
1700  FORMAT(1X,'1 . ENTER THE BULK CRUDE VISCOSITY
     1 AT 25 DEG C, CENTIPOISE, TRY 35.')
      ACCEPT 230, VISZ
      TYPE 1710
1710  FORMAT(1X,'2. ENTER THE VISCOSITY TEMPERATURE SCALING
     1 CONSTANT (ANDRADE), TRY 9000. ')
      ACCEPT 230, MK3
      TYPE 1720
1720  FORMAT(1X,'3. ENTER THE VISCOSITY-FRACTION-OIL
     1-WEATHERED CONSTANT, TRY 10.5')
      ACCEPT 230, MK4
      GO TO 1740
C
```

```
C       USE THE LIBRARY VISCOSITY DATA
C
 1730  VISZ=VISZL(IC)
       MK3=MK3L(IC)
       MK4=MK4L(IC)
C
C       INSERT VISCOSITY CALCULATION ACCORDING TO MASS
C       FRACTION  EVAPORATED.  THIS IS THE VISCOSITY
C       MODIFICATION RELATIVE TO CUTVP1
C
 1740  VSLEAD=VISZ*EXP(MK3*(1./TK-0.003357))
       WRITE (IOU,1750) VISZ,MK3,MK4,VSLEAD
 1750  FORMAT(/,1X,'VISCOSITY ACCORDING TO MASS EVAPORATE:
      1 VIS25C =',1PE9.2,', ANDRADE =',1PE9.2
      2,', FRACT WEATHERED =',1PE9.2,', VSLEAD =',1PE9.2
      3,' CP')
       C2P=1./C2
       WRITE (IOU, 1960) C1,C2P,C4
       NEQ=NCUTS
C
C       SET UP THE DISPERSION PROCESS CONSTANTS.
C       CALCULATE THE FRACTION OF THE SEA SURFACE SUBJECT TO
C       DISPERSIONS/HOUR .
C
       TYPE 1760
 1760  FORMAT(1X,'DO YOU WANT THE WEATHERING TO OCCUR WITH
      1 DISPERSION?')
       ACCEPT 340, ANS
       FRACTS=0.
       IF(ANS.EQ.'N') GO TO 1810
       TYPE 1770
 1770  FORMAT(1X,'DO YOU WANT TO ENTER THE DISPERSION
      1 CONSTANTS?')
       ACCEPT 340, ANS
       IF(ANS.EQ.'N') GO TO 1800
       TYPE 1780
 1780  FORMAT(1X,'ENTER THE WIND SPEED CONSTANT. TRY 0.1')
       ACCEPT 230, KA
       TYPE 1790
 1790  FORMAT(1X,'ENTER THE CRITICAL DROPLET SIZE CONSTANT
      1, TRY 50')
       ACCEPT 230, KB
 1800  FRACTS=KA*(1.+WINDMS)**2
 1810  WRITE (IOU,1820) FRACTS
 1820  FORMAT(/,1X,'THE FRACTIONAL SLICK AREA SUBJECT TO
      1 DISPERSION IS ',1PE8.1,' PER HOUR')
       IF(ANS.EQ.'N') GO TO 1840
       WRITE (IOU, 1830) KA,KB,STEN
 1830  FORMAT(1X,'THE DISPERSION PARAMETERS USED:   KA = '
      1,1PE9.2,', KB = ',1PE9.2,', SURFACE TENSION =',1PE9.2
      2,' DYNES/CM')
C
C       PRINT EVERY XP TIME INCREMENT (HOURS).
C       X1 IS THE  STARTING  TIME=0.
C       X2 IS THE NUMBER OF HOURS FOR WEATHERING TO OCCUR.
C
 1840  XP=1.
       X1=0.
       MOLES(NCUTS+1)=AREA
C
C       PRINT AN OUTPUT FILE FOR 80  COLUMN  OUTPUT, THIS IS
C       THE CUTVP2.TYP FILE.
C
       WRITE (ITY,1850) (ANAME(J),J=1,5)
 1850  FORMAT(/,1X,'OIL WEATHERING FOR ',5A5)
       WRITE (ITY,570)
```

```
      WRITE (I TY, 1860) XPRINT, WINDS
 1860 FORMAT( 1X,'TEMPERATURE= ',F5. 1," DEG F, WIND SPEED= "
     1,F5. 1,' KNOTS")
      WRITE (ITY,1870) BBL
 1870 FORMAT(1X, 'SPILL SIZE= ',1PE10.3,' BARRELS')
      WRITE (ITY,1880) KMTC
 1880 FORMAT(1X, ' MASS-TRANSFER COEFFICIENT CODE= ',I3)
      WRITE (ITY,1890)
 1890 FORMAT(/,1X,'FOR THE OUTPUT THAT FOLLOWS. MOLES
     1=GRAM MOLES*)
      WRITE (ITY,1900)
 1900 FORMAT( 1X, 'GMS=GRAMS, VP=VAPOR PRESSURE IN ATMOSPHERES")
      WRITE (ITY,1910)
 1910 FORMAT( 1X, ' BP=BOILING POINT IN DEG F, API=GRAVITY')
      WRITE (ITY,1920)
 1920 FORMAT(1X,'MW=MOLECULAR WEIGHT')
      WRITE (ITY,1930)
 1930 FORMAT(/,2X , 'CUT' ,3X, 'MOLES' ,6X,'GMS',8X,'VP',8X,'BP '
     1,7X, 'API',5X,'MW')
      DO 1950 I=1,NCUTS
      GMS=MOLES(I )*MW(I)
      IMW=MW(I )
      WRITE (ITY,1940) I,MOLES( I),GMS,VP(I),TB( I),API(I),IMW
 1940 FORMAT(3X,I2,5( 1X,1PE9 .2) ,1X,I3)
 1950 CONTINUE
      WRITE (ITY,1960) C1,C2P,C4
 1960 FORMAT(/,1X , 'MOUSSE CONSTANTS: MOONEY=' ,1PE9.2
     1,", MAX H20=',0PF5.2, ' , WIND**2=',1PE9.2)
      WHITE (ITY,1970) KA,KB,STEN
 1970 FORMAT(1X,'DISPERSION CONSTANTS: KA=' ,1PE9.2
     1,', KB=',1PE9.2,', S-TENSION=' ,1PE9.2)
      WRITE (ITY,1980) VISZ,MK3,MK4
 1980 FORMAT(1X,'VIS CONSTANTS: VIS25C=',1PE9.2
     1,', ANDRADE =',1PE9.2,', FRACT =',1PE9.2)
      WRITE (ITY,1990)
 1990 FORMAT(/,1X, ' FOR THE OUTPUT THAT FOLLOWS. TIME=HOURS')
      WRITE (ITY,2000)
 2000 FORMAT(1X,'BBL=BARRELS , SPGR=SPECIFIC GRAVITY, AREA=M*M' )
      WRITE (ITY.2010)
 2010 FORMAT(1X,'THICKNESS=CM . W=PERCENT WATER IN OIL (
     1MOUSSE)' )
      WRITE (ITY,2020)
 2020 FORMAT(1X,'DISP=DISPERSION RATE IN GMS/M*M/HR')
      WRITE (ITY,2030)
 2030 FORMAT(1X, 'EH.4TE=EVAPORTION RATE IN GMS/M*M/HR')
      WRITE (ITY,2040)
 2040 FORMAT(1X,'M/A=MASS PER M*M OF OIL IN THE SLICK')
      WRITE (ITY,2050)
 2050 FORMAT(1X,'I=FIRST CUT WITH GREATER THAN  1% (MASS)
     1 REMAINING')
      WRITE (ITY,2060)
 2060 FORMAT(1X,'J=FIRST CUT WITH GREATER THAN 50% (MASS)
     1 REMAINING')
      IF(FRACTS.NE.0. ) GO TO 2080
      WRITE (ITY,2070)
 2070 FORMAT( 1X, 'DISPERSION WAS TURNED OFF')
 2080 IF(SPREAD.NE.0. ) GO TO 2100
      WRITE (ITY,2090)
 2090 FORMAT(/,1X,'SPREADING WAS TURNED OFF')
C
C       WRITE SOME INFORMATION TO THE PLOT FILE.
C
 2100 TCODE=KMTC
C
C       XPRINT IS THE ENVIRONMENTAL TEMPERATURF,. DEG F.
C
```

```
       WRITE(IPU,800) XPRINT, WINDS, KA, KB, STEN, BBL, C1,C2, C4
      1,TCODE
C
C         TO THIS POINT IT WAS JUST GETTING READY, NOW
C          INTEGRATE IT.
C
       CALL BRKG4(MOLES,X1,X2,XP,NEQ)
 2110 TYPE 2120
 2120  FORMAT(1X, 'DO IT AGAIN?')
       ACCEPT 340, ANS
       IF(ANS.EQ. 'Y') GO TO 760
 2130  CONTINUE
       END
       SUBROUTINE CHAR(API,TB,A,B,NS,NV)
       REAL*4 MW1
       COMMON ,'COII./ MW1,TC1,VC1,PC1 ,CNUM1 ,VIS1
       DIMENS1ON C(2,6),T(2, 6),P(4),V(2 ,6)
       DATA ((C(I,J),J=1,6),I=1,2)/6 .241E+01, -4.595E-02,-2 .836E-01
      1,3.256E-03 ,4.578E-04, 5.279E-04
      2,4.268E+02,-1 .007, -7.449,1 .38E-02, 1.047E-03,2. 621E-02/
       DATA ((T(I,J),J=1,6),I=1,2)/4 .055E+02, 1.337,-2.662 ,-2.169E-03
      1 ,-4.943E-04,1 .454E-02
      2,412.2,1.276,-2.865,-2 .888E-03 ,-3 .707E-04 ,2 .888E-02/
       DATA P/1.237E-02 ,0 .2516 ,4 .039E-02 , -4 .024E-02/
       DATA ((V(I,J),J=1,6),I=1,2)/ -0.4488, -9.344E-04,0.0 1583
      1,-5.219E-05 ,5.268E-06 ,1.536E-04
      2,-().6()19,1 .793E-03, -3.159E-03 ,-5. 1E-06,9.067E-07 ,3.522E-05/
C
C         THIS SUBROUTINE CHARACTERIZES A CUT OF CRUDE OIL WITH RESPECT
C         TO VAPOR PRESSURE.  THE INPUT REQUIRED IS API GRAVITY AND THE
C         BOILING POINT AT 1 ATMOSPHERE.  THE OUTPUT IS A SWITCH NS
C         WHERE NS=1 MEANS THE VAPOR PRESSURE EQUATION CAN BE USED DOWN TO
C          10NN HG AND NS=2 MEANS THE CLAPEYRON EQUATION SHOULD BE USED.
C
C         THE VAPOR PRESSURE EQUATION IS:
C
C         LOG10(PR) = -A*(1.-TR)/TR - EXP(-20*(TR-B)**2)
C
C         WHERE PR = REDUCED PRESSURE, TR = REDUCED TEMPERATURE AND
C         A AND B ARE RETURNED BY THIS SUBROUTINE.
C
C         API = GRAVITY, TB = BOILING POINT AT 1 ATMOSPHERE IN DEG F.
C         CALCULATE CRITICAL TEMPERATURE AND MOLECULAR WEIGHT.
C
       API2=API*API
       TB2=TB*TB
       CROSS=API*TB
       I=1
       IF(API.GT.35. ) 1=2
       VIS1=V( I, 1)+V(I,2)*TB+V( I,3)*API+V( I,4)*CROSS+V( I,5)*TB2
      1+V(I,6)*API2
       GO TO (10,30), NV
 10    I=1
       IF(TB.GT.500. ) I=2
       MW1=C( I, 1)+C(I,2)*TB+C( I,3)*API+C( I,4)*CROSS+C( I,5)*TB2
      1+C(I,6)*API2
       TC1=T(I ,1)+T(I,2)*TB+T( I,3)*API+T( I,4)*CROSS+T( I,5)*TB2
      1+T(I ,6)*API2
       TCK=(TC1+459. )/1 .8
C
C         CALCULATE THE VISCOSITY OF THE CUT,
C
       I=1
       IF(API.GT.35. ) 1=2
       VIS1=V( 1,1 )+V(I,2)*TB+V( I,3)*API+V( I,4)*CROSS+V( I,5)*TB2
      1+V(I,6)*API2
```

```
C
C         CALCULATE THE CARBON NUMBER
C
      CNUM1=(MW1-2.)/14.
      X=ALOG10(CNUM1)
C
C         CALCULATE B FOR THE VAPOR PRESSURE EQUATION
C
      BPRIME=P(1)+X*(P(2)+X*(P(3)+X*P(4)))
      B=BPRIME-0.02
C
C         CALCULATE THE CRITICAL VOLUME. CC/GMOLE
C
      VW=1.88+2.44*CNUM1
      VC1=VW/0.044
C
C         CALCULATE THE CRITICAL PRESSURE IN ATMOSPHERES
C
      PCP=20.8*TCK/(VC1-8.)
      PC1=PCP+10.
      TR=(TB+459.)/(TC1+459.)
      PR=1./PC1
      NS=1
      IF(TR.LE.B) GO TO 20
      A=(ALOG10(PR)+EXP(-20.*(TR-B)**2))*TR/(TR-1.)
      GO TO 30
   20 NS=2
   30 RETURN
      END
      SUBROUTINE BRKG4(Y,X1,X2,XP,NEQ)
      REAL*4 K1,K2,K3,K4,MTC,MW,MWU,KB,MK4
      COMMON /SPILL/ MTC(30),VP(30),VLOG(30),RHO(30),MW(30)
     1 ,SPGR(30),FRACTS,STEN,KB,DISPER,Z,TERM2,SPREAD,KMTC
      COMMON /PCODE/ VSLEAD,MK4,IOU,IPU,ITY
      COMMON /TALK/ MWU(30),NEQ1,NEQ2,NEQ3
      DIMENSION Y(30),YARG(30),K1(30),K2(30),K3(30),K4(30)
     1 ,GONE(200),YSAVE(30),YF(30),YMSAVE(30),YM(30),YM1(30)
C
C          RUNGA-KUTTA 4-TH ORDER NUMERICAL INTEGRATION FOR SIMULTANEOUS
C          DIFFERENTIAL EQUATIONS, SEE C.R. WYLIE, PAGES 10V-117 OR
C          D. GREENSPAN, PAGES 113-115.
C
C          THIS SUBROUTINE DOES THE PRINTING, THE INITIAL AND FINAL VALUES
C          ARE ALWAYS PRINTED.  PRINT THE RESULTS EVERY XP INCREMENT
C          IN X.
C
C          THE USER MUST WRITE SUBROUTINE FXYZ WHICH CALCULATES THE
C          K1, K2, K3, AND K4 VECTORS AS A FUNCTION OF X AND THE
C          CURRENT Y VECTOR.  INTEGRATION FOLLOWS THE REFERENCES AND
C          WAS TESTED ON PROBLEM 5, PAGE 116 IN WYLIE.
C
C          THE FIRST NCUTS POSITIONS IN THE Y VECTOR ARE THE MOLES
C          OF THE COMPONENTS.  POSITION NCUTS+1 IS THE AREA OF THE
C          SLICK.  POSITION NCUTS+2 IS THE MASS LOST FROM THE SLICK
C          BY DISPERSION ALONE.  POSITION NCUTS+3 IS THE MASS LOST
C          FROM THE SLICK BY EVAPORATION ALONE.
C
C          LINE KEEPS TRACK OF HOW MANY LINES ARE WRITTEN TO THE
C          PLOT FILE.  NEQ1 IS THE NUMBER OF COMPONENTS+1.  NS IS
C          A ROUTING SWITCH TO CHANGE THE PRINT INTERVAL.  TN IS
C          AN INPUT ROUTING SWITCH TO DELETE RAPIDLY CHANGING
C          COMPONENTS.  GONE(LINE) IS THE MASS FRACTION REMAINING
C          AT TIME STEP LINE.  INT IS A SWITCH TO INDICATE WHEN THE
C          INTEGRATION HAS STARTED: INT=1, NOT STARTED; INT=2,
C          STARTED.  ITYP IS A HEADER PRINT SWITCH FOR THE
C          80-COLUMN FILE.
```

```
C
      I NT= 1
      ITYP= 1
      LINE=0
      NEQ1 =NEQ+1
      NEQ2=NEQ+2
      NEQ3=NEQ+3
      NS= 1
      IN=1
      IKEEP=1
      CONE(1)=1.
      DISPER=0.
C
C        TOTAL IS THE INITIAL NUMBER OF MOLES.
C        TSAVE IS THE INITIAL MASS.
C
      TOTAL=0.
      TSAVE=0.
      DO 10 I=1,NEQ
C
C        CALCULATE AND SAVE THE INITIAL CONDITIONS.
C
      YSAVE(I)=Y(I)
      YMSAVE(I)=Y(I)*MW(I)
      MWU(I)=MW(I)
      TSAVE=TSAVE+YMSAVE(I)
      TOTAL=TOTAL+Y(I)
10    CONTINUE
C
C        SAVE THE INITIAL AREA.
c
      YMSAVE(NEQ1)=Y(NEQ1)
C
C        INITIALIZE THE MASS LOST BY DISPERS1ON ALONE AND
C        EVAPORATION ALONE.
C
      Y(NEQ2)=0.
      Y(NEQ3)=0.
C
C        NDEL IS THE NUMBER OF COMPONENTS DELETED BECAUSE THEY
C        EVAPORATE TOO FAST.   NFAST IS THE CURRENT ARRAY LOCATION
C        OF THE FASTEST MOVING COMPONENT.
C
      NDEL=0
      NFAST=0
      X=X1
C
C        INITIALIZE THE PRINT SWITCH TO FORCE A PRINT AND
C        SUBSEQUENT CALCULATIONS THE FIRST TIME THROUGH.
C
      XW=-1 .
      WRITE (IOU,20)
20    FORMAT(/,1X , ‘COUNT THE CUTS IN THE FOLLOWING OUTPUT FROM LEFT
     I TO RIGHT',/)
      WRITE (101J.30)
30    FORMAT(1X,'THE INITIAL GRAM MOLES IN THE SLICK ARE:')
      WRITE (10U.40) (Y(I),I=1,NEQ)
40    FORMAT( 11(1X,1PE10.3))
      WRITE (IOU,50)
50    FORMAT(/,1X,'THE INITIAL MASSEs (GRAMS) IN THE SLICK ARE
     1:')
      WRITE (10IJ,40) (YMSAVE(I),I=1,NEQ)
      WRITE (101J,60) TSAVE
60    FORMAT(1X, ‘THE TOTAL MASS FROM THESE CUTS IS ‘
     1,1PE10.3,' GRAMS’)
      WRITE (10U,70)
```

```
70     FORMAT(/
C
C        CALCULATE DY/DX AND SET THE STEP SIZE TO APPROXIMATE
C        A 5% CHANGE IN THE MOST RAPIDLY CHANGING Y.  WHEN THIS
C        Y DECREASES BY A FACTOR OF 20. RESET THE STEP SIZE
C        ACCORDING TO THE NEXT Y.
C        SOME Y'S WILL CHANGE SO FAST THAT THEY WILL BE GONE
C        IN A FEW MINUTES.  THESE ARE DELETED BEFORE INTEGRATION
C        STARTS AND NOTED ON THE PRINTED RESULTS.
C
C        INITIALIZE OR  NCREMENT NFAST.
C
80     NFAST=NFAST+1
90     CALL FXYZ(X,Y,K1,NEQ)
C
C        THE TIME UNIT IS HOUR.
C        SET THE STEP SIZE TO H=0.05*Y/(DY/DX).
C
       H=0.05*Y(NFAST)/K1(NFAST
       YOLD=Y(NFAST)
       H=ABS(H)
       H2=H/2.
       GO TO (100, 70 ,  N
C
C        IF THERE IS A RAPIDLY MOVING COMPONENT AT THE BEGINNING
C        ITS STEP SIZE WILL BE VERY SMALL. DO NOT LET THE
C        STEP SIZE BE LESS THAN 0.05 HOUR.
C
100     F(H.GT.0.05  GO TO 130
C
C        Y(NFAST) CHANGES TOO FAST TO CALCULATE. DELETE IT AND MOVE
C        EVERYBODY ONE SPACE TO THE LEFT.
C
C        WHEN YOU MOVE THE AREA BE SURE TO SUBTRACT THE CONTRIBUTION
C        OF THE CUT JUST DELETED.
C
       ISTART=1
       NFAST=1
       NDEL=NDEL+
C
C        DECREASE THE NUMBER OF COMPONENTS BY 1
C
       NEQ=NEQ-1
       NEQ1=NEQ+
       NEQ2=NEQ+2
       NEQ3=NEQ+3
       NEQ4=NEQ+4
       AD=Y(1)/RHO(1)/Z
       DO 110 I=1,NEQ
C
C        SHIFT THE ARRAYS.
C
       I1=I+1
       Y(I)=Y(I1)
       VP(I)=VP(I1)
       MTC(I)=MTC(I1)
       YSAVE(I)=YSAVE(I1)
       VLOG(I)=VLOG(I1)
       RHO(I)=RHO(I1)
       MWU(I)=MWU(I1)
       YMSAVE(I)=YMSAVE    )
1 0    CONTINUE
C
C        BE SURE AND DO THE LAST THREE POSITIONS WHEN SHIFTING
C
       Y(NEQ1)=Y(NEQ2)-AD
```

```
         Y(NEQ2)=Y(NEQ3)
         Y(NEQ3)=Y(NEQ4)
         WRITE (IOU,120) NDEL
  20     FORMAT(1X,'CUT ',I2,' GOES AWAY IN MINUTES, THEREFORE IT WAS
        1 DELETED AND THE CUTS RENUMBERED',/)
         WRITE (ITY, 20  NDEL
         GO TO 90
 130     IN=2
         GO TO    0  60   TYP
 140     ITYP=2
         WRITE (ITY,150)
 150     FORMAT(/,1X,'TIME',2X,'BBL',3X,'SPGR',2X,'AREA',2X
        1,'THICKNESS  W',2X,'DISP',4X,'ERATE',4X,'M/A    I  J
 C
 C         THE COMPONENTS THAT MOVE TOO FAST TO CONSIDER (AT TIME
 C         ZERO) HAVE BEEN DELETED AND THE ARRAYS SHIFTED.
 C
 160     NEQ1=NEQ+1
         NEQ2=NEQ+2
         NEQ3=NEQ+3
 C
 C         NEVER LET THE STEP SIZE BE GREATER THAN 0.5
 C
 170     IF(H.GT.0.5) H=0.5
         WRITE (IOU,180) H,NFAST
 180     FORMAT(/,2X,'STEP SIZE OF ',1PE10.3,' IS BASED ON CUT ',I3,/)
 C
 C         CHECK THE PRINT SWITCH.
 C
 190     IF(X.LT.XW) GO TO 380
 C
 C         INCREMENT THE PRINT SWITCH AND CALCULATE INTERMEDIATE
 C         RESULTS NOT CARRIED WITH THE INTEGRATION.
 C
         XW=X+XP
         YTOT=0.
         TMASS=0.
         DO 200 I=1,NEQ
         YF(I)=Y(I)/YSAVE(I)
         YTOT=YTOT+Y(I)
         YM(I)=Y(I)*MWU(I)
         YM1(I)=YM(I)
         TMASS=TMASS+YM(I)
         YM(I)=YM(I)/YMSAVE(
 200     CONTINUE
         YM1(NEQ1)=Y NEQ
 C
 C         CALCULATE THE MEAN MOLECULAR WEIGHT OF THE SLICK.
 C
         WMEANS=0.
         DO 210 I=1,NEQ
         WMEANS=WMEANS+MWU(I)*Y(I)/YTOT
 210     CONTINUE
         LINE=LINE+1
         WRITE (IOU,220) X,LINE
 220     FORMAT(2X,'TIME = ',1PE8.1,' HOURS, MASS FRACTION OF EACH
        1 CUT REMAINING:',65X,I3)
         WRITE (IOU,230) (YM(I),I=1,NEQ)
 230     FORMAT(14(1X,1PE8.1))
         CHECK=TMASS+Y(NEQ2)+Y(NEQ3)
         WRITE (IOU,240) TMASS,Y(NEQ2),Y(NEQ3),CHECK
 240     FORMAT(2X,'MASS REMAINING = ',1PE10.3,', MASS DISPERSED
        1 = ',1PE10.3,', MASS EVAPORATED = ',1PE10.3,'
        2, SUM = ',1PE10.3)
         WRITE (IPU,250) NEQ1
 250     FORMAT(I5)
```

```
      WRITE (IPU,260) X,(YM1(I),I=1,NEQ1)
  260 F01{PLAT( 10( 1X,1I'E10.3))
C
C        WREN THE FR.4CTION REMAINING OF COMPONENT I GETS LOW,
C        SET ITS VAPOR PRESSURE AND MOLESEQUALTO ZERO.
C
      DO 270 I=ISTART,NEQ
      IF(YF(I ).GT.1.0E-08) GO TO 270
      IKEEP=I+1
      VP(I)=0.
      Y(I)=0.
  270 CONTINUE
      ISTART=IKEEP
      NFAST=IKEEP
      CONE(LINE)=TMASS/TSAVE
      ZP=Z*100.
      WRITE (IOU,280) CONE(LINE) ,Y(NEQ1),ZP ,WMEANS
  280 FORMAT(2X, "FRACTION (BASED ON MASS) REMAINING [N THE SLICK
     1=',1PE8. 1,', AREA= ',1PE8. 1,' M**2, THICKNESS='
     2,1PE8. 1,' CM, MOLE WT=',0PF5.1)
C
C        WIO IS THE MOUSSE CALCULATION.
C
      CALL WIO(X,W,VTERM)
C
C        VISCP1 1S THE VISCOSITY OF THE PARENT OIL WITH NO WATER
C        INCORPORATED .
C        VISCP1 IS IN CENTIPOISE, FEVAP IS THE FRACTION OF OIL '
C        EVAPORATED .   NOTE THAT FEVAP IS NOT
C         1 - (FRACTION REMAINING) BECAUSE DIN'ERS1ON LOSSES
C        WOULD BE INCLUDED.  THE FRACTION EVAPORATED MUST
C        CORRECT FOR THE LOSS DUE TO DISPERSION.
C
      FEVAP=1.0-CONE(LINE)
      FEVAP=FEVAP/YM( NEQ)
      VISCP1 =VSLEAD*EXP (MK4*FEVAP)
C
C        VTERMISTHE VISCOSITY J'multiplier FRoM THE MOUSSE
C        CALCULATION.
C
      VISCP=VISCP1 *VTERM
C
C        CALCULATE THE BULK SPGR.
C
      BSPGR=0.
      DO 290 I=ISTART,NEQ
      BSPGR=BSPGR+SPGR(I)*Y(I)/YTOT
  290 CONTINUE
      VISQT=SQRT(VISCP/10.)
C
C        CALCULATE THE DISPERSION FACTOR.
C
      FB=1 ./(1 .+KB*VISQT*Z*STEN/0 .024)
      DISPER=FRACTS*FB
      WRITE (IOU,300) W,VISCP,DISPER
  300 FORMAT(2X,'WEIGHT FRACTION WATER IN OIL = ',1PE8. 1,', VIS
     1COSITY=',1PE8.1 " ,CENTISTOKES, DISPERSION  TERM = '
     2,1PE8.1,' WEIGHT FRACTION/HR')
      CVOLUM=Y(NEQ1 )*Z
      TBBL=CVOLUM/0 .159
      CVOLUM=(1 .0E+06)*CVOLUM
      CSPGR=TMASS/CVOLUM
      WAREA=(1 .0E+06)*Z*CSPGR
      WDISP=WAREA*DISPER
      IF(INT.EQ.1) ERATE=0.
      ERATE=ERATE/Y(NEQ1 )
```

```
      WRITE (IOU,310) WAREA,CSPGR,TBBL,WDISP,ERATE
310   FORMAT(2X,'MASS/AREA=',1PE8.1,' GMS/M*M, SPGR='
     1,1PE8.1,', TOTAL VOLUME=',1PE8.1,' BBL, DISPERSION='
     2,1PE8.1,' GMS/M*M/HR, EVAP RATE=',1PE8.1,' GMS/M*M/HR')
C
C        PRINT AN OUTPUT FILE FOR 80 COLUMN OUTPUT.
C
      DO 320 J= ,NEQ
      JCUT=J
      IF(YM(J .GT.0.5  GO TO 330
320   CONTINUE
330   DO 340 I=1,NEQ
      ICUT=I
      IF(YM(I).GT.0.01) GO TO 350
340   CONTINUE
350   IX=X
      IW=W* 00
      WRITE (ITY,360) IX,TBBL,CSPGR,Y(NEQ1),ZP,IW,WDISP
     1,ERATE,WAREA,ICUT,JCUT
360   FORMAT(1X,I3,1PE8.1,0PF5.2,2(1PE8.1),1X,I3
     1,3(1PE8.1),I2,I3)
      WRITE ( 0,70)
C
C        INCREASE XP TO 10 HOURS AFTER 50 HOURS OF WEATHERING.
C
      GO TO (370,380), NS
370   IF(X.LT.50.) GO TO 380
      NS=2
      XP=10
C
C        TAKE A STEP IN TIME
C
380   XARG=X
      DO 390 I=1,NEQ3
      YARG(I)=Y(I)
390   CONTINUE
C
C        INT IS A SWITCH TO INDICATE THAT THE INTEGRATION WAS
C        INITIATED.
C
      INT=2
      CALL FXYZ(XARG,YARG,K1,NEQ)
      XARG=X+H2
      DO 400 I= ,NEQ3
      YARG(I =Y I)+H*K1(I)/2.
400   CONTINUE
C
C        SAVE THE EVAPORATION RATE FROM THE FIRST TIME
C        THE DERIVATIVES ARE CALCULATED.
C
      ERATE=K1(NEQ3)
      CALL FXYZ(XARG YARG,K2,NEQ
      DO 410 I=1,NEQ3
      YARG(I)=Y(I)+H*K2(I)/2.
410   CONTINUE
      CALL FXYZ(XARG,YARG,K3 NEQ
      XARG=X+H
      DO 420 I=1,NEQ3
      YARG(I)=Y I +H*K3(I)
420   CONTINUE
      CAL  FXYZ(XARG,YARG,K4,NEQ)
      DO 430 I=1,NEQ3
      Y(I)=Y(I)+H*(K1(I)+2.*(K2(I)+K3(I))+K4(I))/6.
430   CONTINUE
C
C          F 10 PER CENT BY MOLES OR LESS OF THE SLICK IS LEFT, STOP
```

```
C         THE CALCULATION BECAUSE STRANGE THINGS HAPPEN CLOSE TO
C         ZERO OIL.
C
        REMAIN=0.
        DO 440 I=1,NEQ
        REMAIN=REMAIN+Y(I)
  440   CONTINUE
        TEST=REMAIN/TOTAL
        IF(TEST.GT.0.1) GO TO 470
        WRITE (IOU,450)
  450   FORMAT(/,1X,'THE SLICK (MOLES) HAS DECREASED TO 10%
       1 OR LESS, THEREFORE THE CALCULATION WAS STOPPED.')
        WRITE (ITY,460)
  460   FORMAT(/,1X,'SLICK DECREASED TO 10% MASS **STOP**')
        GO TO 510
C
C         RECALCULATE THE OVER-ALL MASS-TRANSFER COEFFICIENTS OUTSIDE
C         THE DERIVATIVE SUBROUTINE.  THE DIAMETER DEPENDENCE IS VERY
C         SLOW.  TERM2 IS THE OLD DIA**(-0.11).  SO DIVIDE THE OLD
C         COEFFICIENT BY TERM2 AND MULTIPLY IN THE NEW ONE.
C
C         WHEN YOU CHANGE THE WIND SPEED WITH RESPECT TO TIME,
C         CHANGE THE MASS-TRANSFER COEFFICIENT HERE.  DIVIDE
C         OUT THE OLD WIND TERM AND MULTIPLY IN THE NEW ONE.
C         ALSO, IF THE TEMPERATURE CHANGES, RECALCULATE THE
C         VAPOR PRESSURE HERE.  THIS APPLIES ONLY TO MACKAY
C         AND MATSUGU.
C
  470   GO TO (500,480,500), KMTC
  480   DIA=SQRT(Y(NEQ1)/0.785)
        TNEW=DIA**(-0.11)
        ADJUST=TNEW/TERM2
        DO 490 I=1,NEQ
        MTC(I)=MTC(I)*ADJUST
  490   CONTINUE
        TERM2=TNEW
C
C         CHECK TO SEE IF THE INTEGRATION IS COMPLETED.
C
  500   IF(X.GE.X2) GO TO 510
        X=XARG
C
C         CHECK TO SEE IS THE FIRST NON-ZERO MOLES HAS FALLEN TO
C         0.01 OF ITS STARTING VALUE.  IF IT HAS, RECALCULATE THE
C         STEP SIZE ON THE NEXT NON-ZERO COMPONENT.  NOTE THAT
C         A COMPONENT IS NOT ZEROED UNTIL ITS MOLE NUMBER HAS
C         FALLEN TO LESS THAN 1.0E-08.
C
        TEST=ABS(Y(NFAST)/YOLD)
        IF(TEST.LT.0.01) GO TO 80
        GO TO 190
  510   NDEL=NDEL+1
        WRITE (IOU,520) NDEL
  520   FORMAT(/,1X,'THE CIJ-r NUMBERING BEGINS WITH',I3,' BASED ON
       1 THE ORIGINAL CUT NUMBERS',/)
        LINE=LINE+1
        WRITE (IOU,530) X,LINE
  530   FORMAT(1X,'THE FINAL MASS FRACTIONS FOR THE SLICK AT '
       1,1PE8.1,' HOURS ARE:',65X,I3)
        TYPE 540, LINE
  540   FORMAT(1X,'NUMBER OF LINES WRITTEN TO CUTVP2.PLT = ',I4)
        TMASS=0.
        DO 550 I=1,NEQ
        YM(I)=Y(I)*MWU(I)
        TMASS=TMASS+YM(I)
        YM1(I)=YM(I)
```

```
      YM   )=YM I)/YMSAVE(I
  550 CONTINUE
      YM1(NEQ1)=Y NEQ )
      GONE(LINE)=TMASS/TSAVE
      WRITE (IOU,40) (YM(I),I=1,NEQ)
      WRITE (IPU,250) NEQ1
      WRITE (IPU,260) X,(YM1(I),I=1,NEQ1)
      WRITE (IPU,260) (GONE(I),I=1,LINE)
      ZP=Z*100.
      WRITE (IOU,280) GONE(LINE),Y(NEQ1),ZP,WMEANS
      CHECK=TMASS+Y(NEQ2)+Y(NEQ3)
      WRITE (IOU,240) TMASS,Y(NEQ2),Y(NEQ3),CHECK
      WRITE (IOU,560)
  560 FORMAT(/,1X,'****************************************
     1**************************',/)
      RETURN
      END
      SUBROUTINE FXYZ(XARG,MOLES,K,NEQ)
      REAL*4 MOLES,K,MTC,MW,MWU,KB
      COMMON /SPILL/ MTC(30),VP(30),VLOC(30),RHO(30),MW(30)
     1,SPGR(30),FRACTS,STEN,KB,DISPER,Z,TERM2,SPREAD,KMTC
      COMMON /TALE/ MWU(30),NEQ1,NEQ2,NEQ3
      DIMENSION MOLES(30),K(30),TMPVP(30),TMPDS(30)
C
C        THE VECTOR BEING INTEGRATED RESIDES  N MOLES
C        POSITIONS  =1 THROUGH I=NEQ ARE THE PSEUDO COMPONENTS,
C        POSITION NEQ1=NEQ+1 IS THE AREA
C        POSITION NEQ2=NEQ+2 IS THE MASS LOST BY DISPERSION ALONE.
C        POSITION NEQ3=NEQ+3 IS THE MASS LOST BY EVAPORATION ALONE.
C
C
      SUM=0.
      DO 10 I=1,NEQ
      SUM=SUM+MOLES
   10 CONTINUE
      DO 20 I=1,NEQ
C
C        CALCULATE THE MOLE DERIVATIVES.
C
      TMPVP(I)=MTC(I)*MOLES(NEQ1)*VP(I)*MOLES I)/SUM
      TMPDS(I)=DISPER*MOLES(
      K(I)=TMPVP(I)+TMPDS(I)
      K(I)=-K(  )
   20 CONTINUE
      VOL=0.
      DO 30 I=1,NEQ
      VOL=VOL+MOLES(   /RHO(I)
   30 CONTINUE
C
C        CALCULATE THE AREA DERIVATIVE.
C
      Z=VOL/MOLES(NEQ1)
      K(NEQ1)=(5.4E+05)*(Z**1.33)*MOLES(NEQ1)**0.33
      K(NEQ1)=SPREAD*K(NEQ1)
C
C        CALCULATE THE MASS LOST FROM THE SLICK DUE TO
C        EVAPORATION ALONE AND THEN DISPERSION ALONE.
C
      K(NEQ2)=0.
      K(NEQ3)=0.
      DO 40 I=1,NEQ
      K(NEQ3)=K(NEQ3)+TMPVP(I)*MWU(I)
      K(NEQ2)=K(NEQ2)+TMPDS(I)*MWU(I)
   40 CONTINUE
      RETURN
      END
```

```
      SUBROUTINE WIO(TIME,W,VTERM)
      COMMON /MOOSE/ WINDS,C1,C2,C3,C4
      WFUNC(W)=(1.0-C2*W)*EXP(-2.5*W/(1.0-C1*W))
      VIS(W)=EXP(2.5*W/(1.0-C1*W) )
      DATA WSAVE,C4SAVE/-1.,-1./
C
C       THIS IS THE WATER-IN-OIL (MOUSSE) ROUTINE.
C       W IS THE FRACTIONAL WATER CONTENT IN THE OIL.
C       WINDS IS THE WIND SPEED IN KNOTS.
C       TIME IS IN HOURS.
C       C1 IS A VISCOSITY CONSTANT = 0.65
C       C2 IS AN OIL-COALESCING CONSTANT AND IS OIL
C       DEPENDENT, AND IS THE INVERSE OF THE MAXIMUM WEIGHT
C       FRACTION WATER IN OIL.
C       C3 IS A WATER INCORPORATION RATE (1./HR), USUALLY 0.01*U*U
C
C       THE PREDICTION EQUATION FOR W IS IMPLICIT AND IS
C       SOLVED BY TRIAL AND ERROR.
C
C       REFERENCE:  CHAPTER 4 BY MACKAY IN OIL SPILL PROCESSES
C       AND MODELS.
C
C       DECEMBER, 1981
C
C       IERR IS THE ERROR CODE.
C       IERR=1 IS A NORMAL EXIT, IERR=2 IS A PROBLEM IN THE
C       Till.11.-!lt{l)-k;RItoR ROUTINE, IERR=3 IS A STEADY-STATE
C       MOUSSE EXIT.
C
C       IF THE OIL DOES NOT FORM MOUSSE, C2 WAS SET TO -1.
C
      IF(C2.GT.0. ) GO TO 10
C
C       NO MOUSSE FOR THIS OIL, SET TERMS AND RETURN.
C
      W=0.
      VTERM=1.
      GO TO 90
   10 IERR=1
C
C       CHECK TO SEE IF THE WIND OR INCORPORATION RATE CONSTANT
C       CHANGED.
C
      IF(WINDS.EQ.WSAVE.AND.C4.EQ.C4SAVE) GO TO 20
      WSAVE=WINDS
      C4SAVE=C4
      U2=WINDS*WINDS
      C3=C4*U2
   20 EX=C3*TIME
      IF(EX.GT.20.) GO TO 80
      TEST=EXP(-EX )
C
C       BRACKET THE TIME WITH TWO VALUES OF W.
C
      W=0.
      WMAX=1./C2
      WSTEP=WMAX/ 10.
   30 W=W+WSTEP
      TRY=WFUNC(W)
      IF(TRY.LT.TEST) GO TO 40
      IF(W.LT.WMAX) GO TO 30
      IERR=2
      GO TO 90
C
C       NOW DO INTERVAL HALVING TO FIND W.
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.1o) GO TO 50
17280           VTERM=VIS(W)
17290           GO TO 90
17300    80     IERR=3
17310    90     CONTINUE
17320           RETURN
17330           END
```

APPENDIX B

APPENDIX B

Contract No. NA80RAC00018
Research Unit No. 597

OIL-WEATHERING COMPUTER PROGRAM USER’S MANUAL”

for

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

Submitted to:

Outer Continental Shelf Environmental Assessment Program
National Oceanic and Atmospheric Administration

Submitted by:

Bruce E. Kirstein, James R. Payne,
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July 26, 1983

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LOS ANGELES . MCLEAN ● PALOALTO.SANTA BARBARA-SUNNYVALE ● TUCSON

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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:

- evaporation
- dispersion (oil into water)
- mousse (water into oil)
- 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, '$_1$ is a constant in a viscosity equation due to Mooney (Mooney, 1951), '$_2$ 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

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

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

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

User Input Description

The initial input required to perform an oil-weathering calculation is the distillation characterization of the crude oil. The desired input is termed a true-boiling-point (TBP) distillation and consists of distillate cuts of the oil with each cut characterized by its average boiling point and API gravity. For a description of the TBP distillation see Van Winkle (Van Winkle, 1967). An example of a TBP distillation is shown in Table 1 for a typical crude oil.

TBP distillations of crude oils are not always readily available. The more common inspection on crude oil is termed an ASTM (0.86) 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).

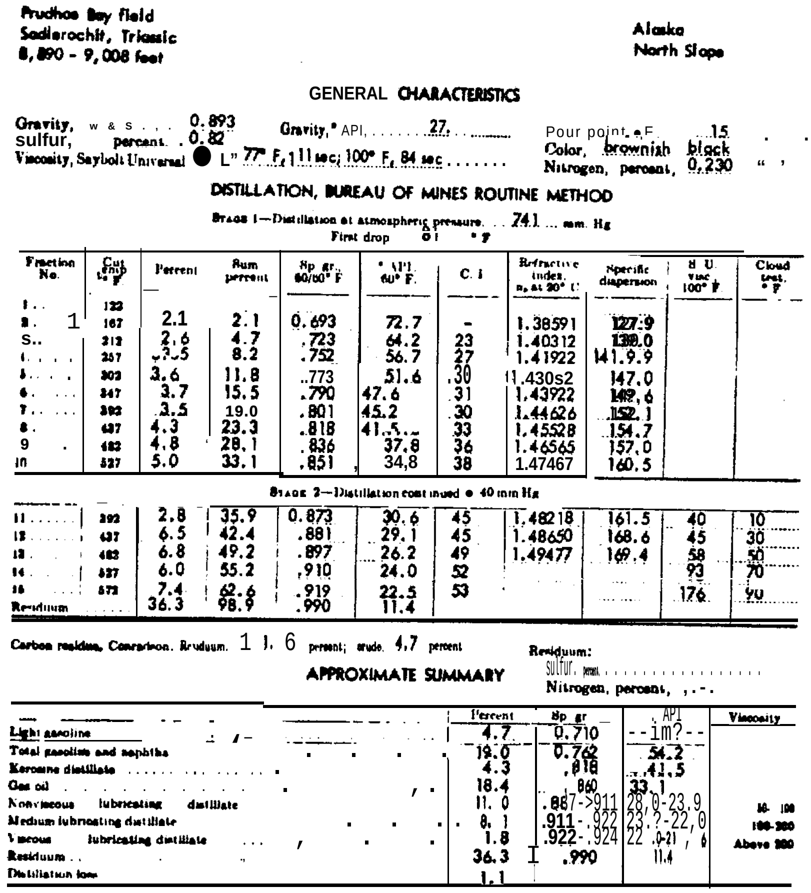
% Distilled	T, °F	API Gravity
0	105	first drop
5	230	63.5
10	300	46.7
20	392	39.0
30	458	34.5
40	505	32.0
50	542	30.8
60	585	27.5
70	640	23.5
80	720	20.4
90	880	13.1
99	1090	----

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 ≥ 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 Atmospheric 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 Gravity, °API, 27. Pour point, °F, 15
Sulfur, percent, 0.82 Color, brownish black
Viscosity, Saybolt Universal at 77° F, 111 sec; 100° F, 84 sec Nitrogen, percent, 0.230

DISTILLATION, BUREAU OF MINES ROUTINE METHOD

Stage 1—Distillation at atmospheric pressure, 741 mm. Hg
First drop [illegible] °F

Fraction No.	Cut temp. °F	Percent	Sum percent	Sp. gr., 60/60° F	°API, 60° F.	C. I	Refractive index, n_D 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	1.43052	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

Fraction No.	Cut temp. °F	Percent	Sum percent	Sp. gr., 60/60° F	°API, 60° F.	C. I	Refractive index, n_D at 20° C	Specific dispersion	S. U. visc., 100° F	Cloud test, °F
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	527	6.0	55.2	.910	24.0	52			93	70
15	572	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	[illegible]	
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.?-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	---

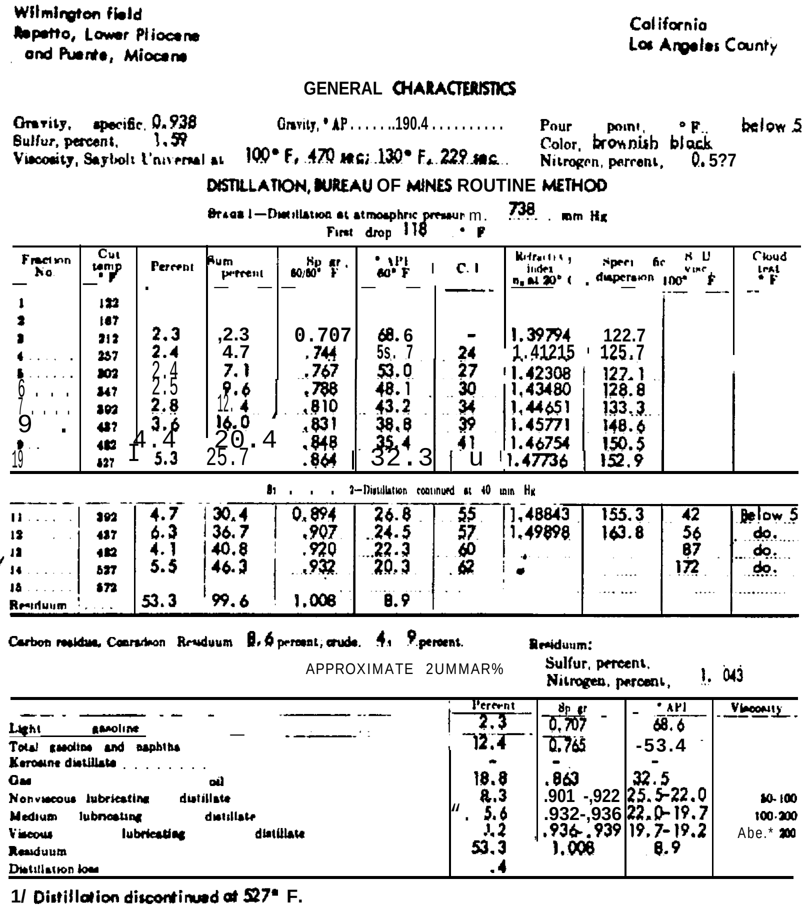
TABLE 3. Distillation Cut Data as Used in Oil-Weathering Calculation (data obtained from Table 2)

```
.EX
LINK:   Loading
[LNKXCT CUTVP2 execution]
ENTER  THE  NUMBER OF TBP  CUTS  TO  BE CHARACTERIZED ON I2
IF  Y(IU  HAVE  NO INPUT DATA  JUST  ENTER  99
A 99 ENTRY  WILL  USE  A LIBRARY  EXAMPLE
9?
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 ....190.4.......... 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, 0.5?7

DISTILLATION, BUREAU OF MINES ROUTINE METHOD

Stage 1—Distillation at atmospheric pressure m. 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, n_D 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	5s. 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		
9	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		
19	527	I 5.3	25.7	.864	32.3	u	1.47736	152.9		

Stage 2—Distillation continued at 40 mm Hg

Fraction No.	Cut temp °F	Percent	Sum percent	Sp. gr. 60/60° F	°API 60° F	C. I.	Refractive index, n_D at 20° C	Specific dispersion	S. U. visc. 100° F	Cloud test °F
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.
1/ 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 8.6 percent; crude 4. 9 percent.

Residuum:
Sulfur, percent,
Nitrogen, percent, 1. 043

APPROXIMATE 2UMMAR%

	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	
Nonviscous lubricating distillate	8.3	.901 -,922	25.5-22.0	50-100
Medium lubricating distillate	// . 5.6	.932-,936	22.0-19.7	100-200
Viscous lubricating distillate	1.2	.936-.939	19.7-19.2	Abe.* 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 FIRESSURE CALCULATION
32.
THE TBP CUTS HAVE BEEN CHARACTERIZED
DO Y(IU 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 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
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
?2222
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 IHE 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 FEE' 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.(5
ENTER VOLUME PER CENT FOR CUT 5
2.

CUT       TB          API        VOL
 1      137.0        71*6        1.5
 2      196.0        5'?*7       2.1
 3      228, 0       55.0        2.0
 4      256.0        53.8        2.0
 5      283.0        4?*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 constants. At this point all input information has been supplied and the calculation proceeds.

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

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

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

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)

$$\mu = \mu_0 \quad \exp \left[\frac{-2.5W}{1-K_1 W} \right]$$

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 $K_2 W < 1$ 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)*

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

TABLE 11. Illustrations of Three 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.
110 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 $\exp(K_4F)$ where F is the fraction weathered (Tebeau, Mackay, et al., 1982) i.e., fresh crude oil has F = O. 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

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

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

TABLE 13. Illustration of Viscosity-Constant Input Options

```
ENTER THE MA SS-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
?
ENTER THE WIND SPEED IN KNOTS
1 0>
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 90
9000,
3.  ENTER  THE  VISCOSITY-FRACTION-OIL-WEATHERED CONSTANT, TRY 10.5
10.5
DO YOU WANT THE  leathering  TO  OCCUR  WITH DISPERSION?
YES
DO Y(IU 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 UISF'ERS1ON 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, U. 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 Dassword must be obtained by calling SAI. Once logged in the code can be executed by typing EX CUTVP2.FOR. The code will then execute and the user will be prompted for input. After an oil-weathering calculation is finished the FORTRAN code will ask the user: DO

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

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

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

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

```
SUMMARY OF TBP CUTS CHARACTERIZATION FOR: PRUDHOE BAY, 0LASKA

CODE VERSION IS CUTVP2 OF  EDR AR  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+02  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  2.80E+00  3  1
10  5.80E+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  3.84E+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
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  5.68E+00  3.17E-01  9.94E+02  4.05E+01  3
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  6

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 H2O= 0.70, WIND**2= 1.00E-03

THE FRACTIONAL SLICK AREA SUBJECT TO DISPERSION IS 4.1 E+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


 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= 7.9 E+03 PI* X2, 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 .   .0E+00 HOURS, MASS FRACTION OF EACH CUT REMAINING:                                                               3
 2.2E-01  6.6E-01  8.1E-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
 1.0E+00
```

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

```
MASS REMAINING =   1.362E+08, MASS 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
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
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
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
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.

```
TIME = 8.2E+01 HOURS, NASS FRACTION OF EACH CUT REMAIRING:                                                                    54
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 13.9 E-01
8.9 E-01
MASS REMAINING = I . 053 E+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
WE IGHT FRACT ION WATER IN 01 L = 7. 0K-0 1, VISCOSITY = 2.2E+05 CENTISTOKES, DISPERSION TERM = 8. 9E-04 WE IGHT FRACTI ON/HR
MASS/ AREA= 4. 5E+02 GMS/M*M , SPGR= 9.1 E-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 S1 ZE OF 5. 000E-01 1S BASED ON CUT 5

TIME = 9.2E+01 HOURS, MASS FRACTION OF EACH CUT REMAINING:                                                                    35
0. 0E+00 O. 0E+00 O. 0E+00 9.1 E-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-0 1
MASS REMA I N I NC =  1 . 040 E+08 , MASS DI SPERSED =  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-0 I , VISCOSITY =  2.6E+05 CENTISTOKES, DISPERSION TERM =  8.8E-04 WEIGHT FRACTION/HR
MASS/AREA= 4. 2E+02 GMS/M*M , SPGR= 9.1 E-0 1 , TOTAL VOLUME= 7.2E+02 BBL, DISPERSION= 3.7E-01 GMS/M*M/HR, EVAP RATE= 1.5E-01 GMS/M*M/HR


TRE CUT NUMBERING BEGINS WITS 1 BASED ON THE ORIGINAL CUT NUMBERS

THE FINAL MASS FRACTIONS FOn TNE SLICK AT 1.0E+02 HOURS ARE:                                                                   56
 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-0 1  8.723E-01  8.725E-01
 8.725E-01  8 . 725E-0 1  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

              V P

 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 INPOT 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          1.932F+01           8.165E+02
   8          1.919E+01           8.112E+02
   9          1.910E+01           8.071E+02
  10          1.1390E+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+01CP

MOUSSE CONSTINTS, MOONEY= 6.20E-01, PIAX H2O= 0.70, WIND**2= 1.00 E-03

THE Factional 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 OUTTUT 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


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= 9.73E-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= 1.7E+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+00GMS/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).

```
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

*****************************************************************
```

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

```
OIL WEATHERING FOR PRUDHOE BAY, ALASKA

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

FOR THE OUTPUT TBAT 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 GRAVIT' , AREA=M*M
THICKNESS=CM, W=PERCENT WATER IN ( IL (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 TEE SL CK
I=FIRST CUT WITH GREATER TBAN 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 $3.90 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 55% (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 leathering 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>
```

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Attachment 1

HOW TO USE TELENET

HOW TO USE TELENET

INFORMATION FOR TERMINAL USERS

WELCOME TO TELENET

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

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

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

TELENET SIGN-ON PROCEDURE

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

STEPS

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

   Example:

   ```
   @ID_LAJOLLA<cr>
   ```

Type in your password:

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

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

Example:

@C_714_20<cr> (for DEC-10]

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

Example:

```
<cr>

SAI banner

PLEASE LOGIN OR ATTACH

LOG_P,PN<cr>

Password . . . . . .<cr>
```

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

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

Hang up the phone to disconnect from Telenet.

* * * $

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

* * * *

CUSTOMER SERVICE

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

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

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

CUSTOMER SERVICE NETWORK ADDRESS - 202 CS

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

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

Boston	(617) 890-0202
Chicago	(312) 298-2188
Los Angeles	(213) 477-2048
New York	(212) 594-6644
Orange County, CA	(714) 891-4481
San Francisco	(415) 854-5845
Washington	(202) 637-7920

EXPLANATION OF NETWORK MESSACES

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 "callerpaid" 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.

LAST UPDATE: 08/09/82

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

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

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

TELENET CUSTOMER SERVICE:
CONTINENTAL USA -- 800/336-0437
IN VIRGINIA -- 800/572-0408
OUTSIDE CONTINENTAL USA -- 703/442-2200

TELEMAIL CUSTOMER SERVICE: 703/442-1900

		300 BPS			1200 BPS
AL%205	BESSEMER	326-3420	{BIRMINGHAM}	(B/V)	326-3420
AL%205	BIRMINGHAM	326-3420		(B/V)	326-3420
AL%205	FLORENCE	766-9101		(B/V)	766-9101
AL 205	HUNTSVILLE	539-2281		(B/V)	539-2281
AL%205	MOBILE	432-1680		(B/V)	432-1680
AL 205	MONTGOMERY	265-1500		(B/V)	265-1500
AL%205	SHEFFIELD	766-9101	<FLORENCE>	(B/V)	766-9101
AK 907	ANCHORAGE	276-0271		(B/V)	276-0271
AK 907	JUNEAU	586-9700		(B/V)	586-9700
AR%501	LITTLE ROCK	372-4616		(B/V)	372-4616
AZ%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

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) (B/V)	694-2710 741-4000
CO#	303	BOULDER	773-8500	{DENVER>	(B/V) (B/V)	694-2710 741-4000
CO%	303	COLORADO SPRINGS	634-5676		(B/V)	635-5361
CO#	303	DENVER	773-8500		(B/V) (B/V)	694-2710 741-4000
CO#	303	LAKEWOOD	773-8500	<DENVER)	(B/V) (B/V)	694-2710 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

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

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		(B/V)	623-0469
NM	505	ALBUQUERQUE	243-7701	<NEWARK)	(B/V)	243-4479
NY	518	ALBANY	445-9111		(B/V)	465-8444
NY	607	BINGHAMTON	772-6642		(B/V)	772-6642
NY	716	BUFFALO	847-0600		(B/V)	847-1440
NY#	516	DEER PARK	667-5566		(B/V)	667-5566
NY	516	HEMPSTEAD	292-0320		(B/V)	292-3800
NY#	212	NEW YORK	785-2540		(B/V)	785-3860
			736-0099		(B/V)	947-9600
NY%	914	POUGHKEEPSIE	473-2240		(B/V)	473-2240

NY 716	ROCHESTER	454-3430		(B/V)	454-1020
NY 518	SCHENECTADY	445-9111	<ALBANY>	(B/V)	465-8444
NY 315	SYRACUSE	472-5503		(B/V)	472-5583
NY 518	TROY	445-9111	<ALBANY>	(B/V)	465-8444
NY 315	UTICA/ROME	797-0920		(B/V)	797-0920
NY 914	WHITE PLAINS	328-9199		(B/V)	328-9199
NC 704	ASHEVILLE	253-3517		(B/V)	253-3517
NC 704	CHARLOTTE	374-0371		(B/V)	332-3131
				(B/V)	377-6065
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)	889-2252
NC 919	RALEIGH	549-8311	<RESEARCH TRI. PARK>	(B/V)	549-813
NC 919	RESEARCH TRI.PARK	549-8311		(B/V)	549-813<
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

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-?907		(B/V)	532-7907
TX 817	FORT WORTH	336-7791		(B/V)	332-4307
TX 7'13	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	7'24-6?17		(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 yes to the question following the echo.

The output presented in Table 2 is the result of the input in Table 1. Reasonable estimates of the input parameters are used in this example from which an important conclusion can be drawn. The important parameters are the (vertical) eddy diffusivity = 185 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 I 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 COEFFICIENTS UNITLESS? TRY 1000
2500.

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

ENTER THE INITIAL OIL-PHASE CONCENTRATIONS 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 = 2 0
9.STEADY STATE APPROXIMATION =  1.00D-02

WANT ?0 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 CM/CC, NUMBER OF TERMS IN THE SERIES = 100, NUMBER OF INTERVAL HALVINGS = [illegible]
SIZE OF LEAD EXPONENTIAL TO APPROXIMATE STEADY STATE =  1.00D-02

      DIMENSIONLESS CONCENTRATIONS AT VARIOUS TIMES AND DEPTHS FOLLOW

      METERS    HOURS      HOURS      HOURS      HOURS      HOURS      HOURS      HOURS      HOURS      HOURS      HOURS
              8.82D-01   2.07D+00   4.86D+00   1.14D+01   2.68D+01   6.30D+01   1.48D+02   3.48D+02   8.17D+02   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   1.88D-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   9.96D-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      HOURS      HOURS      HOURS      HOURS      HOURS      HOURS      HOURS      HOURS      HOURS
              8.82D-01   2.07D+00   4.86D+00   1.14D+01   2.68D+01   6.30D+01   1.48D+02   3.48D+02   8.17D+02   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

     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   5.55D-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 =  20
SIZE OF LEAD EXPONENTIAL TO APPROXIMATE STEADY STATE =  1.00D-02

       DIMENSIONLESS CONCENTRATIONS AT VARIOUS TIMES AND DEPTHS FOLLOW

       METERS   HOURS     HOURS     HOURS     HOURS     HOURS     HOURS     HOURS     HOURS     HOURS     HOURS
               7.01D-01  1.31D+00  2.44D+00  4.55D+00  8.50D+00  1.59D+01  2.96D+01  5.52D+01  1.03D+02  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  ?'.6s0-81  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.am-cl  a.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  4.23041   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  a.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  ?.6s0-48  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     HOURS     HOURS     HOURS     HOURS     HOURS     HOURS     HOURS     HOURS     HOURS
               7.01D-01  1.31D+00  2.44D+00  4.55D+00  8.50D+00  1.59D+01  2.96D+01  5.52D+01  1.03D+02  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  1.750-01  3.10D-01  5.29D-01  8.48D-01  1.22D+00  1.53D+00  1.65D+00
         t.@   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   a.79D-02  5.16D-02  9.48D-02  1.72D-01  3.07D-01  5.27D-01  a.46D-81  1.22D+00  1.53D+00  1.65D+00
         2.5   2.71D-02  5.08D-02  9.40D-02  8.720-61  3.06D-01  5.26D-01  S.46D-61  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  I.53D+00  1.65D+00
         4.0   a.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  9.230-02  1.70D-01  3.05D-01  5.25D-01  8.45D-01  o.22D+00  1.53D+00  1.65D+00
         5.0   a.53D-02  4.89D-02  9.22D-02  1.70D-01  3.05D-01  0.2s0-01  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.   2.722-92  5.14D-02  9.46D-02  1.72D-01  3.07D-01  5.27D-01  8.460-01  1.22D+00  1.53D+00  1.65D+00
     THE MASSES THAT FOLLOW ARE IN GRAMS/CM*CM, THE FLUX 161 IN GRAMS/CM*CM/SEC

      MASS IN
        OIL    4.99D-03  4.97D-03  4.95D-03  4.91D-03  4.85D-03  4.740-02  4.58D-03  4.39D-03  4.24D-03  4.17D-03

      MASS IN
       WATER   1.39D-05  a.57D-05  4.730-06  8.61D-05  1.53D-04  a.63D-04  4.220-84  6.11D-04  7.63D-04  8.25D-04

      MASS FLUX
     AT SURFACE 0.450-99 5.970-49  6.220-09  4.970-69  4.52D-09  3.79D-09  2.73D-09  1.48D-09  4.700-00  5.84D-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.

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

```
      IMPLICIT REAL*8  (A-H,O-Z)
      REAL*8 L,LCM,LCM2,M,KZ,KZS,KH,KPRME,MOIL,MWATER
      REAL*8 LTIME
      COMMON /TRANS/ KH,HCAP
      DIMENSION ALPHA(300),ALPHA2(300),P(300) ,CWP(300)
      DIMENSION CTD(11, 10),XP( 11),TIMEP( 10),COIL(10)
      DIMENSION WATER(10),MWATER(10),MOIL(10) ,FLUX(10)
      DIMENSION A2P(300)
      DATA PIE,ETEST/3.1415926536D0,30.D0/
      OPEN(UNIT=32,DIALOG= 'DSKD:DISOLV.OUT' )
      IOU=32
C
C       THIS CODE CALCULATES THE WATER-COLUMN CONCENTRATION
C       OF A SPECIFIC COMPOUND DISSOLVING INTO TEE WATER
C       FROM AN OIL SLICK
C
C       OCTOBER, 19s2
C
      TYPE 10
10    FORMAT(/,1X,'ENTER THE EDDY DIFFUSIVITY, CM*CM/SEC
     1, TRY 100')
      ACCEPT 20,DW
20    FORMAT(F10.0)
      TYPE    30
30    FORMAT(/,1X,'ENTER THE SLICK THICKNESS, TRY 1 CM*)
      ACCEPT 20, DELTA
      TYPE 40
40    FORMAT(/,1X, 'ENTER THE OCEAN DEPTH, TRY 20 METERS')
      ACCEPT 20, L
      TYPE 50
50    FORMAT(/,1X,'ENTER THE OIL/WATER PARTITION COEFFICIENT
     1, UNITLESS, TRY 1000')
      ACCEPT 20, M
      TYPE 60
60    FORMAT(/,1X,'ENTER TEE OIL-WATER OVER-ALL MASS-
     1TRANSFER COEFFICIENT, TRY 1 CM/HR')
      ACCEPT 20, KZ
      TYPE 70
70    FORMAT(/,1X,'ENTER TEE INITIAL OIL-PEASE CONCENTRATION
     1, GM/CC, TRY 0●el'}
      ACCEPT 20, CZ
      TYPE 80   '
80    FORMAT(/,1X,'ENTER THE NUMBER OF TERM IN THE SERIES
     1, ON I3, TRY 100')
      ACCEPT 90, NTERM
90    FORMAT(I3)
      TYPE 100
100   FORMAT(/,1X,'ENTER TEE NUMBER OF INTERVAL HALVINGS
     1 To USE, ON I2, TRY 20')
      ACCEPT 90, NHALF
      TYPE 110
110   FORMAT(/,1X,'ENTER VALUE FOR LEAD EXPONENTIAL
     1 FOR STEADY STATE APPROXIMATION,',/
     2,1X,'TRY 0.01')
      ACCEPT 20, ELEAD
120   TYPE 130, DW
130   FORMAT(/,1X,'1.  EDDY  DIFFUSIVITY = ',1PD9.2,' CM*CM
     1/SEC') '.
      TYPE 140, DELTA
140   FORMAT(1X,'2. SLICK THICKNESS = ',F5.2,  *  CM')
      TYPE 150, L
150   FORMAT(1X,'3. OCEAN DEPTH          = ',F5.1,' METERS')
      TYPE 160, M
160   FORMAT(1X,'4. OIL/WATER PARTITION = ',1PD9.2,' UNIT
     1LESS' )
      TYPE 170, KZ
```

```
 170   FORMAT(1X,'5. MASS TRANSFER K      = ',1PD9.2', CM
      1/HR')
       TYPE 180, CZ
 180   FORMAT(1X,'6. INITIAL OIL CONC.    = ',1PD9.2,' GM/CC')
       TYPE 190, NTERM
 190   FORMAT(1X,'7. NTERM = ',I3)
       TYPE 200, NHALF
 200   FORMAT(1X,'8. NHALF = ',I3)
       TYPE 210, ELEAD
 210   FORMAT(1X,'9. STEADY STATE APPROXIMATION = ',1PD9.2)
       TYPE 220
 220   FORMAT(/,1X,'WANT TO CHANGE ANY?')
       ACCEPT 230, ANS
 230   FORMAT(A1)
       IF(ANS.EQ.'N') GO TO 350
       TYPE 240
 240   FORMAT(/,1X,'ENTER THE LINE NUMBER TO BE CHANGED')
       ACCEPT 250, LINE
 250   FORMAT(I1)
       GO TO (260,270,280,290,300,310,320,330,340) LINE
 260   TYPE 10
       ACCEPT 20., DW
       GO TO  120
 270   TYPE 30
       ACCEPT 20, DELTA
       GO TO 120
 280   TYPE 40
       ACCEPT 20, L
       GO TO 120
 290   TYPE 50
       ACCEPT 20, M
       GO TO 120
 300   TYPE 60
       ACCEPT 20, KZ
       GO TO 120
 310   TYPE 70
       ACCEPT 20, CZ
       GO TO 120
 320   TYPE 80
       ACCEPT 90, NTERM
       GO TO 120
 330   TYPE 100
       ACCEPT 90, NHALF
       GO TO 120
 340   TYPE 110
       ACCEPT 20, ELEAD
       GO TO 120
C
C        CALCULATE THE PARAMETERS
C
 350   KZS=KZ/3600.D0
       H=KZS/DW
       LCM=100.D0*L
       LCM2=LCM*LCM
       HCAP=LCM*H
       KPRME=LCM/(M*DELTA)
       TDL=DW/LCM2
       HCAP2=HCAP*HCAP
       OSUM=2.D0*KPRME*HCAP2
       WSUM=2.D0*HCAP2
       FLEAD=2.D0*DW*HCAP2/LCM
       CLEAD=1.D0/(1.D0+KPRME)
       XSTEP=LCM/10.D0
       ESIZE=DLOG(ELEAD)
       ESIZE=DABS(ESIZE)
       WRITE (IOU,360)
```

```
 360  FORMAT(1H1 ,5X, 'WELL-STIRRED OIL SLAB
     1 IN CONTACT WITH A DIFFUSION SLAB')
      WRITE(IOU,370) DW,DELTA, L
 370  FORMAT(1X, 'EDDY D IFFUSIVITY = ',1PD10.3
     i,' CM*CM/SEC, OIL SLICK THICKNESS = ', 0PF5.2
     2,' CM, OCEAN DEPTH = ',F5.1,' MEI'ElW')
      WRITE (IOU,380) M,KZ
 380  FORMAT(1X,'OIL/WATER SPECIES PARTITION COEFFICIENT =
     1,1PD10.3,' UNITLESS, OIL-WATER OVER-ALL MASS TRANSFER
     2 COEFFICIENT =● , lPDie.3,' CM/HR')
      WRITE (IOU,390) CZ,NTERM,NHALF
 390  FORMAT(1X,' INITIAL SPECIES OIL-PHASE CONCENTRATION
     1 = ',1PD10.3,' GM/CC, NUMBER OF TERMS IN THE SERIES =
     2,I3,', NUMBER OF INTERVAL HALVINGS = ',I3)
      WRITE (IOU,400) ELEAD
 400  FORMAT(1X,'SIZE OF LEAD EXPONENTIAL TO
     1 APPROXIMATE STEADY STATE= ',1PD9.2)
C
C       CALCULATE THE ROOTS OF THE TRANSCENDENTAL FUNCTION,
C       ORE ROOT PER PIE
C
C       THE TRANSCENDENTAL FUNCTION IS:
C
C       F(X)=X*COTANGENT(X)-(X*X-KH)/HCAP
C
      CMSUM=0 . D0
      P1=KPRME*HCAP*HCAP*(1.D0+KPRME)
      P2=HCAP*HCAP+HCAP-2 .D0*KPRME*HCAP
      WRITE (IOU,410) P2,P1
 410  FORMAT(/,1X,'P = ALPHA**4 + ',1PD13.6,
     1'*ALPHA**2 + ',1PD13.6)
      KH=KPRME*HCAP
      WRITE (IOU,420) HCAP,KPRME,KH
 420  FORMAT(/,1X,'HCAP = ',1PD10.3,', K-PRIME = ',1PD10.3
     1,', KH = ',1PD10.3)
      CNORM=CZ/M
      CNORM6=(1.D+06)*CNORM
      DELTCZ=DELTA*CZ
      CNORML=CNORM*LCM
      FLEAD=FLEAD*CNORM
      WRITE (IOU,430) CNORM,CNORM6
 430  FORMAT(/,1X,'THE NORMALIZING CONCENTRATION IS '
     1,1PD10.3,' GM/CC, OR ',1PD10.3,' PPM')
      WRITE (IOU,440) DELTCZ
 4449 FORMAT(/,1X,'INITIAL MASS/AREA OF TRANSPORTABLE
     1 SPECIES = ',1PD9.2,' GRAM/CM*CM')
      DO 470 N=1,NTERM
      AN=DFLOAT(N)
      AN1=DFLOAT(N-1)
      XL=AN1*PIE
      XL1=XL
      XU=AN*PIE
      XU1=XU
      DO 460 I=1,NHALF
      XT=(XL+XU)/2.D0
      TEST=F(XT)
      IF(TEST.LT.0.D0) GO TO 450
      XL=XT
      GO TO 460
 450  XU=XT
 460  CONTINUE
C
C       CALCULATE OTHER PERTINENT QUANTITIES INVOLVING
C       TEE ALPHA ROOTS
C
      ALPHA(N)=XT
```

```
      CALPHA=DCOS(XT)
      ALPHA2(N)=XT*XT
      P(N)=ALPHA2(N)*(ALPHA2(N)+P2)+P1
      A2P(N)=ALPHA2(N)/P(N)
      CWP(N)=(ALPHA2(N)-KH)/(P(N)*CALPHA)
      CMSUM=CMSUM+1.D0/P(N)
  470 CONTINUE
      CL6=CNORM6*CLEAD
      WRITE (IOU,480) CLEAD,CL6
  480 FORMAT(//,5X,'THE CONSTANT TERM IN THE CONCENTRATION
     1 EXPRESSIONS IS = ',1PD9.2,' UNITLESS, OR ',1PD9.2
     2,' PPM')
      WRITE (IOU,490)
  490 FORMAT(5X,'WHICH IS THE STEADY STATE WATER CON
     1CENTRATION')
      DTIME=ESIZE/ALPHA2(1)
      STIMES=LCM2*DTIME/DW
      STIMEH=STIMES/3600.D0
      WRITE (IOU,500) STIMES,STIMEH
  500 FORMAT(/,5X,'STEADY STATE TIME = ',1PD10.3,' SEC
     1, OR ',1PD10.3,' HOURS')
      CMSUM=2.D0*KPRME*HCAP*HCAP*CMSUM
      CMZERO=CLEAD+CMSUM
      WRITE (IOU,510) CMZERO
  510 FORMAT(/,5X,'THE TIME=0 DIMENSIONLESS CONCENTRATION
     1 IN THE OIL = ',1PD13.6)
C
C         NOW COMPUTE SOME CONCENTRATION PROFILES AT TIMES
C         BEFORE STEADY STATE
C
      XSTEP=L/10.D0
      TSLOG=(DLOG10(DTIME))/10.D0
      TSCALE=LCM2/(3600.D0*DW)
      LTIME=0.D0
      DO 570 ITIME=1,10
      LTIME=LTIME+TSLOG
      TIME=10.D0**LTIME
      TIMEP(ITIME)=TSCALE*TIME
      X=0.D0
      DO 540 JX=1,11
      XARG=1.D0-X/L
      SUM=0.D0
      DO 520 N=1,NTERM
      XCARG=ALPHA(N)*XARG
      COSINE=DCOS(XCARG)
      EARG=ALPHA2(N)*TIME
      IF(EARG.GT.ETEST) GO TO 530
      SUM=SUM+CWP(N)*COSINE*DEXP(-EARG)
  520 CONTINUE
  530 SUM=CLEAD-2.D0*HCAP*SUM
      CTD(JX,ITIME)=SUM
      XP(JX)=X
      X=X+XSTEP
  540 CONTINUE
C
C         CALCULATE THE OIL CONCENTRATION ALSO FOR THE GIVEN
C         TIME, AND THE AVERAGE WATER CONCENTRATION
C
      SUM=0.D0
      FSUM=0.D0
      DO 550 N=1,NTERM
      EARG=ALPHA2(N)*TIME
      IF(EARG.GT.ETEST) GO TO 560
      EXTERM=DEXP(-EARG)
      SUM=SUM+EXTERM/P(N)
      FSUM=FSUM+A2P(N)*EXTERM
```

```
550   CONTINUE
560   COIL(ITIME)=CLEAD+OSUM*SUM
      WATER(ITIME)=CLEAD-WSUM*SUM
      FLUX(ITIME)=FLEAD*FSUM
570   CONTI NUE
      WRITE (IOU, 580)
580   FORMAT(//,5X,'DIMENSIONLESS CONCENTRATIONS AT
     1 VARIOUS TIMES AND DEPTHS FOLLOW')
      WRITE (IOU,590)
590   FORMAT(/,5X,'METERS',3X,'HOURS',9(6X, 'HOURS'))
      WRITE (IOU,600) (TIMEP(I), I=1,10)
600   FORMAT( 10X, 10(2X,1PD9.2) ,/)
      DO 630  JX=1,11
      WRITE (IOU,610) XP(JX), (CTD(JX,I),I=1, 10)
610   FORMAT(5X,F5. 1,10(2X,1PD9.2) )
      DO 620 I=1,10
      CTD(JX, I)=CNORM6*CTD(JX, 13
620   CONTI NUE
630   CONTI  m
      WRITE (IOU,640) (COIL(I),I=1,10)
640   FORMAT(/,6X,'OIL' ,/,5X,'CONC.' ,10(2X,1PD9.2))
      WRITE (IOU,650) (WATER(I), I=1,10)
650   FORMAT(/,4X,'AVERAGE',/,5X, 'WATER',/,5X,'CONC.'
     1,10(2X,1PD9.2))
      WRITE (IOU,660)
660   FORMAT(//,5X,'ACTUAL CONCENTRATIONS IN PPM
     i AT VARIOUS TIMES AND DEPTHS')
      WRITE (IOU,590)
      WRITE (IOU,600) (TIMEP(I),I=1,10)
      DO 670 JX=1,11
      WRITE (IOU,610) XP(JX), (CTD(JX,I),I=1,10)
670   CONTI NUE
C
C       CALCULATE THE OVER-ALL MASS BALANCE TO SEE THAT
C       ALL THE MASS IS ACCOUNTED FOR
C
      CZ6=CZ*(1.D+06)
      DO 680 I=1,10
      MOIL(I)=DELTCZ*COIL(I)
      MWATER(I)=CNORML*WATER(I)
      COIL(I)=CZ6*COIL(I)
      WATER( I)=CNORM6*WATER( I)
680   CONTI NUE
      WRITE (IOU,640) (COIL(I),I=1,10)
      WRITE (IOU,650) (WATER(I),I=1,10)
      WRITE (IOU,690)
690   FORMAT(/,1X,'THE MASSES TEAT FOLLOW ARE IN CRAMS
     1/CM*CM. THE FLUX IS IN GRAMS/CM*CM/SEC')
      WRITE (IOU,700) (MOIL(I), I=1,10)
700   FORMAT(/,4X,'MASS IN',/,6X,'OIL',1X
     1,10(2X,1PD9.2))
      WRITE (IOU,710) (MWATER(I),I=1,10)
710   FORMAT(/,4X,'MASS IN',/,5X,'WATER',10(2X,1PD9.2))
      WRITE (IOU,720) (FLUX(I),I=1,10)
720   FORMAT(/,3X,'MASS FLUX',/,2X,'AT SURFACE'
     1,1PD9.2,9(2X,1PD9.2))
      TYPE 730
730   FORMAT(/,1X,'DO IT AGAIN?')
      ACCEPT 230, ANS
      IF(ANS.EQ.'Y') GO TO 120
      END
      DOUBLE PRECISION FUNCTION F(X)
      IMPLICIT REAL*8 (A-H,O-Z)
      REAL*8 KH
      COMMON /TRANS/ KH,HCAP
      SINE=DSIN(X)
      COSINE=DCOS(X)
      F=X*COSINE/SINE-(X*X-KH)/HCAP
      RETURN
      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 <u>time-varying flux</u> (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 EXPONENTIAL.
AN EXAMPLE DERIVED FROM THE OIL-FEATHERING CODE FOR A
DISPERSION FLUX (20-KNOT WIND)FITTED WITH TWO EXPONENTIAL 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 13
100

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

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

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

 6.  A(1)   = 6.400D-08 GM/CM*CM/SEC

 7* B(1) =  2.030D-06 1/SEC

 8. A(2) =  5.100D-07 GM/CM*CM/SEC

 9. E(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.

```
      IMPLICIT REAL*8 (A-H,O-Z)
      REAL*8 K,L,L2,KP2L,KP2LN
      DIMENSION  AI(5),BI  (5),C(10.10,5)  ,ABL(5),TIME(10)
     1,SINGLE(5),SQRTBK(5) ,SQRTKB(5) ,BD(500,5),KP2LN(500)
     2,RATE( 10),GRAMS(10,5) ,ACONC( 10,5),A10(5).B10( 5)
     3,A20(5) ,B20(5),A40(5)  ,B40{5)  .S(10.10,5),SZERO( 10,5)
     4,CZEIM3( 10,5),XP(11}
      DATA A10/1.89D-07,2.03D-08,3*0.D0/
      DATA B10/1.436D-05,1.02D-06 ,3*0.D0/
      DATA A20/6.4D-08,5.1D-07,3*0 .D0/
      DATA B20/2.03D-06,3.19D-05,3*0 .D0/
      DATA A40/1.12D-07,4.04D-07 ,3*0.D0/
      DATA B40/3.055D-06,9.26D-06 ,3*0.D0/
      DATA ETRAP,PIE,PIE2/50.D0,3  .141592654,9.869604401/
C
C       THIS Is A CODE TO CALCULATE THE WATER-COLUMN
C       CONCENTRATION OF DISPERSED OIL WITH A FLUX BOUNDARY
C       CONDITION
C
C       DECEMBER, 1982
C
      OPEN(UNIT=33,DIALOG= 'DSKD:DSFLUX.OUT' )
      IOU=33
      TYPE 10
10    FORMAT(/,1X,'DO YOU WANT DETAILED INPUT INSTRUCTIONS?')
      ACCEPT 460, ANS
      IF(ANS.EQ. 'N') GO TO 120
      TYPE 20
20    FORMAT(/,1X,'THIS CODE CALCULATES THE WATER-COLUMN
     1 CONCENTRATION OF DISPERSED OIL.')
      TYPE 30
30    FORMAT(1X,'YOU MUST ENTER THE FLUX AT THE SURFACE IN
     1 THE FORM OF A*EXP(-B*TIME).')
      TYPE 40
40    FORMAT(1X, 'YOU CAN ENTER THE FLUX AS A SUM OF THESE
     1 EXPONENTIAL.')
      TYPE 50
50    FORMAT(1X,'AN EXAMPLE DERIVED FROM TRE OIL-WEATHERING
     1 CODE FOR A')
      TYPE 60
60    FORMAT( 1X, 'DISPERSION FLUX (20-KNOT WIND) FITTED WITH
     1 TWO EXPONENTIALS IS:')
      TYPE 70
70    FORMAT( 1X, 'A(1)=6.4D-08 CM/CM*CM/SEC')
      TYPE 80
80    FORMAT(1X, 'B(1 )=2.03D-06 INVERSE SECONDS')
      TYPE 90
90    FORMAT(1X, 'A(2)=5.1D-07')
      TYPE 100
100   FORMAT(1X, 'B(2)=3.19D-05')
      TYPE 110
110   FORMAT(1X,'FOR THE NUMBER OF TERMS IN THE SERIES,
     1 USE 100')
120   TYPE 130
130   FORMAT(/,1X,'ENTER THE VERTICAL DIFFUSIVITY, CM*CM
     1 /SEC ' )
      'ACCEPT 140, K
140   FORMAT(F10.0)
      TYPE 150
150   FORMAT(/,1X,'ENTER THE OCEAN DEPTH, METERS')
      ACCEPT 140, DEPTH
      TYPE 160
160   FORMAT(/,1X,'ENTER THE MAXIMUM TIME. HOURS')
      ACCEPT 140. HOURS
      TYPE  170 '
170   FORMAT(/, 1X,'ENTER THE NUMBER OF TERMS IN THE SERIES
```

TABLE 2. (Continued)

```
      1 ON 13')
       ACCEPT 180, NTERM
180    FORMAT( 13 )
       LIB=1
       TYPE 190
190    FORMAT (/, 1X,'DO YOU WANT PREVIOUSLY STORED DISPERSION
      1 RATE COEFFICIENTS TO BE USED')
       TYPE 200
200    FORMAT(1X,'FOR A 10-, 20-, OR 40-KNOT WIND?')
       ACCEPT 460, ANS
       IF(ANS.EQ.'N') GO TO 270
       NEF=2
       LIB=2
       TYPE 210
210    FORMAT(/,1X,'ENTER 10. 20 OR 40 FOR THE WIND SPEED
      1 YOU WANT')
       ACCEPT 140, WIND
220    IF(WIND.EQ.40. ) GO TO 250
       IF(WIND.EQ.20.) GO TO 260
       IF(WIND.EQ.10. ) GO TO 240
       TYPE 230
230    FORMAT(/,1X,'YOU MUST ENTER 10, 20 OR 40. BUT
      1 YOU CAN ENTER 0 TO ENTER THE DATA YOURSELF')
       ACCEPT 140, WIND
       IF(WIND.EQ.0. ) GO TO 270
       GO TO 220
240    AI(1)=A10(1)
       BI(1)=B10(1)
       AI(2)=A10(2)
       BI(2)=B10(2)
       GO TO 360
250    AI(1)=A40(1)
       BI(1)=B40(1)
       AI(2)=A40(2)
       BI(2)=B40(2)
       GO TO 360
260    AI(1)=A20(1)
       BI(1)=B20(1)
       AI(2)=A20(2)
       BI(2)=B20(2)
       GO TO 360
270    TYPE 280
280    FORMAT(/,1X,'ENTER THE NUMBER OF EXPONENTIAL FITS ON I1')
       ACCEPT 290, NEF
290    FORMAT(I1)
       IF(NEF.LT.5) GO TO 320
       TYPE 300
300    FORMAT(/,1X,'THE NUMBER OF EXPONENTIAL FITS MUST
      1 BE 4 OR LESS.')
       TYPE 310
310    FORMAT(1X,'AND THIS NUMBER HAS BEEN RESET TO 4')
       NEF=4
320    DO 350 I=1,NEF
       TYPE 330, I
330    FORMAT(/,1X,'ENTER A( ',11,'), CM/CM*CM/SEC')
       ACCEPT 140, AI(I)
       TYPE 340, I
340    FORMAT(/,1X,'ENTER B( ',11,"), 1/SEC')
       ACCEPT 140, BI(I)
350    CONTINUE
360    TYPE 37$3, K
370    FORMAT(/,2X,'1.  VERTICAL K = ',1PD1O.3,' CM*CM/SEC')
       TYPE 380, DEPTH
380    FORMAT(2X, '2.  OCEAN DEPTH = ',F5.1,' METERS")
       TYPE 390, HOURS
390    FORMAT(2X, '3.  MAXIMUM TIME = ',F5.0,' HOURS')
```

TABLE 2. (Continued)

```
         TYPE 400, NTERM
  400    FORMAT(2X, '4.  NUMBER OF TERMS IN THE SERIES = '
        1,13)
         TYPE410, NEF
  410    FORMAT(2X,'5.  NUMBER OF EXPONENTIAL FITS = '.12}
         IROW=5
         DO 440 I=1,NEF
         IROW=IROW+1
         TYPE 420, IROW,I,AI(I)
  420    FORMAT(/,1X,I2,'. A( ',11,') = ',1PD10.3.' GM
        1/CM*CM/SEC' )
         IROW=IROW+1
         TYPE 430, IROW,I,BI(I)
  430    FORMAT(/,1X,I2,'. B( ',11,') = ',1PD10.3," 1/SEC')
  440    CONTINUE
         TYPE 450
  4.50   FORMAT(/,1X,'WANT TO CHANGE ANY?')
         ACCEPT 460, ANS
  460    FORMAT(A1)
         IF(ANS.EQ. 'N') GO TO 550
         TYPE 470
  470    FORMAT(/,1X,'ENTER TEE LINE NUMBER TO BE CHANGED')
         ACCEPT 290, ICHNG
         IF(ICHNG.GT.5) GO TO 530
         GO TO (480,490,500,510,520), ICHNG
  480    TYPE 130
         ACCEPT 140, K
         CO TO 360
  490    TYPE 150
         ACCEPT 140, DEPTH
         GO TO 360
  500    TYPE 160
         ACCEPT 140, HOURS
         GO TO 360
  510    TYPE 170
         ACCEPT 180, NTERM
         GO TO 360
  520    TYPE 280
         ACCEPT 290, NEF
         IF(NEF.LT.5) GO TO 360
         TYPE 300
         TYPE 310
         NEF = 4
         GO TO 360
 C
 C          IS ICHNG EVEN OR ODD?
 C
  530    Z=DFLOAT(ICHNG )
         D=Z/2 . D0
         M=D
         E=DFLOAT(M)
         TEST=DABS(E-D )
         IF(TEST.GT.0. 1D0) GO TO 540
 C
 C          ICHNG IS EVEN, ENTER AI(J)
 C
         I=(ICHNG-4)/2
         TYPE 330, I
         ACCEPT 140, AI(I)
         GO TO 360
  540    I=(ICHNG-5)/2
 C
 C          ICHNG IS ODD, ENTER BI(J)
 C
         TYPE 340, I
         ACCEPT 140, BI(I)
```

```
      GO TO 360
550   CONTINUE
      GO TO (560,610) LIB
560   TYPE 570
570   FORMAT(/,1X,'THE WIND SPEED IS USED FOR IDENTIFICATION
     1 PURPOSES, ')
590      TYPE 580
580   FORMAT(1X,'SO ENTER TBE WIND SPEED IN KNOTS')
        ACCEPT 140, WIND
      TYPE 600, WIND
600   FORMAT(/,1X,'YOU ENTERED ',F5.0,' KNOTS. IS THIS
     1 OK?')
      ACCEPT 460, ANS
      IF(ANS.EQ. 'N') GO TO 590
C
C        CALCULATE THE CONTRIBUTION FOR THE WATER-COLUMN
C        CONCENTRATION FOR EACH A,B SET
C
C        THE CONCENTRATION ARRAY IS SET UP SO THAT THE:
C             ROW INDEX IS DEPTH
C             COLUMN INDEX 1S TIME
C             LEVEL INDEX IS A,B SET NUMBER = J
C
C
C        CONVERT THE TIME TO SECONDS
C
610   TSEC=3600.D0*HOURS
      TSTEP=TSEC/ 10.DO
C
C        *************************************************
C
C        WARNING: THE, COORDINATE FRAME FOR THIS PROBLEM IS
C        REVERSED, I.E., THE OCEAN BOTTOM IS AT X=0, THE SURFACE
C        1S AT X=L
C
C        *******************************************************
C
C        CONVERT THE DEPTH TO CENTIMETERS
C
      L=100.D0*DEPTH
      XSTEP=L/10.D0
      L2=L*L
      KP2L=K*PIE2/L2
      PIEL=PIE/L
C
C        THE J INDEX RUNS THE A,B SET NUMBER
C
      WRITE (IOU,620)
620   FORMAT( 1H1,4X, 'CONCENTRATION OF DISPERSED OIL IN THE
     1 WATER COLUMN, CALCULATED BY EXPONENTIAL FITS TO A GIVEN
     2 DISPERS1ON RATE')
      WRITE (IOU,630) K,DEPTH,HOURS
630   FORMAT(/, 5X, 'VERTICAL DIFFUSIVITY = ',1PD10.3
     1.' CM*CM/SEC, DEPTH = ',0PF6.0,' METERS, MAXIMUM
     2 TIME = ',F6.0,' HOURS')
      WRITE (IOU,640) KP2L
640   FORMAT(/,5X,'K*PIE*PIE/L/L = ',1PD10.3
     1,' 1/SEC' )
      WRITE (IOU,650) NTERM,NEF
650   FORMAT(/,5X,'NUMBER OF TERMS IN THE SERIES = '
     1,14,', NUMBER OF EXPONENTIAL FITS = ',I2)
      WRITE (IOU,660)
660   FORMAT(/,5X,'THE EXPONENTIAL FIT COEFFICIENTS
     1 FOR TBE DISPERSION RATE (RATE=A*EXP(-B*TIME)) ARE:')
      WRITE (IOU,670)
670   FORMAT(5X,'UNITS ARE A==GM/CM*CM/SEC, B==1/SEC')
```

```
            WRITE (I OU,680)
      680   FORMAT(/,24X,'AI(J)',15X,'BI(J)')
            DO 700 J=1,NEF
            WRITE (IOU,690) J,AI(J),BI(J)
      690   FORMAT( 10X,I1,2(10X,1PD10 .3))
      700   CONT I RUE
C
C             SET UP THE TIME STEPS FOR PRINTING
C
            TS=HOURS/10 .D0
            T=0.D0
            DO 710 IT=1,10
            T=T+TS
            TIME(IT)=T
      710   CONTINUE
C
C             WRITE OUT WHAT THE DISPERSION RATES ARE FOR THE
C             A,B DATA SETS SO YOU CAN TELL IF YOU GOT
C             THE CORRECT INPUT
C
            WRITE (IOU,720) WIND
      720   FORMAT(/,5X,'THE DISPERSION RATE FROM THE ABOVE
          1 A,B DATA SET FOR A WIND SPEED OF',F5.0,' KNOTS IS:')
            WRITE (IOU,730)
      730   FORMAT(/,18X,'TIME',11X,'RATE")
            WRITE (IOU,740)
      740   FORMAT(18X,'HOUR' ,9X,'GM/M*M/HR' )
            T=0.D0
            DO 770 IT=1,10
            T=T+TSTEP
            RATE (IT)=0.D0
C
C             NOW CALCULATE THE CONTRIBUTIONS TO THE
C             CONCENTRATION PROFILE FOR EACH A,B INPUT SET
C
            DO 750 J=1,NEF
            TARG=T*BI(J)
            IF(TARG.GT.ETRAP) GO TO 750
            RATE(IT)=RATE( IT)+AI(J)*DEXP(-TARG)
      750   CONT I NUE
C
C             CONVERT THE RATE TO GM/M*M/HR AND PRINT IT
C
            RATE(IT)=RATE( IT)*(3.6D+07)
            WRITE (IOU,760) TIME(IT),RATE(IT)
      760   FORNAT(1$3X,2(5X,1 PD10 .3))
      770   CONT I NUE
C
C             BEGIN CALCULATING J CONTRIBUTIONS TO THE WATER-
C             COLUMN CONCENTRATIONS OF DISPERSED OIL
C
            DO 780 I=1,10
            GRAMS(I,5)=0.D0
            ACONC(I,5)=0.D0
            CZERO(I,5)=0.D0
            SZERO(I,5)=0.D0
            DO 780 J=1,10
            C(I,J,5)=0.D0
            S(I,J,5)=0.D0
      780   CONTINUE
            DO 1100 J=1,NEF
C
C             ABL(J) IS TRE LEAD CONSTANT FOR CONCENTRATION
C
            ABL(J)=AI(J)/(BI(J)*L)
            SQRTBK(J )=DSQRT(BI(J )/K)
```

TABLE 2. (Continued)

```
      SQRTKB(J)=DSQRT(K*BI(J))
      ARG=L*SQRTBK(J)
      WRITE (IOU,790) ABL(J)
790   FORMAT(/,5X,'THE TIME = INFINITY WATER-COLUMN
     1 CONCENTRATION OF DISPERSED OIL = ',1PD10.3
     2,' GM/CC')
      WRITE (IOU,800) J
800   FORMAT(/,5X,'A CHECK OF THE INITIAL CONDITIONS FOR
     1 THE J =',I2,'    A,B INPUT SET')
      WRITE (IOU,810)
810   FORMAT(/,15X,'DEPTH',10X,'EBL',12X,'SUM',8X
     1,'CONC AT T=0')
      WRITE (IOU,820)
820   FORMAT(15X,'METER',8X,'COS TERM',8X,'SERIES',/)
C
C       SINGLE(J) IS THE LEAD EXPONENTIAL TERM NOT IN
C       THE SUMMATION
C
C       TRAP ON SIN(ARG)=0
C
      SINGLE(J)=AI(J)/(SQRTKB(J)*DSIN(ARG))
      COSL=DCOS(ARG)
C
C       SLEAD IS THE LEAD COEFFICIENT ON THE SUMMATION
C
      SLEAD=2.D0*AI(J)/L
      DLEAD=AI(J)/(K*DSIN(ARG))
C
C       GENERATE THE TERMS IN THE SERIES FOR J
C
      SIGN=1.D0
      DO 830 N=1,NTERM
      AN=DFLOAT(N)
      SIGN=-1.D0*SIGN
      KP2LN(N)=KP2L*AN*AN
      BD(N,J)=SIGN*SLEAD/(BI(J)-KP2LN(N))
830   CONTINUE
C
C       CHECK THE INITIAL CONDITION
C
      X=L
      DO 860 IX=1,11
      XARG=X*PIEL
      SUM=0.D0
      DO 840 N=1,NTERM
      AN=DFLOAT(N)
      SUM=SUM+BD(N,J)*DCOS(AN*XARG)
840   CONTINUE
      EBL=SINGLE(J)*DCOS(SQRTBK(J)*X)
      CONC=ABL(J)-EBL+SUM
      XP(IX)=(L-X)/100.D0
      WRITE (IOU,850) XP(IX),EBL,SUM,CONC
850   FORMAT(7X,4(5X,1PD10.3))
      X=X-XSTEP
860   CONTINUE
C
C       NOW GENERATE SOME CONCENTRATIONS VERSES TIME
C       AND DEPTH
C
      WRITE (IOU,870)
870   FORMAT(//,5X,'DISPERSED-OIL CONCENTRATIONS, GM/CC
     1, IN THE WATER COLUMN FOR VARIOUS TIMES AND DEPTHS
     2 FOLLOW')
      WRITE (IOU,880)
880   FORMAT(/,50X,'H O U R S')
      WRITE (IOU,890) (TIME(IT),IT=1,10)
```

TABLE 2. (Continued)

```
  890 FORMAT(7X, 'DEPTH',1X,10( 1X,1PD9.2))
      WRITE (IOU,900)
  900 FORMAT(7X, 'METER ')
C
C       DO THE SURFACE OF THE OCEAN FIRST
C
      T=0.D0
      DO 920 IT=1,10
      T=T+TSTEP
      ARG=BI(J)*T
      EX=0.D0
      IF(ARG.LT.ETRAP) EX=DEXP(-ARG)
      CZERO(IT,J)=ABL(J)-SINGLE(J)*COSL*EX
      SIGN=1.D0
      DO 910 N=1,NTERM
      ARG=KP2LN(N) *T
      IF(ARG.GT.ETRAP) GO TO 920
      EX=DEXP(-ARG )
      SIGN=-1.D0*SIGN
      CZERO(IT,J )=CZERO( IT,J)+SIGN*BD(N,J)*EX
  910 CONTINUE
  920 CONTINUE
      WRITE (IOU,960) XP(1), (CZERO(IT,J),IT= 1,10)
      X=L
      DO 970 IX=1,10
      X=X-XSTEP
      CARG=X*PIEL
      XARG=SQRTBK( J)*X
      CTERM1=SINGLE( J)*DCOS(XARG)
      STERM1 =DLEAD*DSIN(XARG)
      T=0.D0
      DO 950 IT=1,10
      T=T+TSTEP
      ARG=BI(J)*T
      EXBT=0.D0
      IF(ARG.LT.ETRAP) EXBT=DEXP(-ARG)
      EBT=EXBT*CTERM1
      STERM2=STERM1*EXBT
      SUM=ABL(J) -EBT
      SLOPE=0.D0
      DO 930 N=1,NTERM
      AN=DFLOAT(N)
      ARG=KP2LN(N)*T
      IF(ARG.GT.ETRAP) GO TO 940
      EX=DEXP(-ARG )
      ANCARG=AN*CARG
      CTERM=DCOS(ANCARG )
      STERM=DSIN(ANCARG )
      SUM=SUM+BD( N,J)*EX*CTERM
      SLOPE=SLOPE-BD( N,J)*EX*STERM*AN*PIEL
  930 CONTINUE
  940 C(IX,IT,J)=SUM
      S(IX,IT,J )=SLOPE+STERM2
  950 CONTINUE
      WRITE (IOU,960) XP(IX+1), (C(IX,IT,J),IT=1,10)
  960 FORMAT(5X,F7.1 ,1X,10(1X, 1PD9.2))
  970 CONTINUE
C
C       WRITE OUT THE WATER-COLUMN CONCENTRATION DERIVATIVE
C       WITH RESPECT TO X, IN GM/(CM**4)
C
      WRITE (IOU,980)
  980 FORMAT(//,5X,'THE DERIVATIVE WITH RESPECT TO X OF
     1 THE WATER COLUMN CONCENTRATION FOLLOWS, IN GM/(CM**4)')
      WRITE (IOU,880)
      WRITE (IOU,890) (TIME(IT), IT=1,10)
```

TABLE 2 . (Continued)

```
      WRITE (10U,900)
      DO 990 IT=1,10
      SZERO(IT,J)=0.D0
  990 CONTI RUE
      T=0.D0
      DO 1000 IT=1,10
      T=T+TSTEP
      ARG=BI(J)*T
      IF(ARG.GT.ETRAP) GO TO 1010
      SZERO(IT,J)=AI (J)*DEXP( -ARG)/K
 1 000 CONTINUE
 1010 WRITE (IOU,960) XP(1), (SZERO(IT,J),IT= 1,10)
      DO 1020 IX=1,10
      WRITE (IOU,960) XP(IX+1 ),(S(IX,IT,J),IT= 1.10)
 1020 CONTI NUE
C
C       CALCULATE THE GRAMS FLUXED INTO THE WATER COLUMN
C       BY INTEGRATING THE SPECIFIED FLUX
C
      AB=AI(J)/BI(J)
      T=0.D0
      DO 1030 IT=1,10
      T=T+TSTEP
      TARG=T*BI(J)
      EX=0.D0
      IF(TARG.LT.ETRAP) EX=DEXP(-TARG)
      GRAMS(IT,J)=AB*(1 .D0-EX)
      ACONC(IT,J)=GRAMS( IT,J )/L
 1 030 CONTINUE
      WRITE (IOU,1040)
 1040 FORMAT(/,3X,'GRAMS OIL')
      WRITE (10U,1050) (GRAMS(IT,J). IT=1,10)
 1050 FORMAT(4X,'IN WATER',1X,10( 1X, 1PD9.2))
      WRITE (IOU,106(3)
 1060 FORMAT(3X,'PER CM*CM')
      WRITE (IOU,1070)
 1 070 FORMAT(/,5X ,'AVERAGE')
      WRITE (IOU,1080I (ACONC(IT,J),IT=1,10)
 1080 FORMAT(7X,'GM/CC',1X,10( lX., 1PD9.2))
      WRITE (IOU,1090) J,J
 1090 FORMAT(/,5X . '*********************X**********%
     1 END OF CALCULATION FOR A( ',11,'), B(',I1 ,')")
 1100 CONTINUE
      IF(NEF.EQ.1) GO TO 1200
C
C       SUM UP THE CONCENTRATION CONTRIBUTIONS FOR EACH
C       SET OF EXPONENTIAL FITS TO THE DISPERSION RATES
C
      Do 1120 I=1,10
      DO 1120 M=1,10
      DO 1110 J=1,NEF
      S(I,M,5)=S( I,M,5)+S(I,M,J )
      C(I,M,5)=C( I,M,5)+C(I ,M,J)
 1110 CONTI RUE
 1120 CONTI NUE
      DO 1140 M=1,10
      DO 1130 J=1,NEF
      CZERO(M, 5)=CZERO(M,5)+CZERO(M,J)
      SZERO(M, 5)=SZERO(M, 5)+SZERO(M,J )
      GRAMS(M,5)=GRAMS(M, 5)+GRAMS(M,J )
      ACONC(M,5)=ACONC(M, 5)+ACONC(M.J )
 1130 CONTINUE
 1140 CONTINUE
      WRITE (IOU,1150) NEF
 1150 FORMAT///. 5X, 'CONCENTRATIONS VERSES TIME AND DEPTH
     1 FOR ',I1,' A,B DATA SETS (ADD UP THE PREVIOUS
```

TABLE 2. (Continued)

```
     2 RESULTS)')
       WRITE (IOU,880)
       WRITE (IOU,890) (TIME(IT), IT=1,10)
       WRITE (IOU,900)
       WRITE (IOU,960) XP(1), (CZERO(IT,5),IT= 1,10)
       DO 1160 IX=1,10
       WRITE (IOU,960) XP(IX+1 ),(C(IX,IT,5),IT= 1,10)
 1160 CONTINUE
       WRITE (IOU,1170) NEF
 1170 FORMAT(/,5X,'THE DERIVATIVE OF THE CONCENTRATION
     1 WITH RESPECT TO X FOR ',11,' A,B DATA SETS')
       WRITE (IOU,880)
       WRITE (IOU,890) (TIME(IT), IT=1,10)
       WRITE (IOU.900)
       WRITE (IOU,960) XP(1), (SZERO(IT,5),IT= 1,10)
       DO 1180 IX=1,10
       WRITE (IOU,960) XP(IX+1 ).(S(IX.IT.5).IT= 1.10)
 1180  CONTINUE
       WRITE (IOU,1040)
       WRITE (IOU,1050) (GRAMS(M,5),M= 1,10)
       WRITE (IOU,1060)
       WRITE (IOU,1070)
       WRITE (IOU,1080) (ACONC(M,5),M=1 ,10)
       WRITE (IOU,1190) NEF
 1190 FORMAT(/,5X,  '*******************************X**
     1  END OF CALCULATION FOR ALL ',11,' OF THE A,B SETS')
 1200 TYPE 1210
 1210 FORMAT(/,1X,'DO IT ACAIN?')
       ACCEPT 460, ANS
       IF(ANS.EQ. 'Y') GO TO 360
       END
```

APPENDIX E

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

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

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

```
.EX CFLUX.FOR
FORTRAN: CFLUX
MAIN.
ERFC1
LINK:   Loading
[LNKXCTCFLUX  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
?9

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 CONCENTRATION PROFILE IN WATER COLUMN FOR A CONSTANT FLUX SOURCE.

```
      IMPLICIT REAL*8 (A-H,O-Z)
      REAL*8 K,L
      COMMON /EXTRA/ ERF,ETRAP,IMAX
      DIMENSION SUM(10),D(11),DP(11),T(10),TP(10)
     1,TIME4(10),TIMEK(10)
      DATA ETRAP/70.D0/
      OPEN(UNIT=32,DIALOG='DSKD:CFLUX.OUT')

C        THIS IS A CODE TO CALCULATE THE WATER-COLUMN
C        CONCENTRATION OF DISPERSED OIL WITH A CONSTANT-
C        FLUX BOUNDARY CONDITION.
C
C        MAY, 1983
C
      IOU=32
      TYPE 10
10    FORMAT(/,1X,'ENTER THE VERTICAL EDDY DIFFUSIVITY
     1, CM*CM/SEC')
      ACCEPT 20, K
20    FORMAT(F10.0)
      TYPE 30
30    FORMAT(/,1X,'ENTER THE CONSTANT FLUX AT THE
     1 SURFACE, GM/CM*CM/SEC')
      ACCEPT 20, W
      TYPE 40
40    FORMAT(/,1X,'ENTER THE OCEAN DEPTH, METERS')
      ACCEPT 20, DM
      TYPE 50
50    FORMAT(/,1X,'ENTER THE MAXIMUM TIME, HOURS')
      ACCEPT 20, HOURS
      TYPE 60
60    FORMAT(/,1X,'ENTER THE NUMBER OF TERMS IN THE I ERFC
     1 SERIES')
      ACCEPT 70, NTERM
70    FORMAT(I2)
      TYPE 80
80    FORMAT(/,1X,'ENTER THE NUMBER OF TERMS IN THE ERF
     1 SERIES')
      ACCEPT 70, IMAX
C
C        ECHO CHECK
C
90    LINE=1
      TYPE 100, LINE,K
100   FORMAT(/,1X,I1,'. VERTICAL DIFFUSIVITY = '
     1,1PD10.3,' CM*CM/SEC')
      LINE=LINE+1
      TYPE 110, LINE,W
110   FORMAT(1X,I1,'. FLUX AT THE SURFACE = ',1PD10.3
     1,' GM/CM*CM/SEC')
      LINE=LINE+1
      TYPE 120, LINE,DM
120   FORMAT(1X,I1,'. OCEAN DEPTH = ',F5.1,' METERS')
      LINE=LINE+1
      TYPE 130, LINE,HOURS
130   FORMAT(1X,I1,'. MAXIMUM TIME = ',F5.1,' HOURS')
      LINE=LINE+1
      TYPE 140, LINE,NTERM
140   FORMAT(1X,I1,'. NUMBER OF TERMS IN IERFC SERIES = ',I2)
      LINE=LINE+1
      TYPE 150, LINE,IMAX
150   FORMAT(1X,I1,'. NUMBER OF TERMS IN ERF SERIES = ',I2)
      TYPE 160
160   FORMAT(/,1X,'WANT TO CHANGE ANY?')
      ACCEPT 170, ANS
170   FORMAT(A1)
```

TABLE 2. (Continued)

```
      IF(ANS.EQ.'N') CO TO 250
      TYPE 180
180   FORMAT(/,1X,'ENTER LINE NUMBER TO BE CHANGED')
      ACCEPT 70, LINE
      GO TO(190,200,210,220,230,240) LINE
190   TYPE 10
      ACCEPT 20, K
      GO TO 90
200   TYPE 40
      ACCEPT 20,W
      GO TO 90
210   TYPE 50
      ACCEPT 20, DM
      GO TO 90
220   TYPE 50
      ACCEPT 20, HOURS
      GO TO 90
230   TYPE 60
      ACCEPT 70, NTERM
      GO TO 90
240   TYPE 80
      ACCEPT 70, IMAX
      GO TO 90
C
C       CALCULATE THE CONCENTRATION PROFILES.
C
250   TSEC=HOURS*3600 .D0
      TS1=TSEC/10.D0
      TS2=HOURS/10 .D0
      DCM=100.D0*DM
      L=DCM
      DS1=DCM/10.D0
      DS2=DM/10.D0
      WRITE (IOU,260)
260   FORMAT( 1H1,'CONCENTRATION PROFILES IN THE WATER
     1 COLUMN FOR DISPERSED OIL (NEUTRAL DENSITY)')
      WRITE (IOU,270)
270   FORMAT(1X,'CALCULATED FOR A CONSTANT FLUX (
     1IERC SOLUTION) AT THE OCEAN SURFACE')
      WRITE (IOU,280)K,W
280   FORMAT(/,1X,'VERTICAL EDDY DIFFUSIVITY = ',1PD9.2,
     1' CM*CM/SEC, DISPERSED OIL FLUX = ',1PD9.2,'
     2 GM/CM*CM/SEC')
      WRITE (IOU,290) DM,HOURS,NTERM
290   FORMAT(1X,'OCEAN DEPTH = ',F5.1,' METERS, MAX
     1IMUM TIME = ',F5.1,' HOURS, NUMBER OF TERMS IN
     2 IERFC SERIES = ',I3)
      WRITE (IOU,300) IMAX
300   FORMAT(1X,'NUMBER OF TERMS IN ERF SERIES = ',I3)
      WRITE (IOU,310)
310   FORMAT(/,1X,'DISPERSED-OIL CONCENTRATIONS,
     1 GM/CC, IN THE WATER COLUMN FOR VARIOUS TIMES
     2 AND DEPTHS FOLLOW*)
      WRITE (IOU,320)
320   FORMAT(/,53X,'H O u R S')
      WRITE (IOU,330)
330   FORMAT(5X,'DEPTH' )
C
C       SETUP TEE DEPTHS.
C
      Do 340 I=1,11
      A=I-1
      D(I)=A*DS1
      DP(I)=A*DS2
340   CONTI NUE
C
```

TABLE 2. (Continued)

```
C         SET UP THE TIMES.
C
        DO 350 I=1,10
        A=I
        T(I)=A*TS1
        TIME4(I)=W*2.D0*DSQRT(T(I)/K)
        TIMEK(I)=2.D0*DSQRT(K*T(I))
        TP(I)=A*TS2
  350   CONTINUE
        WRITE (IOU,360) (TP(I),I=1,10)
  360   FORMAT(5X,'METER',2X,10(2X,1PD9.2),/)
C
C         CALCULATE THE CONCENTRATION PROFILES.
C
        DO 400 I=1,11
        A=I-1
        X=DCM-A*DS1
        DO 380 J=1,10
        SUM(J)=0.D0
        DO 370 N=1,NTERM
        A=2*(N-1)+1
        AL=A*L
        ARG1=(AL-X)/TIMEK(J)
        ARG2=(AL+X)/TIMEK(J)
        E1=ERFC1(ARG1)
        E2=ERFC1(ARG2)
        SUM(J)=SUM(J)+E1+E2
  370   CONTINUE
        SUM(J)=TIME4(J)*SUM(J)
  380   CONTINUE
        WRITE (IOU,390) DP(I),(SUM(J),J=1,10)
  390   FORMAT(5X,F5.1,2X,10(2X,1PD9.2))
  400   CONTINUE
        TYPE 410
  410   FORMAT(/,1X,'DO IT AGAIN?')
        ACCEPT 170, ANS
        IF(ANS.EQ.'Y') GO TO 90
        END
        DOUBLE PRECISION FUNCTION ERFC1(X)
        IMPLICIT REAL*8 (A-H,O-Z)
        COMMON /EXTRA/ ERF,ETRAP,IMAX
        DIMENSION A(100)
C
C         CALCULATE THE FIRST REPEATED INTEGRAL OF THE ERROR
C         FUNCTION ACCORDING TO EQN(11), PAGE 484, IN
C         CARSLAW AND JAEGER, 1967.
C
C         IERFC(X)==(EXP(-X*X))/SQRT(PIE)-X*ERFC(X)
C
C         MAY 13, 1983
C         CALCULATE ERF(X) ACCORDING TO EQN (7.1.6) PAGE 297 IN NBS
C         MATH HANDBOOK BY ABRAMOWITZ AND STEGUN.
C         SYMMETRY IS ERF(-X) = -ERF(X), IF X.GT.3 THEN ERF = 1.
C         20 TERMS IN THE SERIES APPEARS TO BE QUITE SUFFICIENT.
C         THIS ROUTINE RETURNS ERF(X) AND DOES NOT DESTROY X OR THE
C         SIGN OF X.
C
C         MAY 12, 1981
C
        DATA PISQRT,IN/1.7724538509D0,1/
        GO TO (10,30), IN
   10   IN=2
        A(1)=1.0D0
        DO 20 I=1,IMAX
        A(I+1)=2.0D0*A(I)/(2.0D0*DFLOAT(I)+1.0D0)
   20   CONTINUE
```

TABLE 2. (Continued)

```
30    SIGN=1.D0
      IF(X.GT.0.D0) GO TO 4$3
      X=DABS(X)
      SIGN=-1.D0
40    IF(X.GT.3.D0)  GO TO  70
      ERF=A(1)*X
      DO 50 I=1,IMAX
      IPOW=2*I+1
      TEMP=A( I+1)*X**IPOW
      IF(TEMP.LT. 1.0D-10) GO TO 60
50    ERF=ERF+TEMP
60    ERF=2.0D0*DEXP (-X*X)*ERF/PI SQRT
      GO TO 80
70    ERF=1.D0
      X=SIGN*X
80    ERF=SIGN*ERF
C
C       NOW CALCULATE IERFC(X)
C
      XARG= X*X
      EX=0.D0
      IF(XARG.LT.ETRAP) EX=DEXP(-XARG)
      ERFC1=EX/PISQRT-X* (1.D0-ERF)
      RETURN
      END
```

APPENDIX F

METHODS FOR MICROBIAL DEGRADATION STUDIES

^{14}C-Hydrocarbon Mineralization Assay

Three ^{14}C-labeled hydrocarbon substrates were utilized for the determination of hydrocarbon degradation potential, defined here as the Percent mineralization to $^{14}CO_2$: 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) methylnaphthalene (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 concentrations of substrates. Seawater aliquots (50 ml) from each of the experimental tanks and the incoming seawater were transferred to 100 ml sterile serum bottles and spiked with 0.5 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 rectangle 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_2SO_4 (through the sleeve stopper) with a hypodermic syringe. After 2 hours the filter paper was transferred to a second 100 ml serum bottle containing 1 ml of 1N H_2SO_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 Products) and assayed for radioactivity on a Beckman LS100C scintillation counter.

The resulting counts for duplicates were averaged and corrected for the control counts prior to further data treatment. The data (in counts per minute) were converted to 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 μCi/μ 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:

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

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 radiolabeled substrate. To each sample (10 ml for ^3H-Glucose; 15 ml for ^3H-Leucine) 50 μl (1.5 μCi) of radiolabeled compound was added, followed by incubation for 2 hr. in the dark at in situ temperature.

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

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

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 $Na_2B_4O_7$), 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 106/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% formal in) 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 contrast microscopy.

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

METHODS FOR HYDROCARBON ANALYSES AND PHOTOCHEMICAL/MICROBIAL OXIDATION PRODUCT CHARACTERIZATION

Volatile Hydrocarbon Analyses

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

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

Water samples for analysis of dissolved lower-molecular-weight aliphatic and aromatic hydrocarbons are taken in Pierce septum-cawed 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 resorption 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 resorption (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 resorption, 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 chromatography 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 resorption. Typically, 900-1000 scans are acquired for each data file.

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

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

Higher Molecular Weight Petroleum Hydrocarbon Analyses

Water sediment and oil/mousse samples are analyzed by Procedures which basically involve: 1) extraction, 2) fractionation into aliphatic, aromatic and polar constituents by liquid/solid (SiO_2) column chromatography and analysis by FID capillary gas 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 separator 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:

Technology of Materials

Santa Barbara, CA 93103

INTRODUCTION

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

SAMPLES

Samples were received with the following identifications:

BULK SAMPLES:

K-Bay Site #1 OW-1 (Grewingk Glacier Spit)
K-Bay Site #2 OW-2 (China 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.

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

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

A portion of this fine (less than 3 micron) fraction was also studied using long exposure Debye-Scherrer powder camera methods. Specific tests for montmorillonite were also performed on a portion of the clay which was heat treated to 350 degrees C to remove the absorbed water. Portions of this heat treated clay were then subjected to ethylene glycol treatment. A separate portion was modified by strontium ion exchange using strontium chloride. Both of these methods sharpen the (001) diffraction peaks and shift them to a different d-spacing value by interlayer expansion.

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

DISCUSSION

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

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

Sample OW-2B shows a high calcite concentration (probably in the range of 30-40 percent), while the other samples have little or none. Traces of mica are found in many of the samples and a possible trace of gypsum (calcium sulfate dihydrate) may be in OW-3. Certainty cannot be placed on the identification of these trace 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 11,19

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 - mino Gypsom - t

SAMPLE: K Bay Site #4 OW-4

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

SUMMARY OF MINERAL CONTENT (cont.)

March 11,1983

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

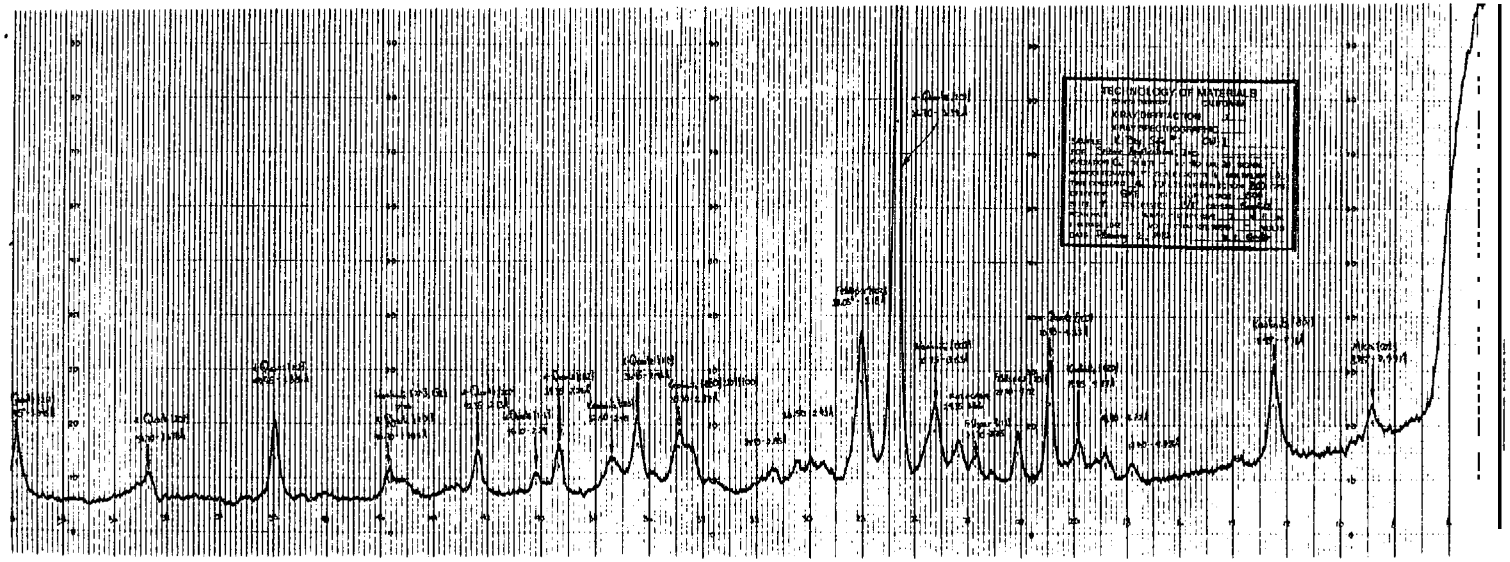
α-Quartz	Kaolinite	Feldspar	Calcite	Other
minor+	major	minor	trace?	Huntite?-t Mica-minor

SUMMARY OF MINERAL CONTENT (cont.)

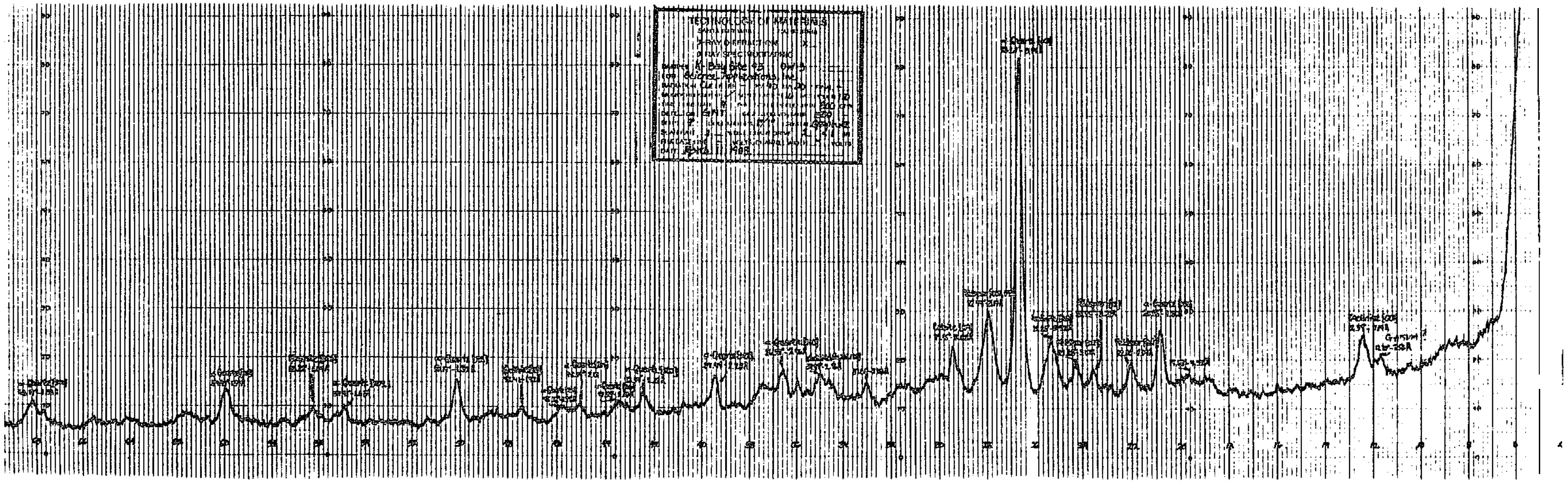
March 11, 19

SAMPLE: Filter 6-M

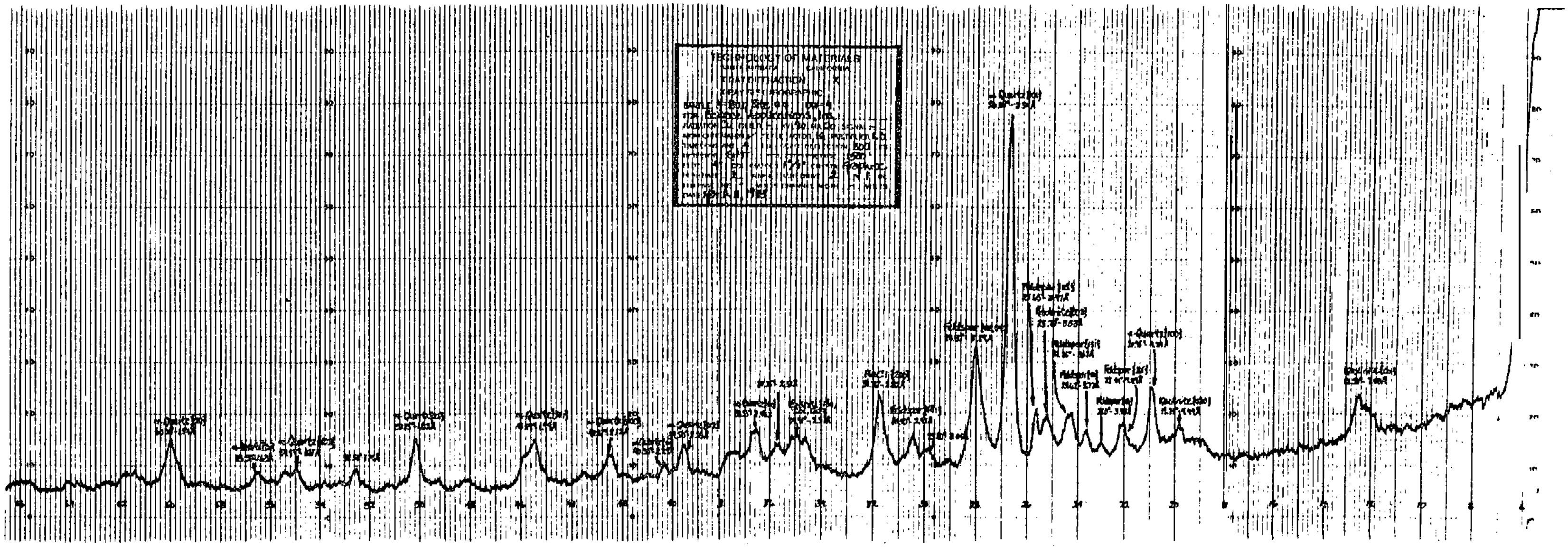
α-Quartz	Kaolinite	Feldspar	Calcite	Other
major	Intermediate	intermediate	none	Mica -tr



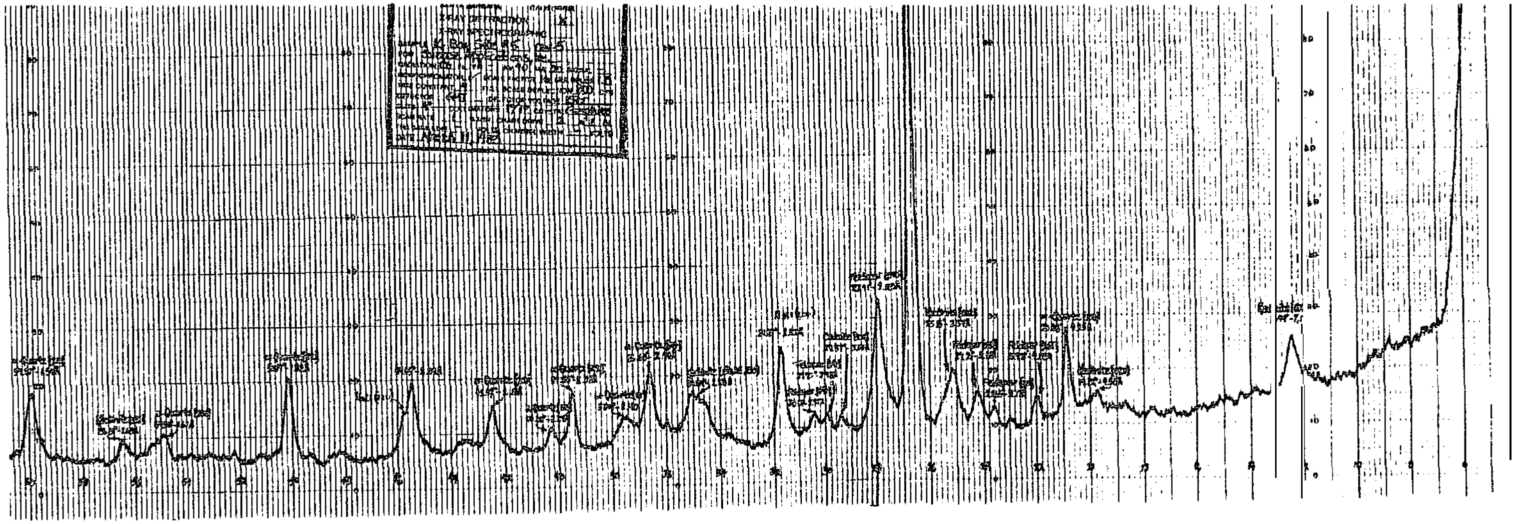
X-ray diffraction spectrograph of sediment from Site KB-1 Grewingk Glacier Spit).



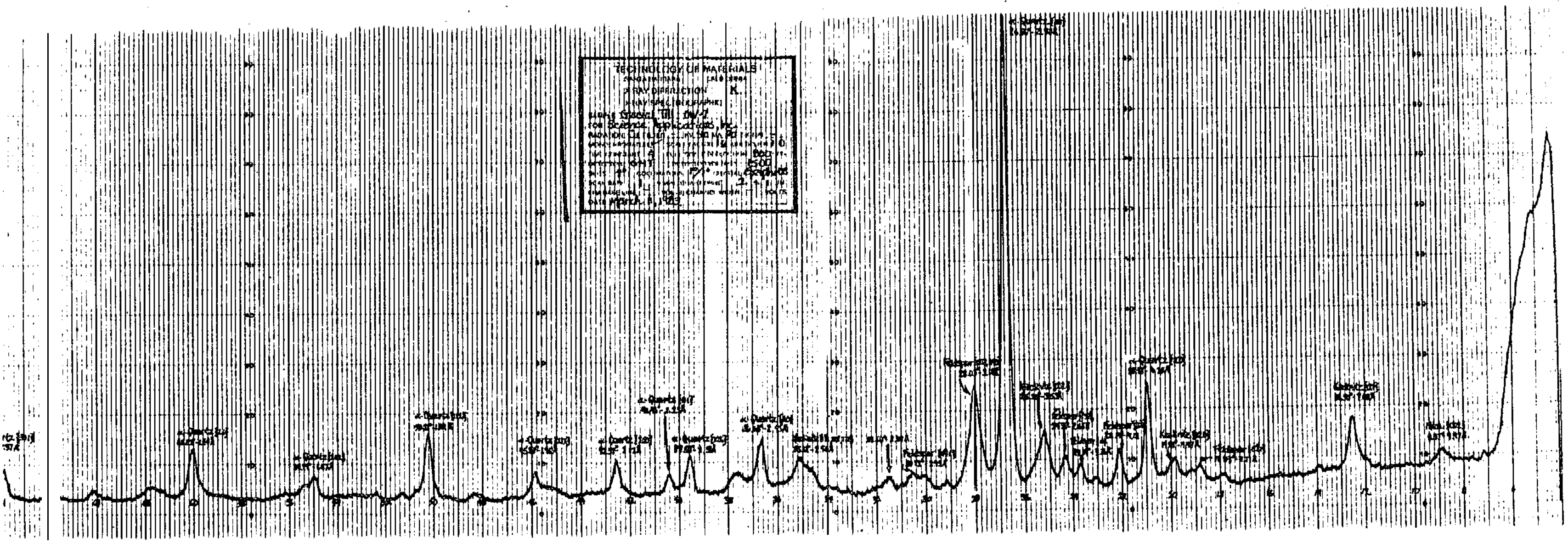
X-ray diffraction spectrograph of sediment from Site KB-3 Kasitsna Bay).



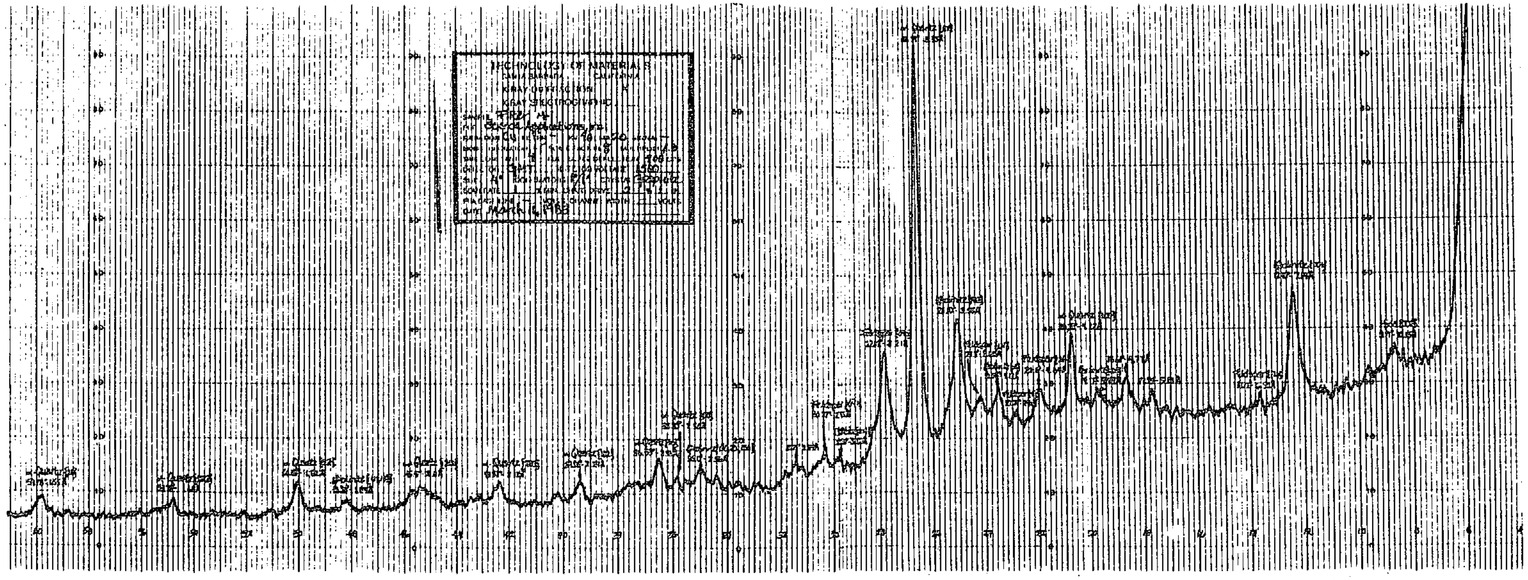
X-ray diffraction spectrograph of sediment from Site KB-4 (Seldovia Salt Marsh).



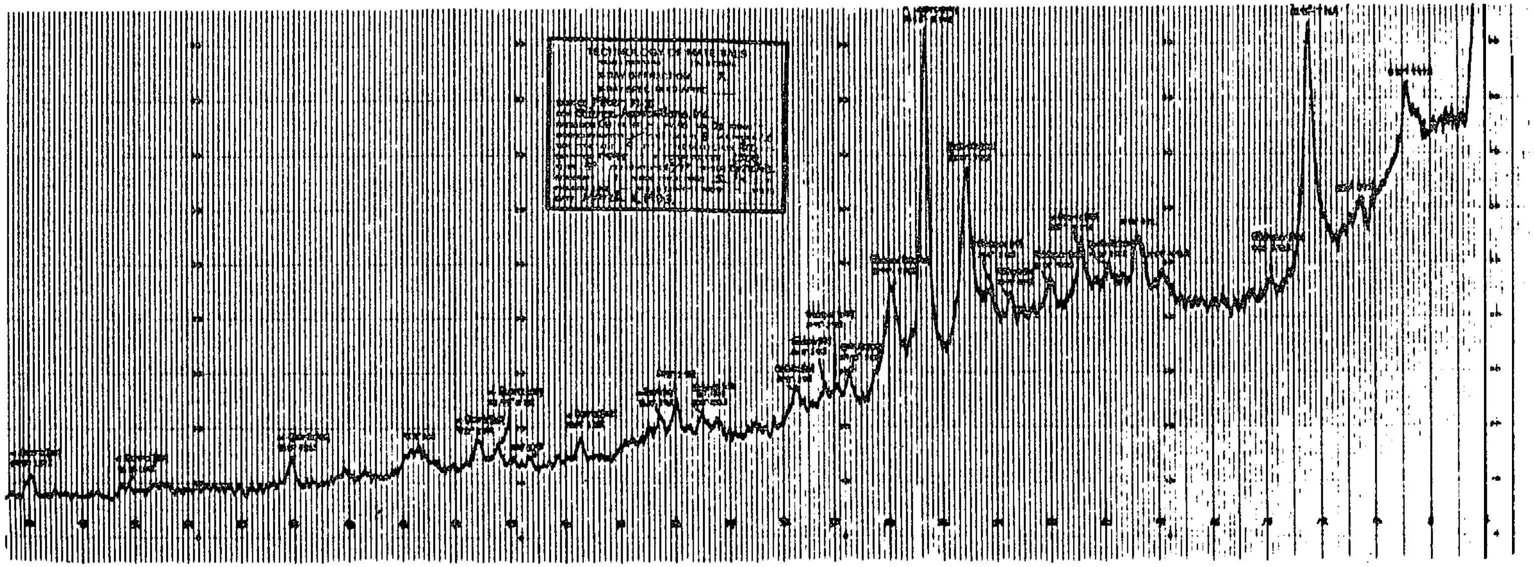
X-ray diffraction spectrograph of sediment from Site KB-5 (Jakolof Bay).



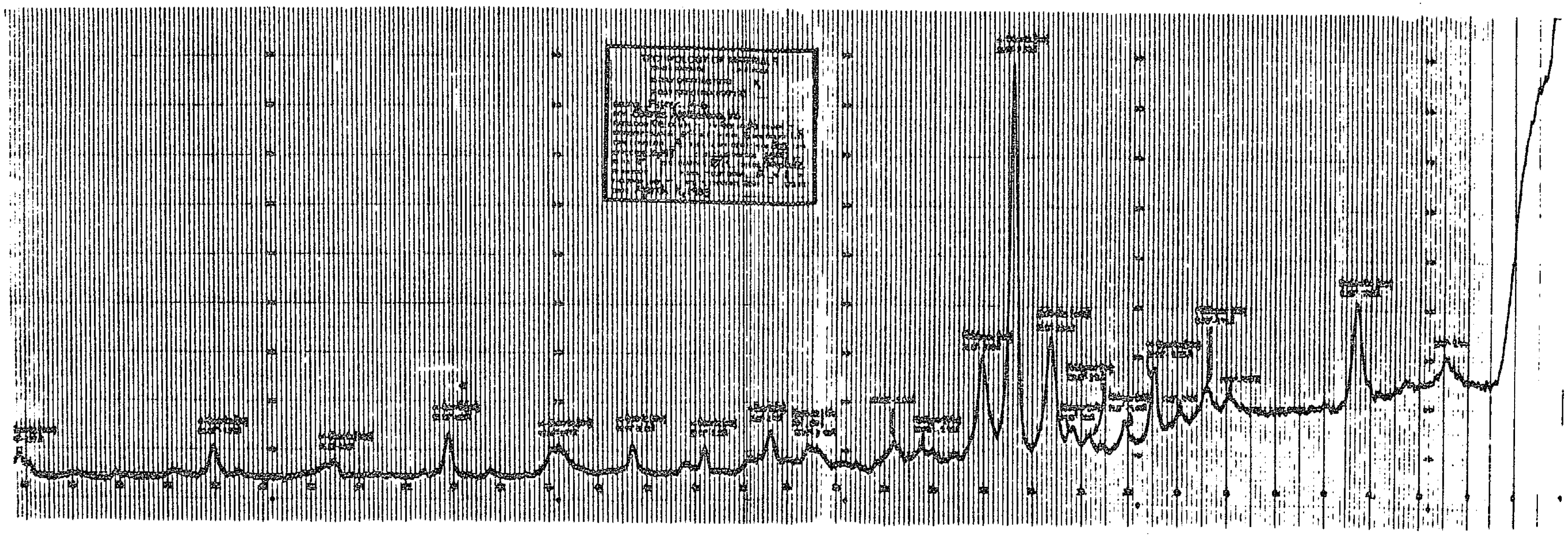
X-ray diffraction spectrograph of sediment collected from the base of Grewingk Glacier.



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



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



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

APPENDIX H

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

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Report Submitted to:

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December, 1980

OBJECTIVES

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

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

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

IMPLICATIONS FOR OFF-SHORE OIL AND GAS DEVELOPMENT

Many investigators have long suspected that spilled oil on the water surface or in the water column does not constitute as great an environmental threat as oil which has been incorporated into sedimentary regimes. Ironically, in the case of most major oil spills and laboratory studies, the sediments have been found to be the ultimate repository or sink for the bulk of the higher molecular weight components in the released oil (Jordan and Payne, 1980, D'Oxouville et al., 1979; Meyers, 1978; Mayo et al., 1978; Gearing et al., 1979; Winters 1978; Meyers and Quinn 1973; Zurcher and Thuer 1978; Bassin and Ichiye 1977). Once incorporated into the sediments, many of the unweathered toxic components of oil are retained unaltered for extended periods (Teal et al., 197$; 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 partitularly 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 separator funnel and back extracted with 400-500 ml of saturated sodium chloride in distilled water which had been previously extracted with hexane. The lower layer (CH_2Cl_2) was removed and the water phase was back extracted with three additional 100 *ml* aliquots of CH_2Cl_2. The combined CH_2Cl_2 extracts were concentrated to approximately 100 ml using a Kuderna-Danish (K-D) apparatus , and dried by passage through a column of sodium sulfate followed by additional elution with CH_2Cl_2. The dried extract was concentrated to about 10 ml using a K-D apparatus and solvent exchanged (3x) into hexane, followed by solvent reduction to 1-2 ml in preparation for column chromatography.

Liquid Column Chromatography

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

Fraction/Solvent	Amount	Compound Class
1. Hexane	30 ml	Aliphatic hydrocarbons
2. Hexane:Benzene 50:50	45 ml	Aromatic hydrocarbons
3. 50% CH_3OH in CH_2Cl_2	60 ml	Polar compounds

Gas Chromatographic Analysis

All gas chrmatographic results were obtained on a Hewlett-Packard 5840A gas chromatography 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.

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

where;

Ax = 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)

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

%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 chromatography 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.

$$\frac{\mu g\ \mathrm{UCM}}{\mathrm{liter}} = \mathrm{Area}_p \times (\mathrm{Conf.\ F}) \times \frac{\mathrm{S.\ Att.}}{\mathrm{Ref.\ Att.}} \times (\overline{\mathrm{R.F.}}_{a-b}) \times [\ldots] \qquad 2$$

where:

Area = UCM area in arbitrary planimeter units,

Conv. F. = a factor for converting arbitrary planimeter units to GC area units at a specific GC attenuation,

S. Att. and Ref. Att. = the GC attenuation at which the sample chromatogram was run and the reference attenuation to determine the conversion factor (Conv. F.), respectively,

$\mathrm{R.F.}_{a\ b}$ = the mean response factor for all sequential n-alkanes (with carbon numbers a to b) whose retention times fall within the retention time window of the UCM, and

[...] = the same parameters enclosed in brackets in equation 1.

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

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

Capillary Gas Chromatography Mass Spectrometry

Selected extractable organic compounds previously analyzed by fused silica capillary column-FID GC were also subjected to fused silica capillary gas chromatography/mass spectrometry (GC/MS). A 30-meter J&W Scientific Co. SE-54 capillary column (0.25-mm I.D. with a film thickness of 25 µm was used to achieve chromatographic separation in a Finnigan 4021 quadruple mass spectrometer. The capillary system was operated in the splitless (Grob-type) mode. The static time upon injection was 0.8 tin, 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/see, 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 spectrometers which was operated in the electron impact mode at 70eV with the lens potentials optimized for maximum ion transmission. The quadruple offset and offset programs were adjusted to yield a fragmentation ratio for perfluorotributylamine m/e 69-to-219 of 4:1. This tuning yields quadruple 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 quadruple 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.SS; 44.75) and nC_{18} and phytane (RT 47.40; 47.83). The three major components at retention times 31.21, 35.77 and 43.08 are internal spikes and a GC recovery standard (triisopropylbenzene, 31.21; n-decylcyclohexane, 43.08; and hexamethylbenzene, 35.77, respectively). There is no apparent evidence of any petroleum contamination and there appears to be a small cluster of branched and unsaturated biogenic hydrocarbons between “20 and nC_{21}. The aromatic fraction chromatogram, B, from this

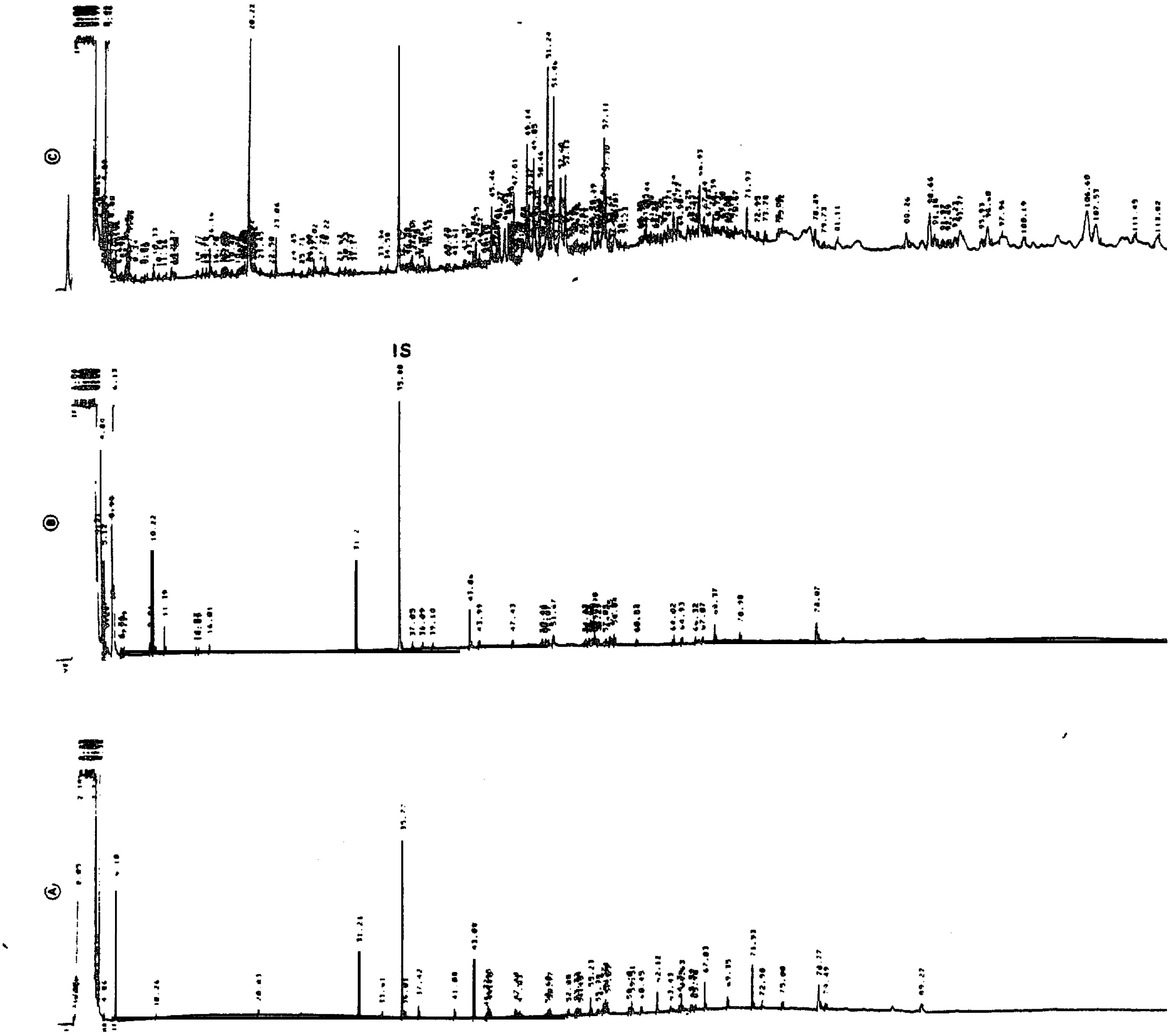

Figure 1. Flame Ionization Detector capillary gaschromatograms of: A, the aliphatic fraction; B, the aromatic fraction and C, the polar fraction extracts obtained from time zero control sediment samples from Kasitsna Bay.

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 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 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.	0.0999	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)	Phenan-threne (1706)	Anthracene	1 Methyl-phenanthrene	Fluoranthene	Pyrene
KASITSNA BAY CONTROL	I	0	1.08	0.	nd	"It	nd	nd	nd	nd	0.0262	nd	nd	nd	0.0392
KA511 SNA BAY CONTROL	625	1	1.212	0.	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd
FRESH CRUDE SPIKE 50ppt	5	0	t460.	1740.	58.0	117.	94.9	16.2	65,4	32.5	66.6	nd	18.0	Ad	nd
FRESH CRUDE SPIKE 1ppt	4	0	12.2	22,3	0.363	0.%0	0.s70	0.0418	0.469	0.120	0.190	nd	0.0658	nd	nd
FRESH CRUDE SPIKE O. 1ppt	3	0	0.0289	0,0259	0. 00025	0. 00064	0.00037	nd	0.0032	nd	O. 00032	nd	nd	0.0021	0.00012
WEATHE RIO CRUDE SPIKE 50	14	0	210.	824.	nd	5.59	4.1)	nd	11.7	4.88	8.65	nd	nd	1.47	nd
WEATHE RED CRUDE SPIKE I	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	23.1	1.48	19.2	4.04	6.7	nd	2.48	I .53	nd
FRESH CRUDE 5P 1 KE 50ppt	629	1	42a.	880.	13.3	35.2	21.0	1.1?	17.9	4.27	5.99	nd	2.4o	0.840	nd
FRESH CRUDE SPIKE 50ppt	630	1	3m.	2020.	9.75	30.4	18.6	nd	17.5	4.44	7.15	nd	2.9s	nd	nd
FRESH CRUDE SPIKE 1ppt	631	1	9.33	29.7	0.163	0.517	0.433	0.0311	0.383	0.101	0.129	nd	0.0621	nd	nd
FRESH CRUDE SPIKE O. 1ppt	634	I	2.23	3.98	nd	0.0251	nd	nd	0.0321	Ad	0.0301	nd	nd	nd	0.0185
WEATHERED CRUDE SPIKE 50	631	1	200.	901.	nd	5.19	4.01	nd	9.58	3.71	6.00	nd	nd	nd	nd
WEATHERED CRUDE SPIKE 1	640	1	12.20	51.84	0.0429	0.243	0.134	0.0234	0.420	0.195	0.137	nd	0.116	0.012	0.0297
SADIE CO/I' CONTROL	206	0	2.92	0	nd	Ad	nd	nd	nd	nd	0.10258	nd	nd	0.02803	0.21013
SADIE COVE 011 & STARCH	782	1	781.	2010.	22.2	51.0	29.5	1.21	22.2	4.50	8.31	nd	2.64	nd	nd
SADIE COVE 011	779	I	812.	2440,	32.6	75.0	43.2	nd	32.3	6.27	10.2	nd	s.71	2.04	nd
SADIE COVE OIL & CHITIN	780	I	1070.	1660.	33.8	71.8	45.7	1.80	11.0	6.24	9.99	nd	6.66	nd	nd
<u>COOK INLET CRUDE OIL</u>															
FRESH		N.A.	34700.	41600.	404,	1110.	644.	nd	S40.	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.

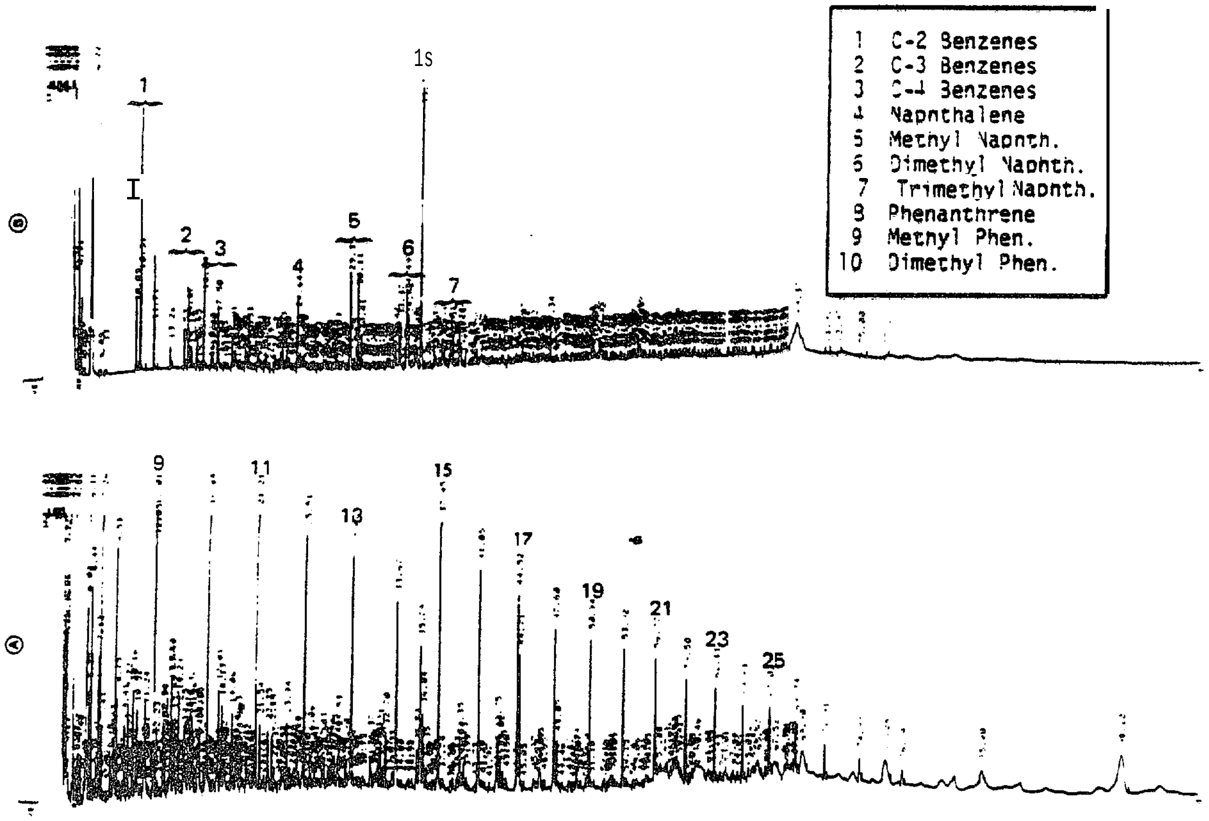

Figure 2. Flame Ionization Detector capillary gas chromatograms of: A, the aliphatic fraction, and B, the aromatic fraction extracts obtained on the fresh Cook Inlet Crude Oil used to spike the Kasitsna Bay sediment samples.

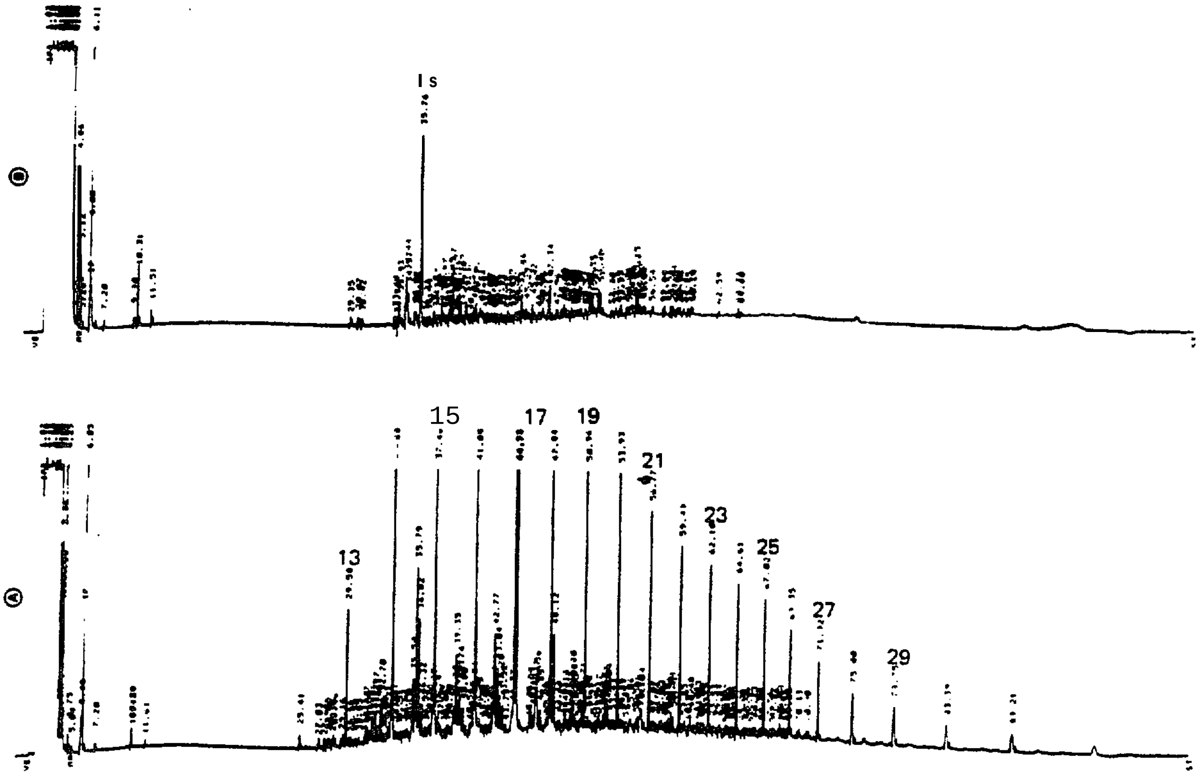

Figure 3. Flame Ionization Detector capillary gas chromatograms of: A. the aliphatic fraction, and B, the aromatic fraction extracts obtained from the Artificially Weathered Cook Inlet Crude Oil used to spike the Kasitsna Bay sediment samples.

although the aliphatic fraction is characterized in general, by n-alkanes from nC_8 through nC_{32}. The aromatic fraction shows a number of lower molecular weight aromatic compounds in the range of KOVAT index 800 to KOVAT index 1500 (RT 10.09 to 35.79). These compounds were identified by GC/MS as alkyl substituted benzenes such as xylenes, ethylbenzene, trimethylbenzene and propylbenzenes. The large peak at RT 35.79 is the GC internal standard hexamethylbenzene. Also in this sample are peaks identified as 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 dimunition 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 fractionof 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

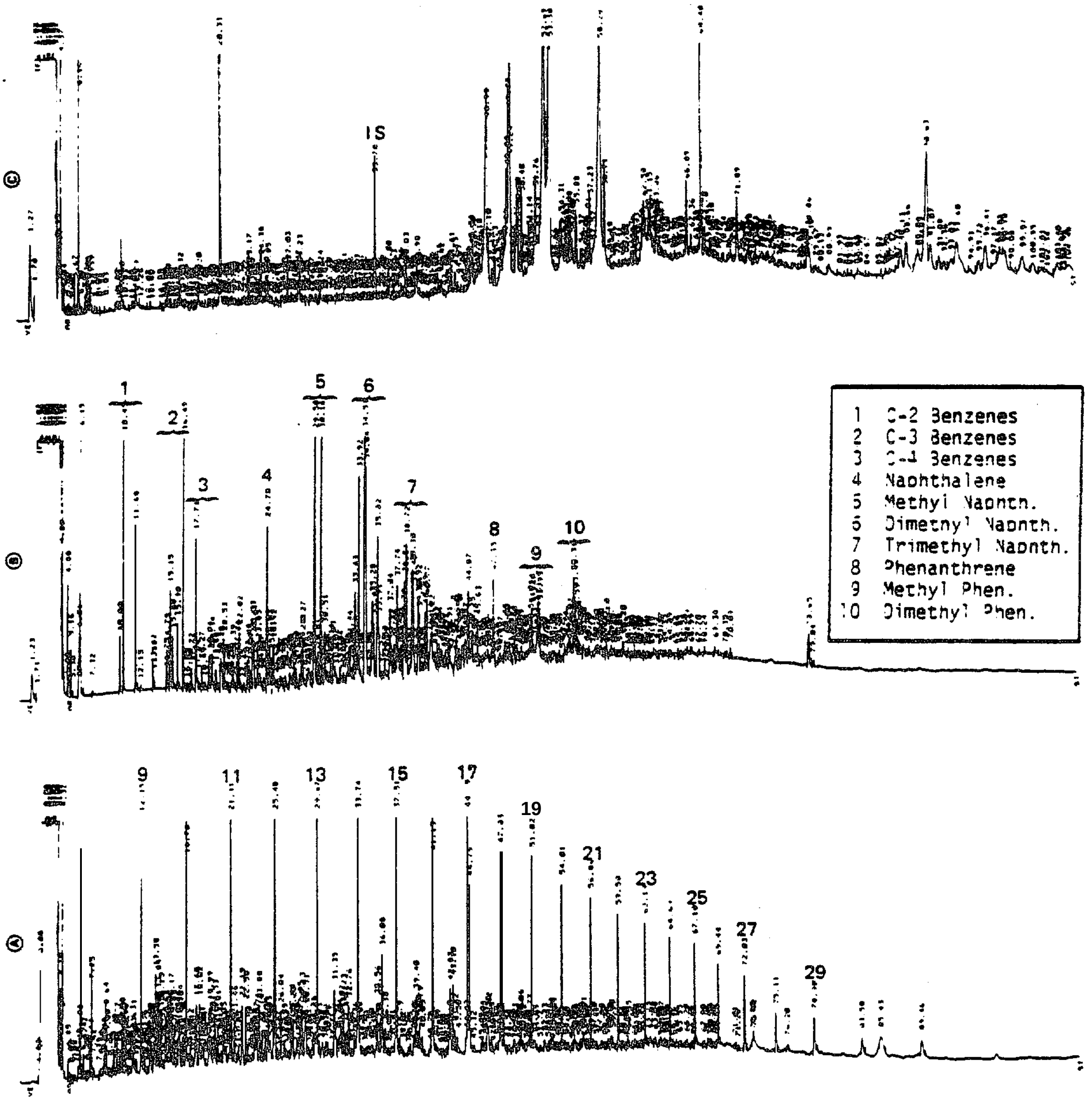

Figure 4. Flame Ionization Detector capillary gas chromatograms of: A, the aliphatic fraction, B, the aromatic fraction, and C, the polar fraction extracts obtained from time zero Kasitsna Bay sediment samples which had been spiked with fresh Cook Inlet Crude Oil at 1 ppt.

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

Figure 5 presents the capillary chromatograms obtained on the time zero sediment samples spiked with artificially weathered crude oil. The chromatograms are qualitatively very similar to those shown in Figure 3 which presented the weathered Cook Inlet crude used to spike the sediment samples. Aliphatics are virtually absent below nC_{13} as are aromatic compounds with KOVAT indices below 1300. A number of higher molecular weight polynuclear aromatic compounds can be identified in the weathered crude, and these are 2-methylnaphthalene at 29.38, 1-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 artificially weathered sediment sample.

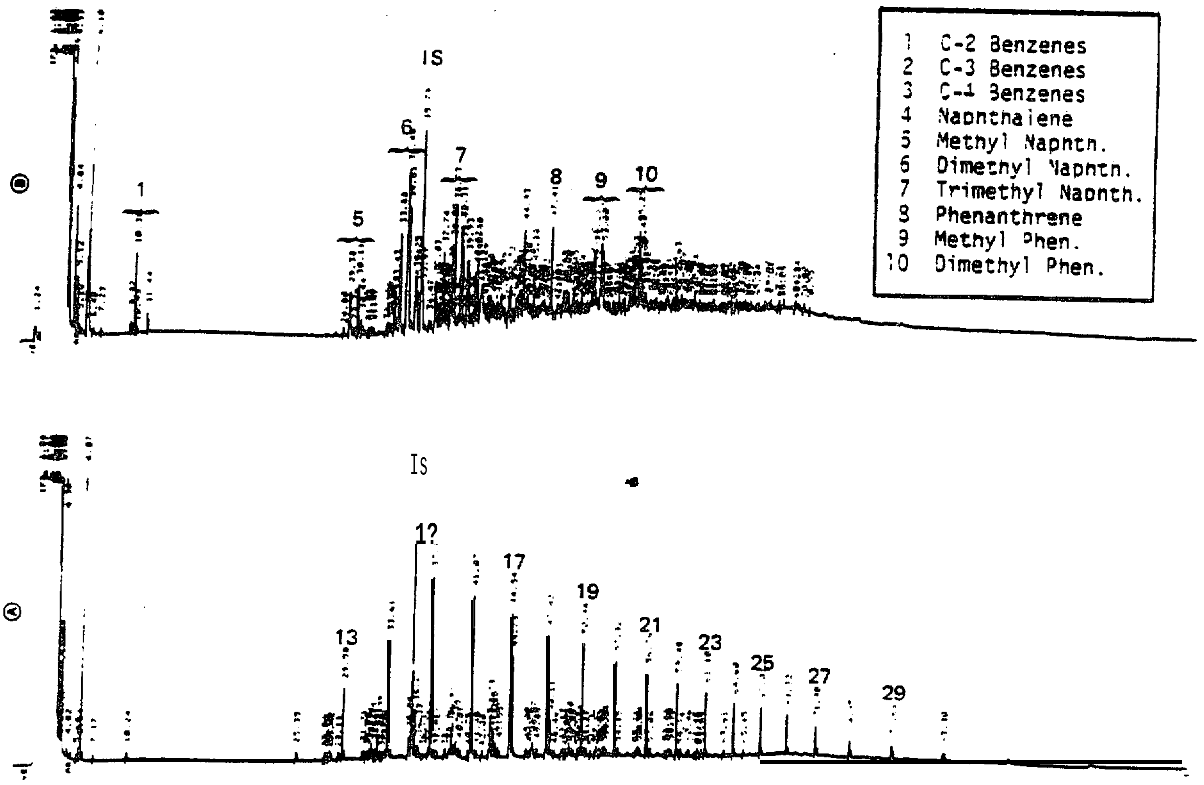

Figure 5. Flame Ionization Detector capillary gas chromatograms of: A, the aliphatic fraction and B, the aromatic fraction extracts obtained from time zero Kasitsna Bay sediment samples spiked with Artificially Weathered Cook Inlet Crude Oil at 50 ppt.

Time One Year Samples

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

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

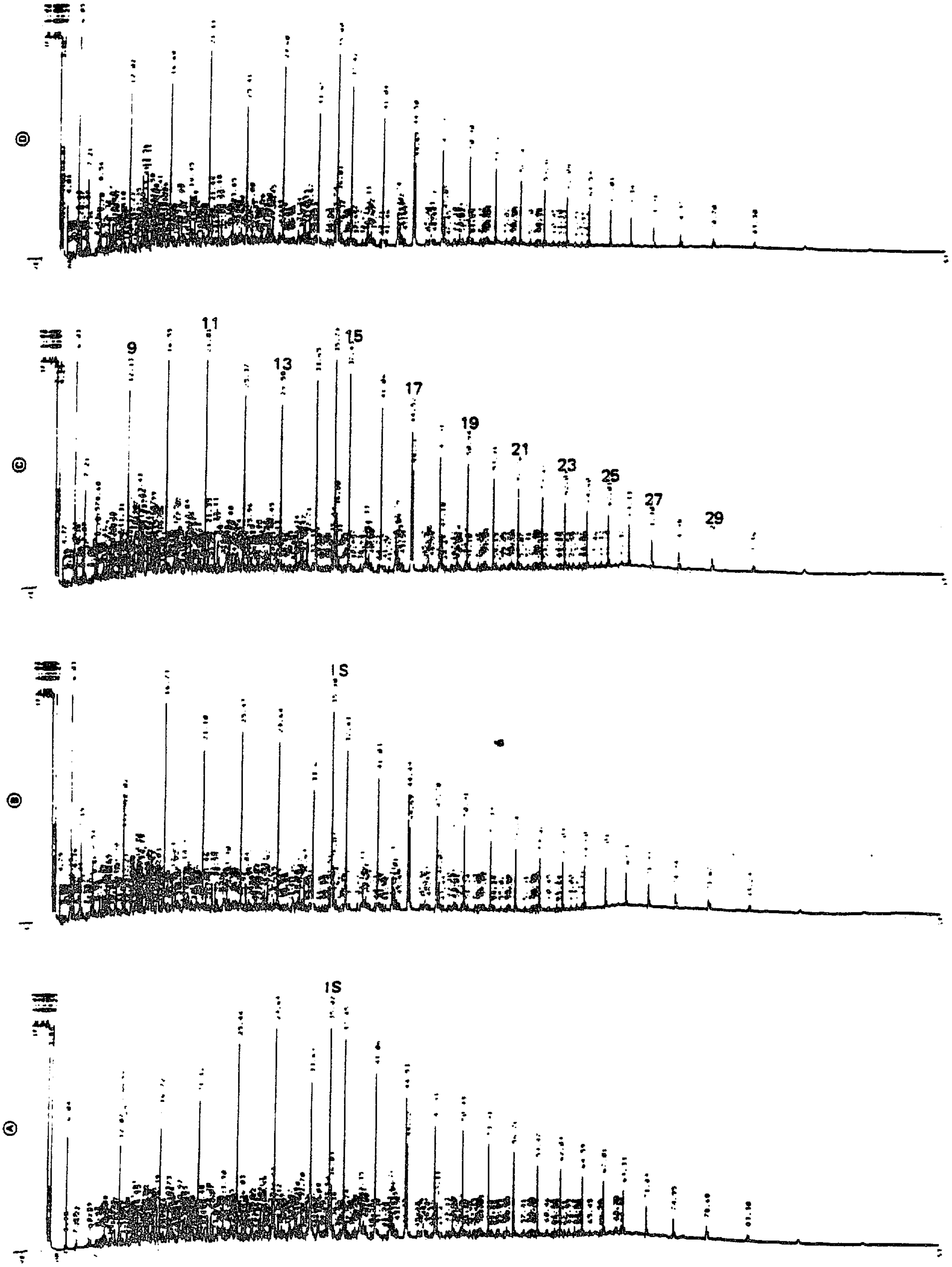

Figure 6. Flame Ionization Detector capillary gas chromatograms of: A, the aliphatic fraction of the 50 ppt fresh Cook Inlet Crude Oil spiked into the sediment at time zero, and B, C, and D, the aliphatic fractions of the triplicate samples examined after one year of natural weathering in Kasitsna Bay.

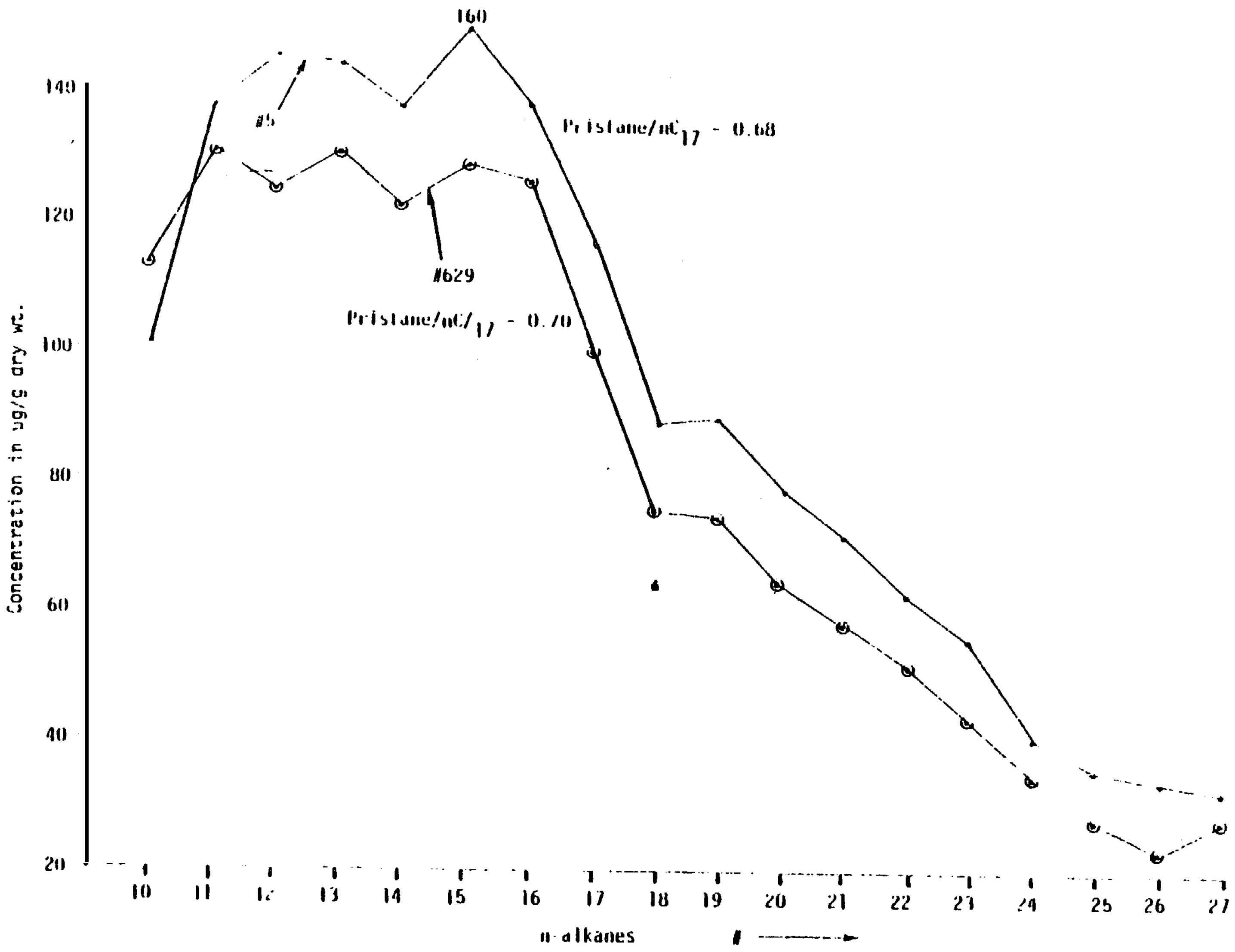

Figure 7. Concentration abundance of the n-alkanes in a sediment sample spiked with 50 parts per thousand fresh crude illustrating the time zero sample (·) and sample after one year of weathering (⊙).

The similarity of the pristane/nC_{17} and phytane/nC_{18} ratios, as observed qualitatively in Figure 6 and Table 1, also illustrates the lack of any appreciable biotic or abiotic weathering in these samples. The chromatographic profiles are essentially superimposable, reflecting the 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

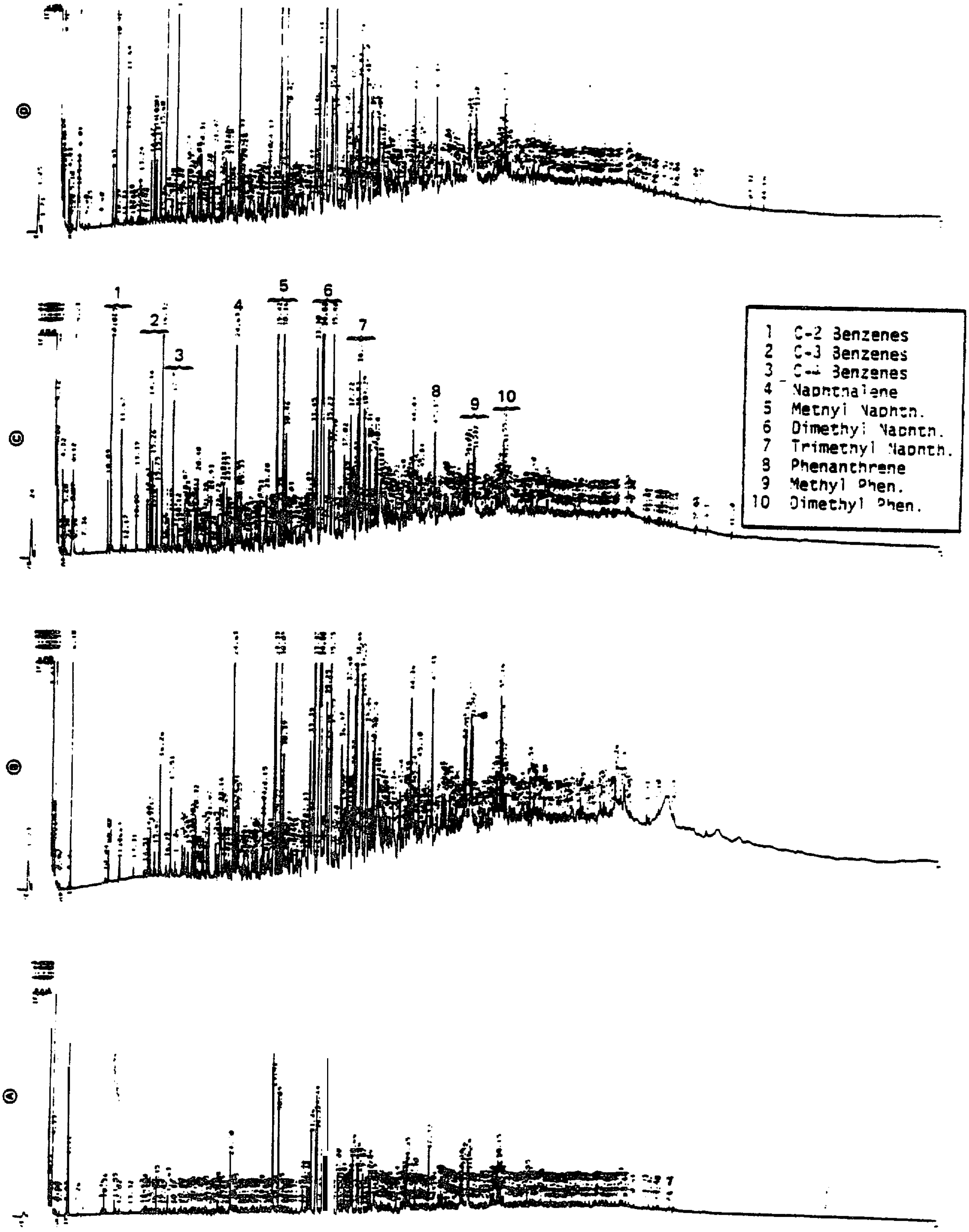

Figure 8. Flame Ionization Detector gas chromatograms of: A, the aromatic fraction of the 50 ppt fresh Cook Inlet Crude Oil spiked into the sediment at time zero and B, C, and D, the aromatic fractions of the triplicate samples examined after one year of natural weathering in Kasitsna Bay.

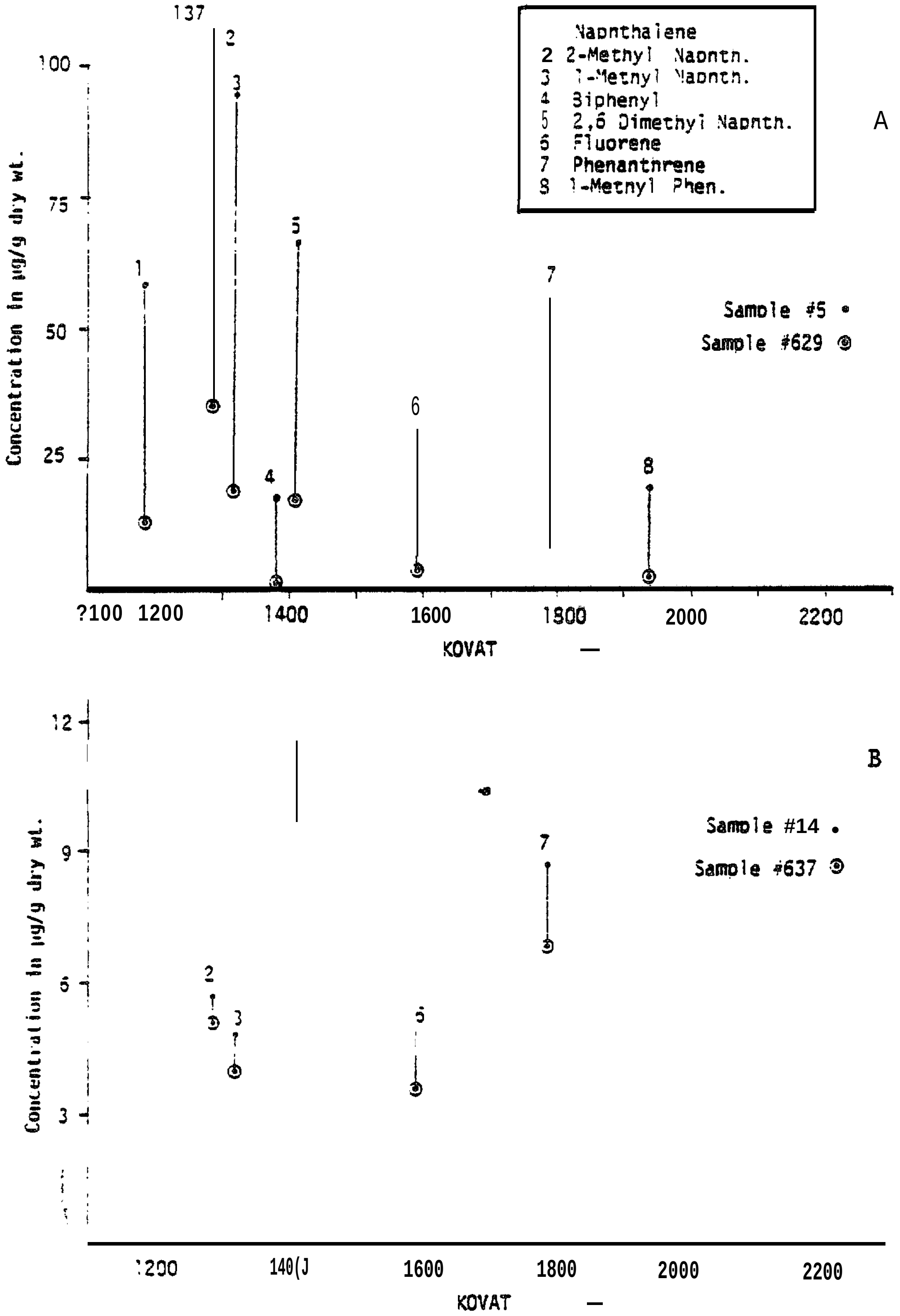

Figure 9. Concentration abundance of selected aromatic hydrocarbons from a 50 parts per thousand spike of fresh crude (Top) showing the time zero sample (•) and sample after one year of weathering (⊙), and bottom, a 50 ppt spike of artificially weathered crude at time zero (·) and after one year of weathering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

spiked sediments at time zero and time one year. While time zero levels of individual aromatic compounds ranged from 50 to 137 micrograms per gram dry weight (for 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 aromatics with Kovat indices ranging from 1500 to 2000. This presumably reflects two things: 1) the greater volatility and water volubility of the lower molecular weight aromatic compounds, and 2) the lower relative abundance of the higher molecular weight aromatics in the crude oil to begin with.

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

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

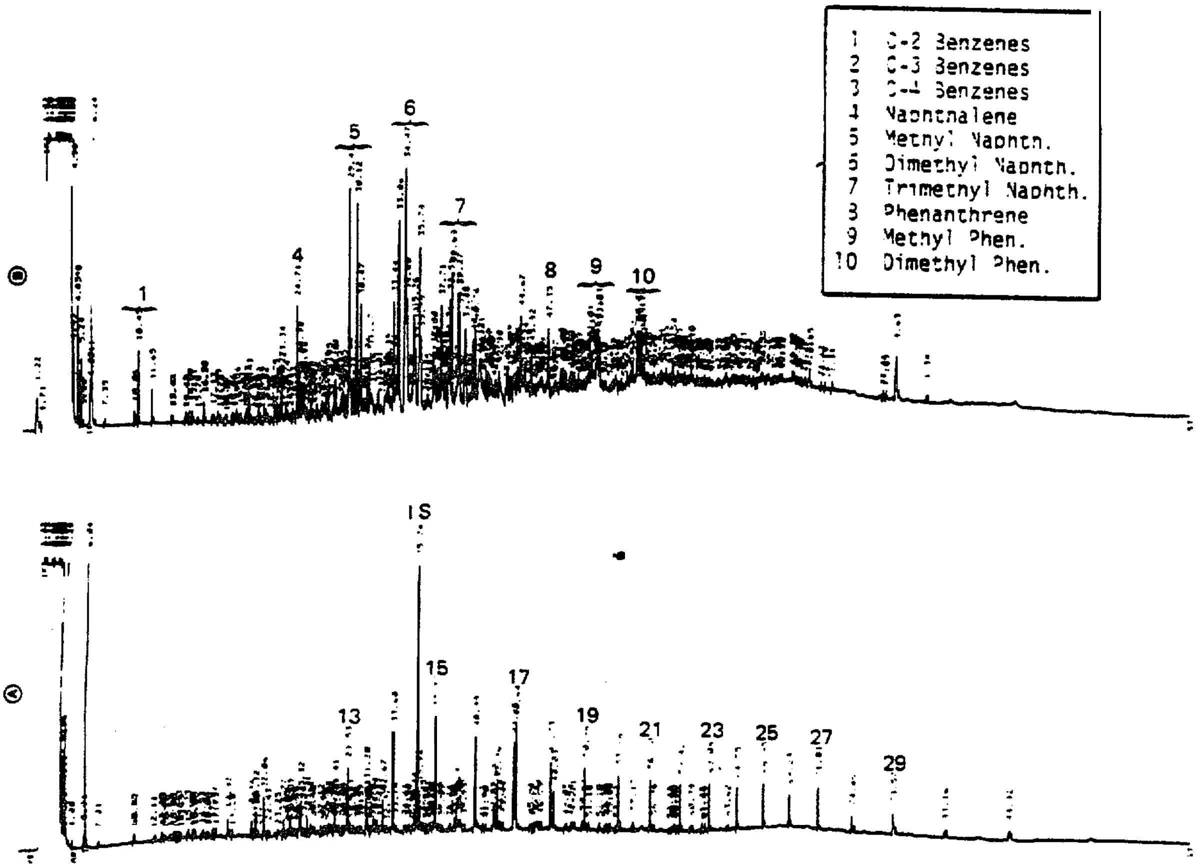

Figure 10. Flame Ionization Detector gas chromatograms of: A, the aliphatic fraction and B, the aromatic fraction extracts obtained from 1 ppt fresh Cook Inlet Crude Oil spiked sediments after one year of weathering in Kasitsna Bay.

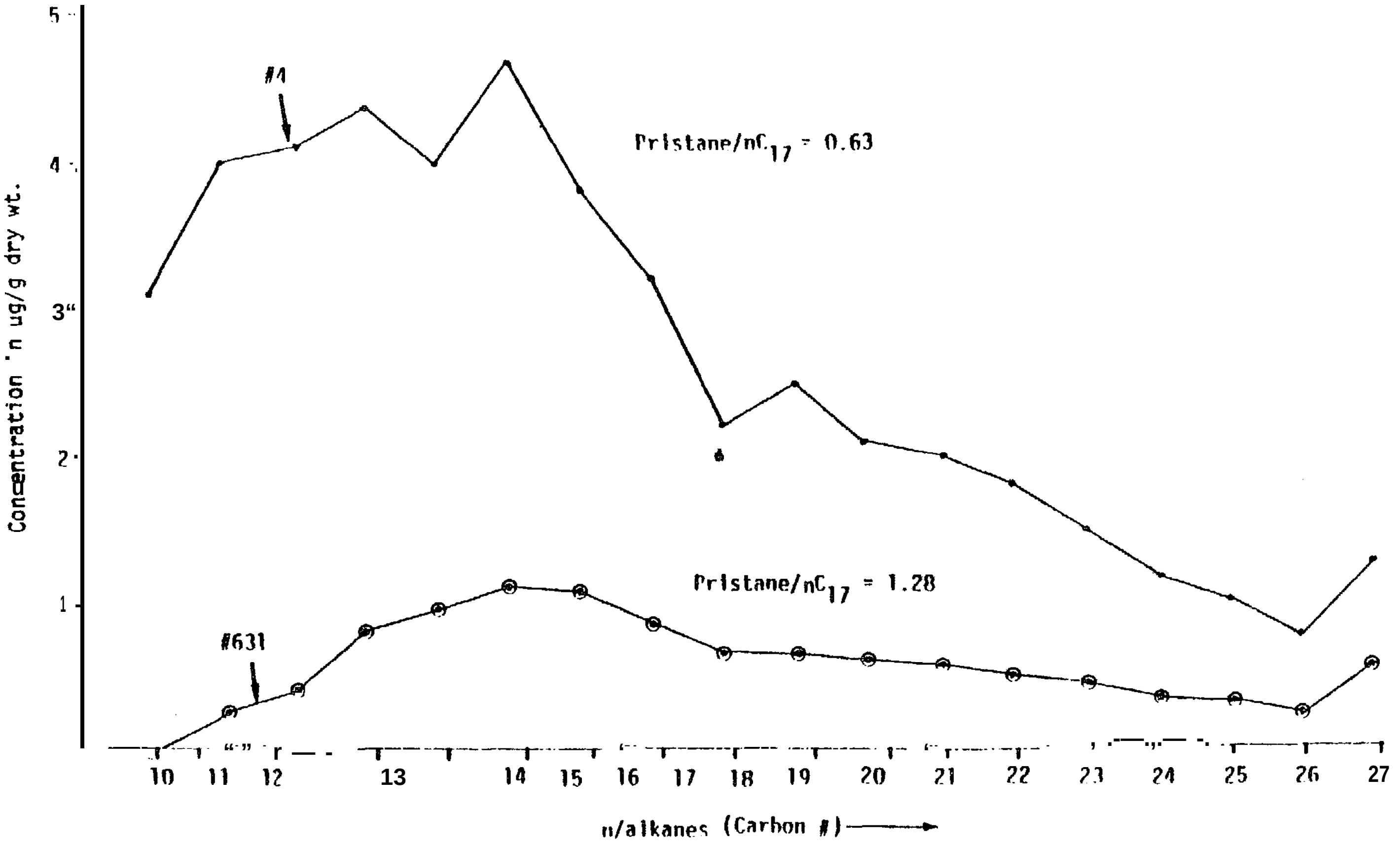

Figure 11. Concentration abundance of the n-alkanes for a sediment oil spike of 1.0 part per thousand fresh crude illustrating the time zero sample (•) and sample after one year of weathering (⊙).

resolved hydrocarbons decreased from 83 to 21 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

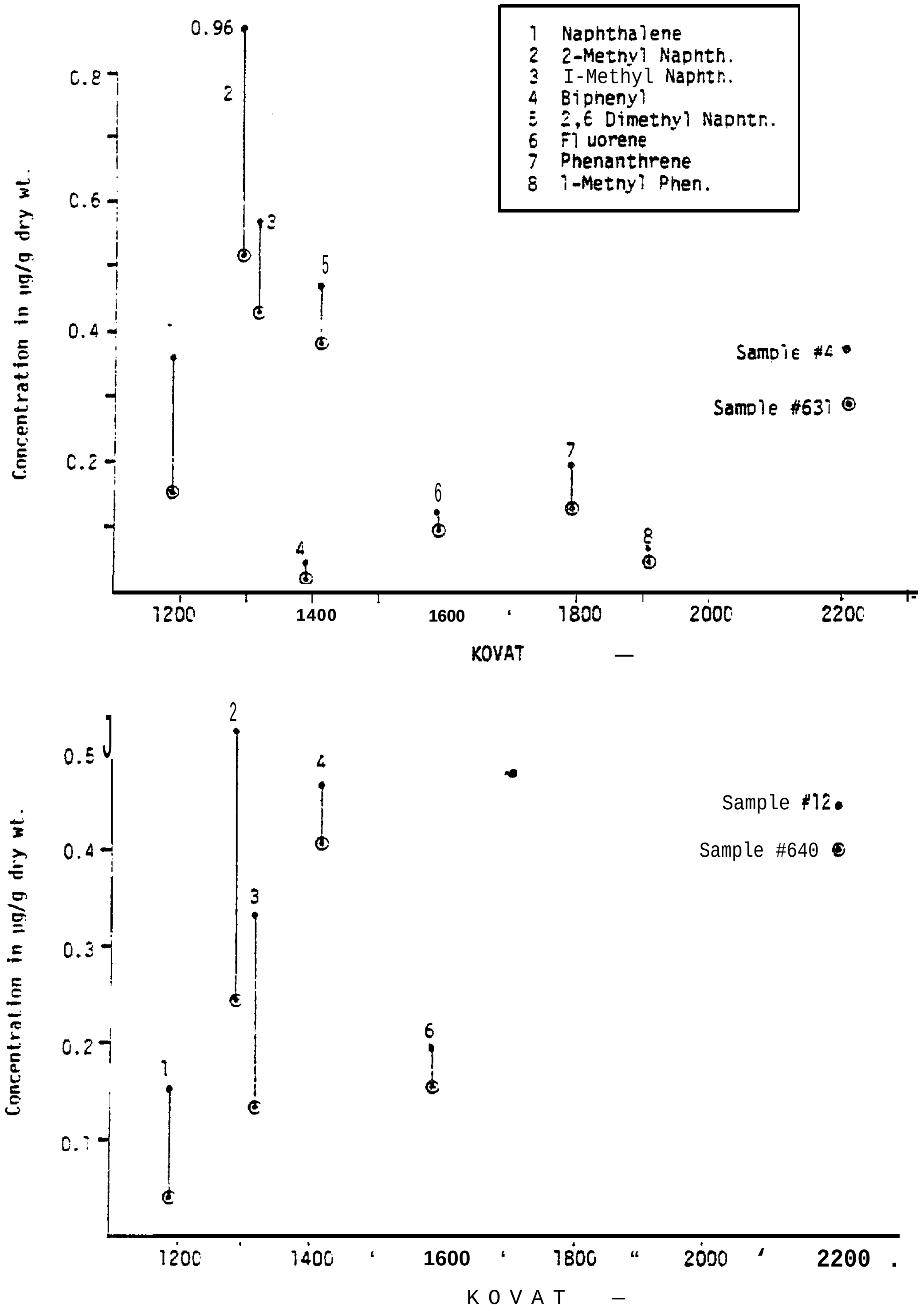

Figure 12. Concentration abundance of selected aromatic hydrocarbons from a 1.0 part per thousand spike of fresh crude (Top) showing the time zero sample (0) and sample after one year of weathering (⊙). Bottom shows a 1.0 ppt spike of artificially weathered crude for the time zero sample (o) and sample after one year of weathering (⊙).

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

Clearly, while biological degradation of the aliphatic hydrocarbons (primarily n-alkane) occurred at the 1 ppt level, concomitant degradation of the higher molecular weight polynuclear aromatics compounds with molecular weights above that of 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 substituted benzenes at retention times 10.45, 11.68, 15.15, 15.90, 16.49 and 17.71 has occurred due to either evaporation or dissolution. Compounds with molecular weights greater than that of 1-methylnapthalene at retention time 29.41 (B) are present in nearly identical relative concentrations. The chromatogram in 13C shows that the same compounds were also

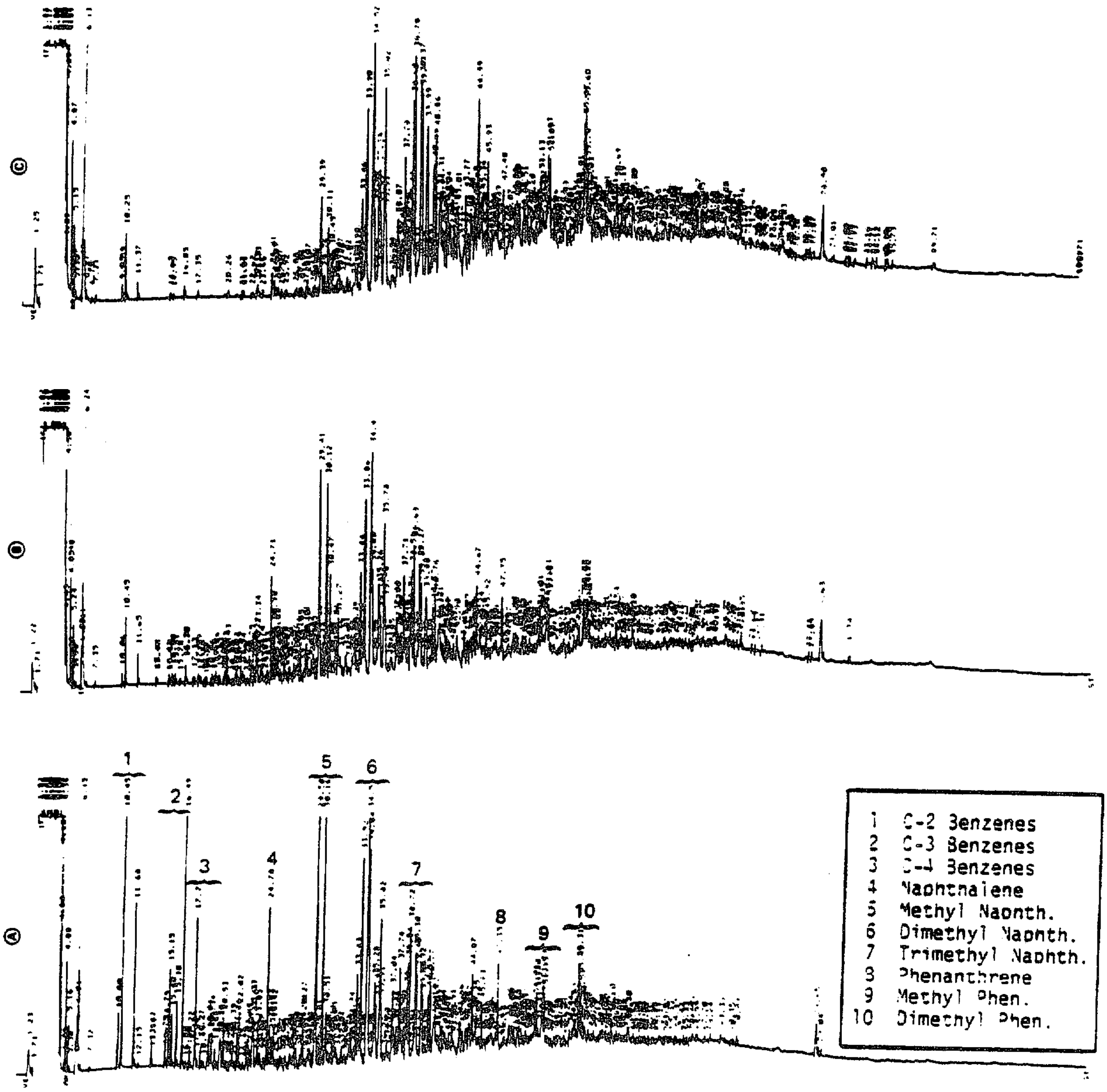

Figure 13. Flame Ionization Detector gas chromatograms of extracts of the aromatic fractions obtained from: A, the sediment spiked with 1 ppt fresh crude oil at time zero; B, the 1 ppt fresh crude sample after one year of natural weathering in Kasitsna Bay and C, the 1 ppt sediment sample spiked with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

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

Figure 14 presents the aliphatic, aromatic and polar fraction chromatograms obtained on the 0.1 ppt fresh crude oil spiked into the sediment at time zero (a) and after one year of weathering in the sediments of Kasitsna Bay (b, aliphatic fraction; c, aromatic fraction; d, polar fraction). Clearly, almost all of the n-alkanes in the starting oil are no longer present in the sediment after one year of weathering. In fact, the only compounds of any significance in the aliphatic fraction of the fully weathered sediment are higher molecular weight odd n-alkanes, nC_{23} , "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

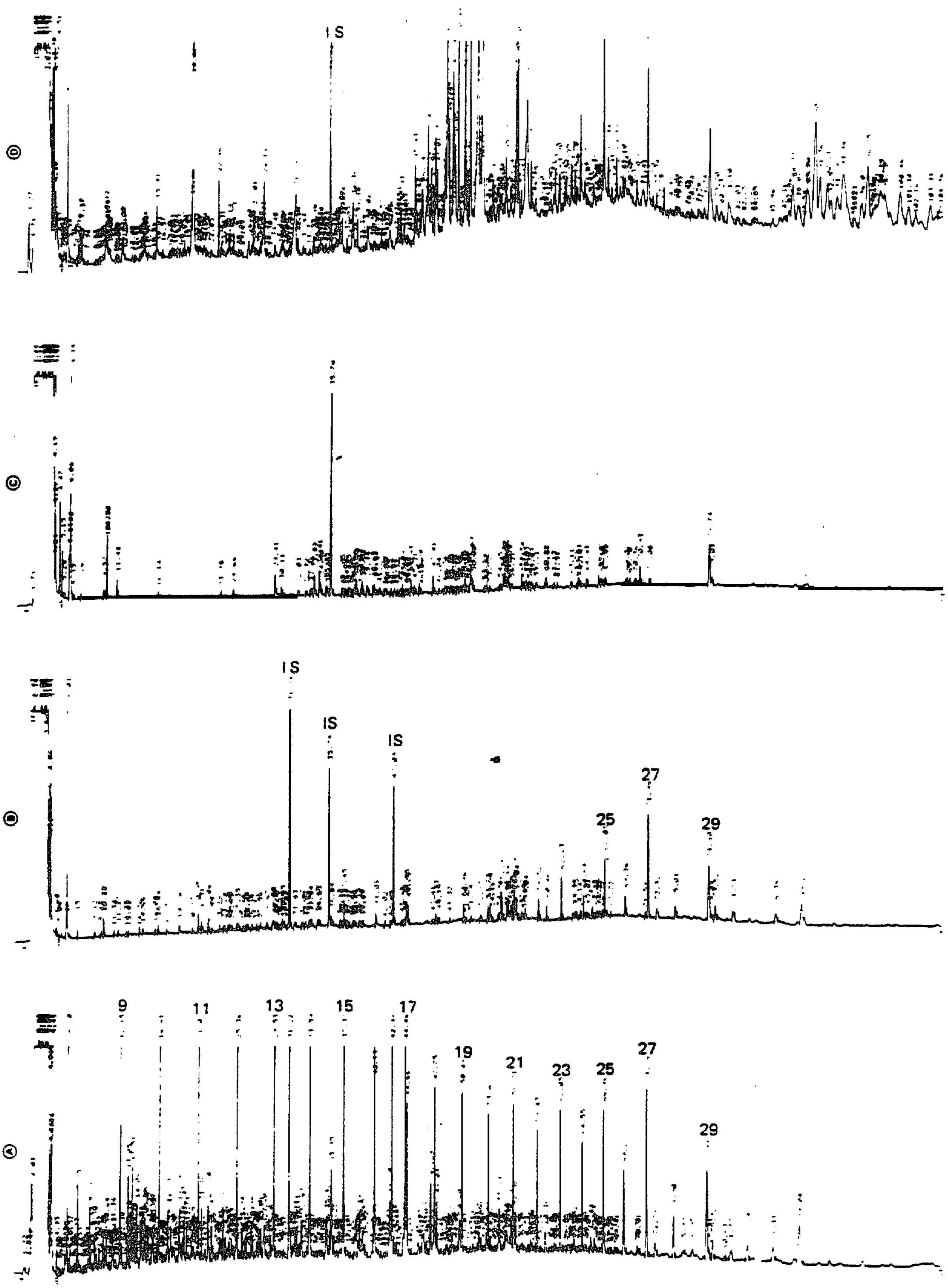

Figure 14. Flame Ionization Detector capillary gas chromatograms of: A, the aliphatic fraction of the sediment spiked with 0.1 ppt Fresh Crude Oil at time zero and B, the aliphatic fraction, C, the aromatic fraction, and i), the polar fraction extracts obtained on the 0.1 ppt Fresh Crude Oil spiked sample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

remain in the sediment after one year, although thee 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 913. These

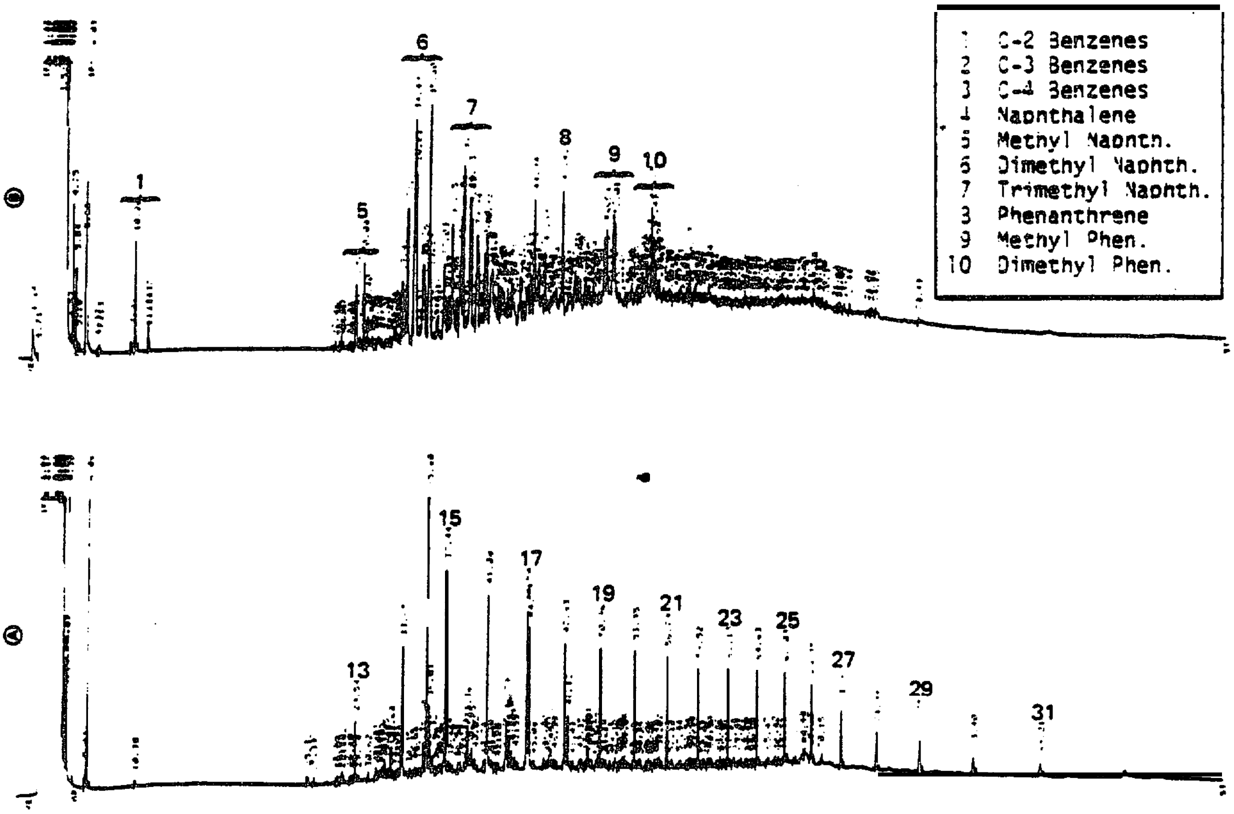

Figure 15. Flame Ionization Detector capillary gas chromatograms of: A, the aliphatic fraction and B, the Aromatic fraction extracts obtained from the time one year Kasitsna Bay sample spiked with Artificially Weathered Cook Inlet Crude Oil at 50 ppt.

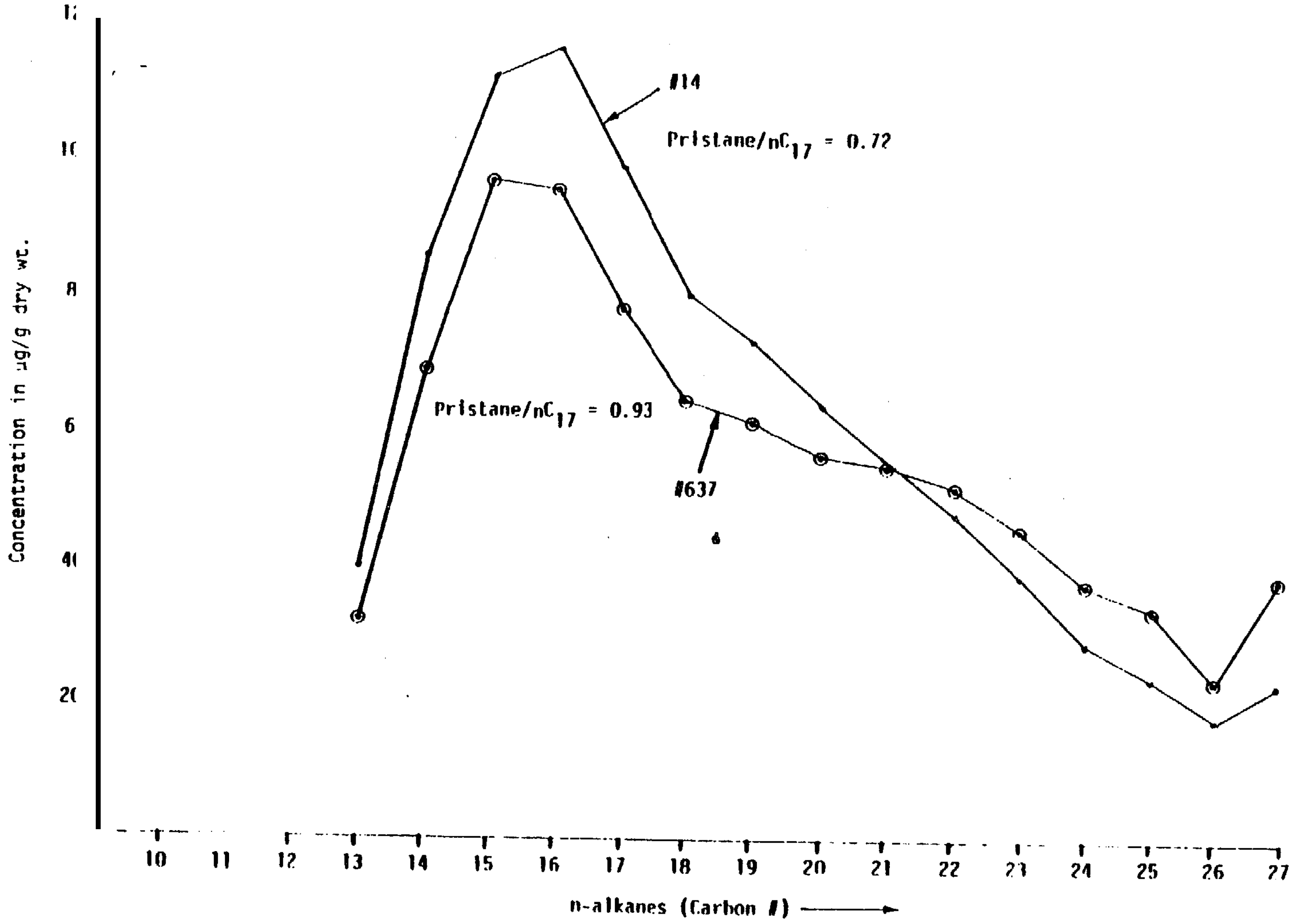

Figure 16. Concentration abundance of the n-alkanes for a sediment oil spike of 50 parts per thousand artificially weathered crude illustrating the time zero sample (•) and sample after one year of weathering (⊙).

show that while the overall concentrations of the lower molecular weight mono and di-cyclic aromatic compounds were reduced in the weathered crude oil compared to the fresh crude oil, once the 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.-

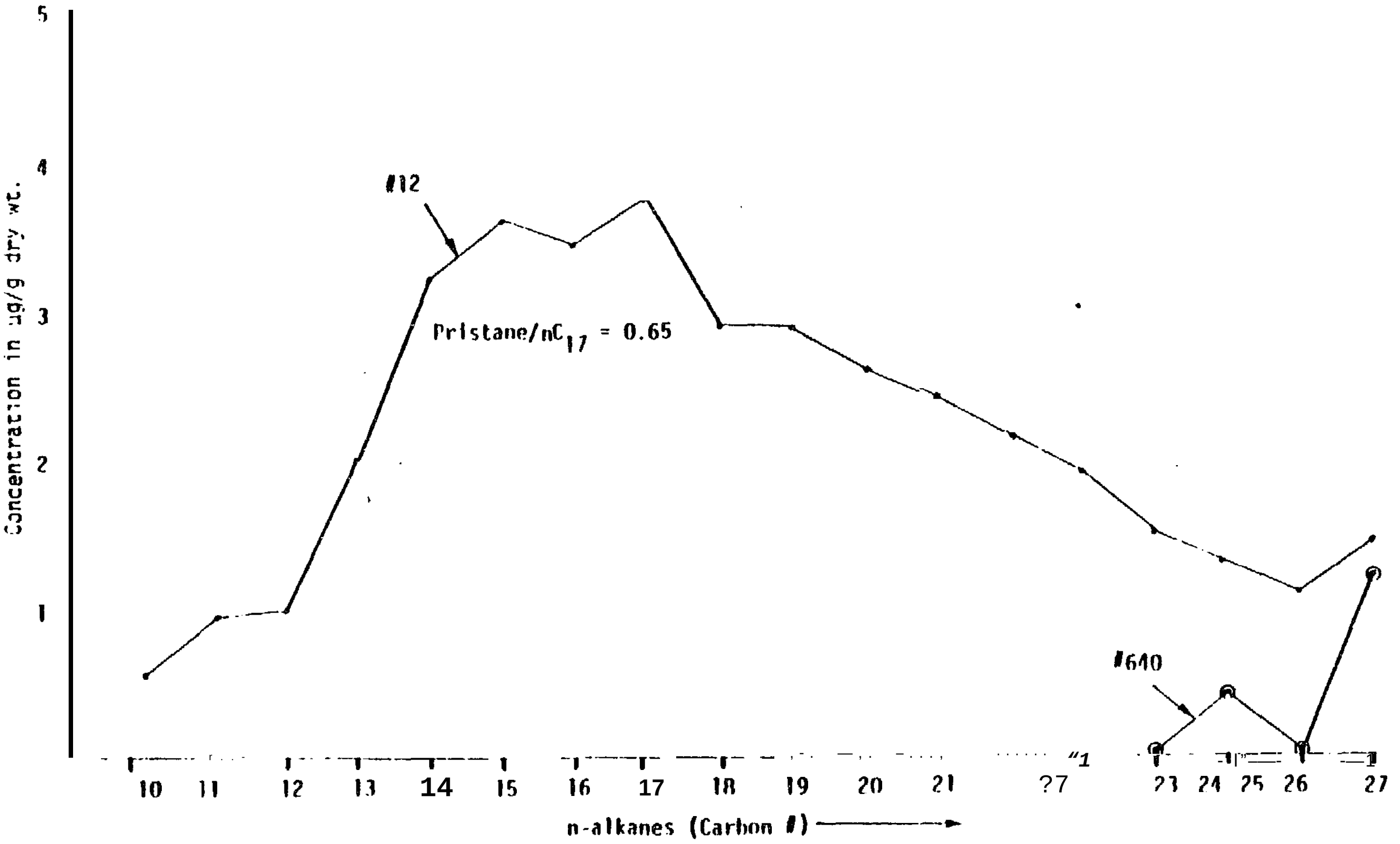

Figure 17. Concentration abundance of the n-alkanes for a sediment oil spike of 1.0 parts per thousand artificially weathered crude illustrating the time zero sample(•) and sample after one year of weathering (⊙).

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 <u>may</u> be some decrease in the levels of aromatic compounds in the oil and starch sample (a). Replicate analyses would be required to determine if the subtle difference in overall aromatic compound levels is statistically significant. Alternatively, it may be prudent to examine 1.0 ppt oil spikes in the presence and absence of nutrients to determine if enhanced aromatic hydrocarbon degradation can be induced to lower overall hydrocarbon levels where the inherent toxicity may be reduced.

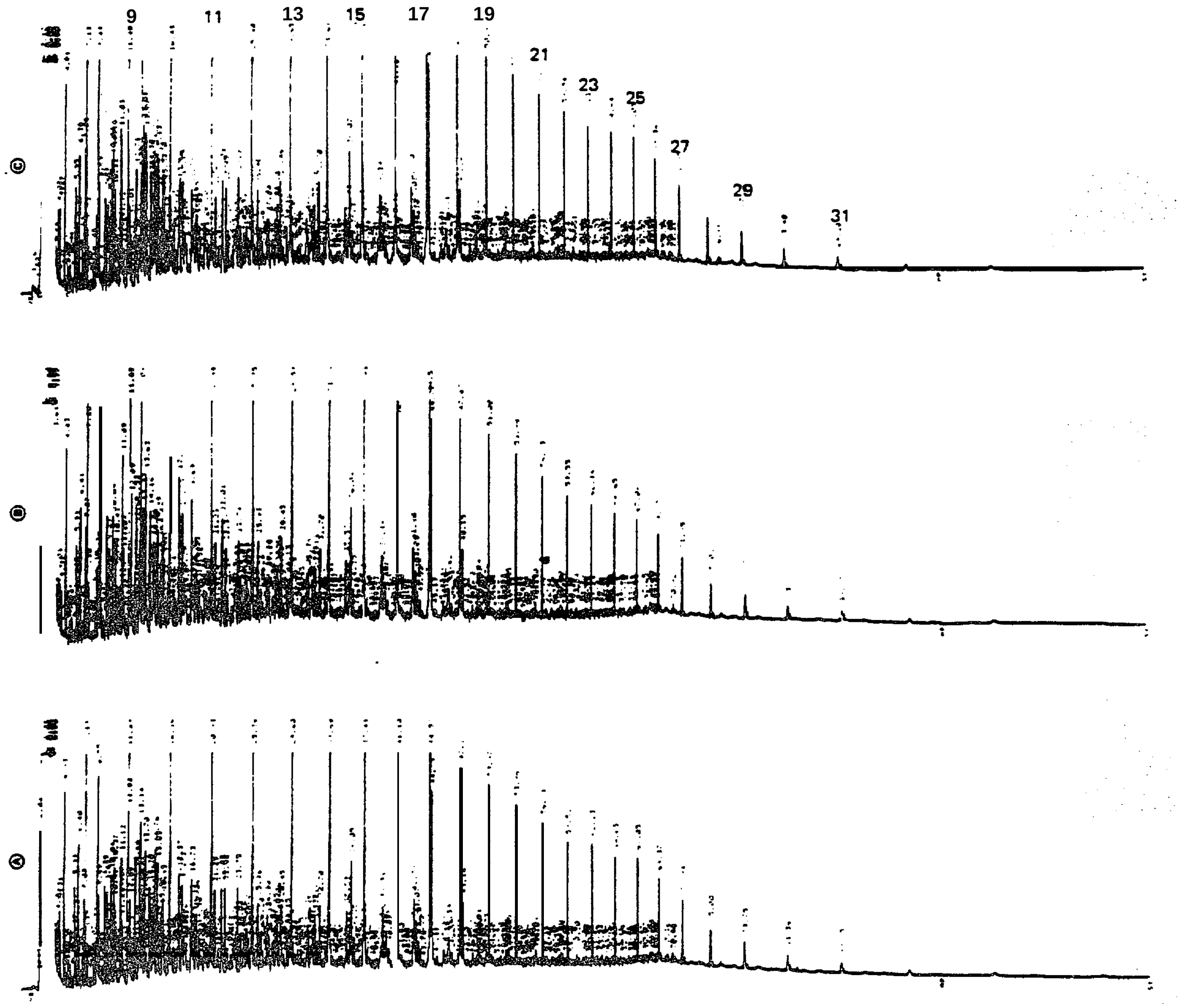

Figure 18. Flame Ionization Detector capillary gas chromatograms of aliphatic fraction extracts obtained on: A, 50 ppt fresh Oil plus starch, B, 50 ppt fresh Oil alone, and C, 50 ppt fresh Oil plus Chitin after one year of natural weathering in the sediments of Sadie Cove.

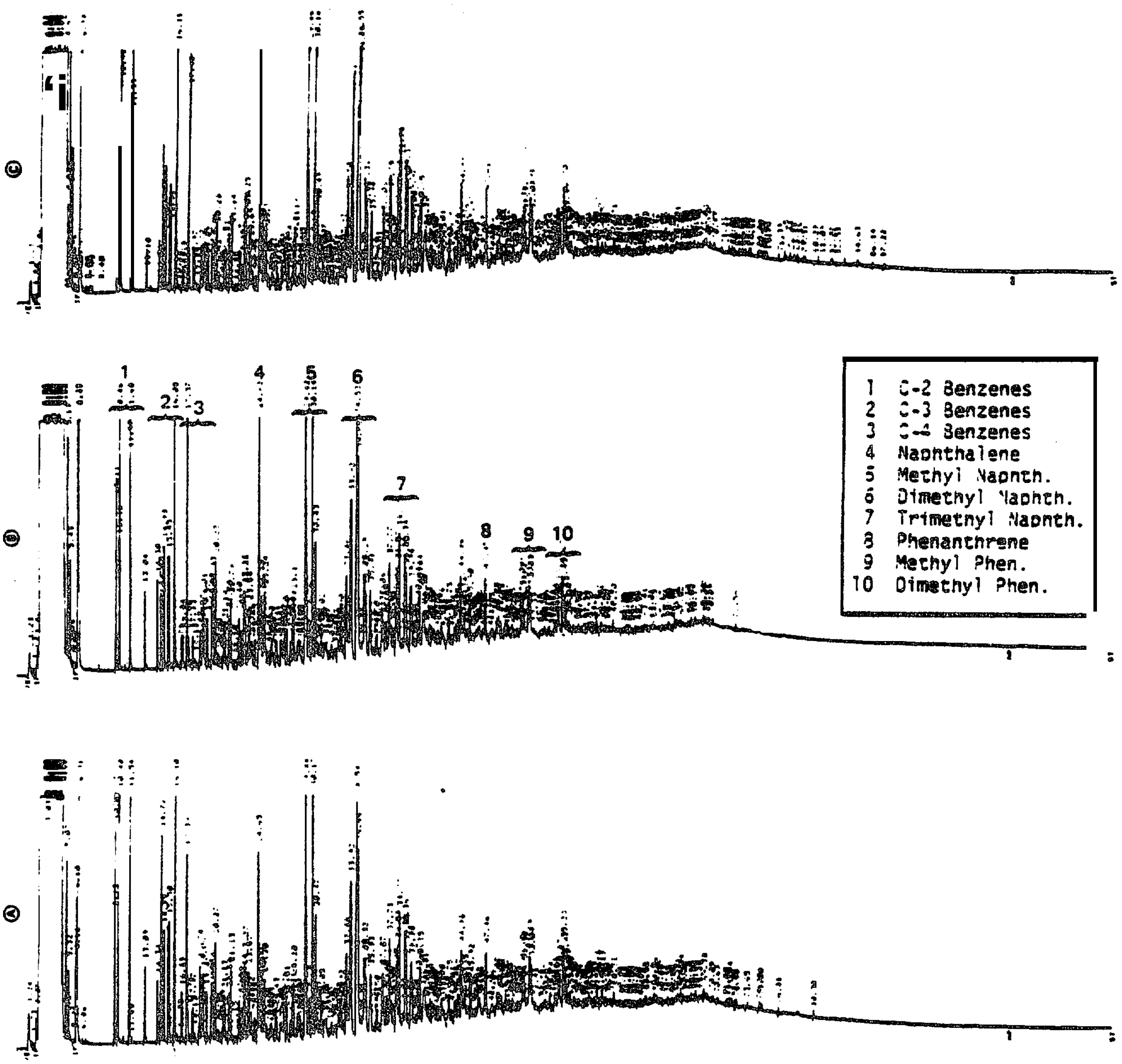

Figure 19. Flame Ionization Detector capillary gas chromatograms of aromatic fraction extracts obtained on: A, 50 ppt fresh Oil plus starch, B, 50 ppt Oil alone, and C, 50 ppt fresh Oil plus Chitin after one year of natural weathering in the sediments of Sadie Cove.

SUMMARY

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

In the study plots which were spiked with 50 ppt oil plus added nutrients (starch and Chitin), there was no evidence of any enhanced biotic recovery or selective hydrocarbon utilization with either fresh or weathered crude oil. This suggests inhibition of biological processes from the high levels of toxic aromatic compounds in the oil itself rather than inhibition from limited nutrient concentrations. To more accurately address the *role* of added nutrients in oil degradation, detailed analyses should be completed on lower spiked oil concentrations in the presence and absence of nutrients. Also, experiments to assess the role of dissolved oxygen, grain-size, the energy (tidal and wave) input to the sedimentary environment, total organic carbon content and other factors such as total bio-mass, could be considered in future studies.

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

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