Section 3

Handling Complex and Large Systems Models

Robustness and Efficiency

- Model must be run with wide ranging data in many combinations
- Model must be executed thousands of times
- model musr be focussed to calculate the desired results and must include the essential features in an efficient way
- judgement is subjective and this is where some of the real skill of modelling lies

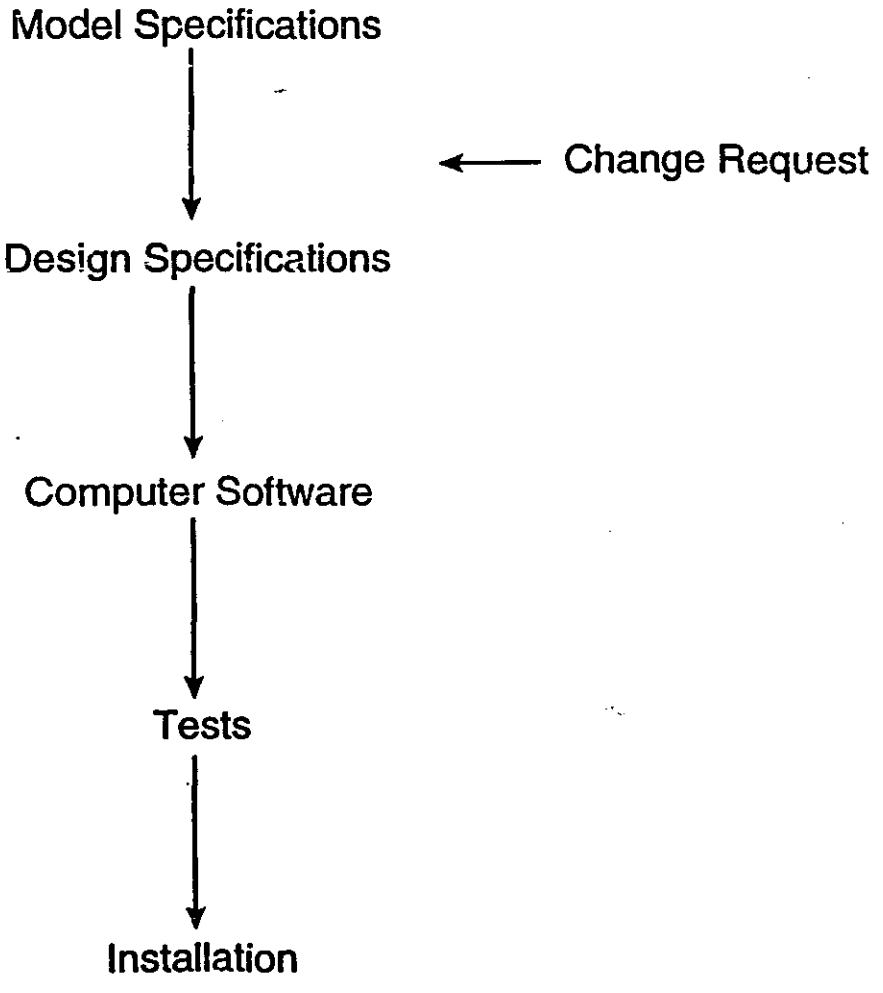
OVERVIEW

Validation - **models and data represent underlying phenomena**

Verification - **computer code accurately represents models and data**

Configuration Control - **audit trail demonstrates code development process**

SOFTWARE DEVELOPMENT CYCLE



Purpose of Configuration Control

- provide an audit trail of all code and data changes
- protect against unauthorized damages

CONFIGURATION CONTROL (1 of 2)

A PROCEDURE FOR STEPWISE MODIFICATION TO A CODE PACKAGE IN A SERIES OF FROZEN VERSIONS

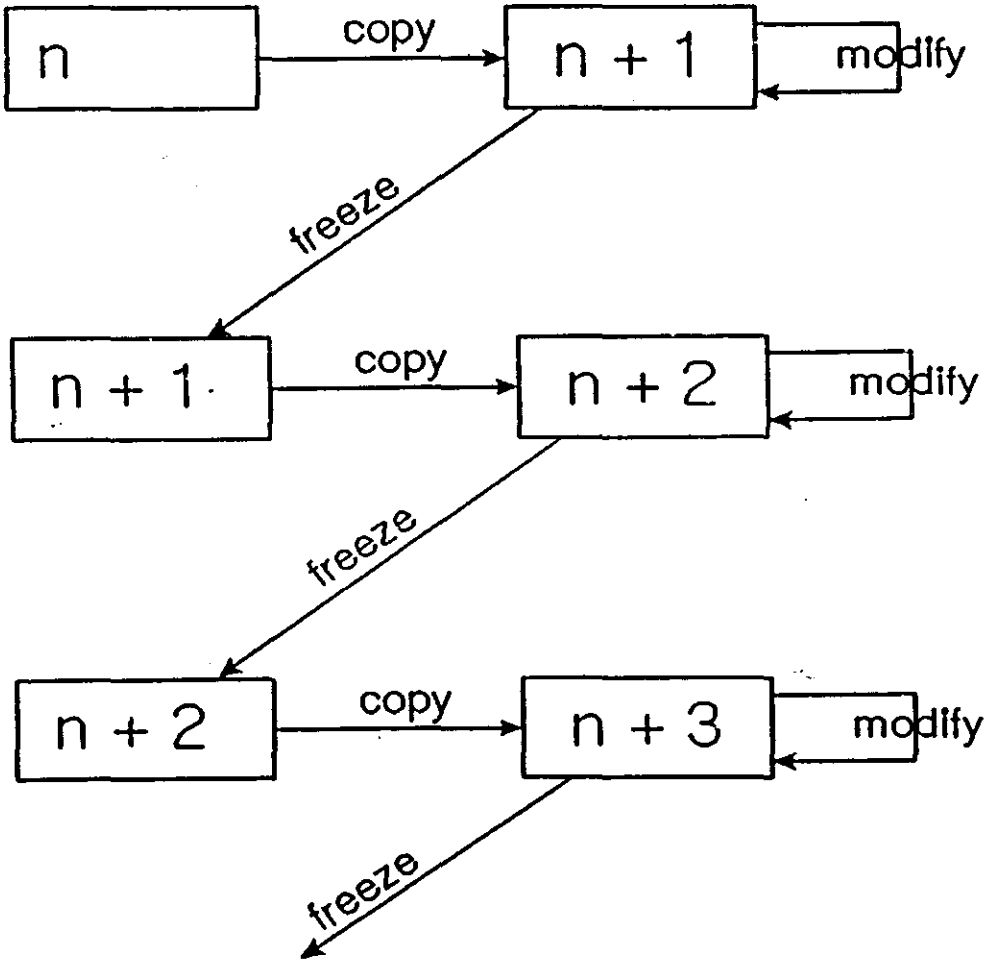
APPLY PROCEDURES FOR FREEZING AND PROCEDURES FOR MODIFYING

ALL APPLICATIONS OR USE OF THE PACKAGE MAKE REFERENCE TO A FROZEN REFERENCE VERSION

CONFIGURATION CONTROL (2 of 2)

FROZEN VERSION

DEVELOPMENT VERSION



CODE PACKAGE CONTENTS

** CODE

** CHANGE SUMMARY

* ARCHIVED CODE FROM CURRENT MODIFICATIONS

* DICTIONARY

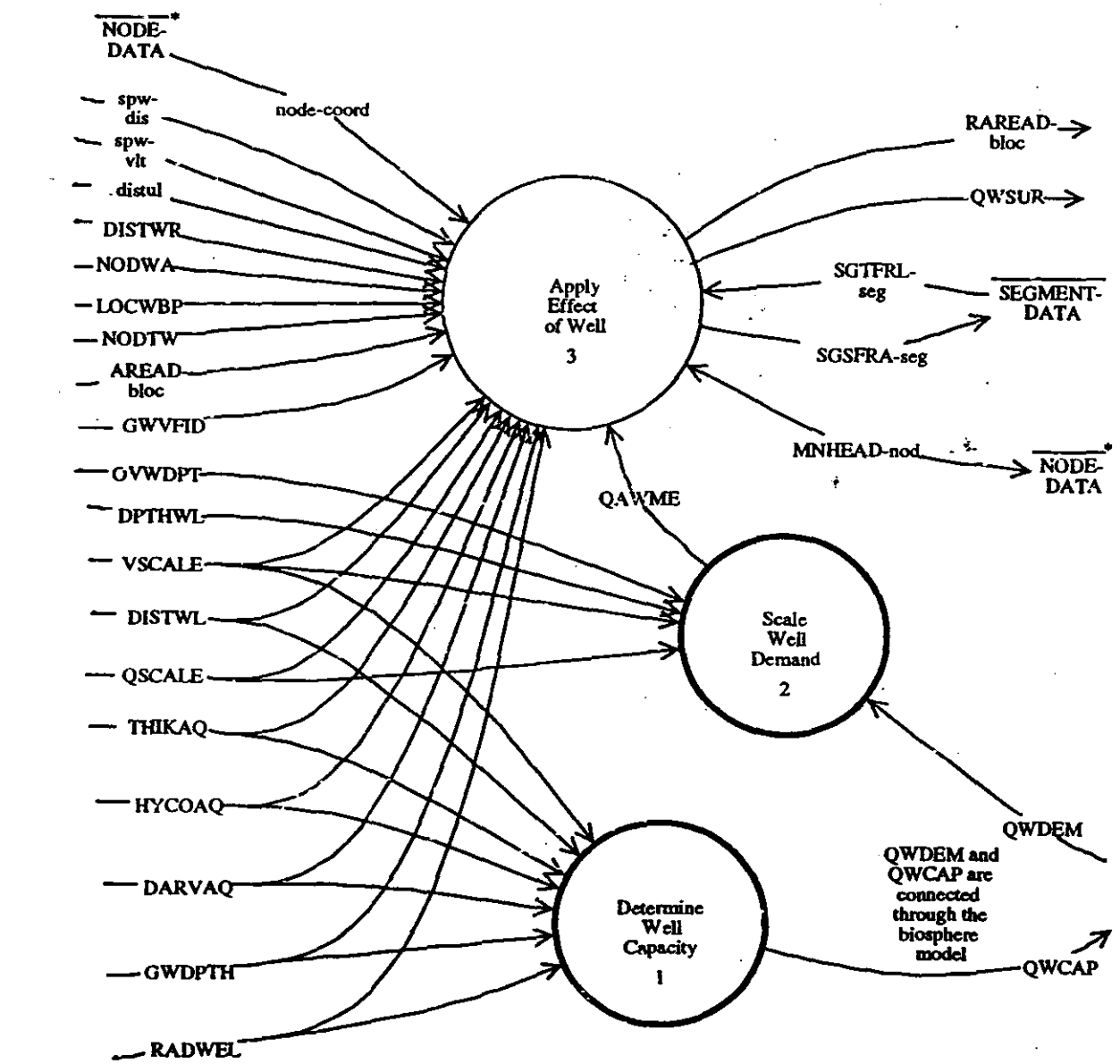
OTHER
- SPECIFICATIONS AND REFERENCES
- DESIGN DOCUMENTS
- STRUCTURE CHARTS
- CROSS REFERENCE DICTIONARIES
- LINKING TEMPLATES
- ETC.

MODEL SPECIFICATIONS

- contribute to validation
- typical elements are:
  - data flow diagram
  - data dependency diagrams
  - data dictionary

DATA FLOW DIAGRAM

Diagram-2.3.1.3
Do-Well-Model-Calculations
94-Oct-04
Version-02A
T-Melnyk



Do Well Model Calculations : Diagram 2.3.1.3

QAWME well demand used in equations Q'_{dem} [m^3/a] Annual volume of water demanded of and supplied by well from the well aquifer, as used in the analytical well model equations. This quantity is obtained from QWDEM after scaling by both QSCALE and VSCALE, but is zero for overburden wells.	Diagram 2.3.1.3.2 Page 1 of 1 Scale Well Demand 1994 October 03 Version 02A TWM

DPTHWL ------> QAWME
OVWDPT
QSCALE
QWDEM
VSCALE

Short Name	Long Name	Mathematical Symbol	Units
DPTHWL	depth of well	d_w	[m]
OVWDPT	overburden well maximum depth	$d_{w,ov}$	[m]
QAWME	well demand used in equations	Q'_{dem}	[m^3/a]
QSCALE	well demand scaling fctr	S_w	[-]
QWDEM	volumetric demand on well	Q_{dem}	[m^3/a]
VSCALE	gw velocity scaling factor	S_v	[-]

If $d_w \geq d_{w,ov}$, then the well demand is scaled by both S_v and S_w:

$$Q'_{dem} = Q_{dem}/(S_v S_w)$$ Eqn. (1)

Section 4.2.2.1, Section 4.2.3

If $d_w < d_{w,ov}$, then the well does not intersect the fracture zone (Section 4.1.5.1) and

$$Q'_{dem} = 0$$ Eqn. (2)

Section 4.1.5.1

Unit Checks:

$$[m^3/a] = [m^3/a]/([-][-])$$ Eqn. (1)

Notes:

none

QAWME

well demand used in equations Q'_{dem} [m^3/a] Annual volume of water demanded of and supplied by well from the well aquifer, as used in the analytical well model equations. This quantity is obtained from QWDEM after scaling by both QSCALE and VSCALE, but is zero for overburden wells. Calculated.

QSCALE

well demand scaling fctr S_w [-] Scaling factor applied to well demand QWDEM to give modified demand QAWME for use in well model equations. This modification is used to adjust demand to account for inaccuracies in simple well model equations to describe full 3D simulations of detailed well models. Sampled.

QWCAP

volumetric well capacity Q_{cap} [m^3/a] The maximum annual capacity of the well to supply water. Calculated, as a function of the well location in the well aquifer, in the geosphere model and passed to the biosphere model. Calculated.

QWCRT

critical well demand Q_{crt} [m^3/a] Well demand at which the stagnation point reaches the constant head boundary at the surface. At larger well demands the stagnation point separates into two stagnation points and capture of infiltrated water from the surface begins. Calculated.

QWDEM

volumetric demand on well Q_{dem} [m^3/a] Annual volume of water demanded of and supplied by well, including both surface water captured and deep groundwater captured. Passed to geosphere model from biosphere model. Calculated.

QWSUR

surface water flow into well Q_{sur} [m^3/a] Annual volume of surface water captured by the well from the constant head boundary which mixes with and dilutes deep groundwater captured by well. This surface water may itself be contaminated but to a different extent than the deep groundwater. Passed to the biosphere model from geosphere model. Calculated.

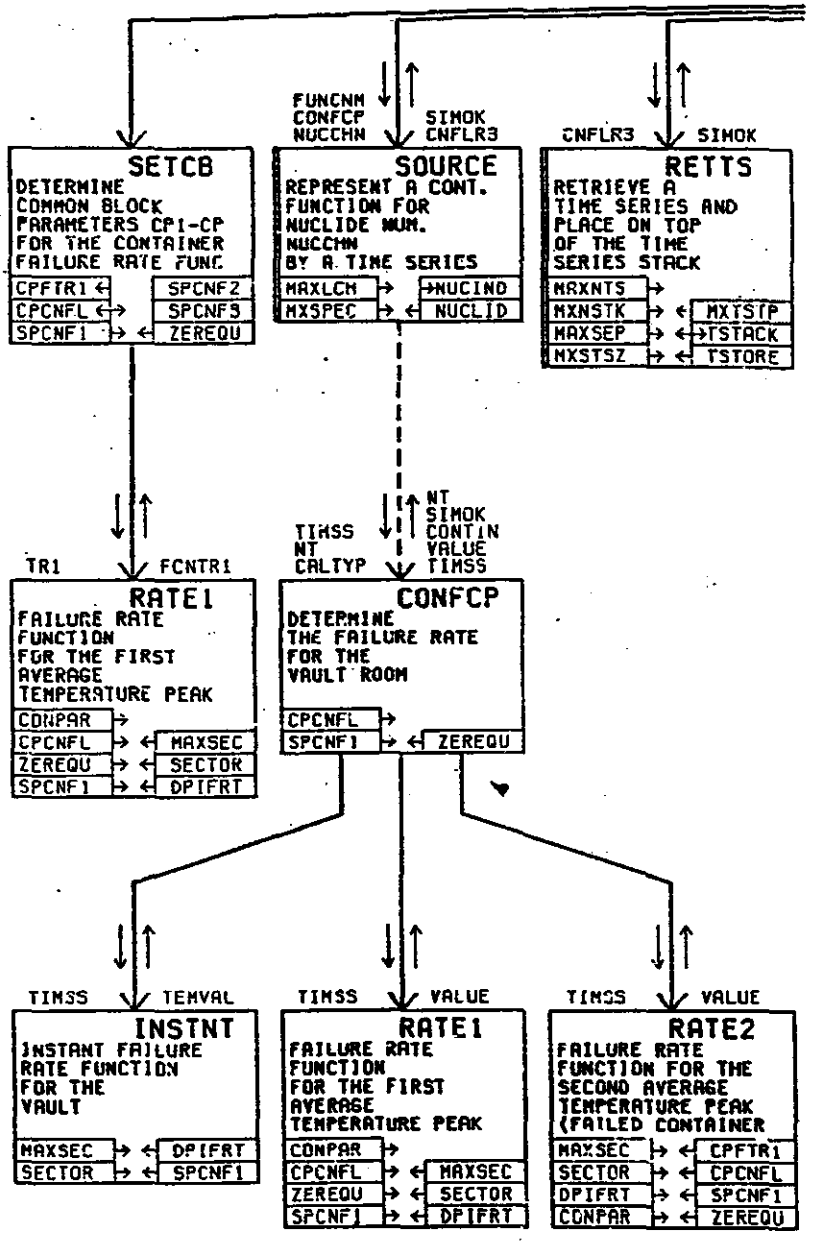
R

RADWEL

well casing radius r_w [m] Radius of well casing, used to determine the maximum drawdown at the well location due to the well demand, QWDEM. Sampled.

RAREAD-bloc

reduced discharge area $A'_{dis,\langle b\rangle}$ [m^2] Discharge area at discharge bloc after modification for influences of the well. Calculated.


SETCB
DETERMINE COMMON BLOCK PARAMETERS CP1-CP FOR THE CONTAINER FAILURE RATE FUNC
CPFTR1
CPCNFL
SPCNF1
SPCNF2
SPCNF3
ZEREQU
FUNCNM
CONFCP
NUCCHN
SIMOK
CNFLR3
SOURCE
REPRESENT A CONT. FUNCTION FOR NUCLIDE NUM. NUCCHN BY A TIME SERIES
MAXLCH
MXSPEC
NUCIND
NUCLID
CNFLR3
SIMOK
RETTS
RETRIEVE A TIME SERIES AND PLACE ON TOP OF THE TIME SERIES STACK
MAXNTS
MXNSTK
MAXSEP
MXSTSZ
MXTSTP
TSTACK
TSTORE
TR1
FCNTR1
RATE1
FAILURE RATE FUNCTION FOR THE FIRST AVERAGE TEMPERATURE PEAK
CONPAR
CPCNFL
ZEREQU
SPCNF1
MAXSEC
SECTOR
DPIFRT
TIMSS
NT
CALTYP
NT
SIMOK
CONTIN
VALUE
TIMSS
CONFCP
DETERMINE THE FAILURE RATE FOR THE VAULT ROOM
CPCNFL
SPCNF1
ZEREQU
TIMSS
TEMVAL
INSTNT
INSTANT FAILURE RATE FUNCTION FOR THE VAULT
MAXSEC
SECTOR
DPIFRT
SPCNF1
TIMSS
VALUE
RATE1
FAILURE RATE FUNCTION FOR THE FIRST AVERAGE TEMPERATURE PEAK
CONPAR
CPCNFL
ZEREQU
SPCNF1
MAXSEC
SECTOR
DPIFRT
TIMSS
VALUE
RATE2
FAILURE RATE FUNCTION FOR THE SECOND AVERAGE TEMPERATURE PEAK (FAILED CONTAINER
MAXSEC
SECTOR
DPIFRT
CONPAR
CPFTR1
CPCNFL
SPCNF1
ZEREQU

PROCEDURES FOR FREEZING

1. DOCUMENT PROCEDURES AND FOLLOW THEM

2. BASIC PROCEDURES
   - BACKUP VERSION
   - ALLOW NO MORE CHANGES
   - COPY TO NEW DEVELOPMENT VERSION

3. EXTRA PROCEDURES
   - MAINTAIN "OTHER" ELEMENTS OF CODE PACKAGE
   - TESTING PROGRAM
   - QUALITY ASSURANCE PROCEDURES
   - DOCUMENTATION/USER'S GUIDE

PROCEDURES

- change control is implemented by completion of a change request

- steps in the change process are submission, analysis, implementation, inspection, integration, review, and installation.

- a person is responsible for one or more steps in the change process

- work is completed in directories assigned to a particular step

PROCEDURES FOR MODIFICATION

1. DOCUMENT PROCEDURES AND FOLLOW THEM

2. BASIC PROCEDURES
   - DESIGN, CODE, IMPLEMENT, TEST, REVIEW, INSTALL MODIFIED CODE
   - KEEP ARCHIVE COPY OF OLD CODE
   - MAINTAIN CHANGE RECORD
   - MAINTAIN DICTIONARY

3. EXTRA PROCEDURES
   - DETAILED DOCUMENTATION OF MODIFICATION
   - QUALITY ASSURANCE PROCEDURES
   - MAINTAIN "OTHER" ELEMENTS OF CODE PACKAGE

Number:_____

SOFTWARE CHANGE REQUEST

LIBRARIAN'S HIP

Submitted by: Date:

Version number of the division(s) affected:
SV3___ ML3___ CC3___ SUP___ TLS___ CFG___ Other_____
Packages or Programs affected:

Modules affected:

Description of the change or problem: (attach if necessary)

Change description summary (for folder records file):

Recorded by: Date:

ANALYSIS

Analysis by: Date:

Comments / Names and versions of analysis products:

Functional Test Data: not required [ ] or attached [ ]

Approved [ ] with priority ____, or terminated [ ](give reason above)

IMPLEMENTATION

Implemented by: Date:

Comments / Names and versions of implementation products:

Implementation completed [ ], or terminated [ ](give reasons above)

FILE IDENTIFICATION

Each source code file (*.FOR and *.INC) and each design document are identified:

1) internally and externally by module name and

2) by an internal version number.

Older files are retired by renaming the file (i.e. *.FOR becomes *.FOR12A).

EXAMPLE:

```
      SUBROUTINE BIOCQ1(NUCCHN, SIMOK)
C*************************************************************** BIOCQ1
C
C Calculate the consequences for the biosphere
C
C  89-JAN-17   VERSION 01A    K. DOUGAN
C  90-MAR-08   VERSION 11A    C.M. SAUNDERS
C  90-MAR-27   VERSION 12A    L. WOJCIECHOWSKI
C
C*****************************************************************
C
```

Number:_____

Inspection by: Date:	INSPECTION
Comments (attach if necessary):	
Inspection completed [ ], or terminated [ ](give reason above)	

Integration by: Date:	INTEGRATION
Run request number _____ Comments / Names and versions of integration products:	
Integration completed [ ], or terminated [ ](give reason above)	

Review by: Date:	REVIEW
Comments (attach if necessary):	
Approved for installation [ ], or terminated [ ](give reason above)	

Computer files installed by: Date:	INSTALLATION
Paper files installed by: Date:	
Version number of the division(s) installed into: SV3___ CC3___ ML3___ SUP___ TLS___ CFG___ Other_____ Comments:	
Installation completed [ ], or terminated [ ](give reason above)	

92-JAN-13 Form ESAH-CR-05A (concluded)

QUALITY ASSURANCE PROCEDURES

1. FOLLOW DOCUMENTED PROCEDURES
   - SYVAC3-CC3 QUALITY CONTROL MANUAL

2. FOLLOW DEVELOPMENT AND CODE STANDARDS
   - SYVAC3-CC3 SOFTWARE STANDARD

3. TEST CODE WITH -
   - NORMAL DATA
   - EXTREME DATA
   - INVALID DATA
   - RETAIN AND DOCUMENT TEST RESULTS

4. OTHER VERIFICATION AND VALIDATION STEPS
   - CODE INTERCOMPARISONS
     - INTRACOIN, BIOMOVS, PSAC
   - SENSITIVITY ANALYSIS
   - PEER REVIEW
   - VALIDATION AGAINST PHYSICAL DATA

EXAMPLES OF TEST PROCEDURES

- inspection
- unit tests
- function tests
- integration tests
- dimensional checks
- FORTRAN standards check

SOFTWARE TOOLS

INSDEF - inserts data dictionary definitions into the code

DDMERG - merges data dictionaries

VAX DIFF - compare code versions

CHECKER - checks ESAB coding standards

UNITCK - checks unit balance in definitions

RESEQ - resequence statement labels

FPE - test code compliance with ANSI FORTRAN 77

SUMMARY

- configuration control maintains the integrity of the software and provides an audit trail

- change control is implemented using the change request process

- files are identified internally and externally

- directories are used to maintain packages of files

- releases are created for several reasons

PSAG

- **Organized in 1985 by the OECD/NEA**
- **Aimed at developing the SVA approach**
- **Code intercomparisons:**

  Level 0
  Level E
  Level 1a
  Level 1b
  (Level 2)

CC3 VERIFICATION STUDIES

- SYVAC2-CC2 and SYVAC3-CC3
- VAULT3 and AREST
- GEONET and INTRACOIN
- BIOTRAC and BIOMOVS

SYVAC-CC3 DATA BASE

- MAINTAINED IN WORD PROCESSOR LIST FORMAT

- DATA SUPPLIED BY R&D GROUPS ON SUBMITTAL FORMS

- COMPLETED FORM IS REVIEWED FOUR TIMES BEFORE DATA IS INSTALLED
  - SUBMITTOR
  - GROUP CHAIRMAN
  - SYVAC3-CC3 MODELLER
  - DATA BASE MANAGER

- DATA IS EXTRACTED FROM DATA BASE DIRECTLY INTO SYVAC3 INPUT FILES USING SOFTWARE TOOLS

Glen Bird

SGPERM(57)

SYVAC3-CC3 Parameter Characteristics for the CAD Post-Closure Assessment

1. Data Authorization
Data submitted by: Glen Bird (signature) Date: 89/05/23

PLEASE TYPE. SEE ESAB GUIDELINES FOR DEFINITIONS OF TERMS.

2. Parameter Full Name, Complete Definition and Mathematical Symbol

Full Name: permeability

Complete Definition:

permeability

Symbol: k

3. SI Units m^2

4. Probability Density Function (PDF) for the Parameter

PDF Type: lognormal

Upper bound: 1.0E-10

Bound Type: value

Lower bound: 1.0E-14

Attributes ($a, b, c, \mu, \sigma, GM, GSD, \alpha_1, \alpha_2, n, \{a_i, b_i, w_i\}$) as appropriate for type:
(List on back of page or on a separate page if you need more space.)

GM	GSD
1.0E-12	10.0

5. Dependence (if any) on Another Parameter via a Correlation Coefficient

Correlated to parameter: THIKSS(02)

with Correlation Coefficient: -0.90

6. Reasons for This Choice of PDF (Please provide justification for the given information, including PDF type, attributes, bounds, the principal sources of uncertainty, underlying assumptions, simplifications and qualifying conditions, and attach a plot of the PDF and data points used. Alternatively, please provide a reference where this information may be found.)

Data for silty sand taken from Groundwater, Freeze and Cherry, (1979), p. 29. See Surface Hodel Submodel Report, Appendix, Table D.

Comments:

89/05/12 T. Melnyk. Sediment layer at boggy creek short time discharge. 89/06/21 T. Chan. It is necessary to limit the permeability of the sediment layers to values greater than or equal to that of the uppermost rock zone. The truncation limits used are consistent with this limitation.

7. SYVAC3-CC3 Information (TO BE COMPLETED BY ESAB)

Short name of the parameter in SYVAC3-CC3: _____

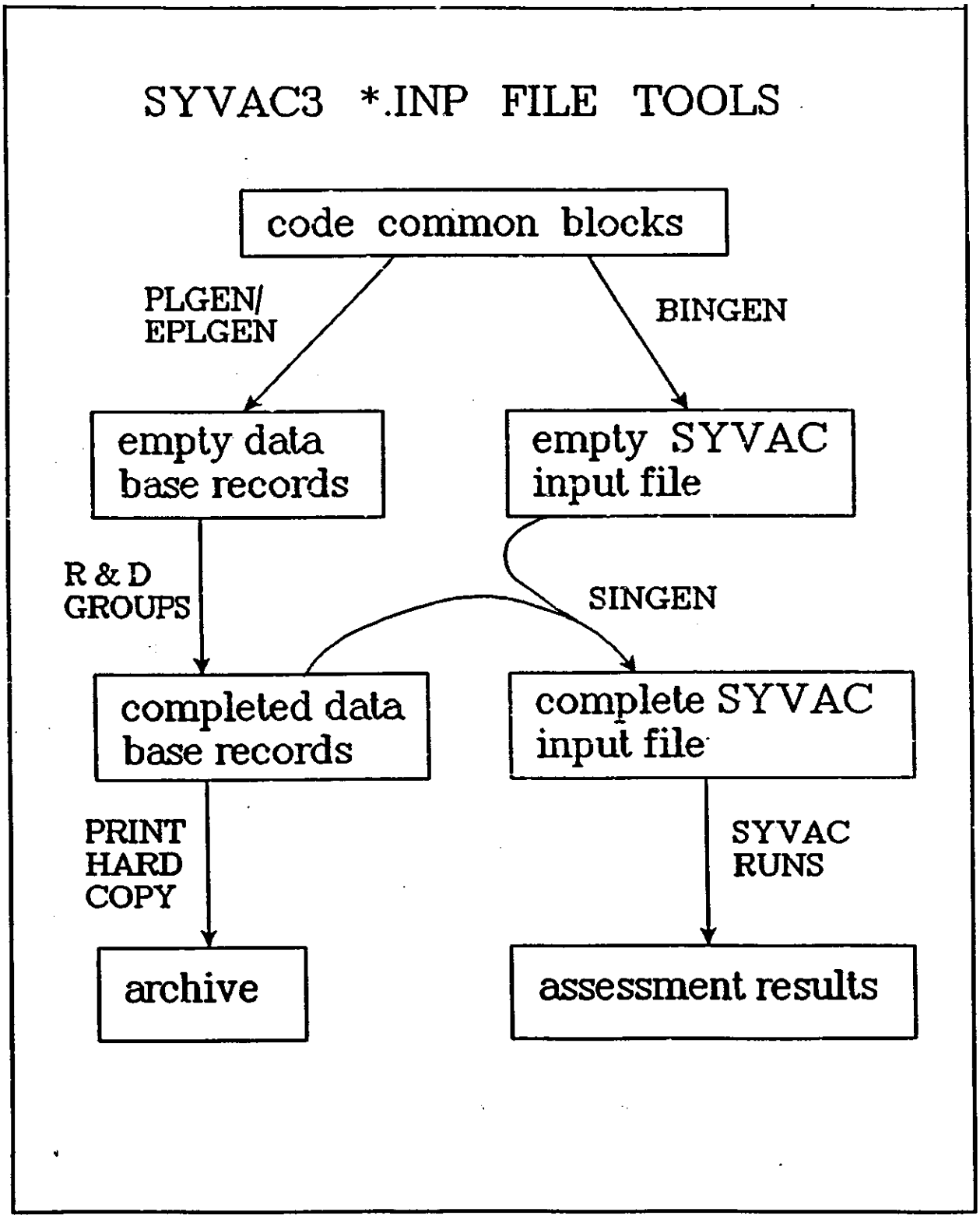
Long name (up to 32 characters): _____

Data are compatible with CC3 model constraints. Checked by: T Melnyk (signature) Date: 89/07/06

Data have been correctly entered into SYVAC3-CC3 data base. Checked by: _____ (signature) Date: _____

DATA BASE RECORD (LIST FORMAT)

<Contributor>Glen Bird
<Long_Name>permeability
<Definition>permeability
<Mathematical_Symbol>k
<SI_Units>m^2
<Subscript1_Label>segment 57
<Subscript2_Label>
<Subscript3_Label>
<Separator_1>***** DATA ENTRY BY CONTRIBUTOR STARTS HERE *****
<Date_Data_Entered>89/05/23
<PDF_Type>Lognormal
<Attribute1_Label>GM
<Attribute1_Value>1.0E-12
<Attribute2_Label>GSD
<Attribute2_Value>10.0
<Attribute3_Label>
<Attribute3_Value>
<Attribute4_Label>
<Attribute4_Value>
<Bound_Type>value
<Lower_Bound>1.0E-14
<Upper_Bound>1.0E-10
<Correlated_to_Parameter>THIKSS(02)
<Correlation_Coefficient>-0.90
<Justification_and_Reference>Data for silty sand taken from Groundwater, Freeze and Cherry, (1979), p. 29. See Surface Model Submodel Report, Appendix, Table D.
<Comments>89/05/12 T. Melnyk. Sediment layer at boggy creek short time discharge. 89/06/21 T. Chan. It is necessary to limit the permeability of the sediment layers to values greater than or equal to that of the uppermost rock zone. The truncation limits used are consistent with this limitation.
<Separator_2>***** DATA ENTRY BY CONTRIBUTOR ENDS HERE *****
<Short_Name>SGPERM(57)
<Include_File_Name>SPSEGS
<Include_File_Description>Sampled physical properties of segments in network.
<Common_Block_Name>SPSEG2
<Model_Compatibility_Checked_by>T.W. Melnyk
<Model_Compatibility_Check_Date>89/07/06
<Correct_Data_Entry_Checked_by>
<Correct_Data_Entry_Check_Date>
<>


SYVAC3 *.INP FILE TOOLS
code common blocks
PLGEN/
EPLGEN
BINGEN
empty data
base records
empty SYVAC
input file
R & D
GROUPS
SINGEN
completed data
base records
complete SYVAC
input file
PRINT
HARD
COPY
SYVAC
RUNS
archive
assessment results

SYVAC3-CC3 Data Base

Summary

- contains data for about 8000 parameters
- about 4000 parameters are constants
- about 4000 parameters are sampled from distributions
- input file generation is almost completely automatic