

Appendix F

<p style="text-align: center;">NUCLEAR WASTE MANAGEMENT PROCEDURE</p> <p><small>Sandia National Laboratories</small></p>	<h2 style="margin: 0;">Implementation Document Criteria</h2>	<p>Form Number: NP 19-1-5</p> <p>Page 1 of 1</p>
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- 1. **Software Name:** BRAGFLO
- 2. **Software Version:** 6.0
- 3. **Document Version:** 6.00
- 4. **ERMS #:** 545017

Prior to sign-off of the ID, all items shall be appropriately addressed by the code sponsor so that "Yes" or "N/A" may be checked. Include this form as part of the ID.

5. Source Code

- Is the source code provided? Yes N/A
- If applicable, is the change documentation in the source code clear and sufficient? Yes N/A

Note: If the source code is not controlled in a configuration management tool then a hardcopy of the source is required. (Check "N/A" for commercially obtained software for which source code was not provided.)

6. Coding Standards Yes N/A

Are the coding standards and conventions which were adhered to in the development of the software identified?

7. Coding Standards Implementation Yes N/A

Does the source code adhere to the coding standards and conventions defined in the ID?

8. Executable Generation Yes N/A

Was the executable generation process documented?

9. Implementation Requirements Yes N/A

Was the code implemented according to the requirements of the RD and where applicable the DD?

Martin Nemer		02/21/2007
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Key for check boxes above:

Check Yes for each item reviewed and found acceptable
Check N/A for items not applicable

WIPP PA

IMPLEMENTATION DOCUMENT

for

BRAGFLO Version 6.0

Document Version 6.00

ERMS #545017

February 12, 2007

Information Only

TABLE OF CONTENTS

1.0	INTRODUCTION	3
1.1	SOFTWARE IDENTIFIER.....	3
1.2	POINTS OF CONTACT.....	3
2.0	SOURCE INFORMATION.....	4
2.1	SOURCE CODE FOR BRAGFLO.....	4
2.2	SUBROUTINE-CALL HIERARCHY FOR BRAGFLO.....	6
2.3	CODING STANDARDS AND CONVENTIONS.....	12
3.0	GENERATION OF EXECUTABLE.....	13
3.1	BUILD SCRIPT.....	13
3.2	BUILD DATA FILE.....	13
3.3	COMPILE AND LINK COMMANDS FOR BRAGFLO BUILD.....	13
3.4	LOG FILES FROM BRAGFLO BUILD.....	14
3.5	PCA BUILD.....	14
4.0	REFERENCES	15

1.0 INTRODUCTION

This document records the creation of the executable for BRAGFLO Version 6.0. This code is used by the Sandia National Laboratories' Performance Assessment (PA) in support of the performance assessment calculations for the Waste Isolation Pilot Plant (WIPP). Using the information contained in this document, qualified personnel can rebuild the executable for BRAGFLO on the existing platform or install it on a similar platform.

1.1 Software Identifier

Code Name:	BRAGFLO
Version:	6.0
WIPP Prefix:	BF2
CMS Library:	BF (WP\$CMSROOT:[BF])
CMS Class:	QB0600
Executable:	BRAGFLO_QB0600.EXE
Executable Identification:	"P QB0600 6.0"
Link Date/Time:	12-FEB-2007 14:57:24.36
Executable Size:	179446 blocks
Platform:	OpenVMS V8.2 hp AlphaServer ES47 7/1150 (node GNR)
Compiler:	HP Fortran V8.0-104655-48F7C
Linker Identification:	A13-03

1.2 Points of Contact

Code Sponsor:	Martin Nemer Sandia National Laboratories (505) 234-0005 mbnemer@sandia.gov
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2.0 SOURCE INFORMATION

This section provides the source code and subroutine-call hierarchy for BRAGFLO.

2.1 Source Code for BRAGFLO

The source code for BRAGFLO is stored in the Software Configuration Management System (SCMS) in class QB0600 of CMS library BF.

The source code for BRAGFLO includes the listed routines, contained in order in the following FORTRAN source file:

```
BF2_BRAGFLO.FOR:
PROGRAM BRAGFLO
SUBROUTINE ADJUSTICS
SUBROUTINE ALI2VAX
SUBROUTINE ALR2VAX
SUBROUTINE BANDIT
SUBROUTINE BANDSTORE
FUNCTION BIOHUM
FUNCTION BIOSAT
SUBROUTINE BIOFES
SUBROUTINE BIOMGO
BLOCK DATA STARTUP
SUBROUTINE BL_INTERP
SUBROUTINE BUBBLE
SUBROUTINE CLOSCHECK
SUBROUTINE CONSOL
SUBROUTINE CONSOL1
FUNCTION CORHUM
FUNCTION CORSAT
SUBROUTINE CORMGO
SUBROUTINE CUMULGEN
DOUBLE PRECISION FUNCTION DASUM
SUBROUTINE DATNTIM
SUBROUTINE DAXPY
DOUBLE PRECISION FUNCTION DDOT
SUBROUTINE DECAY
SUBROUTINE DECBR
SUBROUTINE DELTAMAP
FUNCTION DENGZ
FUNCTION DENGZINT
FUNCTION DENO
SUBROUTINE DENSAT1
SUBROUTINE DEPINVERT
SUBROUTINE DEPINVERT1
SUBROUTINE DGBCO
SUBROUTINE DGBFA
SUBROUTINE DGBSL
SUBROUTINE DISKR
SUBROUTINE DISKW
SUBROUTINE DISOLVGAS
SUBROUTINE DSCAL
FUNCTION FMAX
```

FUNCTION FMIN
SUBROUTINE FUNCT
SUBROUTINE FUNCT7
SUBROUTINE GASC
SUBROUTINE GEN_COEF
SUBROUTINE GEOMETRY
SUBROUTINE GETJAC
SUBROUTINE GETJACINDX
SUBROUTINE GETOLD
SUBROUTINE GETWELLS
SUBROUTINE GETWELLS1
INTEGER FUNCTION IDAMAX
SUBROUTINE INITAL
SUBROUTINE KLINKBERG
SUBROUTINE LABELS
ENTRY LABELS1
SUBROUTINE LOCATE
SUBROUTINE MAPDEP
SUBROUTINE MASSBALNC
SUBROUTINE MATERIALS
SUBROUTINE MEAS_CONV
SUBROUTINE MULTIGRID
SUBROUTINE PERMPHI
SUBROUTINE PERMS
SUBROUTINE POR_SURF
double precision function POROLID
SUBROUTINE PRINTASC
SUBROUTINE PRINTBIN
SUBROUTINE PRINTCONTROL
SUBROUTINE PRINTGRID
SUBROUTINE PRINTHIV
SUBROUTINE PRINTLABS
SUBROUTINE PROPS
SUBROUTINE PROPS1
SUBROUTINE PRORDER
SUBROUTINE PTHRESH
SUBROUTINE QABGNL
SUBROUTINE QAENDL
SUBROUTINE RADIOLYSIS
SUBROUTINE RADTRANS
SUBROUTINE RAPHSON
SUBROUTINE READCLOSURE
SUBROUTINE READCNTRL
SUBROUTINE READFILES
SUBROUTINE READFLUID
SUBROUTINE READICS
SUBROUTINE READMAT
SUBROUTINE READMESH
SUBROUTINE READPRTYPE
SUBROUTINE READRAD
SUBROUTINE READRXGAST
SUBROUTINE READRXN
SUBROUTINE READSTARTUP
SUBROUTINE READWELL
SUBROUTINE READ_DIRICHLET
SUBROUTINE REFCONDS
SUBROUTINE RELPERM
SUBROUTINE RESET
SUBROUTINE RESETMID
SUBROUTINE RESIDUAL

```
SUBROUTINE ROCKCOMP
SUBROUTINE RPGM_INTRFC
SUBROUTINE RXGAST
SUBROUTINE SET_DELTA_DIRICHLET
SUBROUTINE SET_MAIN_DIRICHLET
SUBROUTINE SET_RHS_DIRICHLET
SUBROUTINE SMOOTHPERM
SUBROUTINE SOLER
SUBROUTINE SOLUTION
SUBROUTINE SOLVER
SUBROUTINE SOR
SUBROUTINE STOREINT
SUBROUTINE SUMMARY
SUBROUTINE TIMESTEP
SUBROUTINE TRI_INTERP
SUBROUTINE TSAVG
ENTRY TSAVG0
FUNCTION TTIME
SUBROUTINE UNITSCONV
SUBROUTINE WHERE
SUBROUTINE WHICH
SUBROUTINE WRITBIN
SUBROUTINE WRITEARRAY
SUBROUTINE WRITHIV
```

The source code for BRAGFLO also includes the following FORTRAN INCLUDE file:

```
BF2_PARAMS . INC
```

2.2 Subroutine-Call Hierarchy for BRAGFLO

A subroutine-call hierarchy is output by the Software Coverage Analyzer (SCA) that is run as part of the process of building the executable. This hierarchy, listed below, is stored in the SCMS as file BF2_CALLTREE_QB0600.TXT in class QB0600 of CMS library BF.

```
BRAGFLO procedure calls
  CUMULGEN routine
  DATNTIM routine calls
    . DBLE function
    . EXCPUS routine
    . EXDATE routine
    . EXPARM routine
    . EXTIME routine
    . INT function
    . TTIME routine
  DISKR routine calls
    . GETOLD routine
    . GETWELLS routine
    . MATERIALS routine calls
      . . CLOSCHECK routine calls
        . . . INDEX function
      . . CONSOL routine calls
        . . . MAX function
        . . . MIN function
      . . . POR_SURF routine calls
```

- . . . BL_INTERP routine calls
 - MOD function
- . . . LOCATE routine
- . . . MAX function (See above)
- . . . TRI_INTERP routine calls
 - MOD function (See above)
- . . . CONSOL1 routine calls
 - MAX function (See above)
 - MIN function (See above)
 - POR_SURF routine (See above)
- . . . DENSAT1 routine calls
 - ABS function
- . . . DENGZ routine calls
 - ABS function (See above)
 - EXP function
 - MAX function (See above)
 - SQRT function
- . . . DENGZINT routine calls
 - INT function (See above)
- . . . DENO routine calls
 - EXP function (See above)
 - MIN function (See above)
- . . . DISOLVGAS routine calls
 - BUBBLE routine calls
 - EXP function (See above)
 - LOG function
 - DENO routine (See above)
 - MAX function (See above)
 - MIN function (See above)
- . . . PERMS routine calls
 - KLINKBERG routine
 - LOG function (See above)
- . . . PTHRESH routine
- . . . RELPERM routine calls
 - MAX function (See above)
 - MIN function (See above)
 - SQRT function (See above)
- . . . ROCKCOMP routine calls
 - EXP function (See above)
 - MIN function (See above)
- . . . PERMPHI routine
- . . . PERMS routine (See above)
- . . . TIMESTEP routine calls
 - ABS function (See above)
 - FMIN routine
- . . . GETOLD routine (See above)
- . . . INITAL routine calls
 - ADJUSTICS routine
 - CLOSCHECK routine (See above)
 - GEOMETRY routine
 - GETJACINDX routine
 - GETOLD routine (See above)
 - GETWELLS routine (See above)
 - LABELS1 routine
 - MAPDEP routine
 - MATERIALS routine (See above)
 - PRINTGRID routine calls
 - WRITBIN routine calls
 - ALR2VAX routine calls
 - IAND function

- ISHFT function
- MIN function (See above)
- REAL function
- WRITEARRAY routine
- . PRINTLABS routine calls
 - ALI2VAX routine calls
 - IAND function (See above)
 - ISHFT function (See above)
 - ALR2VAX routine (See above)
 - REAL function (See above)
 - . PROPS routine calls
 - ABS function (See above)
 - BIOFES routine calls
 - EXP function (See above)
 - BIOHUM routine calls
 - EXP function (See above)
 - BIOMGO routine calls
 - EXP function (See above)
 - BIOSAT routine calls
 - EXP function (See above)
 - CLOSCHECK routine (See above)
 - CONSOL routine (See above)
 - CONSOL1 routine (See above)
 - CORHUM routine calls
 - EXP function (See above)
 - CORMGO routine calls
 - EXP function (See above)
 - CORSAT routine calls
 - EXP function (See above)
 - DENGZ routine (See above)
 - DENGZINT routine (See above)
 - DENO routine (See above)
 - DEPINVERT routine
 - DISOLVGAS routine (See above)
 - EXP function (See above)
 - KLINKBERG routine (See above)
 - MAX function (See above)
 - MIN function (See above)
 - PTHRESH routine (See above)
 - RADIOLYSIS routine calls
 - DECAY routine calls
 - WHICH routine calls
 - MIN function (See above)
 - WHERE routine
 - RELPERM routine (See above)
 - ROCKCOMP routine (See above)
 - RPGM_INTRFC routine calls
 - GASC routine
 - SMOOTHPERM routine calls
 - EXP function (See above)
 - LOG function (See above)
 - MAX function (See above)
 - MIN function (See above)
 - . READCLOSURE routine calls
 - MAX function (See above)
 - MIN function (See above)
 - . READCNTRL routine calls
 - ABS function (See above)
 - . READFILES routine calls
 - ALI2VAX routine (See above)

- . . QABGNL routine calls
- . . . DATNTIM routine (See above)
- . READFLUID routine calls
- . . ABS function (See above)
- . . DBLE function (See above)
- . . DENGZ routine (See above)
- . . EXP function (See above)
- . . LOG function (See above)
- . . REFCONDS routine calls
- . . . ABS function (See above)
- . . . DENGZ routine (See above)
- . . . DENGZINT routine (See above)
- . . . DENO routine (See above)
- . READICS routine
- . READMAT routine calls
- . . INDEX function (See above)
- . . LOG10 function
- . . MAX function (See above)
- . . MIN function (See above)
- . READMESH routine calls
- . . COS function
- . . SIN function
- . READPRTYPE routine calls
- . . ALI2VAX routine (See above)
- . . LABELS routine calls
- . . . INDEX function (See above)
- . . . MIN function (See above)
- . . MIN function (See above)
- . . PRORDER routine
- . READRAD routine calls
- . . MAX function (See above)
- . READRXGAST routine
- . READRXN routine calls
- . . ABS function (See above)
- . READSTARTUP routine calls
- . . ABS function (See above)
- . . ALI2VAX routine (See above)
- . READWELL routine
- . READ_DIRICHLET routine
- . REFCONDS routine (See above)
- . RXGAST routine calls
- . . BANDIT routine calls
- . . . DABS function
- . . . MIN0 function
- . . BANDSTORE routine
- . . GEN_COEF routine
- . SET_DELTA_DIRICHLET routine
- . STOREINT routine
- . UNITSCONV routine
- MASSBALNC routine calls
- . . ABS function (See above)
- MATERIALS routine (See above)
- PRINTCONTROL routine calls
- . DISKW routine
- . PRINTASC routine calls
- . . DATNTIM routine (See above)
- . . FLOAT function
- . . MAX function (See above)
- . . PORSOLID routine
- . . WRITEARRAY routine (See above)

- . PRINTBIN routine calls
 - . . ALR2VAX routine (See above)
 - . . DATNTIM routine (See above)
 - . . PORSOLID routine (See above)
 - . . REAL function (See above)
 - . . TSAVG0 routine
 - . . WRITBIN routine (See above)
- . PRINTHIV routine calls
 - . . ALI2VAX routine (See above)
 - . . ALR2VAX routine (See above)
 - . . FLOAT function (See above)
 - . . MAX function (See above)
 - . . MIN function (See above)
 - . . PORSOLID routine (See above)
 - . . REAL function (See above)
 - . . WRITHIV routine calls
 - . . REAL function (See above)
 - . . TSAVG routine
- . QAENDL routine calls
 - . . DATNTIM routine (See above)
- . RADTRANS routine calls
 - . . DECAY routine (See above)
 - . . EXP function (See above)
 - . . FMAX routine
 - . . MAX function (See above)
 - . . MIN function (See above)
- . RESET routine calls
 - . . DENSAT1 routine (See above)
 - . . DISOLVGAS routine (See above)
 - . . PTHRESH routine (See above)
 - . . RELPERM routine (See above)
 - . . ROCKCOMP routine (See above)
- . RESETMID routine calls
 - . . DENSAT1 routine (See above)
 - . . DISOLVGAS routine (See above)
 - . . PTHRESH routine (See above)
 - . . RELPERM routine (See above)
- . SOLVER routine calls
 - . . MAPDEP routine (See above)
 - . . RAPHSON routine calls
 - . . ABS function (See above)
 - . . CLOSCHECK routine (See above)
 - . . DELTAMAP routine
 - . . GETJAC routine calls
 - . . FUNCT7 routine
 - . . GETWELLS1 routine
 - . . PROPS1 routine calls
 - . . . ABS function (See above)
 - . . . BIOFES routine (See above)
 - . . . BIOHUM routine (See above)
 - . . . BIOMGO routine (See above)
 - . . . BIOSAT routine (See above)
 - . . . CONSOL1 routine (See above)
 - . . . CORHUM routine (See above)
 - . . . CORMGO routine (See above)
 - . . . CORSAT routine (See above)
 - . . . DENGZ routine (See above)
 - . . . DENGZINT routine (See above)
 - . . . DENO routine (See above)
 - . . . DEPINVERT1 routine

- . . . DISOLVGAS routine (See above)
- . . . EXP function (See above)
- . . . KLINKBERG routine (See above)
- . . . MAX function (See above)
- . . . MIN function (See above)
- . . . PTHRESH routine (See above)
- . . . RADIOLYSIS routine (See above)
- . . . RELPERM routine (See above)
- . . . ROCKCOMP routine (See above)
- . . . RPGM_INTRFC routine (See above)
- . SET_MAIN_DIRICHLET routine
- GETWELLS routine (See above)
- LOG10 function (See above)
- MEAS_CONV routine calls
 - . ABS function (See above)
- MOD function (See above)
- PROPS routine (See above)
- PROPS1 routine (See above)
- RESIDUAL routine calls
 - . ABS function (See above)
 - . FUNCT routine
- RXGAST routine (See above)
- SET_RHS_DIRICHLET routine
- SOLUTION routine calls
 - . ABS function (See above)
 - DECBR routine calls
 - . ABS function (See above)
 - . MIN0 function (See above)
 - DGBCO routine calls
 - . DABS function (See above)
 - . DASUM routine calls
 - . . ABS function (See above)
 - . . MOD function (See above)
 - . DAXPY routine calls
 - . . MOD function (See above)
 - . DDOT routine calls
 - . . MOD function (See above)
 - . DGBFA routine calls
 - . . DAXPY routine (See above)
 - . . DSCAL routine calls
 - . . . MOD function (See above)
 - . . IDAMAX routine calls
 - . . . ABS function (See above)
 - . . . MAX0 function
 - . . . MIN0 function (See above)
 - . DMAX1 function
 - . DSCAL routine (See above)
 - . DSIGN function
 - . MAX0 function (See above)
 - . MIN0 function (See above)
 - DGBSL routine calls
 - . DAXPY routine (See above)
 - . DDOT routine (See above)
 - . MIN0 function (See above)
 - MAX function (See above)
 - MIN function (See above)
 - MULTIGRID routine
 - SOLBR routine calls
 - . MIN0 function (See above)
 - SOR routine calls

```
.          MAX function  (See above)
SUMMARY routine calls
.  EXP function  (See above)
.  MAX function  (See above)
.  MIN function  (See above)
.  PORSOLID routine  (See above)
TIMESTEP routine  (See above)
```

Note: The notation “(See above)” that follows some routines and/or functions means that the indicated routine/function appears earlier in the call tree. If an expansion of the call tree is associated with that routine/function, the expansion is presented only with its first occurrence.

All routines listed in Section 2.1 should be listed in the subroutine-call hierarchy, with the exception of routines that are never referenced. A list of routines that are never referenced is output by SCA. This list is stored in the SCMS as file BF2_SCA_MOD_NOT_REF_QB0600.TXT in class QB0600 of CMS library BF. SCA did not identify any routines (other than the main program) as never referenced.

The subroutine-call hierarchy includes routines that are not listed in Section 2.1, as follows.

- Intrinsic FORTRAN functions that are called from BRAGFLO are included in the hierarchy. They are identified as “functions” rather than “routines”.
- WIPP PA standard library routines that are called from BRAGFLO are included in the hierarchy. The source code for these libraries (described in Section 2.3) can be found in the related Implementation Documents, which are on file in the Sandia WIPP Central Files. CAMDAT_LIB [1] routines begin with “DB”. CAMCON_LIB [2] routines begin with “QA”, “IQA”, “FF”, “FIL”, “FE”, “STR”, or “ISTR”. CAMSUPES_LIB [3] routines begin with “EX”, “IX”, “MD”, or “MC”.

2.3 Coding Standards and Conventions

Formal software standards were not invoked in developing this software. However, by convention, WIPP PA software that is written in FORTRAN to run on the Compaq Alpha should use software libraries to perform specific functions. Each library is documented in the related User’s Manual, which is on file in the Sandia WIPP Central Files. BRAGFLO uses three of these libraries:

- CAMDAT_LIB [4] reads and writes information to CAMDAT files.
- CAMCON_LIB [5] provides general-use functions, such as the display of standardized output and the free-field parsing of input.
- CAMSUPES_LIB [6] provides machine-dependent functions, especially dynamic memory manipulation.

3.0 GENERATION OF EXECUTABLE

This section provides the necessary files for generating the executable for this version of BRAGFLO. This process is referred to as a "build". For step-by-step instructions regarding how the build is accomplished, please consult the WIPP PA SCMS Plan [7]. See the SCMS Build Consultant for more information.

3.1 Build Script

The build script is invoked to generate the executable for BRAGFLO. The build script is stored in the SCMS as file WP_BUILD.COM in class QB0600 of CMS library WP. For the BRAGFLO build described in this document, WP_BUILD.COM was invoked as follows:

```
$ @WP_BUILD
Code Prefix : BF2
Build type (P=prod, T=test, D=local) : P
Class name (blank for latest generations) : QB0600
Build for SCA? (Y or N) [N] : Y
```

Note that SCA (described in Section 2.2) is run as part of the build.

3.2 Build Data File

The build script reads certain code-specific parameters, such as the compile options and the code version number, from a build data file. The build data file is stored in the SCMS as file WP_BUILD.DAT in class QB0600 of CMS library WP. The following portion of the file is specific to BRAGFLO:

```
BF2      1BRAGFLO
BF2      2/obj=wp_olb:/list/show=include/OPT=LEVEL=5
BF2      36.0      CDB-BRAGFLO
```

3.3 Compile and Link Commands for BRAGFLO Build

The Module Management System (MMS) is invoked by the build script to compile and link BRAGFLO. The MMS description file defines MMS actions and dependencies for BRAGFLO. It is stored in the SCMS as file BF2.MMS in class QB0600 of CMS library BF.

The default MMS rules that apply to all WIPP builds are stored in the SCMS as file WP_MMS\$DEFAULT_RULES.MMS in class QB0600 of CMS library WP.

3.4 Log Files from BRAGFLO Build

The log files from the BRAGFLO build are stored in the SCMS as files BF2_BUILD_QB0600.LOG and BF2_MMS_QB0600.LOG in class QB0600 of CMS library BF.

3.5 PCA Build

Verification and validation of BRAGFLO may involve coverage testing using the Performance Coverage Analyzer (PCA). PCA output is used to identify modules that are not exercised by the test set. To run PCA, a unique PCA executable must be generated.

The PCA executable, BRAGFLO_TEST_PCA_QB0600.EXE, can be generated using the build script WP_BUILD.COM described in Section 3.1. However, the BRAGFLO compile options in WP_BUILD.DAT contain the optimization switch /OPT=LEVEL=5 (see Section 3.2), which overrides the required PCA switch /NOOPT. A correction was made to WP_BUILD.COM to remove the /OPT switch for PCA. This correction appears in WP_BUILD.COM generation 38 and later in CMS library WP; it is not in WP_BUILD.COM in class QB0600 (generation 37) which generated the BRAGFLO executable described in Section 1.1.

To build the PCA executable, WP_BUILD.COM (generation 38 or later) would be invoked as follows:

```
$ @WP_BUILD
Code Prefix : BF2
Build type (P=prod, T=test, D=local) : T
Class name (blank for latest generations) : QB0600
Build from CMS sources? (Y or N) [N] : Y
Build for SCA? (Y or N) [N] : N
Build for PCA? (Y or N) [N] : Y
```

4.0 REFERENCES

1. WIPP PA (Performance Assessment). 2006. Implementation Document for CAMDAT_LIB Version 1.26. Sandia National Laboratories. Sandia WIPP Central Files ERMS #543021.
2. WIPP PA (Performance Assessment). 2006. Implementation Document for CAMCON_LIB Version 2.21. Sandia National Laboratories. Sandia WIPP Central Files ERMS #543029.
3. WIPP PA (Performance Assessment). 2006. Implementation Document for CAMSUPES_LIB Version 2.23. Sandia National Laboratories. Sandia WIPP Central Files ERMS #543023.
4. WIPP PA (Performance Assessment). 1995. User's Manual for CAMDAT_LIB Version 1.22. Sandia National Laboratories. Sandia WIPP Central Files ERMS #227727.
5. WIPP PA (Performance Assessment). 1995. User's Manual for CAMCON_LIB Version 2.16. Sandia National Laboratories. Sandia WIPP Central Files ERMS #227738.
6. WIPP PA (Performance Assessment). 1995. User's Manual for CAMSUPES_LIB Version 2.18. Sandia National Laboratories. Sandia WIPP Central Files ERMS #227745.
7. Long, J. 2003. WIPP Performance Assessment (PA) Software Configuration Management System (SCMS) Plan, Revision 2. Sandia National Laboratories. Sandia WIPP Central Files ERMS #524707.