USER'S MANUAL FOR THE COMPUTER CODES:
OILSPMXS
SPMONLY
OILSPM3

by

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1.0 CODE DESCRIPTIONS

This document is a compilation of the code-user's instructions for the three computer codes OILSPMXS, SPMONLY, and 01LSPM3 described in Chapter 6 of Payne et al. (1989). The intent of this user's manual is to describe how to input data and operate the codes. All internal and external references referred to in this manual are the same as those in Payne et al. (1989). Details of the mathematical bases for these three computer codes can also be found in Chapter 3 of Payne et al. (1989).

OILSPMXS is the coding of an analytical solution for one-dimensional transport of oil and SPM where the SPM concentration exceeds the oil concentration to such an extent that the SPM concentration does not change substantially due to the oil-SPM interactions. Typically, if the number density of SPM particles exceeds the number density of oil droplets by a factor of 10, this code can be used.

SPMONLY is the coding of an analytical solution for one-dimensional transport of sediment in the absence of oil. It **was used primarily to check the numerical** code that follows and to provide a mathematically-consistent SPM concentration profile at steady state to start the numerical integration. Any SPM profile that is "reasonable" can be used. Other SPM profiles not at steady state can also be used, but no coding has been provided to do so.

01LSPM3 is a numerical integration code that solves the one-dimensional transport equations for oil droplets and SPM that are interacting. There are virtually no restrictions on the use of this code.

The choice of a source term for oil is an important consideration. The oil source term used in the codes is a decaying exponential because virtually any time-varying source of oil from the open-ocean oil weathering code has followed this trend. Furthermore, exponential are do-able in a mathematical sense. A series of exponential oil-source terms can **also be used with the requirement that the code be run foreach exponential and the results**

added together. However, a single exponential source term is all that has been used to date.

The codes are one-dimensional. Therefore, the user must recognize that they do not describe any three-dimensional environmental situations. However, this is the only limitation mathematically. Because the describing partial differential equations are linear (i.e., additive and homogeneous), the usual superposition theorem can be used to obtain other results (e.g., the adding of exponential oil-source terms being one).

The sample problems presented herein illustrate the "best" estimate of available input parameters. Additional estimates for input parameters can be extracted from the experimental data in Chapter 5 of Payne et al. (1989), and Chapter 7 (conclusions and major findings) should be consulted by anyone interested in using the model. As users become more experienced with the models and gain real-world experience, better estimates for input parameters should follow. One of the major purposes of a model is to predict reality, or attempt to do so, by adjusting parameters until reality is predicted.

1.1 CODE-USE DESCRIPTION: OILSPMXS

The mathematical model that describes the interaction of oil droplets with excess SPM is coded in BASIC and named OILSPMXS.BAS. The mathematics are described in Section 3.1 of Payne et al. (1989). This code should be run from a compiled and linked executable file. The executable file should be a "stand-alone" and not require a run-time library.

Upon running OILS.PMXS by typing the .EXE file name, the screen will display a prompt asking the user if the parameters are to be "edited" or "entered," as illustrated in Table 1. The user can then enter "edit" as illustrated. Previously stored values of the parameters will be displayed as shown in Table 2. It is recommended that the user "edit" parameters rather than "enter" because' the stored parameters are in the range of interest for environmental applications. Any of the displayed parameters can be changed (i.e., edited by typing "yes" to the prompt), as illustrated in Table 2. Upon

Table 1. Initial Screen Prompt From OILSPMXS.BAS.

```
OIL DROPLETS INTERACTING WITH EXCESS SPM.
CODE NAME IS OILSPMXS.BAS, VERSION OF' 8-3-88@ 0718

WANT TO EDIT OR ENTER INPUT PARAMETERS ? edit
```

Table 2. Screen Display of Parameter Editing From OILSPMXS.BAS.

```
OIL DROPLETS INTERACTING WITH EXCESS SPM.
CODE NAME IS OILSPMXS.BAS, VERSION OF 8-3-88 @ 0718

1.  RISE VELOCITY, CM/SEC =  .001
2.  TURBULENT DIFFUSIVITY,CM*CM/SEC =  100
3.  DEPTH, METERS = 10
4.  NUMBER OF ROOTS = 25
5.  ROOT ERROR LIMIT =  1.000D-06
6.  EXPONENTIAL FLUX TERM, I/SEC =  4.600D-05
7.  INITIAL OIL FLUX, GRAM/(CM*CM*SEC) = 1.800D-05
8.  DISAPPEARANCE RATE CONSTANT, I/SEC = 9.400D-04
9.  NUMBER OF DEPTH VALUES = 27
10. PRINT THE ROOTS? YES

WANT TO CHANGE ANY? yes

ENTER THE LINE NUMBER TO BE CHANGED? 3

ENTER THE DEPTH, METERS ? 20
```

entering "yes" the parameter line number that is to be changed is entered (e.g., in Table 2 the depth is changed to 20 m). After each edit the entire parameter list is displayed. The code will continue execution only after "no" is entered at the parameter-change prompt as illustrated in Table 3.

The code executes in the compiled and linked mode in a few seconds. The initial output is a summary of the input parameters and the roots of the transcendental function (also referred to as eigenvalues) for the problem. Each page of the output begins with a header identifying the code name and version. This information is coded into the source through character strings and any user that changes the code is urged also to make these changes (in the first few lines of the source). By doing this, a record is maintained that can be of great value in documenting results. An example of the first page of output is illustrated in Table 4.

The calculated oil droplet concentration profile for a user-entered time of 1 hr is illustrated in the output in Table 5. The dimensionless time printed just under the time of 1 hr is printed to provide the user with a number that can be used to gauge how close the results are to a steady state value. Typically, dimensionless times greater than 1.0 are indicative of a result that is very close to steady state, and entering a greater time will not markedly change the results. However, this dimensionless time is printed only as a gauge, and in some cases the steady state may be a zero-concentration profile. Note in the calculated results in Table 5 that the oil-droplet concentration varies from 5.04×10^{-5} gm/cm^3 (50.4 ppm) at the surface to 1.05×10^{-5} gm/cm^3 (10.5 ppm) at a depth of 5 m, and to O gm/cm^3 at the bottom. The zero concentration at the bottom is the result of the (imposed) boundary condition described in the derivation.

A summary of the total material balance for oil droplets is printed after the concentration profile. This summary provides information with respect to the quantity of oil droplets dispersed into the water at the surface, in this example (i.e. , Table 5) 0.0597 grams at 1 hour; the mass of unattached oil droplets in the water, 0.0151 grams; oil attached to SPM, 0.0415 grams; and oil attached to the bottom, 0.0032 grams. The latter three masses

Table 3. Screen Display of Parameters to be Used in Calculation, with a Final User Response of "no", From OILSPMXS.BAS.

```
OIL DROPLETS INTERACTING WITH EXCESS SPM.
CODE NAME IS OILSPMXS.BAS, VERSION OF 8-3-88 @ 0718

1.  RISE VELOCITY, CM/SEC =  .001
2.  TURBULENT DIFFUSIVITY,CM*CM/SEC =  100
3.  DEPTH, METERS = 10
4.  NUMBER OF ROOTS = 25
5.  ROOT ERROR LIMIT =  1.000D-06
6.  EXPONENTIAL FLUX TERM,. I/SEC =  4.600D-05
7.  INITIAL OIL FLUX, GRAM/(CM*CM*SEC) = 1.8001)-05
8.  DISAPPEARANCE RATE CONSTANT, 1/SEC = 9.400D-04
9.  NUMBER OF DEPTH VALUES = 27
10. PRINT THE ROOTS? YES

WANT TO CHANGE ANY? no
```

'I'able 4. Printed Output of Problem Parameters From OILSPMXS.BAS.

CODE NAME IS 01 LSPMXS.BAS, VERSION OF 8-3-88 @ 0718
RUN TIME = 07:15:01, RUN DATE = 08-03-1988

THIS CODE SOLVES THE TRANSIENT ADVECTION-DISPERSION EQUATION FOR OIL DROPLETS WITH FIRST-ORDER REACTION LOSS.

PROBLEM IDENTIFICATIONS PRE-LOADED PARAMETER TEST CASE

OIL DROPLET RISE VELOCITY = .001 cM/SEC, DEPTH = 10 METERS

TURBULENT DIFFUSIVITY = 100 CM*CM/SEC

ERROR LIMIT FOR THE ROOTS = 1.000D-06

VX*L/(2*K) = -5.000D-03 UNITLESS

THE 25 ROOTS OF F(BETA) = BETA*COTANGENT(BETA) + VX*L/(2*K)

ROOT	F (BETA)	ERROR CODE
1.568D+00	-4.111D-07	1
4.711D+00	3.831D-07	1
7.853D+00	-7.362D-08	1
1.100D+01	-2.266D-08	1
1.414D+01	4.998D-07	1
1.728D+01	3.937D-07	1
2.042D+01	-4.653D-07	1
2.356D+01	-8.318D-08	1
2.670D+01	2.939D-07	1
2.984D+01	3.739D-07	1
3.299D+01	1.577D-07	1
3.613D+01	-5.745D-07	1
3.927D+01	3.101D-O7	1
4.241D+01	-7.179D-07	1
4.555D+01	6.801D-07	1
4.869D+01	-9.371D-07	1
5.184D+01	5.586D-08	1
5.498D+01	6.808D-07	1
5.812D+01	7.541D-07	1
6.126D+01	5.503D-08	1
6.440D+01	2.015D-07	1
6.754D+01	-9.391D-07	1
7.069D+01	-5.765D-08	1
7.383D+01	9.708D-07	1
7.697D+01	-6.114D-07	1

EXPONENTIAL FLUX TERM = 4.600D-05 I/SEC

INITIAL OIL FLUX = 1.800D-05 GRAMS/(CM*CM*SEC)

FIRST ORDER DISAPPEARANCE RATE CONSTANT, I/SEC = 9.400D-04 1/SEC

ZETA-BAR IS REAL (<> VX/(2*K)) AND EQUAL TO 2.990D-03 1/CM (IZBAR = 1)

Table 5. Calculated Oil-Droplet Concentration Profile at 1 Hour From OILSPMXS.BAS.

```
CODE NAME IS O ILSPMXS .BAS, VERSION OF 8-3-88 @ 0 7 1 8
RUN TIME =  07:15:01,RUN DATE = 08-03-1988

CALCULATED RESULTS ********************************

CONCENTRATION PROFILE(GM/CC)FOR TIME =  1.000D+00 HOURS
DIMENSIONLESS TIME,K*T/L**2 =  3.600D-01
```

DEPTH (CM)	OIL CONC (GM/CC)	
0.000D+00	5.040D-05	(SURFACE)
3.846D+01	4.484D-05	
7.692D+01	3.988D-05	
1.154D+02	3.546D-05	
1.538D+02	3.152D-05	
1.923D+02	2.800D-05	
2.308D+02	2.487D-05	
2.692D+02	2.207D-05	
3.077D+02	1.957D-05	
3.462D+02	1.733D-05	
3.846D+02	1.534D-05	
4.231D+02	1.355D-05	
4.615D+02	1.195D-05	
5.000D+02	1.052D-05	
5.385D+02	9.2250-06	
5.769D+02	8.062D-06	
6.154D+02	7.011D-06	
6.538D+02	6.057D-06	
6.923D+02	5.187D-06	
7.308D+02	4.390D-06	
7.692D+02	3.654D-06	
8.077D+02	2.969D-06	
8.462D+02	2.327D-06	
8.846D+02	1.717D-06	
9.231D+02	1.131D-06	
9.615D+02	5.614D-07	
1.000D+03	0.000D+00	(BOTTOM)

```
TOTAL GRAMS OF OIL DISPERSED INTO THE WATER COLUMN =  5.972D-02

GRAMS OF FREE OIL DROPS IN THE WATER COLUMN  =  1.507D-02
GRAMS OF OIL DROPS ATTACHED TO SPM  =  4.147D-02
GRAMS OF FREE OIL DROPS ATTACHED TO  THE BOTTOM =  3.179D-03

TOTAL GRAMS OF OIL ACCOUNTED FOR IN THE CALCULATION =  5.972D-02
```

must sum to the mass of oil dispersed in order to "close" the material balance. Thus, the last line of output accounts for 0.0597 g of oil. The material balance must close for each calculation; lack of successful closure indicates an error in the calculation.

The oil-droplet concentration profile at 10 hr is presented in Table 6 and is to be compared with the profile at 1 hr in Table 5. Note that the 10-hr concentrations are considerably decreased relative to the l-hr concentrations. This is due to the loss of oil through reaction and loss of oil to the bottom. Note that the dispersion is modeled as a decaying exponential, (line #6 in Table 2) and as a result the oil-droplet flux from the surface goes to zero at large values of time.

The sample problem illustrated in Tables 1 through 6 is based on an $(\epsilon/\nu)^{1/2}$ value of 10 sec^{-1}. However, a review of the literature (Table 7) for energy dissipation rates in the ocean shows that a value of 0.01 erg/cm ^{3}/see can be expected (and down to 0.0003 $erg/cm^3/sec$ also). On a per-unit mass-of-fluid basis this value becomes 0.01 cm^2/sec^3, and dividing by a kinematic viscosity of 0.01 cm^2/sec yields $(\epsilon/\nu)^{1/2} = 1\ sec^{-1}$. The rate constant for oil-droplet loss with an excess SPM load of 100 mg/L then will be 0.000094 sec^{-1} (decreased by a factor of 10 from the previous case). Calculated results for this rate constant at 1 and 10 hr are presented in Tables 8 through 10. Note that the free oil-droplet concentration profile with the decreased α_c in Table 8 is greater than that in Table 5. The reason for this difference is that in the case with a smaller oil-loss rate constant, more oil remains in the water column. This is also illustrated by the mass of oil attached to SPM at 1 hour; for $\alpha_c = 0.00094$ the oil mass attached is 0.0415 grams (Table 5) while for $\alpha_c = 0.000094$ the oil mass attached is 0.00834 grams (Table 9). The corresponding calculation at 10-hr is presented in Table 6-10 and is to be compared with Table 6.

1.2 CODE-USE DESCRIPTION: SPMONLY

The mathematical model which describes the transport of SPM with a first-order reaction loss is coded in BASIC and named SPMONLY.BAS. The

Table 6. Calculated Oil-Droplet Concentration Profile at 10 Hours From OILSPMXS.BAS.

CODE NAME IS OILSPMXS.BAS, VERSION OF 8-3-88 @ 0718
RUN TIME = 07:15:01, RUN DATE = 08-03-1988

CALCULATED RESULTS **********

CONCENTRATION PROFILE (GM/CC) FOR TIME = 1.000D+01 HOURS
DIMENSIONLESS TIME, K*T/L**2 = 3.600D+00

DEPTH (CM)	OIL CONC (GM/CC)	
0.000D+00	1.145D-05	(SURFACE)
3.846D+01	1.020D-05	
7.692D+01	9.083D-06	
1.154D+02	8.087D-06	
1.538D+02	7.197D-06	
1.923D+02	6.404D-06	
2.308D+02	5.695D-06	
2.692D+02	5.062D-06	
3.077D+02	4.496D-06	
3.462D+02	3.990D-06	
3.846D+02	3.537D-06	
4.231D+02	3.131D-06	
4.615D+02	2.767D-06	
5.000D+02	2.439D-06	
5.385D+02	2.144D-06	
5.769D+02	1.877D-06	
6.154D+02	1.636D-06	
6.538D+02	1.416D-06	
6.923D+02	1.215D-06	
7.308D+02	1.030D-06	
7.692D+02	8.583D-07	
8.077D+02	6.984D-07	
8.462D+02	5.478D-07	
8.846D+02	4.046D-07	
9.231D+02	2.667D-07	
9.615D+02	1.325D-07	
1.000D+03	0.000D+00	(BOTTOM)

TOTAL GRAMS OF OIL DISPERSED INTO THE WATER COLUMN = 3.166D-01

GRAMS OF FREE OIL DROPS IN THE WATER COLUMN = 3.459D-03
GRAMS OF OIL DROPS ATTACHED TO SPM = 2.843D-01
GRAMS OF FREE OIL DROPS ATTACHED TO THE BOTTOM = 2.881D-02

TOTAL GRAMS OF OIL ACCOUNTED FOR IN THE CALCULATION = 3.166D-01

Table 7. Observed Energy Dissipation Rates

Depth (m)	ε(ergs/cm³/sec)	References
1	6.4 E-2	Liu (1985)
1-2	3.0 E-2	Stewart &Grant (1962)
15	3.0 E-2	Stewart & Grant (1962)
15	2.5 E-2	Grant et al. (1968)
15	1.0 E-2	Liu (1985)
27	5.2 E-3	Grant et al. (1968)
36	1.5 E-1	Belyaev (1975)*
40	2.65 E-3	Liu (1985)
43	3,0 E-3	Grant et al. (1968)
58	4.8 E-3	Grant et al. (1968)
73	1.9 E-3	Grant et al. (1968)
89	3.4 E-4	Grant et al. (1968)
90	3.1 E-4	Grant et al. (1968)
100	6.25 E-4	Liu (1985)
140	3,7 E-2	Belyaev (1975)*

*In Raj (1977).

Unit Conversions

1 erg/cm³/sec = 1 cm²/sec³ water
= 10^{-4} watts/kg water
= 10^{-7} watts/cm³

Reference:

Kirstein et al., "Observed Energy Dissipation Rates", Interim Report, Integration of Suspended Particulate Matter and Oil Transportation Study, submitted to MMS, November 1, 1985..

Table 8. Printed Output of Problem Parameters From OILSPMXS.BAS (with a_c=0.000094 sec^{-1}).

CODE NAME IS OILSPMXS.BAS, VERSION OF 8-3-88 @ 0718
RUN TIME = 10:42:31, RUN DATE = 08-03-1988

THIS CODE SOLVES THE TRANSIENT ADVECTION-DISPERSION EQUATION FOR OIL DROPLETS WITH FIRST-ORDER REACTION LOSS.

PROBLEM IDENTIFICATION: PRE-LOADED PARAMETER TEST CASE

OIL DROPLET RISE VELOCITY = .001 CM/SEC, DEPTH = 10 METERS

TURBULENT DIFFUSIVITY = 100 CM*CM/SEC

ERROR LIMIT FOR THE ROOTS = 1.000D-06

VX*L/(2*K) = -5.0000-03 UNITLESS

THE 25 ROOTS OF F(BETA) = BETA*COTANGENT(BETA) + VX*L/(2*K)

ROOT	F (BETA)	ERROR CODE!
1.568D+00	-4.111D-07	1
4.711D+00	3.831D-07	1
7.853D+00	-7.362D-08	1
1.100D+01	-2.266D-08	1
1.414D+01	4.998D-07	1
1.728D+01	3.937D-07	1
2.042D+01	-4.6531)-07	1
2.356D+01	-8.318D-08	1
2.670D+01	2.939D-07	1
2.984D+01	3.739D-07	1
3.299D+01	1.577D-07	1
3.613D+01	-5.745D-07	1
3.927D+01	3.101D-07	1
4.241D+01	-7.179D-07	1
4.555D+01	6.801D-07	1
4.869D+01	-9.371D-07	1
5.184D+01	5.586D-08	1
5.498D+01	6.808D-07	1
5.812D+01	7.541D-07	1
6.126D+01	5.503D-08	1
6.440D+01	2.015D-07	1
6.754D+01	-9.391D-07	1
7.069D+01	-5.765D-08	1
7.383D+01	9.708D-07	1
7.697D+01	-6.114D-07	1

EXPONENTIAL FLUX TERM = 4.600D-05 1/SEC

INITIAL OIL FLUX = 1.800D-05 GRAMS/(CM*CM*SEC)

FIRST ORDER DISAPPEARANCE RATE CONSTANT, 1/SEC = 9.400D-05 1/SEC

ZETA-BAR IS REAL (<> VX/(2*K)) AND EQUAL TO 6.928D-04 1/CM (IZBAR = 1)

Table 9. Calculated Oil-Droplet Concentration Profile at 1 Hour From OILSPMXS.BAS (with a_c =0.000094 see-l).

CODE NAME IS OILSPMXS.BAS, VERSION OF 8-3-88 @ 0718
RUN TIME = 10:42:31, RUN DATE = 08-03-1988

CALCULATED RESULTS **********x**********

CONCENTRATION PROFILE (GM/CC) FOR TIME = 1.000D+00 HOURS
DIMENSIONLESS TIME, K*T/L**2 = 3.600D-01

DEPTH (CM)	OIL CONC (GM/CC)	
0.000D+00	9.647D-05	(SURFACE)
3.846D+01	9.068D-05	
7.692D+01	8.512D-05	
1.154D+02	7.977D-05	
1.538D+02	7.463D-05	
1.923D+02	6.970D-05	
2.308D+02	6.498D-05	
2.692D+02	6.044D-05	
3.077D+02	5.61OD-O5	
3.462D+02	5.193D-05	
3.846D+02	4.794D-05	
4.231D+02	4.411D-05	
4.615D+02	4.044D-05	
5.000D+02	3.691D-05	
5.385D+02	3.353D-05	
5.769D+02	3.027D-05	
6.154D+02	2.713D-05	
6.538D+02	2.41OD-O5	
6.923D+02	2.117D-05	
7.308D+02	1.832D-05	
7.692D+02	1.556D-05	
8.077D+02	1.286D-05	
8.462D+02	1.022D-05	
8.846D+02	7.625D-06	
9.231D+02	5.063D-06	
9.615D+02	2.526D-06	
1.000D+03	0.000D+00	(BOTTOM)

TOTAL GRAMS OF OIL DISPERSED INTO THE WATER COLUMN = 5.972D-02

GRAMS OF FREE OIL DROPS IN THE WATER COLUMN = 4.073D-02
GRAMS OF OIL DROPS ATTACHED TO SPM = 8.342D-03
GRAMS OF FREE OIL DROPS ATTACHED TO THE BOTTOM = 1.064D-02

TOTAL GRAMS OF OIL ACCOUNTED FOR IN THE CALCULATION = 5.972D-02

Table 10. Calculated Oil-Droplet Concentration Profile at 10 Hours From OILSPMXS.BAS (with a_c =0.000094 see-l).

CODE NAME IS OILSPMXS.BAS, VERSION OF 8-3-88 @ 0718
RUN TIME = 10:42:31, RUN DATE = 08-03-1988

CALCULATED RESULTS **********

CONCENTRATION PROFILE (GM/CC) FOR TIME = 1.000D+01 HOURS
DIMZNS1ONLESS TIME,K*T/L**2 = 3.600D+00

DEPTH (CM)	OIL CONC (GM/CC)	
0.000D+00	2.988D-05	(SURFACE)
3.846D+01	2.855D-05	
7.692D+01	2.725D-05	
1.154D+02	2.597D-05	
1.538D+02	2.471D-05	
1.923D+02	2.346D-05	
2.308D+02	2.224D-05	
2.692D+02	2.102D-05	
3.077D+02	1.983D-05	
3.462D+02	1.865D-05	
3.846D+02	1.748D-05	
4.231D+02	1.632D-05	
4.615D+02	1.518D-05	
5.000D+02	1.405D-05	
5.385D+02	1.293D-05	
5.769D+02	1.182D-05	
6.154D+02	1.071D-05	
6.538D+02	9.619D-06	
6.923D+02	8.531D-06	
7.308D+02	7.450D-06	
7.692D+02	6.375D-06	
8.077D+02	5.305D-06	
8.462D+02	4.238D-06	
8.846D+02	3.175D-06	
9.231D+02	2.115D-06	
9.615D+02	1.057D-06	
1.000D+03	0.000D+00	(BOTTOM)

TOTAL GRAMS OF OIL DISPERSED INTO THE WATER COLUMN = 3.166D-01

GRAMS OF FREE OIL DROPS IN THE WATER COLUMN = 1.434D-02
GRAMS OF OIL DROPS ATTACHED TO SPM = 1.028D-01
GRAMS OF FREE OIL DROPS ATTACHED TO THE BOTTOM = 1.995D-01

TOTAL GRAMS OF OIL ACCOUNTED FOR IN THE CALCULATION = 3.166D-01

mathematics is described in Section 3.1.2 of Payne et al. (1989). This code should be run from a compiled and linked executable file. The executable file should be a "stand-alone" and not require a run-time library.

Upon running SPMONLY by typing in the .EXE file name, the screen will display a prompt asking the user if the parameters are to be "edited" or "entered". It is recommended that the user enter "edit" because the parameters stored in the code are in the range of interest of environmental applications. Any of the displayed parameters can be changed (i.e., edited) by typing "yes" in response to the prompt. Upon entering "yes" the parameter line number that is to be changed is entered. After each edit the entire parameter list is displayed. The code will continue to execute only after "no" is entered at the parameter-change prompt as illustrated in Table 11.

Upon entering "no" the prompt will ask the user if cotangent values from Abramowitz and Stegun are to be used. The Abramowitz and Stegun cotangent values are double-precision cotangent values as described in the Handbook of Mathematical Functions (M. Abramowitz and I.A. Stegun, page 76). The reason this cotangent calculation was used is the recognition that some BASIC software does not have double-precision trigonometric functions, and in the early stages of coding an error limit of less than 1.D0-05 could not be attained in solving for the roots of the transcendental function (eigenfunction). Most of the time it will make no difference if the Abramowitz and Stegun cotangent values are used or if the single-precision machine function is used. For the example illustrated in Table 11, "no" is entered. The prompt will then ask for a time to calculate the SPM concentration profile.

The results of a calculation are illustrated in Tables 12 through 14. Table 12 provides documentation of the code name and version, an echo of the input parameters, and the roots of the transcendental function (eigenfunction). The code name and version are printed as a header on each page of output to provide a means of documenting results. These two identification items are coded into the source through character strings, and any user that changes the code is urged to make these changes (in the first few lines of the source).

Table 11. Screen Display of Parameter List for SPMONLY.BAS.

```
SUSPENDED-PARTI CULATE-MATTER (SPM) CALCULATION
CODE NAME IS SPMONLY.BAS, VERSION OF 8-4-88 @ 0746

1.  TERMINAL VELOCITY, CM/SEC =  .001
2.  TURBULENT DIFFUSIVITY,CM*CM/SEC =  100
3.  DEPTH, METERS = 10
4.  NUMBER OF ROOTS = 25
5.  ROOT ERROR LIMIT =  1.000D-06
6.  SPM-LOSS RATE CONSTANT, I/SEC =  9.400D-07
7.  FLUX RATE, GM/SEC*CM*CM =  4.600D-05
8.  DEPOSITION RATE, CM/SEC =  4.600D-02
9.  NUMBER OF DEPTH VALUES = 49
10. PRINT THE ROOTS? YES

WANT TO CHANGE ANY? N

DO YOU WANT ABRAMOWITZ&STEGUN COTANGENT VALUES? NO

ENTER THE TIME IN HOURS ? 1.

TIME ENTERED IS 1.000D+00

IS THIS CORRECT ? yes
```

Table 12. Printed Output From SPMONLY Documenting Problem Parameters.

```
CODE NAME IS SPMONLY.BAS, VERSION OF 8-4-88 @ 0746
RUN TIME = 08:12:02, RUN DATE = 08-04-1988

THIS CODE SOLVES THE 1-D TRANSIENT ADVECTION-DISPERSION EQUATION FOR SPM
(ANALYTICAL SOLUTION] WITH FIRST-ORDER REACTION LOSS.

TERMINAL VELOCITY = 1.000D-03 CM/SEC, DEPTH = 10.0 METERS

TURBULENT DIFFUSIVITY = 100.0 CM*CM/SEC

FLUX RATE FROM THE BOTTOM = 4.600D-05 GM/SEC*CM*CM

DEPOSITION RATE = 4.600D-02 CM/SEC

ERROR LIMIT FOR THE ROOTS = 1.000D-06

A = VX/(2*K) = 5.000D-06 1/CM

ROOTS CALCULATED USING MACHINE FUNCTIONS.

THE 25 ROOTS OF F(BETA)=BETA*COTANGENT(BETA)-K*((A*L)^2-A*KS*L+BETA^2)/(KS*L)
```

ROOT	F(BETA)	ERROR CODE
6.319D-01	1.685D-07	1
3.281D+00	9.872D-07	1
6.355D+00	-6.364D-07	1
9.473D+00	-1.659D-07	1
1.260D+01	-8.777D-07	1
1.574D+01	-3.807D-07	1
1.887D+01	4.496D-07	1
2.201D+01	6.450D-07	1
2.515D+01	-7.795D-07	1
2.829D+01	-4.485D-08	1
3.143D+01	-6.668D-07	1
3.457D+01	9.841D-07	1
3.771D+01	1.799D-07	1
4.085D+01	5.034D-07	1
4.399D+01	6.818D-07	1
4.713D+01	-7.496D-07	1
5.027D+01	-3.562D-07	1
5.342D+01	-9.183D-07	1
5.656D+01	-4.542D-07	1
5.970D+01	-8.393D-07	1
6.284D+01	-6.561D-07	1
6.598D+01	7.975D-07	1
6.912D+01	-9.499D-08	1
7.226D+01	5.386D-07	1
7.540D+01	3.503D-07	1

```
INITIAL SPM FLUX = 4.600D-05 GRAMS/(CM*CM*SEC)

FIRST-ORDER SPM DISAPPEARANCE RATE CONSTANT, 1/SEC = 9.400D-07 1/SEC
```

Table 13. Printed Output From SPMONLY, SPM Profile at 1 Hour.

```
CODE NAME IS SPMONLY.BAS, VERSION OF 8-4-88 @ 0746
RUM TIME = 08:12:02, RUN DATE = 08-04-19$8

CONCENTRATION PROFILES AT TIME =  1.000D+00 HOURS •**********************

        DEPTH              SPM CONC.
         CM                GM/CM**3
      0.000D+00          7.772D-05 (SURFACE)
      2.083D+01          7.7810-05
      4.167D+01          7.805D-05
      6.250D+01          7.845D-05
      8.333D+01          7.8990-05
      1.042D+02          7.968D-05
      1.250D+02          8.053D-05
      1.458D+02          8.152D-05
      1.667D+02          8.267D-05
      1.875D+02          8.397D-05
      2.083D+02          8.542D-05
      2.292D+02          8.702D-05
      2.500D+02          8.8770-05
      2.708D+02          9.067D-05
      2.917D+02          9.273D-05
      3.125D+02          9.493D-05
      3.333D+02          9.729D-05
      3.542D+02          9.980D-05
      3.750D+02          1.025D-04
      3.958D+02          1.053D-04
      4.167D+02          1.083D-04
      4.375D+02          1.114D-04
      4.583D+02          1.146D-04
      4.792D+02          1.181D-04
      5.000D+02          1.217D-04
      5.208D+02          1.254D-04
      5.417D+02          1.293D-04
      5.625D+02          1.333D-04
      5.833D+02          1.375D-04
      6.042D+02          1.418D-04
      6.250D+02          1.463D-04
      6.458D+02          1.510D-04
      6.667D+02          1.558D-04
      6.875D+02          1.607D-04
      7.083D+02          1.658D-04
      7.292D+02          1.711D-04
      7.500D+02          1.765D-04
      7.708D+02          1.820D-04
      7.917D+02          1.877D-04
      8.125D+02          1.936D-04
      8.333D+02          1.996D-04
      8.542D+02          2.057D-04
      8.750D+02          2.120D-04
      8.958D+02          2.184D-04
      9.167D+02          2.250D-04
      9.375D+02          2.317D-04
      9.583D+02          2.386D-04
      9.792D+02          2.456D-04
      1.000D+03          2.527D-04 (BOTTOM)

GRAMS OF SP14 (UNATTACHED) IN THE WATER COLUMN = 1.362D-01
GRAMS OF SPM ATTACHED TO OIL = 2.395D-04

GRAMS OF SPM I N WATER + ATTACHED = 1.365D-01

GRAMS 0? SPM FROM THB BOTTOM (FROM VX*C-K*DC/DX) = 1.3650-01
GRAMS OF SPM FROM THE BOTTOM ( F R O M -F0+KS*C) = 1.365D-01
```

Table 14. Printed Output From SPMONLY, SPM Profile at 6 Hours.

```
CODE NAME IS SPMONLY.BAS, VERSION OF 8-4-88 @ 0746
RUN TIME = 08:12:02, RUN DATE = 08-04-1988

CONCENTRATION PROFILES AT TIME= 6.000D+00 HOURS **********************

        DEPTH              SPM CONC.
         CM                GM/CM**3
      0.000D+00          5.395D-04 (SURFACE)
      2.083D+01          5.397D-04
      4.167D+01          5.3990-04
      6.250D+01          5.402D-04
      8.333D+01          5.406D-04
      1.042D+02          5.411D-04
      1.250D+02          5.416D-04
      1.458D+02          5.422D-04
      1.667D+02          5.429D-04
      1.875D+02          5.437)3-04
      2.083D+02          5.445D-04
      2.292D+02          5.455D-04
      2.500D+02          5.465D-04
      2.708D+02          5.4760-04
      2.917D+02          5.487D-04
      3.125D+02          5.500D-04
      3.333D+02          5.513D-04
      3.542D+02          5.527D-04
      3.750D+02          5.541D-04
      3.958D+02          5.557D-04
      4.167D+02          5.573D-04
      4.375D+02          5.590D-04
      4.583D+02          5.608D-04
      4.792D+02          5.626D-04
      5.000D+02          5.645D-04
      5.208D+02          5.665D-04
      5.417D+02          5.686D-04
      5.625D+02          5.708D-04
      5.833D+02          5.730D-04
      6.042D+02          5.753D-04
      6.250D+02          5.776D-04
      6.458D+02          5.801D-04
      6.667D+02          5.826D-04
      6.875D+02          5.852D-04
      7.083D+02          5.879D-04
      7.292D+02          5.906D-04
      7.500D+02          5.934D-04
      7.708D+02          5.963D-04
      7.917D+02          5.992D-04
      8.125D+02          6.0220-04
      8.333D+02          6.053D-04
      8.542D+02          6.0850-04
      8.750D+02          6.1170-04
      8.958D+02          6.150D-04
      9.167D+02          6.183D-04
      9.375D+02          6.217D-04
      9.583D+02          6.252D-04
      9.792D+02          6.288D-04
      1.000D+03          6.324D-04 (BOTTOM)

GRAMS OF SPM (UNATTACHED) IN THE WATER COLUNN = 5.717D-01
GRAMS OF SPM ATTACHED TO OIL =6.677D-03

GRAMS OF SPM IN WATER + ATTACHED = 5.784D-01

GRAMS 0? SPM FROM THE BOTTOM (FROM VX*C-K*DC/DX) = 5.7840-01
GRAMS OF SPM FROM THE BOTTOM (FROM -F0+KS*C)=5.784D-01
```

Tables 13 and 14 illustrate the calculated SPM profiles at 1 and 6 hr, respectively. At 1 hr the SPM concentration varies from 7.7 x 10^{-5} gm/cm^3 (77 ppm) at the surface to 2.5 x 10^{-4} gm/cm^3 (250 ppm) at the bottom, while at 6 hr the SPM at the surface is 5.4 x 10^{-4} gm/cm^3 (540 ppm) and at the bottom 6.3 x 10^{-4} gm/cm^3 (630 ppm). Note that the SPM profile is "flattening out" at 6 hr (i.e., the SPM concentration in the water column is approaching steady state and is expected to be "flat").

A total material balance for the SPM is printed below each concentration profile. SPM can reside in the water column or be removed from the water column through reaction with oil. These two masses must sum to the SPM mass put into the water column at the bottom. This is illustrated in Table 13 where 0.1362 g are in the water column and 0.000239 g are attached to oil (by reaction). These two masses sum to 0.1365 g, which is equal to the SPM mass fluxed into the water at the bottom by -Fo+ksC or the mass fluxed away from the bottom by $\nu_x C - k(dC/dx)$. Similar results are illustrated in Table 14.

1.3 CODE-USE DESCRIPTION: 01LSPM3

The mathematical model that describes the interaction of oil droplets and SPM where SPM is not required to be in excess is coded in BASIC and named OILSPM3.BAS. The "3" in the code name pertains to the fact that this model calculates three changing concentration profiles: oil droplets, SPM, and oil-SPM agglomerate. The mathematics are described in Section 3.1.3 of Payne et al. (1989). This code must be run from a compiled and linked executable file. The executable file should be a "stand-alone" and not require a run-time library.

Upon running OILSPM3 by typing the .EXE file name, the screen will display a prompt asking the user if the parameters are to be "edited" or "entered". It is recommended that the user enter "edit" because the parameters stored in the code are in the range of interest of environmental applications. Any of the displayed parameters can be changed (i.e., edited) by typing "yes" in response to the prompt. Upon entering "yes", the parameter line number that is to be changed is entered. After each edit the entire parameter list is displayed. The code will continue to execute only after "no" is entered at the parameter-change prompt as illustrated in Tables 15a and 15b. These two tables

Table 15a. First (of two) Screen Display of Parameters to be Used in Calculation, with a Final User Response of "no", From OILSPM3.

```
INTERACTING OIL DROPLETS AND SPM CALCULATI ON
CODE NAME IS OILSPM3.BAS, VERSION OF 8-9-88 @ 0643

1.  TURBULENT DIFFUSIVITY,CM*CM/SEC =  1.00D+02
2.  OIL RISING VELOCITY, CM/SEC =  1.00D-02
3.  OIL-SPM RATE CONSTANT FOR OIL LOSS, CC/(GM*SEC) =  9.40D-02
4.  OCEAN DEPTH,METERS =  1.00D+01
5.  NUMBER OF GRID POINTS = 49
6.  INITIAL OIL-DISPERSON FLUX SZERO,GRAMS/(CM*CM*SEC) =  1.80D-05
7.  OIL-DISPERSON GAMMA, 1/SEC =  4.60D-05
8.  MAXIMUM TIME, HOURS =  10.00
9.  PRINT INTERVAL, HOURS = 0.500
10. USE STEADY-STATE OIL PROFILE TO START: NO
11. COUPLE THE CONCENTRATIONS: YES
12. COUPLING ITERATIONS = 3

WANT TO CHANGE ANY? no
```

'I'able 15b. Second Screen Display of Parameters to be Used in Calculation, with a Final User Response of "no", From OILSPM3.

```
INTERACTING OIL DROPLETS AND SPM CALCULATION
CODE NAME IS OILSPM3.BAS, VERSION OF 8-9-88 @ 0643

1.  SPM SETTLING VELOCITY, CM/SEC =  1.00D-03
2.  OIL-SPM AGGLOMERATE SETTLING VELOCITY, CM/SEC =  1.00D-03
3.  OIL-SPM RATE CONSTANT FOR SPM LOSS, CC/(GM*SEC) =  9.40D-02
4.  SPM SOURCE FLUX TERM, GM/(CM^2*SEC) =  4.60D-05
5.  5PM DEPOSITION RATE CONSTANT, CM/SEC =  4.60D-02
6.  USE STEADY-STATE 5PM PROFILE TO START: YES

WANT TO CHANGE ANY? no

TIME FOR UNITY DIMENSIONLESS TIME, HOURS =  2.814D-01

THE TIME STEP WILL BE THE ABOVE TIME DIVIDED BY  20.000

IS THIS ACCEPTABLE? yes
```

illustrate the parameter input list for OILSPM3. Table 15a illustrates mainly oil-related options and integration parameters Such as the number of grid points. Because OILSPM3 is a numerical integration code, it is not possible just to enter a "time" and then calculate the concentration profiles. The code must integrate up to a specified time from an initial condition. The initial condition recommended for oil in the water column is zero (i.e., oil is spilled at time = O. This condition is implemented by line 10 in Table 15a, where a "no" is entered to the prompt: USE STEADY-STATE OIL PROFILE TO START.

The reason this option exists is for material-balance testing calculations only. The user should always make sure that line 10 has a response of "no." Material-balance testing is used to make sure the code calculation accounts for all the masses in the water. This is difficult in numerical integrations because mass transfer changes rapidly in the initial stages of the calculation (i.e., the profiles are quite steep in the early stages of calculation. However, if a "smooth" profile, such as a steady-state profile, is used initially, the early integration errors do not exist; and for purposes of finding programming errors the calculated results are much easier to interpret.

Table 15b illustrates mainly SPM and oil-SPM agglomerate related parameters and the selection of the maximum allowable time step to be used in the Crank-Nicolson integration. Note that line 6 in this table specifies that a steady-state SPM profile is used to start the calculation. In other words, oil is spilled in water that has sediment. The dimensionless time referred to in this table is used as a gauge to select a maximum time step. Experience has resulted in selecting a time step on the order of 1/20 of this dimensionless time. It is recommended that at least 20 be entered. However, if a larger number is entered, compute time will increase accordingly.

The code execute time is on the order of many minutes on a 80286-based personal computer. If an 8088-based machine is used, expect one-half hour or longer. The initial output is illustrated in Table 16 where the code version is documented and the input parameters for the calculation are also documented.

Table 16. Initial Output of Problem Parameters for OILSPM3.

```
FINITE-DIFFERENCE SOLUTION FOR INTERACTING OIL DROPLETS AND SPM.

CODE NAME IS OILSPM3.BAS, VERSION IS 8-9-88@0643
RUN TIME WAS 06:42:48, AND RUN DATE WAS 08-09-1988

PROBLEM PARAMETERS ARE AS FOLLOWS:

VERTICAL TURBULENT DIFFUSIVITY,CM*CM/SEC = 100.00
WATER DEPTH, METERS = 10.0

OIL RISING VELOCITY, CM/SEC = 1.00D-02
OIL-SPM RATE CONSTANT FOR OIL LOSS, CC/(GM*SEC) = 9.400D-02
OIL DISPERSION RATE, GM/(CM*CM*SEC) =(0.18D-04)*EXP((-0.46D-04) *SECONDS)

SPM SETTLING VELOCITY, CM/SEC = 1.00D-03
OIL-SPM RATE CONSTANT FOR SPM LOSS, CC/(GM*SEC) = 9.40D-02
SPM BOTTOM SOURCE FLUX, GM/(CM^2*SEC) = 4.60D-05
SPM DEPOSITION RATE CONSTANT, CM/SEC = 4.60D-02

OIL-SPM AGGLOMERATE SETTLING VELOCITY, CM/SEC = 1.00D-03

TIME STEP, HOURS = 5.62D-03, INTEGRATION TIME, HOURS = 10.00
SPECIFIED PRINT INTERVAL, HOURS = 0.500

THE INITIAL OIL WATER-COLUMN LOADING, GRAMS = 0.000D+00
THE INITIAL SPM WATER-COLUMN LOADING, GRAMS = 9.950D-01
```

Table 17a presents the calculated oil-droplet, SPM and oil-SPM agglomerate concentration profiles at 0.5 hour, and Table 17b presents the total material balance for these species. The SPM concentration profile is close to 0,001 gm/cm^3 because of the values selected for the SPM source flux [at 4.6×10^{-5} $gm/(cm^2$ see)] and the SPM deposition rate constant (4.6×10^{-2} cm/see). The oil-droplet concentration profile ranges from 7.8×10^{-5} gm/cm^3 (78 ppm) at the surface to O at the bottom. The zero concentration at the bottom is an imposed boundary condition and essentially results in an upper bound flux of oil to the. bottom. Likewise, the oil-SPM agglomerate concentration is O at the bottom.

Table 17b -illustrates the total material balance calculation for the three transporting species. Note that the oil fluxed into the water at the surface is 0.03109 g, while the calculation accounted for 0.03091 g as oil that was in the water, lost at bottom (transported to the bottom), and lost through reaction. This difference should be zero; it is not because of numerical integration errors and can be made smaller by decreasing the grid spacing, the time step, or both. The SPM material balance closes by accounting for 0.9950 g, and the oil-SPM agglomerate almost closes by accounting for 0.004827 g in the water and lost to the bottom compared to 0.004825 g produced by reaction. Closing these material balances to four significant digits is considered reasonable given the assumptions and limitation of the data and calculation.

The oil-droplet, SPM and oil-SPM agglomerate concentration profiles and total material balance at 10 hr are presented, in Tables 18a and 18b. Note that the time at the end of the calculation was 7:34 and the start time 6:42 for an integration to 10 hr with a time-step size of 0.00562 hr on a grid size of 20.83 cm (over 10 m, 51 grid points including 1 grid point outside each boundary for central differences). The SPM-concentration profile is still close to 0.001 gm/cm^3 and the oil-droplet 'concentration varies from 3.159×10^{-5} (32 ppm) at the surface to O at the bottom. This concentration is decreasing from the 0.5-hr value because the oil-dispersion source term is a

Table 17a. Calculated Oil-Droplet SPM and Oil-SPM Agglomerate Profiles at 0.5 Hour From OILSPM3.

FINITE-DIFFERENCE SOLUTION FOR INTERACTING OIL DROPLETS AND SPM.

CODE NAME IS OILSPM3.BAS, VERSION IS 8-9-88@ 0643
RUN TIME WAS 06:42:48, AND RUN DATE WAS 08-09-1988

CONCENTRATION PROFILES AT TIME = 0.500 HOURS $**********

DEPTH (CM)	OIL CONC (GM/CC)	SPM CONC (GM/CC)	OIL-SPM CONC (GM/CC)	
0.000D+00	7.832D-05	9.856D-04	8.807D-06	(SURFACE)
2.083D+01	7.476D-05	9.858D-04	8.792D-06	
4.167D+01	7.131D-05	9.860D-04	8.747D-06	
6.250D+01	6.798D-05	9.863D-04	8.675D-06	
8.333D+01	6.476D-05	9.865D-04	8.578D-06	
1.042D+02	6.164D-05	9.868D-04	8.459D-06	
1.250D+02	5.864D-05	9.871D-04	8.320D-06	
1.458D+02	5.574D-05	9.874D-04	8.163D-06	
1.667D+02	5.294D-05	9.877D-04	7.990D-06	
1.875D+02	5.025D-05	9.880D-04	7.803D-06	
2.083D+02	4.765D-05	9.883D-04	7.605D-06	
2.292D+02	4.516D-05	9.886D-04	7.396D-06	
2.500D+02	4.276D-05	9.889D-04	7.179D-06	
2.708D+02	4.045D-05	9.892D-04	6.954D-06	
2.917D+02	3.824D-05	9.895D-04	6.724D-06	
3.125D+02	3.612D-05	9.899D-04	6.490D-06	
3.333D+02	3.408D-05	9.902D-04	6.252D-06	
3.542D+02	3.213D-05	9.905D-04	6.013D-06	
3.750D+02	3.027D-05	9.908D-04	5.772D-06	
3.958D+02	2.848D-05	9.911D-04	5.531D-06	
4.167D+02	2.677D-05	9.915D-04	5.291D-06	
4.375D+02	2.514D-05	9.918D-04	5.052D-06	
4.583D+02	2.358D-05	9.921D-04	4.816D-06	
4.792D+02	2.21OD-O5	9.924D-04	4.5810-06	
5.000D+02	2.068D-05	9.928D-04	4.350D-06	
5.208D+02	1.932D-05	9.931D-04	4.123D-06	
5.417D+02	1.803D-05	9.934D-04	3.899D-06	
5.625D+02	1.680D-05	9.937D-04	3.680D-06	
5.833D+02	1.562D-05	9.940D-04	3.465D-06	
6.042D+02	1.450D-05	9.943D-04	3.254D-06	
6.250D+02	1.343D-05	9.9460-04	3.04$30-06	
6.458D+02	1.241D-05	9.949D-04	2.847D-06	
6.667D+02	1.144D-05	9.952D-04	2.651D-06	
6.875D+02	1.051D-05	9.955D-04	2.4590-06	
7.083D+02	9.622D-06	9.957D-04	2.271D-06	
7.292D+02	8.773D-06	9.9600-04	2.088D-06	
7.500D+02	7.959D-06	9.963D-04	1.91OD-O6	
7.708D+02	7.178D-06	9.966D-04	1.735D-06	
7.917D+02	6.428D-06	9.968D-04	1.564D-06	
8.125D+02	5.705D-06	9.971D-04	1.397D-06	
8.333D+02	5.007D-06	9.974D-04	1.233D-06	
8.542D+02	4.331D-06	9.976D-04	1.073D-06	
8.750D+02	3.674D-06	9.979D-04	9.143D-07	
8.958D+02	3.035D-06	9.981D-04	7.584D-07	
9.167D+02	2.41OD-O6	9.983D-04	6.044D-07	
9.375D+02	1.797D-06	9.986D-04	4.5190-07	
9.583D+02	1.192D-06	9.988D-04	3.006D-07	
9.792D+02	5.942D-07	9.990D-04	1.501D-07	
1.000D+03	0.000D+00	9.992D-04	0.000D+00	(BOTTOM)

Table 17b. Total Material Balance for Oil-Droplets, SPM and Oil-SPM Agglomerate at 0.5 Hour From OILSPM3.

MATERIAL BALANCE INFORMATION (FOR 1CM*CM COLUMN OF WATER) :

OIL IN THE WATER COLUMN, GRAMS = 2.688D-02
OIL LOST TO THE BOTTOM, GRAMS = 1.6120-03
OIL LOST THROUGH REACTION WITH SPM, GRAMS = 2.413D-03

OIL IN WATER + LOST AT BOTTOM + LOST THROUGH REACTION, GRAMS = 3.091D-02
OIL FLUXED INTO WATER + INITIAL LOADING, GRAMS = 3.109D-O2

SPM (UNATTACHED) IN THE WATER COLUMN, GRAMS = 9.926D-01
SPM LOST THROUGH REACTION WITH OIL, GRAMS = 2.413D-03

SPM IN WATER + LOST THROUGH REACTION, GRAMS = 9.950D-01
SPM FLUXED INTO WATER AT BOTTOM + INITIAL LOADING, GRAMS = 9.950D-01

OIL-SPM AGGLOMERATE IN THE WATER COLUMN, GRAMS = 4.496D-03
OIL-SPM AGGLOMERATE FLUXED TO THE BOTTOM, GRAMS= 3.309D-04

OIL-SPM IN WATER + LOST TO BOTTOM, GRAMS = 4.827D-03
OIL-SPM AGGLOMERATE PRODUCED BY REACTION, GRAMS = 4.825D-03

VECTOR CONVERGENCE, OIL = 3.06D-14, SPM = 6.01D-15 ON 3 ITERATIONS.

Table 18a. Calculated Oil-Droplet, SPM and Oil-SPM Agglomerate Profiles at 10 Hours From OILSPM3.

FINITE-DIFFERENCE SOLUTION FOR INTERACTING OIL DROPLETS AND SPM.

CODE NAME IS OILSPM3.BAS, VERSION IS 8-9-88 @ 0643
RUN TIME WAS 06:42:48, AND RUN DATE WAS 08-09-1988

CONCENTRATION PROFILES AT TIME = 10.000 HOURS **********

DEPTH (CM)	OIL CONC (GM/CC)	SPM CONC (GM/CC)	OIL-9PM CONC (GM/CC)	
0.000D+00	3.159D-05	9.366D-04	2.168D-05	(SURFACE)
2.083D+01	3.081D-05	9.368D-04	2.167D-05	
4.167D+01	3.004D-05	9.371D-04	2.163D-05	
6.250D+01	2.927D-05	9.373D-04	2.157D-05	
8.333D+01	2.852D-05	9.375D-04	2.148D-05	
1.042D+02	2.777D-05	9.378D-04	2.136D-05	
1.250D+02	2.702D-05	9.381D-04	2.121D-05	
1.458D+02	2.629D-05	9.384D-04	2.105D-05	
1.667D+02	2.556D-05	9.387D-04	2.086D-05	
1.875D+02	2.483D-05	9.390D-04	2.064D-05	
2.083D+02	2.411D-05	9.393D-04	2.040D-05	
2.292D+02	2.340D-05	9.396D-04	2.014D-05	
2.500D+02	2.269D-05	9.400D-04	1.986D-05	
2.708D+02	2.199D-05	9.403D-04	1.955D-05	
2.917D+02	2.130D-05	9.407D-04	1.923D-05	
3.125D+02	2.061D-05	9.411D-04	1.888D-05	
3.333D+02	1.992D-05	9.415D-04	1.851D-05	
3.542D+02	1.924D-05	9.419D-04	1.813D-05	
3.750D+02	1.857D-05	9.423D-04	1.773D-05	
3.958D+02	1.790D-05	9.4270-04	1.731D-05	
4.167D+02	1.723D-05	9.432D-04	1.687D-05	
4.375D+02	1.657D-05	9.436D-04	1.641D-05	
4.583D+02	1.591D-05	9.441D-04	1.594D-05	
4.792D+02	1.526D-05	9.445D-04	1.546D-05	
5.000D+02	1.461D-05	9.450D-04	1.496D-05	
5.208D+02	1.397D-05	9.455D-04	1.444D-05	
5.417D+02	1.333D-05	9.460D-04	1.391D-05	
5.625D+02	1.269D-05	9.465D-04	1.337D-05	
5.833D+02	1.206D-05	9.470D-04	1.282D-05	
6.042D+02	1.143D-05	9.475D-04	1.225D-05	
6.250D+02	1.081D-05	9.480D-04	1.167D-05	
6.458D+02	1.019D-05	9.485D-04	1.108D-O5	
6.667D+02	9.566D-06	9.490D-04	1.048D-05	
6.875D+02	8.950D-06	9.496D-04	9.876D-06	
7.083D+02	8.337D-06	9.501D-04	9.259D-06	
7.292D+02	7.727D-06	9.507D-04	8.633D-06	
7.500D+02	7.120D-06	9.512D-04	7.999D-06	
7.708D+02	6.515D-06	9.518D-04	7.358D-06	
7.917D+02	5.913D-06	9.523D-04	6.711D-06	
8.125D+02	5.313D-06	9.529D-04	6.057D-06	
8.333D+02	4.715D-06	9.535D-04	5.398D-06	
8.542D+02	4.119D-06	9.541D-04	4.734D-06	
8.750D+02	3.526D-06	9.546D-04	4.066D-06	
8.958D+02	2.934D-06	9.552D-04	3.394D-06	
9.167D+02	2.344D-06	9.558D-04	2.719D-06	
9.375D+02	1.756D-06	9.564D-04	2.042D-06	
9.583D+02	1.169D-06	9.570D-04	1.362D-06	
9.792D+02	5.839D-07	9.576D-04	6.8140-07	
1.000D+03	0.000D+00	9.582D-04	0.000D+00	(BOTTOM)

Table 18b. Total Material Balance for Oil-Droplets, SPM and Oil-SPM Agglomerate at 10 Hours From 01LSPM3.

MATERIAL BALANCE INFORMATION (FOR 1CM*CM COLUMN OF WATER):

OIL IN THE WATER COLUMN, GRAMS = 1.501D-02
OIL LOST TO THE BOTTOM, GRAMS = 2.001D-01
OIL LOST THROUGH REACTION WITH SPM, GRAMS = 1.013D-01

OIL IN WATER + LOST AT BOTTOM + LOST THROUGH REACTION, GRAMS = 3.164D-01
OIL FLUXED INTO WATER + INITIAL LOADING, GRAMS = 3.166D-01

SPM (UNATTACHED) IN THE WATER COLUMN, GRAMS = 9.458D-01
SPM LOST THROUGH REACTION WITH OIL, GRAMS = 1.013D-01

SPM IN WATER + LOST THROUGH REACTION, GRAMS = 1.047D+00
SPM FLUXED INTO WATER AT BOTTOM + INITIAL LOADING, GRAMS = 1.047D+00

OIL-SPM AGGLOMERATE IN THE WATER COLUMN, GRAMS = 1.358D-02
OIL-SPM AGGLOMERATE FLUXED TO THE BOTTOM, GRAMS = 1.890D-01

OIL-SPM IN WATER + LOST TO BOTTOM, GRAMS = 2.026D-01
OIL-SPM AGGLOMERATE PRODUCED BY REACTION, GRAMS = 2.025D-01

VECTOR CONVERGENCE, OIL = 9.98D-16, SPM = 6.55D-16 ON 3 ITERATIONS.

END OF RUN WAS 07:34:47

decaying exponential. The oil-SPM agglomerate concentration varies from 2.168 x 10^{-5} gm/cm^3 to O; also, note this oil-SPM agglomerate concentration(s) is higher than the 0.5-hr value because the oil-SPM agglomerate has been produced over the 9.5 hr interval.

The total material balance at 10 hours presented in Table 18b illus-crates that numerical integration errors improve (i.e. , decrease) as the calcu-lation "steps out" in time. Note that the oil put into the water from the surface is 0.3166 g while the calculation accounts for 0.3164 g. The material balances for the other two species close to four digits.

The vector convergence numbers that appear at the end of each of the material balance calculations are the average final errors in trial vectors used in the calculation. In other words, to solve for an oil-droplet concentration profile, the SPM concentration (vector) must be "guessed." Likewise, to solve for the SPM-concentration profile the oil-droplet concentration (vector) must be guessed. The average error in the concentrations is printed to indicate how well (or not) the calculation proceeded. For the case illustrated here the average error between "guessed" and "calculated" concentrations is 9.9 x 10-16 g/cm^3 for oil and 6.55 x 10^{-16} for SPM, which is considered sufficiently small.

1.4 CODE LIMITATIONS AND PERSPECTIVE

An important aspect of the three calculations described here is that they are one dimensional. For the sample problems discussed, a water-column depth of 10 m is used with an area (top or bottom) of 1 cm^2. Note that if 0.5 cm of oil is spilled and this oil transports into the water, the oil droplet concentration could be $0.4gm/1000cm^3$ or 400 ppm if there are no oil-loss mechanisms. For the case where oil is removed at the bottom the resulting concentrations will be lower. Clearly this oil concentration is much higher than ever observed in the ocean. The main reason for not predicting a lower oil concentration is that the one-dimensional calculation does not

consider horizontal dispersion or spreading of the oil. Thus, the one-dimensional calculations are conservatively too high. Then the question arises: What good are the calculations?

Besides providing upper bound estimates of concentrations, these calculations also provide an estimate of the time required for things to happen in the water column. Also, the sensitivity of the input parameters can be investigated to learn what is or is not important with respect to a specific objective. For example, the oil deposition mechanisms are the boundary conditions at the bottom for the oil and the oil-SPM agglomerate, and the *relative* importance of these two processes can be investigated with respect to the parameters that will affect them (i.e., oil rise velocity, oil-SPM reaction rate, and oil-SPM settling velocity).

These calculations (codes) *are* not usable by interfacing them with other codes (i.e., with an ocean circulation code). The only part of the calculation that is usable is the oil-SPM reaction rate that is of the form: $\alpha_c CS$. This reaction rate is written on a per-unit volume basis, and an ocean-circulation model in three dimensions must then integrate this expression for the loss of oil, loss of SPM, and production of oil-SPM agglomerate. Thus, the relatively simple reaction rate expression is quite difficult to use in an environmental situation, if for no other reason than the environmental situations of interest are three dimensional.

APPENDIX A

CODE LISTING FOR OILSPMXS.BAS

```
100 DEFDBL A-H,K-Z
110 REM THIS CODE SOLVES THE ADVECTION-DISPERSION EQUATION FOR OIL
120 REM DROPS WITH EXCESS SPM AND FIRST-ORDER REACTION LOSS.
130 DIM BETA(50),C(50),XDEPTH(50),PT(50),COSR(50),SINR(50)
140 DIM EXPTERM(50),CONTERM(50 ), MASTERM(50),REATERM(50),FLXTERM(50)
150 DIM ICHECK(50)
160 PIE=3.1415926536#
170 PIE2=PIE/2#
180 TOF$=CHR$(12)
130 CODE$="OILSPMXS.BAS"
200 VER$="8-3-88@ 0718"
210 RTIME$=TIME$
220 RDATES=DATES
230 REM ITIME=1
240 REM EBIG IS THE MAXIMUM ARGUMENT AN EXPONENTIAL IS ALLOWED TO BE
250 EBIG=30#
260 VXIN=.001#:K=100#:L=10#:RERROR=.000001#:GAMMA=.000046#
270 ALPHA=.00094#:NZERO=.000018#:NROOT=25:IEX=27:AN1$="YES"
280 HEADS="PRE-LOADED PARAMETER TESTCASE"
290 CLS
300 GOSUB 4020
310 PRINT:INPUT"WANT TO EDIT OR ENTER INPUT PARAMETERS ";AN2$
320  TEST2S=LEFTS(AN2S,2)
330 IF TEST2$="ED" GOTO 560
340 IF TEST2$="ed" GOTO S60
350 PRINT:INPUT"ENTER AN IDENTIFICATION LINE: ";HEAD$
360 PRINT: INPUT"ENTER THE OIL-DROP RISE VELOCITY, CM/SEC (TRY -0.001) ";VX
370 REM SEE THE LETTER TO MAURI PELTO FROM BRUCE KIRSTEIN,28 JULY 1987
380 REM FOR THE VERTICAL TURBULENT DIFFUSIVITY
390 PRINT: INPUT"ENTER THE TURBULENT DIFFUSIVITY,CM*CM/SEC (TRY 100) ";K
400 PRINT: INPUT"ENTER THE DEPTH, METERS (TRY 10.0) ";L
410 PRINT: INPUT"ENTER THE NUMBER OF ROOTS TO BE DETERMINED (TRY 25) ";NROOT
420 PRINT:PRINT"ENTER THE ERROR LIMIT FOR THE ROOTS (TRY 1.0D-06)";
430 INPUT RERROR
440 REM SEE THE LETTER TO DAVE LIU FROM BRUCE KIRSTEIN, I-JULY-83 FOR
450 REM CALCULATION OF THE DISPERSION RATE CONSTANTS
460 PRINT: INPUT"ENTER THE EXPONENTIAL FLUX TERM, 1/SEC (TRY 4.6D-05)";GAMMA
470 PRINT:PRINT"ENTER THE INITIAL OIL FLUX, GRAM/(CM*CM*SEC) (TRY 1.8D-05)";
480 INPUT NZERO
490 PRINT:PRINT"ENTER THE DISAPPEARANCE RATE CONSTANT, I/SEC (TRY 0.00094) ";
500 INPUT ALPHA
510 PRINT:INPUT"ENTER THE NUMBER OF DEPTH VALUES TO EVALUATE (TRY 29) ";IEX
520 IF IEX<50 GOTO 550
530 PRINT:PRINT"NUMBER OF DEPTH VALUES MUST BE LESS THAN 50, RE-ENTER."
540 GOTO 510
550 PRINT:INPUT"WANT TO PRINT THE ROOTS (SAY NO) ";AN1$
560 CLS
570 GOSUB 4020
580 PRINT:PRINT"1.  RISE VELOCITY, CM/SEC = ";VXIN
590 PRINT"2.  TURBULENT DIFFUSIVITY,CM*CM/SEC = ";K
600 PRINT"3.  DEPTH, METERS = ";L
610 PRINT"4.  NUMBER OF ROOTS = ";NROOT
620 PRINT"5.  ROOT ERROR LIMIT = ";
630 PRINT USING"##.###^^^^";RERROR
640 PRINT"6.  EXPONENTIAL FLUX TERM, I/SEC = ";
650 PRINT USING"##.###^^^^";GAMMA
660 PRINT"7.  INITIAL OIL FLUX, GRAM/(CM*CM*SEC) = ";
670 PRINT USING"##.###^^^^";NZERO
680 PRINT"*8.  DISAPPEARANCE RATE CONSTANT, I/SEC = ";
690 PRINT USING"##.###^^^^";ALPHA
700 PRINT"9.  NUMBER OF DEPTH VALUES = ";IEX
710 PRINT"10. PRINT THE ROOTS? ";AN1$
720 PRINT:INPUT"WANT TO CHANGE ANY";AN$
730 TEST$=LEFT$(AN$,1)
```

```
740 IF TEST $="N" GOTO 980
750 IF TEST $="n" GOTO 980
760 PRINT: INPUT"ENTER THE LINE NUMBER TO BE CHANGED";IL
770 ONIL GOTO 780,800,820,840,860 ,880,900,920,940,960
780 PRINT: INPUT"ENTER THE RISE VELOCITY, CM/SEC ";VXIN
790 GOTO 560
800 PRINT: INPUT"ENTER THE TURBULENT DIFFUSIVITY,CM*CM/SEC ";K
810 GOTO 560
820 PRINT: INPUT"ENTER THE DEPTH, METERS ";L
830 GOTO 560
840 PRINT:INPUT"ENTER THE NUMBER OF ROOTS TO BE DETERMINED ";NROOT
850 GOTO 560
860 PRINT: INPUT"ENTER THE ERROR LIMIT FOR THE ROOTS ";RERROR
870 GOTO 580
880 PRINT: INPUT"ENTER THE EXPONENTIAL FLUX TERM, I/SEC ";GAMMA
890 GOTO S60
900 PRINT: INPUT"ENTER THE INITIAL OIL FLUX, GRAM/(CM*CM*SEC)";NZERO
910 GOTO 560
920 PRINT:INPUT"ENTER THE DISAPPEARANCE RATE CONSTANT, I/SEC ";ALPHA
930 GOTO 560
940 PRINT:INPUT"ENTER THE NUMBER OF DEPTH VALUES TO EVALUATE ";IEX
950 GOTO 560
960 PRINT:INPUT"WANT TO PRINT THE ROOTS? ";AN1$
970 GOTO 560
980 REM BEGIN THE CALCULATION
990 TEST1$=LEFT$(AN1$,1)
1000 LCM=100#*L
1010 LCM2=LCM*LCM
1020 VX=-VXIN
1030 A=VX/(2#*K)
1040 A2=A*A
1050 AL=A*LCM
1060 AL2=AL*AL
1070 EAL=EXP(AL)
1080 EMAL=1#/EAL
1090 VX2=VX/2#
1100 VXLK=VX*LCM+2#*K
1110 K2=2#*K
1120 IEARLY=1
1130 IPAGE=0
1140 GOSUB 4070
1150 LPRINT:LPRINT"THIS CODE SOLVES THE TRANSIENT ADVECTION-DISPERSION";
1160 LPRINT" EQUATION FOR"
1170 LPRINT"OIL DROPLETS WITH FIRST-ORDER REACTION LOSS."
1180 LPRINT:LPRINT"PROBLEM IDENTIFICATION: ";HEAD$
1190 LPRINT:LPRINT"OIL DROPLET RISE VELOCITY = ";VXIN;
1200 LPRINT" CM/SEC, DEPTH = ";L;
1210 LPRINT" METERS"
1220 LPRINT:LPRINT"TURBULENT DIFFUSIVITY = ";K;
1230 LPRINT" CM*CM/SEC"
1240 LPRINT:LPRINT"ERROR LIMIT FOR THE ROOTS = ";
1250 LPRINT USING"##.###^^^^";RERROR
1260 LPRINT:LPRINT"VX*L/(2*K 1 = ";
1270 LPRINT USING"##.###^^^^";AL;
1280 LPRINT" UNITLESS"
1290 IF TEST1$="N" GOTO 1350
1300 IF TEST1$="n" GOTO 1350
1310 LPRINT:LPRINT"THE ";
1320 LPRINT USING"##";NROOT;
1330 LPRINT" ROOTS OF F(BETA) = BETA*COTANGENT(BETA) + VX*L/(2*K)"
1340 LPRINT:LPRINT"          ROOT          F ( BETA)        ERROR CODE"
1350 FOR I = 1 TO NROOT
1360 ICHECK(I)=1
1370 XR=PIE*CDBL(I)
1380 XL=XR-PIE
1390 FOR IHALF = 1 TO 50
```

```
1410 X=(XL+XR)/2#
1411 FX=X*COS(X)/SIN(X)+AL
1420 TEST=ABS(FX)
1430 IF TEST<RERROR GOTO 1510
1440 IF FX>0# GOTO 1470
1450 XR=X
1460 GOTO 1480
1470 XL=X
1480 NEXT IHALF
1490 ICHECK(I)=2
1500 REM STORE CONVENIENT FORMS OF THE ROOTS
1510 x2=x*x
1520 BETA(I)=X
1530 EXPTERM(I)=ALPHA+K*(A2+X2/LCM2)
1540 COSR(I)=COS(X)
1550 SINR(I)=SIN(X)
1560 REM SEE PAGE 15 FOR THE SERIES CONCENTRATION TERM
1570 CONTERM(I)=X/((GAMMA-EXPTERM(I))*(VXLK*COSR(I)-K2*X*SINR(I)))
1580 REM SEE PAGE 42 FOR THE SERIES MASS-IN-WATER TERM
1590 MASTERM(I)=X*CONTERM(I)*(1#-EMAL*(AL*SINR(I)/X+COSR(I)))/(X2+AL2)
1600 REM SEE PAGE 43 FOR THE SERIES MASS-LOST-BY-REACTION TERM
1610 REATERM(I)=MASTERM(I)/EXPTERM(I)
1620 REM SEE PAGE 33 FOR THE SERIES MASS-LOST-AT-THE-BOTTOM TERM
1630 FLXTERM(I)=X*CONTERM(I)/EXPTERM(I)
1640 IF TEST1$="N" GOTO 1710
1650 LPRINT TAB(S);
1660 LPRINT USING"##.###^^^^";BETA(I);
1670 LPRINT TAB(19);
1680 LPRINT USING"##.###^^^^";FX;
1690 LPRINT TAB(36);
1700 LPRINT USING"##";ICHECK(I)
1710 NEXT I
1720 LPRINT:LPRINT"EXPONENTIAL FLUX TERM = ";
1730 LPRINT USING"##.###^^^^";GAMMA;
1740 LPRINT" I/SEC"
1750 LPRINT:LPRINT"INITIAL OIL FLUX = ";
1760 LPRINT USING"##.###^^^^";NZERO;
1770 LPRINT"GRAMS/(CM*CM*SEC)"
1780 LPRINT:LPRINT"FIRST ORDER DISAPPEARANCE RATE CONSTANT, I/SEC = ";
1790 LPRINT USING"##.###^^^^";ALPHA;
1800 LPRINT"1/SEC"
1810 NZL=4#*NZERO*K/LCM
1820 REM SEE PAGE 25 OF THE DERIVATION NOTES FOR ZETA-BAR.
1830 ALPHAK=ALPHA/K
1840 GAMMAK=GAMMA/K
1850 REM ZGAMMA2 IS ZETA-BAR SQUARED ON PAGE 25.
1860 ZGAMMA2=A2+ALPHAK-GAMMAK
1870 REM THIS ZERO-SWITCH WAS INSTALLED 8-3-88, TO REMOVE, JUST REMOVE
1880 REM THE REM'S DOWN TO ZGAMMA2=0#
1890 IF ABS(ZGAMMA2)<1D-20 THEN ZGAMMA2=0#
1900 REM PRINT:PRINT"ZGAMMA2 = ";
1910 REM PRINT USING"##.######^^^^";ZGAMMA2
1920 REM PRINT:INPUT"WANT TO ZERO IT (YES IF LESS THAN 1.0D-20)";AN$
1930 REM TEST$=LEFT$(AN$,1)
1940 REM IF TEST$="N" GOTO 1940
1950 REM IF TEST$="n" GOTO 1940
1960 REM ZGAMMA2=0#
1970 REM SET THE ZETA-BAR SWITCH FOR REAL (=1), REAL 'A' WHICH MEANS
1980 REM THAT GAMMA=ALPHA(=2), IMAGINARY (=3), OR A HARD ZERO (=4)
1990 REM SEE PAGES 25-27 FOR THE SPECIAL CASES OF ZETA-BAR.
2000 IF ZGAMMA2<>0# GOTO 2030
2010 IZBAR=4
2020 GOTO 2170
2030 IF ALPHA<>GAMMA GOTO 2070
2040 IZBAR=2
2050 ZGAMMA=A
```

```
2060 GOTO 2140
2070 IF ZGAMMA2>0# GOTO 2100
2080 IZBAR=3
2090 GOTO 2120
2100 IZBAR=1
2110 GOTO 2130
2120 ZGAMMA2=-ZGAMMA2
2130 ZGAMMA=SQR(ZGAMMA2)
2140 ARG=ZGAMMA*LCM
2150 COSZ=COS(ARG)
2160 SINZ=SIN(ARG)
2170 ON IZBAR GOTO 2180,2200,2220,2240
2180 LPRINT:LPRINT"ZETA-BAR IS REAL ( <> VX/(2*K))";
2190 GOTO 2260
2200 LPRINT:LPRINT"ZETA BAR IS REAL ( = VX/(2*K))";
2210 GOTO 2260
2220 LPRINT:LPRINT"ZETA-BAR IS IMAGINARY";
2230 GOTO 2260
2240 LPRINT:LPRINT"ZETA-BAR IS EQUAL TO ZERO";
2250 GOTO 2290
2260 LPRINT" AND EQUAL TO ";
2270 LPRINT USING"##.###^^^^";ZGAMMA;
2280 LPRINT"1/CM";
2290 LPRINT"(IZBAR =";
2300 LPRINT USING"##";IZBAR;
2310 LPRINT")"
2320 ON IZBAR GOTO 2330,2330,2390,2410
2330 EXP1=EXP(ARG)
2340 EXP2=1#/EXP(ARG)
2350 SINH=(EXP1-EXP2)/2#
2360 COSH=(EXP1+EXP2)/2#
2370 LTERM=NZERO/(VX2*SINH+K*ZGAMMA*COSH)
2380 GOTO 2420
2390 LTERM=NZERO/(VX2*SINZ+K*ZGAMMA*COSZ)
2400 GOTO 2420
2410 LTERM=2#*NZERO/VXLK
2420 GOSUB 4070
2430 LPRINT:LPRINT"CALCULATED RESULTS ********************************u
2440 PRINT:INPUT"ENTER THE TIME, HOURS ";TH
2450 PRINT:PRINT"TIME ENTERED IS ";
2460 PRINT USING"##.###^^^^";TH
2470 PRINT:INPUT"IS THIS CORRECT ";AN$
2480 TEST$=LEFT$(AN$,1)
2490 IF TEST$="N" GOTO 2440
2500 IF TEST$="n" GOTO 2440
2510 T=3600#*TH
2520 DTIME=K*T/LCM2
2530 EGAMT=EXP(-GAMMA*T)
2540 IF IEX=0 GOTO 3030
2550 REM LOAD THE X VALUES
2560 XSTEP=LCM/CDBL(IEX-1)
2570 FOR I = 1 TO IEX
2580 XDEPTH(I)=(I-1)*XSTEP
2590 NEXT I
2600 FOR I = 1 TO IEX
2610 X=XDEPTH(I)
2620 EAX=EXP(A*X)
2630 ARG=ZGAMMA*(LCM-X)
2640 ON IZBAR GOTO 2650,2650,2680,2700
2650 EXP1=EXP(ARG)
2660 CLEAD=EAX*LTERM*EGAMT*(EXP1-1#/EXP1)/2#
2670 GOTO 2710
2680 CLEAD=EAX*LTERM*EGAMT*SIN(ARG)
2690 GOTO 2710
2700 CLEAD=EAX*LTERM*EGAMT*(LCM-X)
2710 SUM1=0#
```

```
2720 FOR IROOT = 1 TO NROOT
2730 ARG=EXPTERM(IROOT)*T
2740 IF ARG>EBIG GOTO 2780
2750 TEMP1=CONTERM(IROOT)*EXP(-ARG)*SIN(BETA(IROOT)*(1#-X/LCM))
2760 SUM1=SUM1+TEMP1
2770 NEXT IROOT
2?80 c(I) =CLEAD-NZL*EAX*SUM1
2790 REM NOW INCREMENT TO NEXT X
2800 NEXT I
2810 REM CHECK FOR NEGATIVE CONCENTRATIONS WHICH CAN OCCUR FOR TIMES
2820 REM TOO SMALL, I.E., THE CONCENTRATION PROFILE HAS NOT HAD TIME
2830 REM TO TOUCH THE BOTTOM
2840 REM IEARLY IS THE SWITCH THAT DENOTES WHEN THE TIME IS TOO SMALL
2850 IEARLY=1
2860 FOR I = 1 TO IEX
2870 IF C(I)<0# GOTO 2910
2880 PT(I)=C(I)
2890 NEXT I
2900 GOTO 2970
2910 IEARLY=2
2920 IEX1=I
2930 FOR I = IEX1 TO IEX
2940 C(I)=0#
2950 PT(I)=C(I)
2960 NEXT I
2970 LPRINT:LPRINT"CONCENTRATION PROFILE (GM/CC) FOR TIME = ";
2980 LPRINT USING"##.###^^^^";TH;
2990 LPRINT" HOURS"
3000 LPRINT"DIMENSIONLESS TIME, K*T/L**2 = ";
3010 LPRINT USING"##.###^^^^";DTIME
3020 GOSUB 3790
3030 REM CALCULATE "THE MASS OF OIL IN THE WATER AT TIME T, THE LOSS OF OIL
3040 REt4 THROUGH REACTION, AND THE LOSS OF OIL AT THE BOTTOM
3050 ON IZBAR GOTO 3060,3080,3100,3120
3060 CWLEAD=LTERM*(ZGAMMA*EAL-A*SINH-ZGAMMA*COSH)/(A2-ZGAMMA2)
3070 GOTO 3170
3080 CWLEAD=LTERM*(LCM*EAL-SINH/A)/2#
3090 GOTO 3170
3100 CWLEAD=LTERM*(ZGAMMA*EAL-A*SINZ-ZGAMMA*COSZ)/(A2+ZGAMMA2)
3110 GOTO 3170
3120 REM CHECK FOR A-O OR GAMMA=0.
3130 IF A<>0# GOTO 3160
3140 CWLEAD=NZERO*LCM2/VXLK
3150 GOTO 3170
3160 CWLEAD=-2#*NZERO*(LCM/A+(1#-EAL)/A2)/VXLK
3170 IF GAMMA>0# GOTO 3200
3180 CRLEAD=CWLEAD*T
3190 GOTO 3220
3200 CRLEAD=CWLEAD*(1#-EGAMT)/GAMMA
3210 CWLEAD=CWLEAD*EGAMT
3220 ON IZBAR GOTO 3230,3230,3230,3280
3230 IF GAMMA>0# GOTO 3260
3240 CFLEAD=LTERM*K● ZGAII?4A*EAL*T
3250 GOTO 3320
3260 CFLEAD=LTERM*K● ZGA14MA*EAL* (1#-EGAMT)/GAMMA
3270 GOTO 3320
3280 IF GAMMA>0# GOTO 3310
3290 CFLEAD=K2*NZERO*EAL*T/VXLK
3300 GOTO 3320
3310 CFLEAD=K2*NZERO*EAL*(1#-EGAMT)/(GAMMA*VXLK)
3320 SUM1=0#
3330 SUM2=0#
3340 SUM3=0#
3350 FOR I = 1 TO NROOT
3360 ARG=EXPTERM( I)*T
3370 EXP1=0#
```

```
3380 IF ARG<EBIG THEN EXP1=EXP(-ARG)
3390 SUM1=SUM1+EXP1*MASTERM(I)
3400 SUM2=SUM2+(1#-EXP1)*REATERM(I)
3410 SUM3=SUM3+(1#-EXP1)*FLXTERM(1)
3420 NEXT I
3430 CWMASS=CWLEAD-4#*NZERO*K*EAL*SUM1
3440 CRMASS=(CRLEAD-4#*NZERO*K*EAL*SUM2)*ALPHA
3450 CFMASS=CFLEAD-4#*NZERO*K*K*EAL*SUM3/LCM2
3460 IF IEX>0 GOTO 3510
3470 LPRINT:LPRINT"TIME = ";
3480 LPRINT USING" ##.###^^^^";TH;
3490 LPRINT"HOURS, DIMENSIONLESS TIME, K*T/L**2 = ";
3500 LPRINT USING"##.###^^^^";DTIME
3510 IF GAMMA>0# GOTO 3540
3520 FLUXED=NZERO*T
3530 GOTO 3550
3540 FLUXED=NZERO*(1#-EGAMT)/GAMMA
3550 LPRINT:LPRINT"TOTAL GRAMS OF OIL DISPERSED INTO THE WATER COLUMN = ";
3560 LPRINT USING"##.###^^^^";FLUXED
3570 LPRINT:LPRINT"GRAMS OF FREE OIL DROPS IN THE WATER COLUMN=";
3580 LPRINT USING"##.###^^^^";CWMASS
3590 LPRINT"GRAMS OF OIL DROPS ATTACHED TO SPt4 = ";
3600 LPRINT USING"##.###^^^^";CRMASS
3610 ON IEARLY GOTO 3660,3620
3620 LPRINT"THE CONCENTRATION PROFILE HAS NOT 'TOUCHED' THE ";
3630 LPRINT"BOTTOM YET"
3640 CFMASS=0#
3650 GOTO 3690
3660 LPRINT"GRAMS OF FREE OIL DROPS ATTACHED TO THE BOTTOM = ";
3670 IF CFMASS<0# THEN CFMASS=0#
3680 LPRINT USING"##.###^^^^";CFMASS
3690 TOTOIL=CFMASS+CRMASS+CWMASS
3700 LPRINT:LPRINT"TOTAL GRAMS OF OIL ACCOUNTED FOR IN THE CALCULATION = ";
3710 LPRINT USING"##.###^^^^";TOTOIL
3720 CLS
3730 PRINT:INPUT"WANT TO DO IT AGAIN ";AN$
3740 TEST$=LEFT$(AN$,1)
3750 IF TEST$="Y" GOTO 2420
3760 IF TEST$="y" GOTO 2420
3770 LPRINT TOF$
3780 END
3790 REt4 PRINT SUBROUTINE
3800 LPRINT:LPRINT"        DEPTH";
3810 LPRINT TAB(21);
3820 LPRINT"OIL CONC"
3830 LPRINT"        (CM)";
3840 LPRINT TAB(22);
3850 LPRINT"(GM/CC)"
3860 FOR I = 1 TO IEX
3870 LPRINT TAB(5);
3880 LPRINT USING"##.###^^^^";XDEPTH(I);
3890 LPRINT TAB(20);
3900 LPRINT USING"##.###^^^^";PT(I);
3910 IF 1>1 GOTO 3950
3920 LPRINT TAB(36);
3930 LPRINT"(SURFACE )"
3940 GOTO 4000
3950 IF I<IEX GOTO 3990
3960 LPRINT TAB(36);
3970 LPRINT"(BOTTOM)"
3980 GOTO 4000
3990 LPRINT" "
4000 NEXT I
4010 RETURN
4020 REM SUBROUTINE TO PRINT SCREEN HEADER.
4030 PRINT"OIL DROPLETS INTERACTING WITH EXCESS SPM.
```

```
4040 PRINT"CODE NAME IS ";CODE$;
4050 PRINT", VERSION OF";VER$
4060 RETURN
4070 REM SUBROUTINE TO PRINT PAGE HEADER.
4080 LPRINT TOF$
4090 LPRINT"CODE NAME IS ";CODE$;
4100 LPRINT", VERSION OF";VER$
4110 LPRINT"RUN TIME = ";RTIME$;
4120 LPRINT", RUN DATE = ";RDATE$;
4130 IPAGE=IPAGE+1
4140 LPRINT TAB(65);
4150 LPRINT"PAGE ";
4160 LPRINT USING"##";IPAGE
4170 RETURN
```

APPENDIX B

CODE LISTING FOR SPMONLY.BAS

```
100 DEFDBL A-H,K-Z
110REM THIS CODE SOLVES THE ADVECTION-DISPERSION EQUATION FOR OIL
120REM DROPS wITH EXCESS SPM AND FIRST-ORDER REACTION LOSS.
130 DIM BETA(50),C(50),XDEPTH( 50), PT(50),COSR(50),SINR(50)
140 DIM EXPTERM(50),CONTERM(50 I, MASTERM(50),REATERM(50),FLXTERM(50)
150DIM ICHECK(5O)
160 PIE=3.1415926536#
170 PIE2=PIE/2#
180 TOF$=CHR$(12)
190 CODE$="OILSPMXS .BAS"
200 VER$="8-3-88@ 0718"
210 RTIME$=TIME$
220 RDATE$=DATE$
230 REM ITIME=1
240 REM EBIG IS THE MAXIMUM ARGUMENT AN EXPONENTIAL IS ALLOWED TO BE
250 EBIG=30#
260 VXIN=.001#:K=100#:L=10#:RERROR=.000001#:GAMMA=.000046#
270 ALPHA=.00094#:NZERO=.000018#:NROOT=25:IEX=27:AN1$="YES"
280 HEAD$="PRE-LOADED PARAMETER TEST CASE"
290 CLS
300 GOSUB 4020
310 PRINT:INPUT"WANT TO EDIT OR ENTER INPUT PARAMETERS ";AN2$
320 TEST2$=LEFT$(AN2$,2)
330 IF TEST2$="ED" GOTO 560
340 IF TEST2$="ed" GOTO 560
350 PRINT:INPUT"ENTER AN IDENTIFICATION LINE: ";HEAD$
360 PRINT:INPUT"ENTER THE OIL-DROP RISE VELOCITY, CM/SEC (TRY -0.001) ";VX
370 REM SEE THE LETTER TO MAURI PELTO FROM BRUCE KIRSTEIN,28 JULY 1987
380 REM FOR THE VERTICAL TURBULENT DIFFUSIVITY
390 PRINT: INPUT"ENTER THE TURBULENT DIFFUSIVITY,CM*CM/SEC (TRY 100) ";K
400 PRINT: INPUT"ENTER THE DEPTH, METERS (TRY 10.0) ";L
410 PRINT: INPUT"ENTER THE NUMBER OF ROOTS TO BE DETERMINED (TRY 25) ";NROOT
420 PRINT:PRINT"ENTER THE ERROR LIMIT FOR THE ROOTS (TRY 1.00-06) ";
430 INPUT RERROR
440 REM SEE THE LETTER TO DAVE LIU FROM BRUCE KIRSTEIN, l-JULY-83 FOR
450 REM CALCULATION OF THE D1SPERS1ON RATE CONSTANTS
460 PRINT:INPUT"ENTER THE EXPONENTIAL FLUX TERM, 1/SEC (TRY 4.60-05) ";GAMMA
470 PRINT:PRINT"ENTER THE INITIAL OIL FLUX, GRAM/(CM*CM*SEC) (TRY 1.8D-05) ";
480 INPUT NZERO
490 PRINT:PRINT"ENTER THE DISAPPEARANCE RATE CONSTANT, 1/SEC (TRY 0.00094) ";
500 INPUT ALPHA
510 PRINT: INPUT"ENTER THE NUMBER OF DEPTH VALUES TO EVALUATE (TRY 27) ";IEX
520 IF IEX<50 GOTO 550
530 PRINT:PRINT"NUMBER OF DEPTH VALUES MUST BE LESS THAN 50, RE-ENTER."
540 GOTO 510
550 PRINT:INPUT"WANT TO PRINT THE ROOTS (SAY NO) ";AN1$
560 CLS
570 GOSUB 4020
580 PRINT:PRINT"1.  RISE VELOCITY, CM/SEC = ";VXIN
590 PRINT"2.  TURBULENT DIFFUSIVITY,CM*CM/SEC = ";K
600 PRINT"3.  DEPTH, METERS = ";L
610 PRINT*4.  NUMBER OF ROOTS = ";NROOT
620 PRINT"5.  ROOT ERROR LIMIT = ";
630 PRINT USING"##.###^^^^";RERROR
640 PRINT*6.  EXPONENTIAL FLUX TERM, I/SEC = ";
650 PRINT USING"##.###^^^^";GAMMA
660 PRINT"7.  INITIAL OIL FLUX, GRAM/(CM*CM*SEC) = ";
670 PRINT USING"##.###^^^^";NZERO
680 PRINT"8.  DISAPPEARANCE RATE CONSTANT, I/SEC = ";
690 PRINT USING"##.###^^^^";ALPHA
700 PRINT"9.  NUMBER OF DEPTH VALUES = ";IEX
710 PRINT"1O. PRINT THE ROOTS? ";AN1$
720PRINT:INPUT"WANT TO CHANGE ANY";AN$
730 TEST$=LEFT$(AN$,1)
```

```
740 IF TEST$="n" GOTO 970
750 PRINT:INPUT"ENTER THE LINE NUMBER TO BE CHANGED";IL
760 ON IL GOTO 770,790,810,830,850, 870,890,910,930,950
770 PRINT:INPUT"ENTER THE TERMINAL VELOCITY, CM/SEC ";VX
790 GOTO 550
790 PRINT:INPUT"ENTER THE TURBULENT DIFFUSIVITY,CM*CM/SEC";K
800 GOTO 550
810 PRINT: INPUT"ENTER THE DEPTH, METERS ";L
820 GOTO 550
830 PRINT: INPUT"ENTER THE NUMBER OF ROOTS TO BE DETERMINED ";NROOT
840 GOTO 550
850 PRINT:INPUT"ENTER THE ERROR LIMIT FOR THE ROOTS ";RERROR
860 GOTO 570
870 PRINT:INPUT"ENTER THE SPM-LOSS RATE CONSTANT, 1/SEC";ALPHA
880 GOTO 550
890 PRINT:INPUT"ENTER THE FLUX RATE, GM/SEC*CM*CM ";FO
900 GOTO 550
910 PRINT:INPUT"ENTER THE DEPOSTION RATE, CM/SEC ";KS
920 GOTO 550
930 PRINT:INPUT"ENTER THE NUMBER OF DEPTH VALUES TO EVALUATE ";IEX
940 GOTO 550
950 PRINT:INPUT"WANT TO PRINT THE ROOTS? ";AN1$
960 GOTO 550
970 REt4 BEGIN THE CALCULATION
980 TEST1$=LEFT$(AN1$,1)
990 PRINT:INPUT"DO YOU WANT ABRAMOWITZ & STEGUN COTANGENT VALUES";AN$
1000 TEST$=LEFT$(AN$, L)
1010 IF TEST$="N" THEN AANDS=1
1020 IF TEST$="n" THEN AANDS=1
1030 LCM=100#*L
1040 LCM2=LCM*LCM
1050 A=VX/(2#*K)
1060 A2=A*A
1070 AL=A*LCM
1080 AL2=AL*AL
1090 EAL=EXP(AL)
1100 EMAL=1#/EAL
1110 VX2=VX/2#
1120 VXLK=VX*LCM+2#*K
1130 K2=2#*K
1140 K2L=K2/LCM
1150 TERM2=A*KS*LCM
1160 TERM3=LCM*KS-2#*K
1170 TERM4=A*KS*LCM2/K
1180 TERM5=KS*LCM/K
1190 TERM6=LCM*KS+K2
1200 IEARLY=1
1210 IPAGE=0
1220 GOSUB 4030
1230 LPRINT:LPRINT"THIS CODE SOLVES THE 1-D TRANSIENT ADVECTION-";
1240 LPRINT"DISPERSION EQUATION FOR SPM"
1250 LPRINT"(ANALYTICAL SOLUTION) WITH FIRST-ORDER REACTION LOSS."
1260 LPRINT:LPRINT"TERMINAL VELOCITY = ";
1270 LPRINT USING"##.###^^^^";VX;
1280 LPRINT"CM/SEC, DEPTH = ";
1290 LPRINT USING"###.#";L;
1300 LPRINT" METERS"
1310 LPRINT:LPRINT"TURBULENT DIFFUSIVITY = ";
1320 LPRINT USING"####.#";K;
1330 LPRINT" CM*CM/SEC"
1340 LPRINT:LPRINT"FLUX RATE FROM THE BOTTOM = ";
1350 LPRINT USING"##.###^^^^";FO;
1360 LPRINT" GM/SEC*CM*CM"
1370 LPRINT:LPRINT"DEPOSITION RATE = ";
1380 LPRINT USING"##.###^^^^";KS;
1390 LPRINT" CM/SEC"
```

```
1400 LPRINT:LPRINT"ERROR LIMIT FOR THE ROOTS = ";
1410 LPRINT USING"##.###^^^^";RERROR
1420 LPRINT:LPRINT"A = VX/(2*K) = ";
1430 LPRINT USING"##.###^^^^";A;
1440 LPRINT" 1/CM"
1450 IF TEST1$="N" GOTO 1580
1460 IF TEST1$="n" GOTO 1580
1470 LPRINT:LPRINT"ROOTS CALCULATED USING";
1480 IF AANDS=2 THEN LPRINT"ABRAMOWITZ AND STEGUN."
1490 IF AANDS=1 THEN LPRINT" MACHINE FUNCTIONS."
1500 LPRINT:LPRINT"THE ";
1510 LPRINT USING"##";NROOT;
1520 LPRINT" ROOTS OF F(BETA) =BETA*COTANGENT( BETA)-";
1530 LPRINT"K*((A*L)^2-A*KS*L+BETA^2)/(KS*L)
1540 LPRINT:LPRINT"        ROOT        F(BETA)        ERRORCODE"
1550 GOTO 1610
1560 LPRINT:LPRINT"THE NUMBER OF ROOTS USED IS ";
1570 LPRINT USING"####";NROOT
1580 REM START ON THE FIRST ZERO-PIE INTERVAL
1590 TESTI=(AL2-TERM4)/TERM5
1600 REt4 IF TESTI>1 THERE IS NO ROOT.
1610 FOR I=1 TO NROOT
1620 IF I>1 GOTO 1650
1630 NOROOT=1#
1640 IF TESTI<=1# THEN NOROOT=0#
1650 ICHECK(I)=1
1660 XR=PIE*CDBL(I+NOROOT)
1670 XL=XR-PIE
1680 FOR IHALF = 1 TO 50
1690 X=(XL+XR)/2#
1700 IF AANDS=2 GOTO 1730
1710 FX=COS(X)/SIN(X)-((AL2/X)-(TERM4/X)+X)/TERM5
1720 GOTO 1750
1730 GOSUB 3530
1740 FX=FCOTX-((AL2/X)-(TERM4/X)+X)/TERM5
1750 TEST=ABS(FX)
1760 ICHECK(I)=IHALF
1770 IF TEST<RERROR GOTO 1850
1780 IF FX>0# GOTO 1810
1790 XR=X
1800 GOTO 1820
1810 XL=X
1820 NEXT IHALF
1830 ICHECK(I)=99
1840 REt4 STORE CONVENIENT FORMS OF THE ROOTS.
1850 X2=X*X
1860 BETA(I)=X
1870 PEXPT(I)=K*(A2+X2/LCM2)
1880 EXPTERM(I)=ALPHA+PEXPT( I)
1890 SUMTEMP(I)=LCM*(KS-LCM*PEXPT(I)+TERM2)
1900 COSR(I)=COS(X)
1910 SINR(I)=SIN(X)
1920 REM SEE PAGE 29 FOR THE SERIES CONCENTRATION TERM
1930 CONTERM(I)=X/(EXPTERM(I)*(TERM6*X*SINR(I)-SUMTEMP(I)*COSR(I)))
1940 RE14 SEE PAGE 9 CC FOR THE SERIES MASS-IN-WATER TERM
1950 MASTERM(I)=CONTERM(I)*(VX*AL+K2L*X2)*SINR(I)/((LCM/K)*PEXPT(I))
1960 REM SEE PAGE 12(CC) FOR THE SERIES MASS-LOST-BY-REACTION TERM
1970 REATERM(I)=MASTERM(I)/EXPTERM(I)
1980 REM SEE PAGE 19(CC) FOR THE SERIES MASS-LOST-AT-THE-BOTTOM TERM
1990 FLXTERM(I)=((K2L/2#)*K2L*X2+VX*VX2)*SINR(I)*CONTERM(I)/EXPTERM(I)
2000 BFLUX(I)=(VX*SINR(I)+K2L*X*COSR(I))*CONTERM(I)/EXPTERM(I)
2010 IF TEST1$="N" GOTO 2100
2020 IF TEST1$="n" GOTO 2100
2030 LPRINT TAB(5);
2040 LPRINT USING"##.###^^^^";BETA(I);
2050 LPRINT TAB(19);
```

```
2060 LPRINT USING" ##.###^^^^";FX;
2070 LPRINT TAB(38);
2080 IF ICHECK(I)<51 THEN ICHECK(I)=1
2090 LPRINT USING"##";ICHECK(I)
2100 NEXT I
2110 LPRINT:LPRINT"INITIAL SPM FLUX = ";
2120 LPRINT USING"##.###^^^^";F0;
2130 LPRINT" GRAMS/(CM*CM*SEC)"
2140 LPRINT:LPRINT"FIRST-ORDER SPM DISAPPEARANCE RATE CONSTANT,1/SEC=";
2150 LPRINT USING"##.###^^^^";ALPHA;
2160 LPRINT" I/SEC"
2170 ALPHAK=ALPHA/K
2180 ZETA2=A2+ALPHAK
2190 ZZETA=SQR(ZETA2)
2200 ARG=ZZETA*LCM
2210 EXP1=EXP(ARG)
2220 EXP2=1#/EXP(ARG)
2230 SINH=(EXP1-EXP2)/2#
2240 COSH=(EXP1+EXP2)/2#
2250 ZHYP=2#*K*ALPHA+VX*KS
2260 LTERM=1#/(K2*KS*ZZETA*COSH+ZHYP*SINH)
2270 BLEAD=(VX*SINH+K2*ZZETA*COSH)*LTERM
2280 REM START THE CALCULATION.
2290 PRINT:INPUT"ENTER THE TIME IN HOURS ";TYME
2300 PRINT:PRINT"TIME ENTERED IS ";
2310 PRINT USING"##.###^^^^";TYME
2320 PRINT:INPUT"IS THIS CORRECT ";AN$
2330 TEST$=LEFT$(AN$, I)
2340 IF TEST$="N" GOTO 2290
2350 IF TEST$="n" GOTO 2290
2360 T=3600#*TYME
2370 REM LOAD THE X VALUES
2380 XSTEP=LCM/CDBL(IEX-1)
2390 FOR I= 1 TO IEX
2400 XDEPTH(I)=(I-1)*XSTEP
2410 NEXT I
2420 FOR I = 1 TO IEX
2430 X=XDEPTH(I)
2440 EAX=EXP(-A*(LCM-X))
2450 ARG=ZZETA*X
2460 EXP1=EXP(ARG)
2470 EXP1R=1#/EXP(ARG)
2480 CLEAD2=K2*ZZETA*(EXP1+EXP1R)/2#
2490 CLEAD1=LTERM*((VX*(EXP1-EXP1R)/2#)+CLEAD2)
2500 SUM1=0#
2510 FOR IROOT = 1 TO NROOT
2520 ARG=EXPTERM(IROOT)*T
2530 IF ARG>EBIG GOTO 2600
2540 TRIGARG=BETA(IROOT)*X/LCM
2550 SINTERM=VX*SIN(TRIGARG)
2560 COSTERM=K2L*BETA( ROOT) *COS(TRIGARG)
2570 TEMP1=CONTERM(IROOT)*EXP(-ARG)*(SINTERM+COSTERM)
2580 SUM1=SUM1+TEMP1
2590 NEXT IROOT
2600 C(I)=F0*EAX*(CLEAD1-SUM1)
2610 REM NOW INCREMENT TO NEXT X
2620 NEXT I
2630 REM CHECK FOR NEGATIVE CONCENTRATIONS WHICH CAN OCCUR FOR TIMES
2640 REM TOO SMALL, I.E., THE CONCENTRATION PROFILE HAS NOT HAD TIME
2650 REM TO TOUCH THE BOTTOM.
2660 REM IEARLY IS THE SWITCH THAT DENOTES WHEN THE TIME IS TOO SMALL.
2670 IEARLY=1
2680 FOR I = 1 TO IEX
2690 J=IEX-I+1
2700 IF C(J)<0# GOTO 2720
2710 NEXT I
```

```
2720 IEARLY=2
2730 IEX1=I
2740 FOR I = IEX1 TO IEX
2750 J=IEX-I+1
2760 C(J)=0#
2770 NEXT I
2780 REM NOW PRINT THE CONCENTRATION PROFILES
2790 GOSUB 4030
2800 LPRINT:LPRINT"CONCENTRATION PROFILES AT TIME = ";
2810 LPRINT USING"##.###^^^^";TYME;
2820 LPRINT" HOURS ******************* ***"
2830 LPRINT:LPRINT TAB(9);
2840 LPRINT"DEPTH";
2850 LPRINT TAB(27);
2860 LPRINT"SPM CONC."
2870 LPRINT TAB(10);
2880 LPRINT"CM";
2890 LPRINT TAB(27);
2900 LPRINT"GM/CM**3"
2910 FOR I=1 TO IEX
2920 LPRINT"      ";
2930 LPRINT USING"##.###^^^^";XDEPTH( I);
2940 LPRINT"          ";
2950 LPRINT USING"##.###^^^^";C(I);
2960 IF I>1 GOTO 3000
2970 LPRINT TAB(36);
2980 LPRINT"(SURFACE)"
2990 GOTO 3050
3000 IF I<IEX GOTO 3040
3010 LPRINT TAB(36);
3020 LPRINT"(BOTTOM)"
3030 GOTO 3050
3040 LPRINT" "
3050 NEXT I
3060 REM CALCULATE THE MASS OF OIL IN THE WATER AT TIME T, THE LOSS OF OIL
3070 REM THROUGH REACTION, AND THE LOSS OF OIL AT THE BOTTOM.
3080 CWLEAD=LTERM*K2*SINH
3090 CRLEAD=ALPHA*CWLEAD
3100 CFLEAD=CRLEAD
3110 SUM1=0#
3120 SUM2=0#
3130 SUM3=0#
3140 SUM4=0#
3150 FOR I = 1 TO NROOT
3160 ARG=EXPTERM(I)*T
3170 EXP1=0#
3180 IF ARG<EBIG THEN EXP1=EXP(-ARG)
3190 SUM1=SUM1+EXP1*MASTERM( I)
3200 EXPM1=1#-EXP1
3210 SUM2=SUM2+EXPM1*REATERM( I)
3220 SUM3=SUM3+EXPM1*FLXTERM( I)
3230 SUM4=SUM4+EXPM1*BFLUX(I)
3240 NEXT I
3250 CWMASS=F0*(CWLEAD-SUM1)
3260 CRMASS=F0*(CRLEAD*T-ALPHA*SUM2)
3270 CFMASS=F0*(CFLEAD*T+SUM3)
3280 IF IEX>0 GOTO 3330
3290 LPRINT:LPRINT"TIME = ";
3300 LPRINT USING"##.###^^^^";TYME
3310 LPRINT" HOURS, DIMENSIONLESS TIME,K*T/L**2 = ";
3320 LPRINT USING"##.###^^^^";DTIME
3330 LPRINT:LPRINT"GRAMS OF SPM (UNATTACHED) IN THE WATER COLUMN = ";
3340 LPRINT USING"##.###^^^^";CWMASS
3350 LPRINT"GRAMS OF SPt4 ATTACHED TO OIL = ";
3360 LPRINT USING"##.###^^^^";CRMASS
3370 TOTSPM=CRMASS+CWMASS
```

```
3380 LPRINT:LPRINT"GRAMS OF SPM IN WATER + ATTACHED = ";
3390 LPRINT USING"##.###^^^^";TOTSPM
3400 LPRINT:LPRINT"GRAMS OF SPM FROM THE BOTTOM (FROM VX*C-K*DC/DX)=";
3410 LPRINT USING"##.###^^^^";CFMASS
3420 SEDIMENT=F0*T-KS*F0*(BLEAD*T-SUM4)
3430 LPRINT"GRAMS OF SPM FROM THE BOTTOM (FROM-F0+KS*C) = ";
3440 LPRINT USING"##.###^^^^";SEDIMENT
3450 CLS
3460 PRINT:INPUT"WANT TO DO IT AGAIN ";AN$
3470 TEST$=LEFT$(AN$, 1)
3480 IF TEST$="Y" GOTO 2280
3490 IF TEST$="y" GOTO 2280
3500 LPRINT TOFS
3510 LPRINT TOF$
3520 END
3530 REM SUBROUTINE TO CALCULATE COTANGENT FROM M. ABRAMOWITZ
3540 REM AND I.R.STEGUN, HANDBOOK OF MATHEMATICAL FUNCTIONS,
3550 RE14 SEE PAGE 76, EQUATION 4.3.103.
3560 FLIP=0
3570 REM THIS CALCULATES THE SERIES APPROX FOR XCOT(X).
3580 AC2=-.333333341#:AC4=-.02222202871 :AC6=-.0021177168#
3590 AC8=-.00020785041) :AC10=-.0000262619#
3600 REM UNWIND THE ARGUMENT TO LESS THAN PIE/4.
3610 REM ADJUST X TO A 2PI FRAME.
3620 YI=(X/TWOPIE-CDBL(INT(X/TWOPIE)))*TWOPIE
3630 IF (YI>0)AND(YI<PIE2) THEN IQUAD=1
3640 IF (YI>PIE2)AND(YI<PIE) THEN IQUAD=2
3650 IF (YI>PIE)AND(YI<PIE*1.5# ) THEN IQUAD=3
3660 IF (YI>PIE*1.5#)AND(YI<TWOPIE) THEN IQUAD=4
3670 IF (YI=PIE2) OR (YI=PIE*1.5#) THEN IQUAD=5
3680 IF (YI=PIE)OR(YI=TWOPIE)OR(YI=0) THEN IQUAD=6
3690 ON IQUAD GOTO 3700,3720,3740,3760,3940, 3960
3700 Y=YI
3710 GOTO 3770
3720 Y=PIE-YI
3730 GOTO 3770
3740 Y=YI-PIE
3750 GOTO 3770
3760 Y=TWOPIE-YI
3770 TEST=PIE4-Y
3780 IF TEST>0# GOTO 3820
3790 XI=Y
3800 Y=PIE2-XI
3810 FLIP-1
3820 YSQ=Y*Y
3830 SREMAIN=YSQ*(AC8+(AC10)*YSQ)
3840 SCOTX=1#+YSQ*(AC2+YSQ*(AC4+YSQ*(AC6+SREMAIN)))
3850 TCOTX=SCOTX/Y
3860 IF IQUAD=2 THEN TCOTX=-TCOTX
3870 IF IQUAD=4 THEN TCOTX=-TCOTX
3880 REM SO NOW WE REALLY HAVE COTX FOR THE ZERO TO PIE/4 WEDGE.
3890 IF FLIP=1 GOTO 3920
3900 FCOTX=TCOTX
3910 GOTO 3970
3920 FCOTX=1#/TCOTX
3930 GOTO 3970
3940 FCOTX=0#
3950 GOTO 3970
3960 FCOTX=1D+21
3970 RETURN
3980 REM SUBROUTINE TO PRINT SCREEN HEADER.
3990 PRINT"SUSPENDED-PARTICULATE-MATTER(SPM) CALCULATION
4000 PRINT"CODE NAME IS ";CODEN$;
4010 PRINT", VERSION OF ";VER$
4020 RETURN
4030 REM SUBROUTINE TO PRINT PAGE HEADER.
```

```
4040 LPRINT TOF$
4050 LPRINT"CODE NAME IS ";CODEN$;
4060 LPRINT", VERSION OF ";VER$
4070 LPRINT"RUN TIME = ";RTIME$;
4080 LPRINT",RUN DATE = ";RDATE$;
4090 IPAGE=IPAGE+1
4100 LPRINT TAB(65);
4110 LPRINT"PAGE ";
4120 LPRINT USING"##";IPAGE
4130 RETURN
```

APPENDIX C

CODE LISTING FOR OILSPM3BAS

```
10  REM
110 DEFDBL A-H, O-Z
120 REM THIS CODE IS THE SIMULTANEOUS OIL-SPM SOLVER AND CAN BEUSED
130 REMTO SOLVE FOR OIL ALONE OR SPMALONE WITH AN ARBITRARY INITIAL
140 REM CONDITION.  CRANK-NICOLSON INTEGRATION IS USED.
150  D I M  A(3,101),C(101),U(101),Y(101),X(101),PNT(101)
160 DIM B(3,101),S(101),V(101),Z(101),CG(101),SG(101)
170 DIM D(3,101),W(101),Q(101),G(101),R(101)
180 CODEN$="OILSPM3.BAS"
190 VER$="8-9-88 @ 0643"
200 TOF$=CHR$(12)
210 RTIME$=TIME$: RDATE$=DATE$
220 CLS
230 GOSUB 9250
240 REM SET THE PAGE COUNTER TO ZERO.
250 IPAGE=0
260 REM SPECIFY SOME OIL PARAMETERS:
270 VDIFFA=100#:VOIL=.01#:ALPHO=.094#:DEPTH=10#:NPOINTSA=49
280 SZER=.000018#:GAMM=.000046#:TYMEMAX=.5#:PINT=.5#:TDIVIDE=20#
290 REM SPECIFY SOME SPM PARAMETERS:
300 VSPM=.001#:ALPHS=.094#:FZER=.000046#:SKZER=.046#:PIE2=9.869589#
310 VASPM=.001#:SECONDS=3600#:IEULER=1:ICRATE=3
320 ANSP$="YES":ANOP$="NO":ANCP$="YES"
330 PRINT:PRINT"WANT TO 'ENTER' NEW PARAMETERS OR 'EDIT' RECOMMENDED";
340 INPUT" VALUES";ANS$
350 TESTA$=LEFT$(ANS$, 2)
360 IF TESTA$="EN" GOTO 390
370 IF TESTA$="en" GOTO 390
380 GOTO 610
390 CLS
400 GOSUB 9250
410 PRINT: PRINT"ENTER THE vERTICAL-TURBULENT DIFFUSIVITY,CM*CM/SEC";
420 INPUT", (TRY 100)";VDIFFA
430 PRINT: PRINT"ENTER THE OIL RISING VELOCITY, CM/SEC, (TRY0.001)";
440 INPUT VOIL
450 PRINT: PRINT"ENTER THE OIL-SPM RATE CONSTANT FOR OIL LOSS, CC/(GM*SEC)";
460 INPUT", i TRY .094)";ALPHO
470 PRINT: INPUT"ENTER THE OCEAN DEPTH, METERS, (TRY10)";DEPTH
480 PRINT:PRINT"ENTER THE NUMBER OF GRID POINTS (MAXIMUM '3'3,";
490 PRINT" MUST BE ODD, TRY 49)";
500 REMTHIS IS THE NUMBER OF POINTS WITHIN THE WATER COLUMN AND DOES
510 REM NOT INCLUDE THE EXTERIOR TWO POINTS.
520 INPUT NPOINTSA
530 PRINT:PRINT"THE OIL-Dispersion FLUX IS:SZERO*EXP(-GAMMA*TIME) "
540 PRINT:INPUT"ENTER SZERO,GRAMS/(CM*CM*SEC) . (TRY 1.8D-05)";SZER
550 PRINT: INPUT"ENTER GAMMA, 1/SEC, (TRY 4.6D-05)";GAMM
560 PRINT: INPUT"ENTER THE MAXIMUM TIME, HOURS";TYMEMAX
570 PRINT: INPUT"ENTER THE PRINT INTERVAL, HOURS";PINT
580 PRINT: INPUT"USE STEADY-STATE OIL PROFILE TO START (SAYNO):";ANOP$
590 PRINT: INPUT"COUPLE THE CONCENTRATIONS: ";ANCP$
600 PRINT: INPUT"COUPLING ITERATIONS (TRY5)";ICRATE
610 CLS
620 GOSUB '32S0
630 PRINT:PRINT"1.  TURBULENT DIFFUSIVITY,CM*CM/SEC = ";
640 PT=VDIFFA
650 GOSUB 7210
660 PRINT"2.  OIL RISING VELOCITY, CM/SEC = ";
670 PT=VOIL
680 GOSUB 7210
690 PRINT"3.  OIL-SPM RATE CONSTANT FOR OIL LOSS, CC/(GM*SEC) = ";
7(>0 PT=ALPHO
710 GOSUB 7210
720 PRINT"4.  OCEAN DEPTH, METERS = ";
730 PT=DEPTH
740 GOSUB 7210
```

```
750 PRINT"5.  NUMBER OF GRID POINTS =  ";
760 IPT=NPOINTSA
770 GOSUB 7240
780 PRINT"6.  INITIAL OIL-DISPERSON FLUX SZERO,GRAMS/(CM*CM*SEC) = ";
790 PT=SZER
800 GOSUB 7210
810 PRINT"7.  OIL-DISPERSON GAMMA, I/SEC = ";
820 PT=GAMM
830 GOSUB 7210
840 PRINT"8.  MAXIMUM TIME, HOURS = ";
850 PRINT USING"###.##";TYMEMAX
860 PRINT"9.  PRINT INTERVAL, HOURS = ";
870 PRINT USING"#.###";PINT
880 PR1NT"10. USE STEADY-STATE OIL PROFILE TO START: ";ANOP$
890 PRINT"11. COUPLE THE CONCENTRATIONS: ";ANCP$
900 PRINT"12. COUPLING ITERATIONS = ";
910 PRINT USING"##";ICRATE
920 PRINT: INPUT"WANT TO CHANGE ANY";ANS$
930 TESTB$=LEFT$(ANS$,1)
940 IF TESTB$="N" GOTO 1230
950 IF TESTB$="n" GOTO 1230
960 PRINT: INPUT"ENTER THE LINE NUMBER TO BE CHANGED";LN
970 ON LN GOTO 980,1000,1020,1040,1060,1090,1110,1130,1150,1170,1190,1210
980 PRINT: INPUT"ENTER THE TURBULENT DIFFUSIVITY,CM*CM/SEC";VDIFFA
990 GOTO 610
1000 PRINT: INPUT"ENTER THE OIL RISING VELOCITY, CM/SEC";VOIL
1010 GOTO 610
1020 PRINT: INPUT"ENTER THE OIL-SPM RATE CONSTANT,CC/(GM*SEC)";ALPHO
1030 GOTO 610
104o PRINT: INPUT"ENTER THE OCEAN DEPTH, METERS";DEPTH
1050 GOTO 610
1060 PRINT: PRINT"ENTER THE NUMBER OF GRID POINTS ('MAXIMUM 99,";
1070 INPUT" MAKE IT ODD, TRY 49)";NPOINTSA
1080 GOTO 610
1090 PRINT: INPUT"ENTER SZERO, GRAMS/(CM*CM*SEC) ";SZER
1100 GOTO 610
1110 PRINT:INPUT"ENTER GAMMA, 1/SEC";GAMM
1120 GOTO 610
1130 PRINT: INPUT"ENTER THE MAXIMUM TIME, HOURS";TYMEMAX
1140 GOTO 610
1150 PRINT: INPUT"ENTER THE PRINT INTERVAL, HOURS";PINT
1160 GOTO 610
1170 PRINT: INPUT"USE STEADY-STATE OIL PROFILE TO START:";ANOP$
1180 GOTO 610
1190 PRINT: INPUT"COUPLE THE CONCENTRATIONS: ";ANCP$
1200 GOTO 610
1210 PRINT: INPUT"COUPLING ITERATIONS (TRY5)"; CRATE
1220 GOTO 610
1230 REM CHECK THE NUMBER OF GRID POINTS.
1240 IF NPOINTSA<100 GOTO 1300
1250 CLS
1260 PRINT:PRINT"THE NUMBER OF GRID POINTS EXCEEDS ARRAY CAPACITY";
1270 PRINT" OF 99."
1280 PRINT: INPUT"ENTER THE NUMBER OF GRID POINTS(MAKE IT ODD)";NPOINTSA
1290 GOTO 610
1300 REM ENTER OR EDIT THE SPM parameters
1310 CLS
1320 IF TESTA$="EN" GOTO 1350
1330 IF TESTA$="en" GOTO 1350
1340 GOTO 1460
1350 GOSUB 9250
1360 PRINT: INPUT"ENTER THE SPM SETTLING VELOCITY, CM/SEC (TRY 0.001)";VSPM
1370 PRINT: PRINT"ENTER THE OIL-SPM AGGLOMERATE SETTLING VELOCITY,";
1380 INPUT" CM/SEC ITRY 0.0001)";VASPM
1390 PRINT: PRINT"ENTER THE OIL-SPM RATE CONSTANT FOR SPM LOSS,";
1400 INPUT" CC/(GM*SEC), TRY 0.094";ALPHS
```

```
1410 PRINT: PRINT"ENTER THE SPM BOTTOM SOURCE FLUX TERM, GM/(CM-*S E  ,
1420 INPUT" (TRY4.6D-05)";FZER
1430 PRINT: PRINT"ENTER THE 5PM BOTTOM DEPOSITION RATE CONSTANT, CM/SEC,;
1440 INPUT" (TRY 0.046)";SKZER
1450 PRINT: INPUT"WANT TO START OFF WITH STEADY-STATE SPM";ANSP$
1460 CLS
1470 GOSUB 9250
1480 PRINT:PRINT"1.  SPM SETTLING VELOCITY, CM/SEC = ";
1490 PT=VSPM
1500 GOSUB 7210
1510 PRINT"2.  OIL-SPM AGGLOMERATE SETTLING VELOCITY, CM/SEC = ";
1520 PT=VASPM
1530 GOSUB 7210
1540 PRINT"3.  OIL-SPM RATE CONSTANT FOR SPM LOSS, CC/(GM*SEC) = ";
1550 PT=ALPHS
1560 GOSUB 7210
1570 PRINT"4.  SPM SOURCE FLUX TERM, GM/(CM^2*SEC)";
1580 PT=FZER
1590 GOSUE 7210
1600 PRINT"5.  SPM DEPOSITION RATE CONSTANT, CM/SEC = ";
1610 PT=SKZER
1620 GOSUB 7210
1630 PRINT"6.  uSE STEADY-STATE SPMPROFILE TO START:";ANSP$
1640 PRINT:INPUT"WANT TO CHANGE ANY";ANS$
1650 TESTB$=LEFT$(ANS$,1)
1660 IF TESTB$="N" GOTO 1830
1670 IF TESTB$="n" GOTO 1830
1680 PRINT: INPUT"ENTER THE LINE NUMBER TO BE CHANGED";LN
1690 ON LN GOTO 1700,1720,1730,1770,1750, 1S10
1700 PRINT: INPUT"ENTER THE SPM SETTLING VELOCITY, CM/SEC";VSPM
1710 GOTO 1460
1720 PRINT:PRINT"ENTER THE OIL-SPM AGGLOMERATE SETTLING VELOCITY,";
1730 INPUT" CM/SEC ";VASPM
1740 GOTO 1460
1750 PRINT: INPUT"ENTER THE OIL-SPM RATE CONSTANT FOR SPMLOSS";ALPHS
1760 GOTO 1460
1770 PRINT: INPUT"ENTER THE SPM BOTTOM SOURCE FLUX TERM";FZER
1780 GOTO 1460
1790 PRINT: INPUT"ENTER THE SPMBOTTOM DEPOSITION RATE CONSTANT";SKZER
1800 GOTO 1460
1810 PRINT: INPUT"USE STEADY-STATE SPM PROFILE TO START: ";ANSP$
1820 GOTO 1460
1830 REM INITIALIZE THE SPM  CONCENTRATION  PROFILE.
1840 TESTSPM$=LEFT$(ANSP$,1)
1850 ISPM=1
1860 IF TESTSPM$="Y" THEN ISPM=2
1870 IF TESTSPM$="y" THEN ISPM=2
1880 TESTOIL$=LEFT$(ANOP$,1)
1890 IOIL=1
1900 IF TESTOIL$="Y" THEN IOIL=2
1910 IF TESTOIL$="y" THEN IOIL=2
1920 REM IS COUPLING ON"?
1930 ICPLE=1
1940 TESTCPL$=LEFT$(ANCP$,1)
1950 IF TESTCPL$="N" THEN ICPLE=2
1960 IF TESTCPL$="n" THEN ICPLE=2
1970 REM THE ACTUAL NUMBER OF POINTS IS NPOINTSA+2 BECAUSE THERE IS
1980 REMA POINT AT -DX ON THE LEFT BOUNDARY AND A POINT AT +DX ON
1990 REM THE RIGHT BOUNDARY.  THE REASON FOR DOING THIS IS THAT
2000 REM CENTRAL DIFFERENCE APPROXIMATIONS ARE USED FOR THE DERIVATIVES
2010 REM AT THE SOUNDARIES.
2020 NPOINTS=NPOINTSA+2
2030 APOINTS=CDBL(NPOINTS)
2040 NPOINTS1=NPOINTS-1
2050 NPOINTS2=NPOINTS-2
2060 NPOINTS3=NPOINTS-3
```

```
2070 REM THE BOTTOM BOUNDARY CONDITION IS C=0 FOR OIL ALWAYS,
2080 C(NPOINTS1)=0#
2090 REM AS IS W=0 FOR THE OIL-SPM AGGLOMERATE.
2100 Q(NPOINTS1)=0#
2110 REM START THE CALCULATION.
2120 REM THE WORKING UNITS ARE GRAM-CENTIMETER-HOUR.
2130 DEPTH1=DEPTH*100#
2140 DEPTH2=DEPTH1*DEPTH1
2150 REM EXAMINE K*T*PIE2/L2 TO DETERMINE THE TIME REQUIRED
2160 REM FOR UNIT DIMENSIONLESS TIME, SEE SECTION 3.8, PAGE 113
2170 REM OF CARSLAW AND JAEGER FOR A SIMILAR PROBLEM.
2180 VDIFF=VDIFFA*SECONDS
2190 TUNITY=DEPTH2/VDIFF/PIE2
2200 PRINT: PRINT"TIME FOR UNITY DIMENSIONLESS TIME, HOURS = ";
2210 PRINT USING"##.###^^^^";TUNITY
2220 PRINT:PRINT"THE TIME STEP WILL BE THE ABOVE TIME DIVIDED BY";
2230 PRINT USING"####.###";TDIVIDE
2240 PRINT: INPUT"IS THIS ACCEPTABLE";ANS$
2250 TESTB$=LEFT$(ANS$, 1)
2260 IF TESTB$="Y" GOTO 2310
2270 IF TESTB$="y" GOTO 2310
2280 PRINT: INPUT"ENTER THE VALUE YOU WANT";TDIVIDE
2290 GOTO 2220
2300 REM SET THE TIME STEP.
2310 DT=TUNITY/TDIVIDE
2320 REPI NOW COMPUTE THE REQUIRED TIME STEP WHICH IS LESS THAN
2330 REM THE CURRENT VALUE OF DT TO 'STEP' ON A PRINT INTERVAL.
2340 TYME=0#
2350 TYME9=.9999#*TYMEMAX
2360 PINT9=.9999#*PINT
2370 NSTEPS=FIX(PINT/DT)+1
2380 ASTEPS=CDBL(NSTEPS)
2390 DT=PINT/ASTEPS
2400 RDT=1#/DT
2410 REM SET THE FINAL PRINT SWITCH.
2420 IPFINAL=1
2430 REM SET UP THE PARAMETERS IN THE CORRECT UNITS OF GRAM-CM-HOUR.
2440 REM USE CM/HOUR FOR THE RISING OR SETTLING VELOCITY.
2450 REM THE OIL RISING VELOCITY IS NEGATIVE BECAUSE THE UP-DIRECTION
2460 REM IS NEGATIVE, POSITIVE IS DOWN.
2470 VROIL=-VOIL*SECONDS
2480 VRSPM=VSPM*SECONDS
2490 VRAGG=VASPM*SECONDS
2500 REM USE 1/HOUR FOR THE RATE CONSTANT WITH UNIT SPM concentration
2510 REM OR GM/(CM^3*HOURS) WHEN A REAL SPM concentration IS USED.
2520 ALPHAO=ALPHO*SECONDS
2530 ALPHAS=ALPHS*SECONDS
2540 REM THE RATE CONSTANT FCIR THE APPEARANCE OF THE OIL-SPM AGGLOMERATE
2550 REM IS THE SUM OF THE TWO Individual RATE CONSTANTS.
2560 ALPHAB=ALPHAO+ALPHAS
2570 SZERO=SZER*SECONDS
2580 FZERO=FZER*SECONDS
2590 SKZERO=SKZER*SECONDS
2600 GAMMA=GAMM*SECONDS
2610 REM NUMBER OF UNKNOWN OIL CONCENTRATIONS SOLVED FOR MUST BE SET
2620 REM TO L FOR THE SPARSE-MATRIX SOLVING ROUTINE. THIS ROUTINE
2630 REM SOLVES FOR THE N-2 UNKNOWNS AND THE OTHER UNKNOWN IS SOLVED
2640 REM FOR 'OFF-LINE.' THE REASON FOR THIS IS AS FOLLOWS:
2650 REM THE NUMBER OF GRID POINTS IS NPOINTS, HENCE THE NUMBER OF
2660 REM OF UNKNOWN OIL concentrations IS NPOINTS. BUT, THE OIL
2670 REM CONCENTRATION AT THE OCEAN BOTTOM IS O., I.E., C(NPOINTS1)=0.
2680 REM BECAUSE OF THIS PARTICULAR ZERO OIL CONCENTRATION, THE 'OIL'
2690 REM SYSTEM OF EQUATIONS IS SOLVED THROUGH NPOINTS-2 ONLY, AND THE
2700 REM LAST UNKNOWN OIL CONCENTRATION IS SOLVED FOR AT THE 'END.'
2710 REM SOLVING SUBROUTINE.
2720 L=NPOINTS2
```

```
2730 LM1=L-1
2740 LM2=L-2
2750 APOINTS1=CDBL(NPOINTS3 )
2760 DX=DEPTH1/APOINTS1
2770 DX2=DX*DX
2780 DX4=4#*DX
2790 REM CALCULATE THE EULER INTEGRATION PARAMETERS
2800 REM FOR THE INTEGRATION OF rHE FLUX OF 011. TO THE BOTTOM,
2810 REM THE OIL REACTION LOSS, THE NET SPM FLUX AND THE SPM
2820 REM REACTION LOSS.
2830 EDTDX=VDIFF*DT/DX
2840 REM AND FOR THE REACTION LOSS.
2850 EDT=DT
2860 REM SETUP THE SIMPSONS INTEGRATION PARAMETERS.   DO NOT INCLUDE
2870 REM C(1) AND C(N) IN THE [INTEGRATION BECAUSE THEY ARE OUTSIDE THE
2880 REM BOUNDARIES.
2890 ISMP42=(NPOINTSA-3)/2
2900 HSMP3=DX/3#
2910 ALPHAO2=ALPHAO/2#
2920 ALPHAS2=ALPHAS/2#
2930 ALPHAB2=ALPHAB/2#
2940 DOILDX=VDIFF/DX
2950 DOILDX2=VDIFF/DX2
2960 DOILDX22=DOILDX2/2#
2970 V4XO=VROIL/DX4
2980 V4XS=VRSPM/DX4
2990 V4XB=VRAGG/DX4
3000 REM THE C(I) ARRAY STORES THE OIL CONCENTRATION PROFILE AT THE
3010 REM CURRENT TIME, THE U(I) ARRAY STORES THE CALCULATED OIL
3020 REM Concentration PROFILE AT THE NEXT TIME (STEP).
3030 REM THE A(3,N) ARRAY STORES THE COEFFICIENTS FOR THE CRANK-
3040 REM NICOLSON ALGORITHM FOR THE OIL.
3050 REM ALSO, THE S(I) ARRAY STORES THE SPM CONCENTRATION PROFILE AT THE
3060 REM CURRENT TIME, THE V(I) ARRAY STORES THE CALCULATED SPM
3070 REM CONCENTRATION PROFILE AT THE NEXT TIME (STEP).
3080 REM THE B(3,N) ARRAY STORES THE COEFFICIENTS FOR THE CRANK-
3090 REM NICOLSON ALGORITHM FOR THE SPM.
3100 REM THE MAIN DIAGONAL ELEMENT IS 'DIAGC1' FOR THE C(I,J+1).
3110 REM THE MAIN DIAGONAL ELEMENT IS 'DIAGC2' FOR THE C(I,J).
3120 DIAGC1=DOILDX2+RDT
3130 DIAGC2=DOILDX2-RDT
3140 REM THE MAIN DIAGONAL ELEMENT IS 'DIAGS1' FOR THE S(I,J+1).
3150 REM THE MAIN DIAGONAL ELEMENT IS 'DIAGS2' FOR THE S(I,J).
3160 DIAGS1=DIAGC1
3170 DIAGS2=DIAGC2
3180 REM THE MAIN DIAGONAL ELEMENT IS'DIAGB1' FOR THE W(I,J+1).
3190 REM THE MAIN DIAGONAL ELEMENT [S 'DIAGB2' FOR THE W(I,J)
3200 DIAGB1=DIAGC1
3210 DIAGB2=DIAGC2
3220 REM THE UPPER DIAGONAL IS 'UDIAG'
3230 UDIAGC=DOILDX22-V4XO
3240 UDIAGS=DOILDX22-V4XS
3250 UDIAGB=DOILDX22-V4XB
3260 REM THE LOWER DIAGONAL IS 'BDIAG'
3270 BDIAGC=DOILDX22+V4XO
3280 BDIAGS=DOILDX22+V4XS
3290 BDIAGB=DOILDX22+V4XB
3300 GOSUB 9300
3310 LPRINT:LPRINT"PROBLEM PARAMETERS ARE AS FOLLOWS:"
3320 LPRINT:LPRINT"VERTICAL TURBULENT DIFFUSIVITY,CM*CM/SEC = ";
3330 LPRINT USING"####. ##";VDIFFA
3340 LPRINT"WATER DEPTH, METERS = ";
3350 LPRINT USING"###. #";DEPTH
3360 LPRINT: LPRINT"OIL RISING VELOCITY, CM/SEC  =  ";
3370 LPRINT USING"##.##^^^^";vOIL
3380 LPRINT"OIL-SPM RATE CONSTANT FOR OIL LOSS, CC/(GM*SEC)= ";
```

```
3390 LPRINT USING"##.###^^^^ ";ALPHO
3400 LPRINT"OIL 2I3PERSION RATE, GM/(CM*CM*SEC)=(";
3410 LPRINT USING"#.##^^^^ ";SZER;
3420 LPRINT")*EXP(( -";
3430 LPRINT USING"#.##^^^^ ";GAMM;
3440 LPRINT")● SECOND51"
3450 LPRINT:LPRINT"SPM SETTLING VELOCITY, CM/SEC = ";
3460 LPRINT USING"##.##^^^^ ";VSPM
3470 LPRINT"OIL-SPM RATE CONSTANT FOR SPM LOSS, CC/(GM*SEC) = ";
3480 LPRINT USING"##.##^^^^";ALPHS
3490 LPRINT"SPM BOTTOM SOURCE FL U X, GM/(CM^2*SEC) = ";
3500 LPRINT USING"##.##^^^^ ";FZER
3510 LPRINT"SPM DEPOSITION RATE CONSTANT, CM/SEC = ";
3520 LPRINT USING"##.##^^^^ ";SKZER
3530 LPRINT:LPRINT"OIL-SPM AGGLOMERATE SETTLING VELOCITY, CM/SEC=";
3540 LPRINT USING"##.##^^^^^^";VASPM
3550 LPRINT:LPRINT"TIME STEP, HOURS = ";
3560 LPRINT USING"##.##^^^^^^";DT;
3570 LPRINT", INTEGRATION TIME, HOURS = ";
3580 LPRINT USING"###.##";TYMEMAX
3590 LPRINT"SPECIFIED PRINT INTERVAL, HOURS = ";
3600 LPRINT USING"##.###";PINT
3610 REM SAVE THE DEPTHS.
3620 FOR I = 1 TO NPOINTS2
3630 X(I)=(I-1)*DX
3640 NEXT I
3650 REM ZERO THE ARRAYS.
3660 FOR I = 1 TO NPOINTS
3670 S(I)=0#
3680 C(I)=0#
3690 W(I)=0#
3700 SG(I)=0#
3710 CG(I)=0#
3720 NEXT I
3730 REM IF THE REACTION RATE CONSTANTS ARE GREATER THAN ZERO,
3740 REM TURN ON THE CROSS TERMS.
3750 IF ALPHAO=0# GOTO 3790
3760 FOR I = 1 TO NPOINTS
3770   SG(I)=1#
3780 NEXT I
3790 IF ALPHAS=0# GOTO 3830
3800 FOR I = 1 TO NPOINTS
3810 CG(I)=1#
3820 NEXT I
3830 OILZERO=0#
3840 ON IOIL GOTO 3930,3850
3850 REM CALCULATE A STEADY STATE (GAMMA=0) OIL CONCENTRATION PROFILE.
3860 GOSUB 8830
3870 FOR I = 1 TO NPOINTSA
3880 PNT(I)=C(I+1)
3890 NEXT I
3900 REM INTEGRATE THE INITIAL NONZERO OIL PROFILE.
3910 GOSUB 8330
3920 OILZERO=SUM1
3930 LPRINT:LPRINT"THE INITIAL OIL WATER-COLUMN LOADING, GRAMS = ";
3940 LPRINT USING"##.###^^^^^^";OILZERO
3950 SPMZERO=0#
3960 ON ISPM GOTO 4060,3970
3970 REM CALCULATE A STEADY-STATE SPM CONCENTRATION PROFILE.
3980 GOSUB 8460
3990 REM AND LOAD THE SPM STEADY-STATE PROFILE.
4000 FOR I = 1 TO NPOINTSA
4010 PNT(I)=S(I+1)
4020 NEXT I
4030 REM INTEGRATE THE INITIAL NONZERO SPM PROFILE.
4040 GOSUB 8330
```

```
4060 SPMZERO=SUM1
4060 LPRINT"THE INITIAL SPM WATER-COLUMN LOADING,GRAMS";
4070 LPRINT USING"##.###    ";SPMZERO
4080 REM FILL IN SOME ELEMENTS WHICH DO NOT CHANGE.
4090 AEXTRA=-DOILDX/2#
4100 DEXTRA=AEXTRA
4110 A(2,1)=-AEXTRA
4120 A(1,1)=VROIL
4130 B(1,1)=VRSPM
4140 BEXTRA2=DOILDX/2#
4150 BEXTRA1=-BEXTRA2
4160 B(2,1)=BEXTRA2
4170 B(1,1)=VRSPM
4180 Z(1)=0#
4190 REM THE NEXT THREE STATEMENTS REFER TO THE OIL-SPM AGGLOMERATE.
4200 D(2,1)=-DEXTRA
4210 D(1,1)=VRAGG
4220 G(1)=0#
4230 REM INTEGRATE THE INITIAL OIL CONCENTRATION PROFILE.
4240 FOR I = 1 TO NPOINTSA
4250 PNT(I)=C(I+1)
4260 NEXT I
4270 GOSUB 8330
4280 OILP=SUM1
4290 REM INTEGRATE THE INITIAL SPM CONCENTRATION PROFILE.
4300 FOR I = 1 To NPOINTSA
4310 PNT(I)=S(I+1)
4320 NEXT I
4330 GOSUB 8330
4340 SPMP=SUM1
4350 REM THE INITIAL OIL-SPM AGGLOMERATE CONCENTRATION PROFILE IS
4360 REM ALWAYS ZERO,
4370 AGLP=0#
4380 REM AS IS THE INTEGRAL OF THE FLUX TO THE BOTTOM.
4390    AGFLUX=0#
4400 REM THE INTEGRATION OF THE PROFILES IS DONE AT EACH TIME
4410 REM INCLUDING T=0.  THIS IS THE START OF THE EULER INTEGRATION.
4420 OILFLUX=(C(NPOINTS2)-C(NPOINTS))/4#
4430 OILLOSS=OILP/2#
4440 SPMCONC=S(NPOINTS1)/2#
4450 SPMLOSS=SPMP/2#
4460 REM IS COUPLING ON?
4470 ONICPLE GOTO 4480,4600
4480 REM INTEGRATE THE INITIAL OIL*SPM CONCENTRATION PROFILE.
4490 FOR I = 1 TO NPOINTSA
4500 PNT(I)=C(I+1)*S(I+1)
4510 NEXT I
4520 GOSUB 8330
4530 REM AND INTEGRATE WITH RESPECT TO TIME.
4540 CROSS=SUM1/2#
4550 ICNT=0
4560 FOR I = 1 TO NPOINTS
4570 CG(I)=C(I)
4580 SG(I)=S(I)
4590 NEXT I
4600 REM DO AN INITIAL PRINT.
4610 GOSUB 6230
4620 REM START THE CALCULATION.
4630 REM FILL IN THE OIL AND SPM TRIDIAGONAL ELEMENTS INTO THE
4640 REM A(3,NPOINTS) AND B(3,NPOINTS) ARRAYS.
4650 REM FILL THE UPPER OIL DIAGONAL STARTING WITH A(1,2) AND RUNNING
4660 REM THROUGH NPOINTS3.
4670 FOR I = 2 TO NPOINTS3
4680 A(1,I)=UDIAGC
4690 NEXT I
4700 REM FILL THE MAIN OIL DIAGONAL STARTING WITH A(2,2) AND RUNNING
```

```
4730 REM THROUGH NPOINTS2.
4740 FOR I = 2 TO NPOINTS2
4750 REM NOW GUESS THE SEDIMENT VECTOR AND COMPUTE ALPHA-PRIME
4760 REM FOR EACH POSITION IN THE WATER COLUMN.
4770 REM LEAVE AT UNITY FOR NOW, 2-13-88.
4780 A(2,I)=-DIAGC1-ALPHAO2*SG(I)
4790 NEXT I
4800 REM FILL THE LOWER OIL DIAGONAL STARTING WITH A(3,1) AND RUNNING
4810 REM THROUGH NPOINTS3.
4820 FOR I = 1 TO NPOINTS3
4830 A(3,I)=BDIAGC
4840 NEXT I
4850 REM FILL Y(1) WITH THE OIL BOUNDARY CONDITION AT THE TYME+DT STEP.
4860 Y(1)=SZERO*EXP(-GAMMA*(TYME+DT))
4870 REM FILL Y(I) VECTOR STARTING WITH Y(2) AND RUNNING THROUGH NPOINTS1.
4880 FOR I = 2 TO NPOINTS1
4890 IM=I-1
4900 IP=I+1
4910 Y(I)=-BDIAGC*C(IM)+(DIAGC2+ALPHAO2*SG(I))*C(I)-UDIAGC*C(IP)
4920 NEXT I
4930 REM FILL THE UPPER SPM DIAGONAL STARTING WITH B(1,2) AND RUNNING
4940 REM THROUGH NPOINTS1.  FILL THE MAIN SPM DIAGONAL STARTING
4950 REM WITH B(2,2) AND RUNNING THROUGH NPOINTS1 WITH THE GUESS
4960 REM OF THE OIL CONCENTRATION.
4970 FOR I = 2 TO NPOINTS1
4980 B(1,I)=UDIAGS
4990 B(2,I)=-DIAGS1-ALPHAS2*CG(I)
5000 NEXT I
5010 REM FILL IN THE LAST B(2,NPOINTS) ELEMENT.
5020 B(2,NPOINTS)=BEXTRA1
5030 REM FILL THE LOWER SPM DIAGONAL STARTING WITH B(3,1) AND RUNNING
5040 REM THROUGH NPOINTS2.
5050 FOR I = 1 TO NPOINTS2
5060 B(3,I)=BDIAGS
5070 NEXT I
5080 B(3,NPOINTS1)=VRSPM-SKZERO
5090 REM FILL Z(I) VECTOR STARTING WITH Z(2) AND RUNNING THROUGHT
5100 REM NPOINTS1, NOTE THAT' Z(1) IS ALWAYS 0.
5110 FOR I = 2 TO NPOINTS1
5120 IM=I-1
5130 IP=I+1
5140 Z(I)=-BDIAGS*S(IM)+(DIAGS2+ALPHAS2*CG(I))*S(I)-UDIAGS*S(IP)
5150 NEXT I
5160 REM AND FILL IN Z(NPOINTS).
5170 Z(NPOINTS)=-FZERO
5180 REM NOW SOLVE THE SYSTEM OF EQUATIONS.
5190 GOSUB 7640
5200 GOSUB 7850
5210 REM IS COUPLING ON"?
5220 ONICPLE GOTO 5210,5400
5230 ICNT=ICNT+1
5240 IF ICNT>ICRATE GOTO 5380
5250 ERROIL=0#
5260 ERRSPM=0#
5270 FOR I = 1 To NPOINTS
5280 ERROIL=ERROIL+ABS(CG(I)-U(I))
5290 ERRSPM=ERRSPM+ABS(SG(I)-V(I))
5300 CG(I)=U(I)
5310 SG(I)=V(I)
5320 NEXT I
5330 ERROIL=ERROIL/APOINTS
5340 ERRSPM=ERRSPM/APOINTS
5350 PRINT:PRINT"OIL ERROR = ";
5360 PRINT USING"##.##^^^^"; ERROIL;
5370 PRINT", SPM ERROR = ";
5380 PRINT USING"##.##^^^^";ERRSPM
```

```
5370 GOTO 4820
5380 REM RESET THE ITERATION COUNTER.
5390 ICNT=0
5400 REM INCREMENT TIME, IPNTED=1 MEANS A PRINT AT THIS TIME
5410 REM HAS NOT OCCURRED.
5420 TYME=TYME+DT
5430 PRINT:PRINT"TIME = ";
5440 PRINT USING"##. ###^^^^";TYME
5450 IPNTED=1
5460 REM RELOAD THE CONCENTRATION VECTORS AND SAVE THE AVERAGE OIL-SPM
5470 REM CONCENTRATION PRODUCT.
5480 FOR I = 1 TO NPOINTS
5490 R(I)=C(I)*S(I)+U(I)*V(I)
5500 C(I)=U(I)
5510 S(I)=V(I)
5520 NEXT I
5530 REM NOW SOLVE FOR THE OIL-SPM AGGLOMERATE CONCENTRATION PROFILE.
5540 REM FILL IN THE OIL-SPM AGGLOMERATE TRIDIAGONAL ELEMENTS INTO THE
5550 REM D(3,NPOINTS) ARRAY.
5560 REM FILL THE uppER OIL-SPM DIAGONAL STARTING WITH D(1,2) AND RUNNING
5570 REM THROUGH NPOINTS3.
5580 FOR I = 2 TO NPOINTS3
5590 D(1,I)=UDIAGB
5600 NEXT I
5610 REM FILL THE MAIN OIL-SPM DIAGONAL STARTING WITH D(2,2) AND RUNNING
5620 REM THROUGH NPOINTS2.
5630 FOR I = 2 TO NPOINTS2
5640 D(2,I)=-DIAGB1
5650 NEXT I
5660 REM FILL THE LOWER OIL-SPM DIAGONAL STARTING WITH D(3,1) AND RUNNING
5670 REM THROUGH NPOINTS3.
5680 FOR I = 1 TO NPOINTS3
5690 D(3,I)=BDIAGB
5700 NEXT I
5710 REM FILL G(1) WITH THE OIL-SPM BOUNDARY CONDITION AT THE TYME+DT STEP.
5720 G(1)=0#
5730 REM FILL G(I) VECTOR STARTING WITH G(2) AND RUNNING THROUGH NPOINTS1.
5740 FOR I = 2 TO NPOINTS1
5750 IM=I-1
5760 IP=I+1
5770 G(I)=-BDIAGB*W(IM)+DIAGB2*W(I)-UDIAGB*W(IP)-ALPHAB2*R(I)
5780 NEXT I
5790 REM NOW SOLVE FOR THE OIL-SPM AGGLOMERATE CONCENTRATION PROFILE.
5800 GOSUB 8080
5810 REM AND STORE THE NEW VECTOR IN W(I).
5820 FOR I = 1 TO NPOINTS
5830 W(I)=Q(I)
5840 NEXT I
5850 REM INTEGRATE THE OIL CONCENTRATION PROFILE.
5860 FUR I = 1 TO NPOINTSA
5870 PNT(I)=C(I+1)
5880 NEXT I
5890 GOSUB S330
5900 OILP=SUM1
5910 REM INTEGRATE THE SPM CONCENTRATION PROFILE.
5920 FOR I = 1 TO NPOINTSA
5930 PNT(I)=S(I+1)
5940 NEXT I
5950 GOSUB 8330
5960 SPMP=SUM1
5970 REM INTEGRATE THE OIL-SPM AGGLOMERATE CONCENTRATION PROFILE.
5980 FOR I = 1 TO NPOINTSA
5990 PNT(I)=W(I+1)
6000 NEXT I
6010 GOSUB 8330
6020 AGLP=SUM1
```

```
6030 ON ICPLE GOTO 6040, 6120
6040 REM INTEGRATE THE OIL+SPM CONCENTRATION PROFILE.
6050 FOR I = 1 TO NPOINTSA
6060 PNT(I)=C(I+1)+S(I+1)
6070 NEXT I
6080 GOSUB 8330
6090 REM AND INTEGRATE WITH RESPECT TO TIME.
6100 CROSSL=SUM1
6110 CROSS=CROSS+CROSSL
6120 REM INTEGRATE THE FLUX OF OIL TO THE BOTTOM AND REACTION LOSS,
6130 REM SPM DEPOSITION AND REACTION LOSS.
6140 OILFLUX=OILFLUX+(C(NPOINTS2)-C(NPOINTS))/2#
6150 OILLOSS=OILLOSS+OILP
6160 SPMCONC=SPMCONC+S(NPOINTS1)
6170 SPMLOSS=SPMLOSS+SPMP
6180 REM INTEGRATE THE OIL-SPM AGGLOMERATE FLUX TO THE BOTTOM.
6190 AGFLUX=AGFLUX+(W(NPOINTS2)-W(NPOINTS))/2#
6200 REM IS IT TIME TO PRINT'?
6210 IF TYME<=PINT9 GOTO 6980
6220 PINT9=.9999#*(PINT+TYME)
6230 REM DO A PRINT.
6240 GOSUB 9300
6250 LPRINT:LPRINT
6260 LPRINT: LPRINT"CONCENTRATION PROFILES AT TIME=";
6270 LPRINT USING"##.###";TYME;
6280 LPRINT" HOURS  ***************************"
6290 GOSUB 7270
6300 LPRINT:LPRINT"MATERIAL BALANCE INFORMATION ";
6310 LPRINT"(FOR 1 CM*CM COLUMN OF WATER):"
6320 REM CALCULATE THE TOTAL MASS OF OIL IN THE WATER COLUMN,
6330 REM WHICH WAS DONE ABOVE.
6340 LPRINT:LPRINT"OIL IN THE WATER COLUMN, GRAMS =";
6350 LPRINT USING"##.###^^^^";OILP
6360 REM CALCULATE THE MASS OF OIL FLUXED TO THE BOTTOM.
6370 BMASSO=(OILFLUX-(C(NPOINTS2)-C(NPOINTS))/4#)*EDTDX
6380 LPRINT"OIL LOST TO THE BOTTOM, GRAMS = ";
6390 LPRINT USING"##.###^^^^"; BMASSO
6400 ON ICPLE GOTO 6410,6440
6410 CROSS2=(CROSS-CROSSL/2#)*EDT
6420 AMASSO=ALPHAO*CROSS2
6430 GOTO 6450
6440 AMASSO=ALPHAO*(OILLOSS-OILP/2#)*EDT
6450 LPRINT"OIL LOST THROUGH REACTION WITH SPM, GRAMS = ";
6460 LPRINT USING"##.###^^^^";AMASSO
6470 TOTALO=AMASSO+BMASSO+OILP
6480 LPRINT:LPRINT"OIL IN WATER + LOST AT BOTTOM + LOST THROUGH Reaction, ";
6490 LPRINT" GRAMS = ";
6500 LPRINT USING"##.###^^^^"; TOTALO
6510 REM CALCULATE THE OIL FLUXED INTO THE WATER AT THE SURFACE.
6520 IF GAMMA=0# GOTO 6550
6530 SURFACE=SZERO*(1#-EXP(-GAMMA*TYME))/GAMMA
6540 GOTO 6560
6550 SURFACE=SZERO*TYME
6560 SURFACE=SURFACE+OILZERO
6570 LPRINT"OIL FLUXED INTO WATER + INITIAL LOADING,";
6580 LPRINT" GRAMS = ";
6590 LPRINT USING"##.###^^^^";SURFACE
6600 LPRINT:LPRINT:LPRINT"SPM (UNATTACHED) IN THE WATER COLUMN, GRAMS = ";
6610 LPRINT USING"##.###^^^^"; SPMP
6620 ON ICPLE GOTO 6630,6650
6630 SPMREAC=ALPHAS*CROSS2
6640 GOTO 6660
6650 SPMREAC=ALPHAS*(SPMLOSS-SPMP/2#)*EDT
6660 LPRINT"SPM LOST THROUGH REACTION WITH OIL, GRAMS = ";
6670 LPRINT USING"##.###^^^^";SPMREAC
6680 TOTALS=SPMREAC+SPMP
```

```
6700 LPRINT:LPRINT"SPM IN WATER + LOST THROUGH REACTION";
6710 LPRINT", GRAMS = ";
6720 LPRINT USING"##.###^^^^";TOTALS
6730 SPMFLUX=FZERO*TYME-SPZERO*(SPMCONC-S(NPOINTS1))/2#)*EDT
6740 LPRINT"SPM FLUXED INTO WATER AT BOTTOM + INITIAL LOADING";
6750 LPRINT", GRAMS = ";
6760 SPMFLUX=SPMFLUX+SPMZERO
6770 LPRINT USING"##.###^^^^";SPMFLUX
6780 REMPRINT THE OIL-SPM AGGLOMERATE INFORMATION.
6790 LPRINT:LPRINT:LPRINT"OIL-SPM AGGLOMERATE IN THE WATER COLUMN, GRAMS = ";
6800 LPRINT USING"##.###^^^^";AGLP
6810 BMASSA=(AGFLUX-(W(NPOINTS2)-W(NPOINTS))/4#)*EDTDX
6820 LPRINT"OIL-SPM AGGLOMERATE FLUXED TO THE BOTTOM, GRAMS = ";
6830 LPRINT USING"##.###^^^^";BMASSA
6840 TOTALA=AGLP+BMASSA
6850 LPRINT:LPRINT"OIL-SPM IN WATER + LOST TO BOTTOM,GRAMS = ";
6860 LPRINT USING"##.###^^^^";TOTALA
6870 AGRATE=ALPHAB*CROSS2
6880 LPRINT"OIL-SPM AGGLOMERATE PRODUCED BY REACTION, GRAMS = ";
6890 LPRINT USING"##.###^^^^";AGRATE
6900 ON ICPLE GOTO 6900,6970
6910 LPRINT:LPRINT:LPRINT"VECTOR CONVERGENCE, OIL =";
6920 LPRINT USING"##.##^^^^";ERROIL;
6930 LPRINT". SPM =";
6940 LPRINT USING"##.##^^^^";ERRSPM;
6950 LPRINT" ON ";
6960 LPRINT USING"##";ICRATE;
6970 LPRINT" ITERATIONS."
6980 IPNTED=2
6990 REM HAS THE SPECIFIED INTEGRATION TIME BEEN ATTAINED"?
7000 IF TYME>=TYME9 GOTO 7030
7010 REM THE INTEGRATION TIME HAS NOT BEEN ATTAINED,
7020 REM TAKE ANOTHER STEP.
7030 GOTO 4620
7040 REM CHECK TO SEE IF A FINAL PRINT IS REQUIRED.
7050 IF IPNTED=2 GOTO 7120
7060 REM DO A FINAL PRINT.
7070 ON IPFINAL GOTO 7070,7120
7080 IPFINAL=2
7090 LPRINT:LPRINT
7100 LPRINT:LPRINT"FINAL PRINT FROM LAST TIME STEP";
7110 LPRINT" (NOT NECESSARILY ON A PRINT INTERVAL) : "
7120 GOTO 6260
7130 LPRINT:LPRINT"END OF RUN WAS ";TIME$
7140 CLS
7150 LPRINT:INPUT"WANT TO DO ANOTHER CALCULATION" ;AGAIN$
7160 TESTC$=LEFT$(AGAIN$,1)
7170 IF TESTC$="Y" GOTO 610
7180 IF TESTC$="y" GOTO 610
7190 LPRINT TOF$
7200 LPRINT TOF$
7210 END
7220 REM PRINT 3-PLACE SCIENTIFIC NOTATION.
7230 PRINT USING"##.##^^^^"; PT
7240 RETURN
7250 REM PRINT 3-PLACE FIXED NOTATION.
7260 PRINT USING"###"; IPT
7270 RETURN
7280 REM THIS IS THE RESULT PRINTING ROUTINE.
7290 REM PRINT THE HEADER.
7300 LPRINT:LPRINT"          DEPTH";
7310 LPRINT TAB(21);
7320 LPRINT"OIL CONC";
7330 LPRINT TAB(36);
7340 LPRINT"SPM CONC";
7350 LPRINT TAB(50);
```

```
      LPRINT"OIL-SPM CONC"
      LPRINT"          SPM";
7370 LPRINT TAB(22);
7380 LPRINT"(GM/CC)";
7390 LPRINT TAB(37);
7400 LPRINT"(GM/CC)";
7410 LPRINT TAB(52);
7420 LPRINT"(GM/CC)"
7430 FOR I = 1 TO NPOINTSA
7440 J=I+1
7450 LPRINT TAB(5);
7460 LPRINT USING"##.###    ";X(I);
7470 LPRINT TAB(20);
7480 LPRINT USING"##.###    ";C(J);
7490 LPRINT TAB(35);
7500 LPRINT USING"##.###    ";S(J);
7510 LPRINT TAB(50);
7520 LPRINT USING"##.###    ";W(J);
7530 IF I. 1 GOTO 7570
7540 LPRINT TAB(63);
7550 LPRINT"(SURFACE)"
7560 GOTO 7620
7570 IF INPOINTSA GOTO 7610
7580 LPRINT TAB(63);
7590 LPRINT"(BOTTOM)"
7600 GOTO 7620
7610 LPRINT
7620 NEXT I
7630 RETURN
7640 REM THIS IS THE SPARSE MATRIX SOLVING ROUTINE FOR THE OIL
7650 REM CONCENTRATION VECTOR.
7660 REM SEE THE DERIVATION NOTES OF 7-14-86.
7670 A(1,2)=A(1,2)-AEXTRA*A(3,1)/A(2,1)
7680 FOR I = 2 TO L
7690 IM1=I-1
7700 ATEMP=A(3,IM1)/A(2,IM1)
7710 A(2,I)=A(2,I)-A(1,IM1)*ATEMP
7720 Y(I)=Y(I)-Y(IM1)*ATEMP
7730 NEXT I
7740 REM NOW PICK UP U(N).
7750 Y(NPOINTS1)=Y(NPOINTS1)-Y(NPOINTS2)*BDIAGC/A(2,NPOINTS2)
7760 U(NPOINTS)=Y(NPOINTS1)/UDIAGC
7770 REM NOW BACKSUBSTITUTE AND STORE THE SOLUTION IN THE U VECTOR.
7780 U(L)=Y(L)/A(2,L)
7790 FOR I = 1 TO LM2
7800 IN=L-I
7810 U(IN)=(Y(IN)-A(1,IN)*U(IN+1))/A(2,IN)
7820 NEXT I
7830 U(1)=(Y(1)-A(1,1)*U(2)-AEXTRA*U(3))/A(2,1)
7840 RETURN
7850 REM THIS IS THE SPARSE MATRIX SOLVING ROUTINE FOR THE SPM
7860REM CONCENTRATION VECTOR.
7870 B(1,2)=B(1,2)-BEXTRA1*B(3,1)/B(2,1)
7880 FOR I = 2 TO NPOINTS1
7890 IM1=I-1
7900 BTEMP=B(3,IM1)/B(2,IM1)
7910 B(2,I)=B(2,I)-B(1,IM1)*BTEMP
7920 Z(I)=Z(I)-Z(IM1)*BTEMP
7930 NEXT I
7940 B(3,NPOINTS1)=B(3,NPOINTS1)-BEXTRA2*B(1,NPOINTS2)/B(2,NPOINTS2)
7950 Z(NPOINTS)=Z(NPOINTS)-BEXTRA2*Z(NPOINTS2)/B(2,NPOINTS2)
7960 B(2,NPOINTS)=B(2,NPOINTS)-B(3,NPOINTS1)*B(1,NPOINTS1)/B(2,NPOINTS1)
7970 Z(NPOINTS)=Z(NPOINTS)-B(3,NPOINTS1)*Z(NPOINTS1)/B(2,NPOINTS1)
7980 V(NPOINTS)=Z(NPOINTS)/B(2,NPOINTS)
7990 FOR I = 1 TO NPOINTS2
8000 IN=NPOINTS-I
```

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8010 V(IN)=(Z(IN)-B(1,IN)*V(IN+1))/B(2,IN)
8020 NEXT I
8030 REM NOW PICK UP THE EXTRA TERM AT THE TOP OF THE MATRIX, NOTE
8040 REM THAT Z(1)=0.
8050 V(1)=(B(1,1)*V(2)+BEXTRA1*V(3))/B(2,1)
8060 V(1)=-V(1)
8070 RETURN
8080 QEM THIS IS THE SPARSE MATRIX SOLVING ROUTINE FOR THE OIL-SPM
8090 REM AGGLOMERATE CONCENTRATION VECTOR.
8100 REM THE COLUMN VECTOR CONTAINING THE 'LAST-TIME-STEP' INFORMATION
8110 REM IS G(I), I.E., THIS IS 'Y'
8120 REM SEE THE DERIVATION NOTES OF 7-1-$-86.
8130 D(1,2)=D(1,2)-DEXTRA*D(3,1)/D(2,1)
8140 FOR I = 2 TO L
8150 IM1=I-1
8160 DTEMP=D(3,IM1)/D(2,IM1)
8170 D(2,I)=D(2,I)-D(1,IM1)*DTEMP
8180 G(I)=G(I)-G(IM1)*DTEMP
8190 NEXT I
8200 REM THE NEW OIL-SPM AGGLOMERATE CONCENTRATION PROFILE IS
8210 REM STORED IN Q(I).
8220 REM NOW PICK UP Q(N).
8230 G(NPOINTS1)=G(NPOINTS1)-G(NPOINTS2)*BDIAGB/D(2,NPOINTS2)
8240 Q(NPOINTS)=G(NPOINTS1)/UDIAGB
8250 REM NOW BACK SUBSTITUTE AND STORE THE SOLUTION IN THE Q VECTOR.
8260 Q(L)=G(L)/D(2,L)
8270 FOR I = 1 TO LM2
8280 IN=L-I
8290 Q(IN)=(G(IN)-D(1,IN)*Q(IN+1))/D(2,IN)
8300 NEXT I
8310 Q(1)=(G(1)-D(1,1)*Q(2)-DEXTRA*Q(3))/D(2,1)
8320 RETURN
8330 REM INTEGRATION OF THE PNT(I) VECTOR BY SIMPSONS RULE.
8340 REM THE PARAMETERS ISMP42 AND HSMP3 MUST BE CALCULATED IN
8350 REM THE MAIN ROUTINE BEFORE THE FIRST CALL.
8360 REM ISMP42 IS THE NUMBER OF (4,2) PAIRS IN THE INTEGRATION SUM
8370 REM AND IS EQUAL TO (NPOINTSA-4)/2, AND HSMP3 IS THE INTERVAL
8380 REM DELTA-X DIVIDED BY 3.
8390 SUM1=PNT(1)
8400 FOR I = 1 TO ISMP42
8410 K=2*I
8420 SUM1=SUM1+4##PNT(K)+2##PNT(K+1)
8430 NEXT I
8440 SUM1=(SUM1+4##PNT(K+2)+PNT(K+3))*HSMP3
8450 RETURN
8460 REM SUBROUTINE TO CALCULATE THE STEADY STATE SPM PROFILE.
8470 REM CALCULATE SOME TERMS USED THROUGHOUT. THERE IS NO REACTION-
8480 REM RATE CONSTANT FOR SPM LOSS IN THE STEADY-STATE SPM PROFILE
8490 REM BECAUSE THERE MUST BE AN OIL CONCENTRATION, AND THERE IS NOT.
8500 REM IF THERE IS A NEED TO PUT A REACTION-LOSS TERM IN,
8510 REM ADD ALPHAS*OILCONC/VDIFF TO SQRARG, AND ADD
8520 REM 2*VDIFF*ALPHAS*OILCONC TO BRACKET (SEE BELOW). BUT, OILCONC
8530 REM MUST BE DEFINED AND IT MUST BE UNIFORM IN THE WATER COLUMN.
8540 VX2K=VRSPM/(2##VDIFF)
8550 SQRARG=VX2K*VX2K
8560 REM IF THE SQUARE-ROOT ARGUMENT IS ZERO, THE STEADY-STATE SPM
8570 REM PROFILE IS FZERO/SKZERO.
8580 IF SQRARG<>0# GOTO 8640
8590 CSPM=FZERO/SKZERO
8600 FOR I = 1 TO NPOINTS
8610 S(I)=CSPM
8620 NEXT I
8630 GOTO 8820
8640 ZETAZ=SQR(SQRARG)
8650 TWOKZ=2##VDIFF*ZETAZ
8660 TWOKKZ=TWOKZ*SKZERO
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8670 BRACKET=VRSPM*SKZERO
8680 REM CALCULATE THE DENOMINATOR ONL% ONCE.
8690 EXPTERM=EXP(ZETAZ*DEPTH1)
8700 SINHL=(EXPTERM-1#/EXPTERM)/2#
8710 COSHL=(EXPTERM+1#/EXPTERM)/2#
8720 DENOM=(TWOKKZ*COSHL+BRACKET*SINHL)/FZERO
8730 FOR I = 1 TO NPOINTS
8740 X=CDBL(I-2)*DX
8750 HARG=ZETAZ*X
8760 EXPTERM=EXP(HARG)
8770 SINHX=(EXPTERM-1#/EXPTERM)/2#
8790 COSHX=(EXPTERM+1#/EXPTERM)/2#
8790 EXPLEAD=EXP(VX2K*(X-DEPTH1))
8800 S(I)=EXPLEAD*(VRSPM*SINHX+TWOKZ*COSHX)/DENOM
8810 NEXT I
8820 RETURN
8830 REM SUBROUTINE TO CALCULATE A STEADY-STATE OIL PROFILE
8840 REM WITH EXPONENTIAL DISERSION(GAMMA)SET TO ZERO,
8850 REM OTHERWISE THERE IS ND STEADY STATE PROFILE, SEE
8860 REM PAGE 25 OF 12-9-87.
8870 REM IT IS RECOMMENDED THAT A STEADY-STATE OIL PROFILE NOT BE USED.
8880 REM USING SUCH A STEADY-STATE OIL PROFILE IS SOMEWHAT ODD, I.E.,
8890 REM THE WATER USUALLY HAS SPM IN IT TO START WITH AND OIL IS
8900 REM THEN SPILLED. IT IS DIFFICULT TO CONCEIVE OF A SITUATION WHERE
8910 REM OIL IS AT STEADY STATE IN THE WATER, BUT THIS SUBROUTINE IS HERE
8920 REM ANYWAY, MAINLY AS A TESTING ROUTINE TO GET THINGS GOING IN
8930 REM MATHEMATICAL SENSE.
8940 REM CHECK TO SEE IF VROIL=0.
8950 IF VROIL<>0# GOTO 9030
8960 IF ALPHAO>0# GOTO 9030
8970 SSOIL=SZERO/VDIFF
8980 FOR I = 1 TO NPOINTS
8990 X=CDBL(I-2)*DX
9000 C(I)=SSOIL*(DEPTH1-X)
9010 NEXT I
9020 GOTO 8820
9030 AOIL=VROIL/(2#*VDIFF)
9040 REM USE THE CORRECT REACTION CONSTANT FOR OIL LOSS, NOTE THAT THERE
9050 REM MUST BE AN SPM CONCENTRATION ASSOCIATED WITH THE OIL-LOSS CONSTANT.
9060 REM SEE PAGES 25A OF 12-"3-87 AND 25B OF 8-8-88 OF THE DERIVATION
9070 REM NOTES FOR COMMENTS ON THIS AND ALSO A SPECIAL CASE WHEN
9080 REM THE REACTION CONSTANT IS LARGE.
9090 ALPHAU=ALPHAO*FZER/SKZER
9100 ZETAO2=AOIL*AOIL+ALPHAU/VDIFF
9110 ZETAO=SQR(ZETAO2)
9120 EXP1=EXP(ZETAO*DEPTH1 1
9130 EXP2=1#/EXP1
9140 SINHO=(EXP1-EXP2)/2#
9150 COSHO=(EXP1+EXP2)/2#
9160 SSOIL=SZERO/(VDIFF*ZETAO*COSHO+SINHO*VROIL/2#)
9170 FOR I = 1 TO NPOINTS
9180 X=CDBL(I-2)*DX
9190 EXPLEAD=EXP(AOIL*X)
9200 EXP1=EXP(ZETAO*(DEPTH1-X))
9210 SINH=(EXP1-1#/EXP1)/2#
9220 CC I) =SSOIL*EXPLEAD*SINH
9230 NEXT I
9240 RETURN
9250 REM Subroutine To PRINT HEADER ON THE SCREEN.
9260 PRINT" INTERACTING OIL DRopLETs AND SPMCALCULATION"
9270 PRINT"CODE NAME IS ";CODEN$;
9280 PRINT", VERSION OF ";VER$
9290 RETURN
9300 REM Subroutine TO PRINT PAGE HEADER.
9310 LPRINT TOF$
9320 LPRINT"FINITE-DIFFERENCE SOLUTION FOR INTERACTING OIL DROPLETS";
```

```
9330 LPRINT" AND SPM."
9340 LPRINT: LPRINT"CODE NAME IS ";CODEN$;
9350 LPRINT", VERSION IS ";VER$
9360 LPRINT"RUN TIME WAS";RTIME$;
9370 LPRINT", AND RUN DATE WAS";RDATE$;
9380 IPAGE=IPAGE+1
9390 LPRINT TAB(65);
9400 LPRINT"PAGE ";
9410 LPRINT USING"###"; IPAGE
9420 RETURN
```