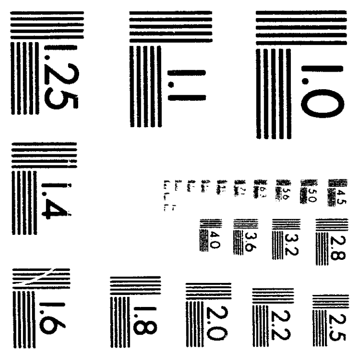
1.0
1.1
1.25
1.4
1.6
1.8
2.0
2.2
2.5
2.8
3.2
3.6
4.0
4.5
5.0

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Software Verification and Validation Plan for the GWSCREEN Code

A. S. Rood

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Idaho National Engineering Laboratory
EG&G Idaho Inc.
PO Box 1625
Idaho Falls Idaho, 83415

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APPROVALS

[signature]

Author

[signature] 06/25/93

Technical Review

Quality Engineering Reviewer

CONTENTS

Software Verification and Validation Plan for the GWSCREEN Code

1. Purpose

1.1 Introduction

The purpose of this Software Verification and Validation Plan (SVVP) is to prescribe steps necessary to verify and validate the GWSCREEN code, version 2.0 (Reference 7) to Quality level B standards. GWSCREEN output is to be verified and validated by comparison with hand calculations, and by output from other Quality Level B computer codes. Verification and validation will also entail performing static and dynamic tests on the code using several analysis tools (Reference 9 and 10). This approach is consistent with guidance in the ANSI/ANS-10.4-1987., "Guidelines for Verification and Validation of Scientific and Engineering Computer Programs for the Nuclear Industry".

The intended audience for this SVVP includes:

1. Quality auditors whose function is to verify compliance with requirements of Reference 1 and Reference 2, section 6.3-4.

2. The cognizant engineer in the EG&G Idaho Subsurface and Environmental Modeling (SEM) Unit (B670) in charge of quality level B analysis.

This plan conforms with the requirements of IEEE std. 1012-1986, and considers the Scientific Computing Unit's Software Quality Engineering reference. Compliance with Reference 3 must be included in this plan. Where a section is not applicable to this plan, the statement *This section /paragraph is not applicable to this plan* appears.

1.2 Scope

This plan provides the single, complete source for all activities involved in the verification and validation of the above listed computer codes and their output data as required for quality level B.

The computer code to which this plan applies (GWSCREEN version 2.0) is in the test phase of the software life-cycle. This plan does not apply to the software life-cycle items 5.1 thru 5.5 since these phases were completed before this plan was written. Procedures will be described in this document to:

1. Perform test phase V & V
2. Perform Installation and Checkout V & V
3. Perform Operation and Maintenance Phase V & V.

Version 1.5 of the code is in-use and procedures will be described to verify and validate the *output* from the code by comparison to similar output from GWSCREEN version 2.0. Thus the life cycle portion to which the plan applies is the operation and maintenance phases for GWSCREEN version 1.5 and the test , installation and checkout, and operation and maintenance phase for version 2.0.

2. References

1. EG&G Idaho Inc., Quality Manual, December, 1989.

2. EG&G Idaho, Inc., Engineering Standard Practice Engineering Analysis," ESP 3.2.1 Rev. B, DRREG-866, May 30, 1991.

3. ANSI/IEEE Std. 1012-1986, IEEE Standard for Software Verification and Validation Plans, Institute of Electrical and Electronic Engineers.

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5. Rood, A. S., GWSCREEN: A Semi-Analytical Model for Assessment of the Groundwater Pathway from Surface or Buried Contamination: Theory and Users Manual. EGG-GEO-10158, March, 1992, Revised, November, 1992.

6. Codell, R. B. et al., A Collection of Mathematical Models for Dispersion in Surface Wate: and Groundwater. U.S. Nuclear Regulatory Commission, NUREG-0868, 1982.

7. Rood, A. S., GWSCREEN: A Semi-Analytical Model for Assessment of the Groundwater Pathway from Surface or Buried Contamination: Version 2: Theory and Users Manual. EGG-GEO-10797, May, 1993.

8. Runchal, A. K., Sagar, B., PORFLO-3: A Mathematical Model for Fluid Flow, Heat and Mass Transport in a Variably Saturated Geologic Media. Westinghouse Hanford Corporation, WHC-WP-0041, July, 1989.

9. Marshal, N. H., E. S. Marwil, Cross Reference Analysis of FORTRAN (CRAFT). EG&G Idaho Inc, EGG-CATT-9198, 1981

10. National Bureau of Standards, FORTRAN-77 Analyzer User's Manual. NBS GCR81-359., 1981.

11. Matthews, S. D., Software Configuration Management Plan for Controlled Code Support System. EGG-CATT-10196, April, 1992.

12. Magnuson, S. O., R.G. Baca, A.J. Sondrup, Independent Verification and Benchmark Testing of the PORFLO-3 Computer Code, Version 1.0 EGG-BG-9175, August, 1990.

3.Definitions

Definitions, acronyms and abbreviations typical to a SVVP and to the life cycle approach to software development in general are provided in detail in Reference 4. In particular, the following terms are used in this document.

Acceptance Testing. Formal testing conducted to determine whether or not a system satisfies its acceptance criteria and to enable the customer to determine whether or not to accept the system.

Operation and Maintenance Phase. The period of time in the software life cycle during which a software product is employed in its operational environment, monitored for satisfactory performance, and modified as necessary to correct problems or to respond to changing environments.

Quality Level B. Software whose failure or defects would degrade the performance or reliability of operations, data acquisition, or deliverable products; or any software whose result is relied upon by the customer.

Software Verification and Validation Plan. A plan for the conduct of software verification and validation.

Software Verification and Validation Report. Documentation of the V & V results and appropriate software quality assurance results.

Validation. The process of evaluating software at the end of the software development process to ensure compliance with software requirements.

Verification. The process of determining whether or not the products of a given phase of the software development cycle fulfill the requirements established during the previous phase.

4. Verification and Validation Overview

4.1 Organization

The participating organizations include the Subsurface and Environmental modeling unit, which provides this plan's author and reviewer. The verification and validation report will be performed and produced by Applied Geosciences unit.

4.2 Master Schedule

The verification and validation of the GWSCREEN code is to be performed in the time frame from March, 1993 to the end of June, 1993. The verification and validation report is to be produced during the month of June 1993 (Table 1).

Item	Begin Date	End Date	Comments
Software Development: 1. Software Requirements 2. Theory of Operation 3. Users Manual	3-91	3-92	Requirements, theory of operation and users manual in Reference 5.
Release of version 1.3	3-91		
Release of version 1.4	10-92		
Release of version 1.5	11-92		Version 1.5 released with revised theory and users manual.
Begin development of version 2.0. Revise software requirements, theory user's manual documentation	1/93	7-93	
Develop Software verification and validation test plan	1/93	6/93	
Perform verification and validation and generate report	4/93	7/93	

4.3 Resource Summary

Resources required to perform the verification and validation tasks shall be assigned on an as needed, case by case basis. As a minimum, these will include an analyst, independent reviewer, independent approver, hardware and software necessary to execute the codes, and a report of the application of the acceptance criteria.

4.4 Responsibilities

A. S. Rood is responsible for producing this document, C. S. Smith of the Applied Geosciences Unit, EG&G Idaho, is responsible for performing the verification and validation tests and producing the verification and validation report (SVVR). S. J. Maheras is responsible for providing independent review and A. S. Rood, code author, custodian, and customer, is responsible for approval and acceptance of this document and the verification validation report.

4.5 Tools, Techniques, and Methodologies

This section/paragraph is not applicable to this plan

5. Life-Cycle Verification and Validation

5.1 Management of V&V

Management of the verification and validation of GWSCREEN requires this plan, the Theory and Users Manual (Reference 5), an independent review of this plan, and independent documentation of the performance of GWSCREEN using the verification/validation exercises described in this document. Independent documentation of the performance of this code will be completed after the completion of this document.

5.2 Concept Phase V & V

This section/paragraph is not applicable to this plan.

5.3 Requirements Phase V & V

This section/paragraph is not applicable to this plan.

5.4 Design Phase V & V

This section/paragraph is not applicable to this plan.

5.5 Implementation Phase V & V

This section/paragraph is not applicable to this plan.

5.6 Test Phase V & V

5.5.1 Verification -- Verification is the process of determining whether or not the products of a given phase of the software development cycle fulfill the requirements established during the previous phase. Computational and modeling requirements for the GWSCREEN code are stated in Section 2 of the GWSCREEN Theory and user's manual (Reference 7). Verification will entail examination of the GWSCREEN code and comparison of GWSCREEN output to the requirements stated in section 2 of the GWSCREEN Theory and User's Manual. The sample problems in the GWSCREEN theory and users manual will serve as the test cases. Additional test cases may be added at the discretion of the person generating the verification and validation report. The attached hand calculation worksheets will assist in this task. Equations implemented in the code and stated in the theory and user's manual will be checked against hand calculations performed on the work sheets, and if necessary, comparison with other numerical routines to insure accurate coding. Output from the following parts of the code should be explicitly checked using the hand calculation worksheets (Appendix A) and reported in the SVVR.

- Source term model Check GWSCREEN output in test problems with hand calculations produced in worksheets for the surface and buried source model (version 1.5 and 2.0) and pond model (version 2.0, only).

- Unsaturated model Check GWSCREEN output in test problems with hand calculations produced in work sheets.

- Saturated zone model Verify the numerical integration routines using a spreadsheet or other numerical integration tools. A benchmark using a code with a similar algorithm may also be used but groundwater concentrations, not radiological dose or other byproducts of the calculation, should be compared (see Reference 6).

- Limiting soil concentration Check GWSCREEN output in test problems with hand calculations produced in work sheets.

The difference between hand calculations and computer output should be no greater that 1%. The 1% value was chosen somewhat arbitrarily but was intended to account for machine dependent differences in computations (personnel computer vs. hand calculator) in addition to a limited number of significant digits reported in the GWSCREEN output. The difference shall be calculated by

$$\% \text{ difference} = \frac{O_c - O_h}{O_h} \times 100$$

where O_c = output from GWSCREEN computer code

O_h = output from hand calculations

The difference between GWSCREEN numerical integration output compared with other numerical integration routines shall be evaluated on a case by case basis. The complexity of the problem, sophistication of the computer algorithm, and applicability of the code to the problem shall be considered when a comparison is made. A difference goal of +/- 5% is desirable. This difference goal was chosen somewhat arbitrarily but was intended to account for differences in the computational methodology.

5.5.2 Validation -- Validation is the process of evaluating software at the end of the software development process to ensure compliance with software requirements. Validation will be performed by a series of benchmark exercises using several other codes. The validation exercise should include the following problems in these benchmarks:

1. Comparison of maximum concentration and time of maximum for the following types of contaminants:

   a) A non-decaying, non sorbing contaminant

b) A decaying, non-sorbing contaminant

d) A decaying, sorbing contaminant with radioactive progeny

Mass flux from the source, unsaturated travel time, and mass flux to the aquifer may be computed on a spread sheet and checked against GWSCREEN output. The codes, PORFLO-3 (Reference 8) and GRDFLX (Reference 6) are to be used to compute groundwater concentrations. PORFLO-3 has been verified and validated (reference 12), is a quality level B code, and has been used extensively in the Department of Energy for performing solute transport calculations.

Differences found between GWSCREEN results and results from other codes should be investigated on a case by case basis. The complexity of the problem, sophistication of the computer algorithm, and applicability of the code to the problem shall be considered when a comparison is made.

2. Coverage analysis of the GWSCREEN test problems will be performed using a coverage analysis tool provided by the EG&G Scientific Computing unit (Reference 10). The coverage analysis tool determines the percentage of code segments that were activated while running a simulation. In addition, a static analysis of the code using the CRAFT software (Reference 9) shall be performed. Results of these two tests will be published in the verification and validation report.

5.7 Installation and Checkout Phase V & V.

Proper installation of the GWSCREEN code will be verified and validated by execution of the 9 test problems presented in Appendix A of Reference 7. Results should be compared with the published results. Some minor differences may be expected between the published results and results generated from other machines other than an IBM 486 SX, which the published results were computed on.

5.8 Operation and Maintenance Phase V & V.

Normal operation of the code shall entail proper installation followed by a running of the 9 test problems presented in Appendix A of Reference 7 and comparison with published results. Any future modification of the code will require appropriate testing depending on the nature of the modification. These modification can be classified as follows

1. A correction in the computations
2. A change in the computational method
3. A change in the structure of the code
4. A cosmetic change in the output.

For item 1 and 2, the nine test problems shall be run with the corrected version of the code and compared with the published results. Differences are to be documented in an Engineering Design File and a new version of the code issued. The theory and users manual (Reference 7) shall be revised to reflect the corrections and re-issued.

For item 3, the complete V & V test plan presented in this document shall be repeated and documented in a new V & V report. The theory and users manual shall be revised to reflect the changes and re-issued.

For item 4, the nine test problems will be re-run and compared with the published results. The results will be documented in an engineering design file and a new version of the code issued.

Output from GWSCREEN version 1.5 (Reference 5) may be compared with output from version 2.0 for test problems that are applicable. Since version 2.0 contains additional computations and features compared to version 1.5, not all test problems can be compared directly. Test problems 2, 3a, 3b, and 4 may be compared directly and the results should not differ significantly, however some differences can be expected since a greater number of integration points are used in version 2.0 in addition to changes in the peak finding routine and the solubility limited release time for a decaying source.

6. Software Verification and Validation Reporting

Verification and validation of the Test Phase will be reported in a verification and validation report generated by personnel from the Applied Geosciences unit. Verification and validation of each new installation of GWSCREEN on another machine where compilation is required, will require an generation of an EDF showing the nine test problems published in Reference 7 and the corresponding I/O for the new installation. Any modifications to the code, such as system dependent time and date routines will also be noted. If installation requires only coping an executable file and test problems to a hard disk on a computer with an MS DOS operating system, then no formal reporting is required.

7. Verification and Validation Administrative Procedures.

Configuration control functions for this plan and each subsequent SVVR will be controlled as set out in Reference 11 by the current GWSCREEN code custodian. Procedures are those described in Section 5.6, 5.7 and 5.8. No other information is applicable to this section.

APPENDIX A

GWSCREEN HAND CALCULATION WORKSHEETS

GWSCREEN VERSION 2.0 HAND CALCULATION WORKSHEETS

CODE VARIABLE: C(I) **TEXT VARIABLE:** C **EQUATION IN TEXT:** 32

DESCRIPTION: CONCENTRATION FOR iTH PROGENY. WHERE QDX = THE DECAY INGROWTH FACTORS

SUBROUTINE CALCULATED IN: MAXRAD, RAD and CTIME

SUBROUTINE(S) USED IN:

EQUATION (CODE VARIABLES):

$$\underset{C(I)}{\boxed{c}}\ \frac{CI}{m^{**}3} = \underset{C(1)}{\boxed{c}}\ \frac{CI}{m^{**}3} \cdot \frac{\underset{ARD(1)}{\boxed{c}}}{\underset{ARD(I)}{\boxed{c}}} \cdot \frac{\underset{QDX(I)}{\boxed{c}}\ CI}{\underset{QDX(1)}{\boxed{c}}\ CI}$$

QDX = the decay ingrowth factor (DIF in text).

Parameter Source Legend:

i = GWSCREEN Input Value
c = Calculated Value

CODE VARIABLE: RELSRC **TEXT VARIABLE:** NONE **EQUATION IN TEXT:** NONE

DESCRIPTION: CUMULATIVE SOURCE FLUX FOR SURFICIAL OR BURIED SOURCES (IMODEL=1) IF TSL=0

SUBROUTINE CALCULATED IN: FLUXES

SUBROUTINE(S) USED IN: FLUXES

EQUATION (CODE VARIABLES):

$$\underset{\text{RELSRC}}{\boxed{c}}\ \text{M} = \underset{\text{QI}}{\boxed{i}}\ \text{M} \cdot \frac{\underset{\text{SLEACH}}{\boxed{c}}\ \frac{1}{\text{Y}}}{\underset{\text{SLEACH}}{\boxed{c}}\ \frac{1}{\text{Y}} + \underset{\text{DLR}}{\boxed{c}}\ \frac{1}{\text{Y}}}$$

$$\left[1 - \text{EXP}\left| - \left[\left[\underset{\text{SLEACH}}{\boxed{c}}\ \frac{1}{\text{Y}} + \underset{\text{DLR}}{\boxed{c}}\ \frac{1}{\text{Y}} \right] \cdot \underset{\text{TIME}}{\boxed{i}}\ \text{Y} \right] \right]$$

M = mg or Ci

Parameter Source Legend:

i = GWSCREEN Input Value
c = Calculated Value

CODE VARIABLE: RELSRC **TEXT VARIABLE:** NONE **EQUATION IN TEXT:** NONE

DESCRIPTION: CUMULATIVE SOURCE FLUX FOR SURFACE OR BURIED SURFACES (IMODEL=1) AND TSL>0 AND T<TSL

SUBROUTINE CALCULATED IN: FLUXES

SUBROUTINE(S) USED IN: FLUXES

EQUATION (CODE VARIABLES):

$$\underset{\text{RELSRC}}{[\;c\;]}\ \text{mg} = \underset{\text{WFLUX}}{[\;c\;]}\ \frac{L}{Y} \bullet \underset{\text{SL}}{[\;i\;]}\ \frac{mg}{L} \bullet \underset{\text{TIME}}{[\;i\;]}\ Y$$

Parameter Source Legend:

i = GWSCREEN Input Value
c = Calculated Value

CODE VARIABLE: RELSRC **TEXT VARIABLE:** NONE **EQUATION IN TEXT:** NONE

DESCRIPTION: CUMULATIVE SOURCE FLUX FOR SURFICIAL OR BURIED SOURCES (IMODEL=1) IF TSL>0 AND T>TSL

SUBROUTINE CALCULATED IN: FLUXES

SUBROUTINE(S) USED IN: FLUXES

EQUATION (CODE VARIABLES):

$$\underset{\text{RELSRC}}{\boxed{c}}\ \text{mg} = \underset{\text{WFLUX}}{\boxed{c}}\ \frac{\text{L}}{\text{Y}} \cdot \underset{\text{SL}}{\boxed{i}}\ \frac{\text{mg}}{\text{L}} \cdot \underset{\text{TSL}}{\boxed{c}}\ \text{Y} + \underset{\text{QSL}}{\boxed{c}}\ \text{mg} \cdot \frac{\underset{\text{SLEACH}}{\boxed{c}}\ \frac{1}{\text{Y}}}{\underset{\text{SLEACH}}{\boxed{c}}\ \frac{1}{\text{Y}} + \underset{\text{DLR}}{\boxed{c}}\ \frac{1}{\text{Y}}} \cdot$$

$$\left[1 - \text{EXP}\left[- \left[\underset{\text{SLEACH}}{\boxed{c}}\ \frac{1}{\text{Y}} + \underset{\text{DLR}}{\boxed{c}}\ \frac{1}{\text{Y}} \right] \cdot \left[\underset{\text{TIME}}{\boxed{c}}\ \text{Y} - \underset{\text{TSL}}{\boxed{c}}\ \text{Y} \right] \right] \right]$$

Parameter Source Legend:

i = GWSCREEN Input Value
c = Calculated Value

CODE VARIABLE: QSL **TEXT VARIABLE:** Q_{SL} **EQUATION IN TEXT:** 13

DESCRIPTION: Solubility limited source mass. The mass such that the equilibrium concentration does not exceed the solubility limit of the contaminant.

SUBROUTINE CALCULATED IN: SOURCEX

SUBROUTINE(S) USED IN: FLUXES, SRCTERM

EQUATION (CODE VARIABLES):

$$\underset{QSL}{\boxed{}}\ mg = \underset{SL}{\boxed{}}\ \frac{mg}{L} \cdot \underset{AL}{\boxed{}}\ m \cdot \underset{WA}{\boxed{}}\ m \cdot \underset{THICKS}{\boxed{}}\ m \cdot \underset{THETAS}{\boxed{}} \cdot$$

$$\left[1 + \underset{ZKDS}{\boxed{i}}\ \frac{mL}{G} \cdot \underset{RHOS}{\boxed{i}}\ \frac{g}{mL} + \underset{THETAS}{\boxed{i}} \right] \cdot 1000\ L/m^{**}3$$

Parameter Source Legend:

i = GWSCREEN Input Value
c = Calculated Value

CODE VARIABLE: FRAC and FRACD **TEXT VARIABLE:** f **EQUATION IN TEXT:** 23

DESCRIPTION: Fraction of source that decays during unsaturated transit.

SUBROUTINE CALCULATED IN: SOURCEX

SUBROUTINE(S) USED IN: SRCTERM

EQUATION (CODE VARIABLES):

$$\underset{FRAC}{\boxed{c}} = EXP\left[-\underset{ADLR(1)}{\boxed{c}}^{\frac{1}{Y}} \cdot \underset{TRANSIT}{\boxed{c}}^{Y}\right]$$

$$\underset{FRACD}{\boxed{c}} = 1 - \underset{FRAC}{\boxed{c}}$$

Parameter Source Legend:

i = GWSCREEN Input Value
c = Calculated Value

CODE VARIABLE: TRANSIT **TEXT VARIABLE:** T **EQUATION IN TEXT:** 20

DESCRIPTION: Transit time in unsaturated zone.

SUBROUTINE CALCULATED IN: SOURCEX

SUBROUTINE(S) USED IN: FLUXES

EQUATION (CODE VARIABLES):

$$\underset{\text{TRANSIT}}{[\,c\,]}\ \text{Y} = \frac{\underset{\text{DEPTH}}{[\,i\,]}\ \text{M}}{\underset{\text{UX}}{[\,c\,]}\ \frac{\text{M}}{\text{Y}}} \cdot \underset{\text{RDU}}{[\,c\,]}$$

Parameter Source Legend:

i = GWSCREEN Input Value
c = Calculated Value

CODE VARIABLE: QM **TEXT VARIABLE:** QMASS **EQUATION IN TEXT:** 15

DESCRIPTION: Initial mass in source volume. Calculated only if IMODE≤3 (radiological source term).

If IMODE ≥ than 3 (non-radiological contaminant) then QM=QI.

SUBROUTINE CALCULATED IN: GWS6

SUBROUTINE(S) USED IN: SOURCEX

EQUATION (CODE VARIABLES):

$$\underbrace{[\ c\ ]}_{QM}\ mg = \frac{\underbrace{[\ i\ ]}_{QI}\ Ci \bullet 3.7E10\ \frac{ATOMS}{sec\ Ci} \bullet 3.1536E7\ \frac{s}{Y} \bullet \underbrace{[\ \ ]}_{MW}\ \frac{mg}{MOLE}}{\underbrace{[\ c\ ]}_{DLR} \bullet 6.023E23\ ATOMS/MOLE}$$

Parameter Source Legend:

i = GWSCREEN Input Value
c = Calculated Value

CODE VARIABLE: RDU **TEXT VARIABLE:** Rd_u **EQUATION IN TEXT:** 22

DESCRIPTION: Retardation in the unsaturated zone.

SUBROUTINE CALCULATED IN: SOURCEX

SUBROUTINE(S) USED IN: SOURCEX

EQUATION (CODE VARIABLES):

$$\underset{RDU}{\boxed{c}} = 1 + \frac{\underset{ZKDU}{\boxed{i}}\ \frac{mL}{g} \bullet \underset{RHOU}{\boxed{i}}\ \frac{g}{mL}}{\underset{THETAU}{\boxed{i}}}$$

Parameter Source Legend:

i = GWSCREEN Input Value
c = Calculated Value

GWSCREEN VERSION 2.0 HAND CALCULATION WORKSHEETS

CODE VARIABLE: ARD(J) and RD **TEXT VARIABLE:** Rd **EQUATION IN TEXT:** 26

DESCRIPTION: Retardation factor in the aquifer. Array of NPROG+1 elements. RD = the parent retardation factor, AKD(1) = ZKDA, RD = ARD(1)

SUBROUTINE CALCULATED IN: SOURCEX

SUBROUTINE(S) USED IN: TIME, RAD, MAXRAD, AREA, LIMITS

EQUATION (CODE VARIABLES):

$$\underset{c}{\mathrm{ARD(J)}} = 1 + \frac{\underset{i}{\mathrm{AKD(J)}}\ \left[\frac{mL}{g}\right] \cdot \underset{i}{\mathrm{RHOA}}\ \left[\frac{g}{mL}\right]}{\underset{i}{\mathrm{PHI}}}$$

Parameter Source Legend:

i = GWSCREEN Input Value
c = Calculated Value

GWSCREEN VERSION 2.0 HAND CALCULATION WORKSHEETS

CODE VARIABLE: ADLR(J) and DLR **TEXT VARIABLE:** λ_D **EQUATION IN TEXT:** 4

DESCRIPTION: Decay rate constant. Array of NPROG+1 elements where DLR=ADLR(1)

SUBROUTINE CALCULATED IN: SOURCEX

SUBROUTINE(S) USED IN: RDK, AREA, LIMITS

EQUATION (CODE VARIABLES):

$$\underset{\text{ADLR(J)}}{\boxed{c}}\ \frac{1}{Y} = \frac{0.693}{\underset{\text{ATHALF(J)}}{\boxed{i}}\ Y}$$

Parameter Source Legend:

i = GWSCREEN Input Value
c = Calculated Value

GWSCREEN VERSION 2.0 HAND CALCULATION WORKSHEETS

CODE VARIABLE: UX **TEXT VARIABLE:** U_u **EQUATION IN TEXT:** 21

DESCRIPTION: Unsaturated pore velocity for pond model (IMODEL=2) and surface model (IMODEL=1).

SUBROUTINE CALCULATED IN: SOURCEX

SUBROUTINE(S) USED IN: CTIME, SOURCEX

EQUATION (CODE VARIABLES):

FOR IMODEL=1

$$\underset{\text{UX}}{[\ c\ ]}\ \frac{m}{Y} = \frac{\underset{\text{PERC}}{[\ i\ ]}}{\underset{\text{THETAU}}{[\ i\ ]}}$$

FOR IMODEL=2

$$\underset{\text{UX}}{[\ c\ ]}\ \frac{m}{Y} = \frac{\underset{\text{PNDFLX}}{[\ i\ ]}\ \frac{m**3}{Y} + \left[\underset{\text{AL}}{[\ i\ ]}\ m \cdot \underset{\text{WA}}{[\ i\ ]}\ m\right]}{\underset{\text{THETAU}}{[\ i\ ]}}$$

Parameter Source Legend:

i = GWSCREEN Input Value
c = Calculated Value

CODE VARIABLE: SLEACH **TEXT VARIABLE:** λ_l **EQUATION IN TEXT:** 4

DESCRIPTION: Leach rate constant for waste at surface or buried or after discharge to a pond ends. Not used if IMODEL=3

SUBROUTINE CALCULATED IN: SOURCEX

SUBROUTINE(S) USED IN: SRCTERM, FLUXES

EQUATION (CODE VARIABLES):

$$\underset{\text{SLEACH}}{\boxed{c}}\ \frac{1}{Y} = \frac{\underset{\text{PERC}}{\boxed{i}}\ \frac{m}{Y}}{\underset{\text{THETAS}}{\boxed{i}} \bullet \underset{\text{THICKS}}{\boxed{i}}\ m \bullet \left[1 + \underset{\text{ZKDS}}{\boxed{i}}\ \frac{mL}{g} \bullet \underset{\text{RHOS}}{\boxed{i}}\ \frac{g}{mL} + \underset{\text{THETAS}}{\boxed{i}} \right]}$$

Parameter Source Legend:

i = GWSCREEN Input Value
c = Calculated Value

GWSCREEN VERSION 2.0 HAND CALCULATION WORKSHEETS

CODE VARIABLE: PLEACH **TEXT VARIABLE:** λ_l **EQUATION IN TEXT:** 17

DESCRIPTION: Leach rate constant for pond sediments during the operational period of the pond.

SUBROUTINE CALCULATED IN: SOURCEX

SUBROUTINE(S) USED IN: SRCPOND, FLUXES

EQUATION (CODE VARIABLES):

$$\underset{\text{PLEACH}}{\boxed{c}}\ \frac{1}{Y} = \frac{\underset{\text{PNDFLX}}{\boxed{i}}\ \frac{m^{**}3}{Y} \div \left[\underset{\text{AL}}{\boxed{i}}\ m \bullet \underset{\text{WA}}{\boxed{i}}\ m \right]}{\underset{\text{THETAP}}{\boxed{i}}\ m \bullet \underset{\text{THICKS}}{\boxed{i}}\ m \bullet \left[1 + \underset{\text{ZKDS}}{\boxed{i}}\ \frac{mL}{g} \bullet \underset{\text{RHOS}}{\boxed{i}}\ \frac{g}{mL} + \underset{\text{THETAP}}{\boxed{i}} \right]}$$

Parameter Source Legend:

i = GWSCREEN Input Value
c = Calculated Value

GWSCREEN VERSION 2.0 HAND CALCULATION WORKSHEETS

CODE VARIABLE: CL **TEXT VARIABLE:** C_l **EQUATION IN TEXT:** 36

DESCRIPTION: Limiting groundwater concentration for contaminants regulated by radiological dose.

SUBROUTINE CALCULATED IN: RAD

SUBROUTINE(S) USED IN: RAD

EQUATION (CODE VARIABLES):

$$\underset{CL}{\boxed{c}}\ \frac{Ci}{L} = \frac{\underset{DLIM}{\boxed{i}}\ \frac{rem}{Y}}{\underset{CDCF}{\boxed{i}}\ \frac{rem}{Ci} \cdot \underset{WI}{\boxed{i}}\ \frac{L}{d} \cdot \underset{EF}{\boxed{i}}\ \frac{d}{Y}}$$

Parameter Source Legend:

i = GWSCREEN Input Value
c = Calculated Value

CODE VARIABLE: CL **TEXT VARIABLE:** C_l **EQUATION IN TEXT:** 37

DESCRIPTION: Limiting groundwater concentration for contaminants regulated by carcinogenic risk

SUBROUTINE CALCULATED IN: CARCIN

SUBROUTINE(S) USED IN: CARCIN

EQUATION (CODE VARIABLES):

$$\underset{\text{CL}}{\boxed{c}}\ \frac{mg}{L} = \frac{\underset{\text{CRISK}}{\boxed{i}} \cdot \underset{\text{BW}}{\boxed{i}}\ kg \cdot \underset{\text{AT}}{\boxed{i}}\ d}{\underset{\text{SFACTOR}}{\boxed{i}}\ \frac{kg\text{-}d}{mg} \cdot \underset{\text{WI}}{\boxed{i}}\ \frac{L}{d} \cdot \underset{\text{ED}}{\boxed{i}}\ y \cdot \underset{\text{EF}}{\boxed{i}}\ \frac{d}{y}}$$

Parameter Source Legend:

i = GWSCREEN Input Value
c = Calculated Value

CODE VARIABLE: TSL, R, and WFLUX **TEXT VARIABLE:** t_{sl} **EQUATION IN TEXT:** 14

DESCRIPTION: The solubility limited release time (TSL) when DLR + RC2 > 1 x 10^{-10}; Mass flux from the source volume while under solubility limited release control (R); Water flux from the source (WFLUX) Calculated only if QSL<QM, else TSL=0.

SUBROUTINE CALCULATED IN: SOURCEX

SUBROUTINE(S) USED IN: SRCTERM, FLUXES

EQUATION (CODE VARIABLES):

$$\underset{TSL}{[c]} = \frac{-LN\left[\underset{X1}{[c]}\ mg + \underset{X2}{[c]}\ mg\right]}{\underset{DLR}{[c]}\ \frac{1}{y} + \underset{RC2}{[i]}\ \frac{1}{y}}$$

$$\underset{X1}{[c]}\ mg = \underset{QSL}{[c]}\ mg + \underset{R}{[c]}\ \frac{mg}{y} \div \left[\underset{DLR}{[c]}\ \frac{1}{y} + \underset{RC2}{[i]}\ \frac{1}{y}\right]$$

$$\underset{X2}{[c]}\ mg = \underset{QM}{[c]}\ mg + \underset{R}{[c]}\ \frac{mg}{y} \div \left[\underset{DLR}{[c]}\ \frac{1}{y} + \underset{RC2}{[i]}\ \frac{1}{y}\right]$$

$$\underset{R}{[c]}\ \frac{mg}{y} = \underset{WFLUX}{[c]}\ \frac{L}{y} \bullet \underset{SL}{[i]}\ \frac{mg}{L}$$

$$\underset{WFLUX}{[c]}\ \frac{L}{Y} = \underset{PERC}{[i]}\ \frac{m}{Y} \bullet \underset{AL}{[i]}\ m \bullet \underset{WA}{[i]}\ m \bullet 1000\ L/m^{**}3$$

CODE VARIABLE: CL **TEXT VARIABLE:** C_L **EQUATION IN TEXT:** A-1

DESCRIPTION: Maximum allowable parent concentration adjusted for progeny ingrowth. ARADMAX(1)=MAXIMUM ALLOWABLE PARENT NUCLIDE CONCENTRATION; QDX(J)=THE DECAY INGROWTH FACTOR FOR THE JTH PROGENY

SUBROUTINE CALCULATED IN: MAXRAD

SUBROUTINE(S) USED IN: MAXRAD

EQUATION (CODE VARIABLES):

for j=1 to NN number of members in the radioactive decay chain

$$\underset{\text{CL}}{\boxed{c}\ \frac{Ci}{L}} = \frac{\underset{\text{DAIC(1)}}{\boxed{c}\ \frac{Ci}{L}}}{\dfrac{\underset{\text{DAIC(1)}}{\boxed{c}\ \frac{Ci}{L}}}{\underset{\text{ARADMAX(1)}}{\boxed{c}\ \frac{Ci}{L}}} + \dfrac{\underset{\text{DAIC(2)}}{\boxed{c}\ \frac{Ci}{L}}}{\underset{\text{ARADMAX(2)}}{\boxed{c}\ \frac{Ci}{L}}} + \dfrac{\underset{\text{DAIC(3)}}{\boxed{c}\ \frac{Ci}{L}}}{\underset{\text{ARADMAX(3)}}{\boxed{c}\ \frac{Ci}{L}}} \cdots \dfrac{\underset{\text{DAIC(J)}}{\boxed{c}\ \frac{Ci}{L}}}{\underset{\text{ARADMAX(J)}}{\boxed{c}\ \frac{Ci}{L}}}}$$

Where DAIC(J) = Average integrated concentration of the Jth member of the decay chain

Parameter Source Legend:

i = GWSCREEN Input Value
c = Calculated Value

GWSCREEN VERSION 2.0 HAND CALCULATION WORKSHEETS

CODE VARIABLE: CL **TEXT VARIABLE:** C_L **EQUATION IN TEXT:** 41

DESCRIPTION: Limiting groundwater concentration for non-radiological, non-carcinogenic contaminants based on the Hazard Quotient

SUBROUTINE CALCULATED IN: NCARCIN

SUBROUTINE(S) USED IN: NCARCIN

EQUATION (CODE VARIABLES):

$$\underset{CL}{\square}\ \frac{mg}{L} = \frac{\underset{HQ}{\square} \cdot \underset{BW}{\square}\ kg \cdot \underset{AT}{\square}\ d \cdot \square\ \frac{mg\ d}{kg}}{\underset{WI}{\square}\ \frac{L}{d} \cdot \underset{EF}{\square}\ \frac{d}{y} \cdot \underset{ED}{\square}\ y}$$

Parameter Source Legend:

i = GWSCREEN Input Value
c = Calculated Value

CODE VARIABLE: TSL **TEXT VARIABLE:** t_{sl} **EQUATION IN TEXT:** 14

DESCRIPTION: Solubility release time when DRL + RC2 < 1 x 10^{-10}

SUBROUTINE CALCULATED IN: SOURCEX

SUBROUTINE(S) USED IN: SRCTERM AND FLUXES

EQUATION (CODE VARIABLES):

$$\underset{TSL}{\boxed{c}}\ y = \frac{\underset{QM}{\boxed{c}}\ mg - \underset{QSL}{\boxed{c}}\ mg}{\underset{R}{\boxed{c}}\ \frac{mg}{y}}$$

Parameter Source Legend:

i = GWSCREEN Input Value
c = Calculated Value

GWSCREEN VERSION 2.0 HAND CALCULATION WORKSHEETS

CODE VARIABLE: FAQU, QMASS **TEXT VARIABLE:** q_a **EQUATION IN TEXT:** 19, 24

DESCRIPTION: Mass flux to the aquifer from the pond model (IMODEL=2) and T < TOPPER and QI=0.0

SUBROUTINE CALCULATED IN: SRCPOND, FLUXES

SUBROUTINE(S) USED IN: QGAUS2, TRAPZD

EQUATION (CODE VARIABLES):

$$\underset{\text{FAQU}}{\boxed{c}}\ \frac{M}{y} = \underset{\text{QMASS}}{\boxed{c}}\ M \bullet \underset{\text{PLEACH}}{\boxed{c}}\ \frac{1}{y} \bullet \underset{\text{FRAC}}{\boxed{c}}$$

$$\underset{\text{QMASS}}{\boxed{c}}\ M = \frac{\underset{\text{RMI}}{\boxed{i}}\ \frac{M}{y} \bullet \left[1 - EXP\left[- \left[\left[\underset{\text{EVAP}}{\boxed{i}}\ \frac{1}{y} + \underset{\text{DLR}}{\boxed{c}}\ \frac{1}{y} + \underset{\text{PLEACH}}{\boxed{c}}\ \frac{1}{y} \right] \underset{\text{T*}}{\boxed{c}}\ y \right] \right] \right]}{\underset{\text{EVAP}}{\boxed{i}}\ \frac{1}{y} + \underset{\text{DLR}}{\boxed{c}}\ \frac{1}{y} + \underset{\text{PLEACH}}{\boxed{c}}\ \frac{1}{y}}$$

$$\underset{\text{T*}}{\boxed{c}}\ y = \underset{\text{TIME}}{\boxed{c}}\ y - \underset{\text{TRANSIT}}{\boxed{c}}\ y$$

Parameter Source Legend:

M = contaminant mass or activity (mg or Ci)
i = GWSCREEN Input Value
c = Calculated Value

GWSCREEN VERSION 2.0 HAND CALCULATION WORKSHEETS

CODE VARIABLE: CS TEXT VARIABLE: C_s EQUATION IN TEXT: 34

DESCRIPTION: Limiting Soil Concentration

SUBROUTINE CALCULATED IN: RAD, CRAD, MAXRAD, MAXNRAD, CARCIN, NCARCIN

SUBROUTINE(S) USED IN: GWS6

EQUATION (CODE VARIABLES):

$$\underset{CS}{[\ ]_c}\ \frac{M}{m^{**}3} = \frac{\underset{CL}{[\ ]_c}\ \frac{M}{m^{**}3}}{\underset{CU}{[\ ]_c}\ \frac{M}{m^{**}3}} \times \frac{1.0\ M}{\underset{AL}{[\ ]}\ m \times \underset{WA}{[\ ]}\ m \times \underset{THICK}{[\ ]}\ m}$$

$$\underset{CU}{[\ ]}\ \frac{M}{m^{**}3} = \frac{\underset{C}{[\ ]}\ \frac{M}{m^{**}3}}{\underset{QI}{[\ ]}\ M} \times 1.0\ M$$

Parameter Source Legend:

i = GWSCREEN Input Value
c = Calculated Value
M = mg or Ci

GWSCREEN VERSION 2.0 HAND CALCULATION WORKSHEETS

CODE VARIABLE: CE **TEXT VARIABLE:** C_E **EQUATION IN TEXT:** 35

DESCRIPTION: Limiting Pond Effluent Concentration

SUBROUTINE CALCULATED IN: RAD, CRAD, MAXRAD, MAXNRAD, CARCIN, NCARCIN

SUBROUTINE(S) USED IN: GWS6

EQUATION (CODE VARIABLES):

$$\underset{CE}{\boxed{c}\ \frac{M}{m^{**}3}} = \frac{\underset{CL}{\boxed{c}\ \frac{M}{m^{**}3}} \times \underset{RMI}{\boxed{i}\ \frac{M}{y}}}{\underset{C}{\boxed{c}\ \frac{M}{m^{**}3}} \times \underset{PNDFLX}{\boxed{i}\ \frac{m^{**}3}{y}}}$$

Parameter Source Legend:

i = GWSCREEN Input Value
c = Calculated Value
M = mg or Ci

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END