

**Final Deliverables for the ACTIV Code Project
(Project No. 05-07741)**

Appendix I

Release of Version 2 of the ACTIV Code

Release of Version 2 of the ACTIV Code

Dr. John R. White
Chemical and Nuclear Engineering Department
University of Massachusetts Lowell
August 31, 1997

Enclosed for general use at Yankee Atomic is the release of Version 2 of the ACTIV code system. Packaged as part of this release are the source code for all the modules of the ACTIV system, a variety of input, output, and library files used in the sample problems, and a set of selected files used and generated as part of the activation library development and the JPDR benchmark calculations. This information is contained on three distribution diskettes as a series of archived files (*.zip files).

The first disk contains the source code for the ACHAIN, ACTMAT and ACTIV modules and associated sample problem files. The function of these three modules is as follows:

- ACHAIN - This routine automatically generates the chain data necessary for setting up the activation calculations in ACTIV. It generates all possible parent-daughter-process relationships consistent with the available base cross section library and the materials to be irradiated. It writes a chain library file that can be input directly to ACTIV. It can also generate a filtered dataset containing only those parent-daughter-process relationships that eventually lead to a selected list of activation products. The full or filtered chain library can be easily modified as needed by the user to specialize a particular calculation.
- ACTMAT - This is a small utility routine that uses nominal information about the materials to be irradiated (including impurity information) and creates a dataset of initial conditions for the nuclide vector for direct application within ACTIV.
- ACTIV - This is the main computational routine within the ACTIV system and it performs the space-energy activation analysis calculations on a pointwise and/or zone-averaged basis. It uses the space-energy scalar neutron flux information from a DORT calculation (or other suitable transport code) and other data libraries from ACHAIN, ACTMAT, and ACTXS (the code used for generating the activation library). The focus in this version of ACTIV is on the activation of excore structural materials.

The remaining two diskettes contain a lot of detailed information that might assist the interested reader in reproducing many of the computations needed to generate the ACTXS47.LIB activation library and in rerunning the JPDR benchmark calculations (if desired). However, no attempt at completeness was made - since many of the codes needed here are separate from the ACTIV system (i.e. several modules of the SCALE system are needed for use with the ACTXS code, and the DORT, GIP, and PROCESS codes were used as part of the JPDR analysis (and Matlab was used for most of the post processing and comparative analyses of the JPDR results). Many of the files have been included primarily as illustrative examples and they have not been fully documented. The intent here is to be as informative as possible, and these files do indeed contain a lot of information. The reader can extract as much or as little of this

material as needed for his or her own use. Note, however, that the source code and an example application of the ACTXS code is present on Disk #2. ACTXS is considered an integral part of the ACTIV system, even though most users will never have to work directly with this code - since a suitable activation library for use with ACTIV is already available.

A summary of the contents of the distribution diskettes is included in a text file called VER2.RME. This readme file is in the root directory of each diskette and a listing is given in Table I as part of this code release summary. This internal documentation summarizes the overall directory structure and it gives a brief description of the files included in this distribution. The information contained here should allow the implementation of Version 2 of the ACTIV system at Yankee. Verification of the local implementation can be made by comparison to several of the output files that have been included for this purpose. The primary ACHAIN, ACTMAT, and ACTIV modules are written in Fortran and they have been tested on a Unix workstation and on a Pentium PC (with the Lahey Fortran-90 compiler). The ACTXS code (also written in Fortran) has been used exclusively with a PC version of the SCALE 4.3 package. It is anticipated that the complete ACTIV system can be installed on any computer system with little difficulty.

Table I. Listing of the VERS2.RME file.

VERS2.RME (August 1997)

This readme file gives a brief overview of the material associated with the release of Version 2 of the ACTIV code and its associated processing codes.

All the known bugs from Version 1 have been eliminated and several new features relative to Version 1 have been added. The most important features are the new restart capability and a complete overhaul of the edit control in ACTIV (with some new edit), a change in the format of the chnlib & matlib files read by ACTIV (from ACHAIN and ACTMAT), and a new filter option in ACHAIN that only includes the parent-daughter-process triplets that eventually lead to a specified set of activation products. Documentation in the form of a "User Guide and Sample Problems for the ACTIV System" is also available.

Also in this release is Version 2 of the ACTXS code and a sample sequence that shows the development of an ACTXS47.LIB activation library that is fully consistent with the BUGLE96 shielding library. Full documentation of the library generation process is also available (see "Development of Activation Analysis Libraries for Use with the ACTIV Code").

A full re-analysis of the JPDR benchmark was also completed using the new BUGLE96-compatible library. Full documentation of these results is also available in a report titled, "Summary Results for the JPDR Activation Analysis Benchmark Using VITAMIN-B6 and BUGLE96 Data."

Further verification with additional benchmarks, as well as a host of additional enhancements, are still needed. However, this version of the codes and documentation represent a fully functional activation analysis system.

The system is distributed on THREE (3) diskettes, as follows:

Disk #1

The ACHAIN, ACTMAT, and ACTIV codes and three sample problem sequences are included on Disk #1 as follows:

SRC1 directory

achain.f	- source code for ACHAIN Ver. 2
activ1/2/3/4/5.f	- source code for ACTIV Ver. 2
actmat.f	- source code for ACTMAT Ver. 2
sfidas.f	- source code for FIDAS input processor and associated routines
lnachain.bat	- sample DOS bat file to create ACHAIN executable
lnactiv.bat	- sample DOS bat file to create ACTIV executable
lnactmat.bat	- sample DOS bat file to create ACTMAT executable

XSLIB directory

actxs47.lib	- 47n group activation library based on VITAMIN-B6 and BUGLE96 (created by ACTXS code) This library is included here (and on Disk #2) since it is needed to run the sample problems.
-------------	---

MYRUNS directory (needs BUGLE96 shielded library - not included)

- dorno.sub - sample script file to run DORT & GIP on Unix machine
- myfno.gin/got - input and output from GIP case to mix macros for the 1D MY model
- dgamf01.din/dot - input and output from 1D MY model (forward neutron only case)
- dgamf01.flx2 - ascii version of scalar flux file from DORT/PROCESS
 Note: ACTIV has been modified to read this file so that the sample problems can be run on the PC independent of the DORT case. For DOS compatibility, this file was renamed to dgamf01.asc.
- prono.sub - sample script file to run PROCESS
- myfno.pin - input for PROCESS to edit spatial flux profiles for three broad groups (for comparison in ACTIV)
- respfl145.g47 - response file used by PROCESS (data from BUGLE-96)
- dgamf01.pot - PROCESS output file for dgamf01 case

SMPL0_PC directory (activation of only thermal shield in 1D MY model)

- chn0.lib - chain library data with parent-daughter-process information for a select set of processes (new format)
- mat0.* - files for ACTMAT run to generate initial nuclide densities for MY model [needs chn0.lib]
- act0.* - ACTIV files that use 11 isotopes in the nuclide vector with 9 parent-daughter-process relationships (only 2 timesteps) [needs chn0.lib & mat0.lib]
- smpl0.m/smpl0f.m - Matlab m-files that independently verify the matrix exponential solution technique implemented within ACTIV

SMPL1_PC directory (include all excore structure in MY model - no impurities)

- chn1*.* - batch, input, and output files for ACHAIN run to generate parent-daughter-process chain information for structures in MY model (no impurities)
 *** This run generates two chain libraries - a full library and a filtered library (only the filtered library named chn1part.lib is used here).
- mat1.* - files for ACTMAT run to generate initial nuclide densities for MY model (no impurities) [needs chn1part.lib file]
- act1.* - files for ACTIV run that uses 40 isotopes in the nuclide vector with 95 parent-daughter-process relationships (no impurities) [needs chn1part.lib & mat1.lib] (this run contains a full power burn to 7300 days and a 1200 day shutdown run)
- act1a.* - same as case act1 except only the full power burn is completed to 7300 days and a restart density file is saved.
- act1b.* - same geometry setup as above but now only the 1200 day shutdown interval is processed starting from the restart file written in case act1a.
 *** The self consistency of cases 1, 1a, and 1b validate the new restart capability built into this version of ACTIV.

SMPL2_PC directory (include all excore structure in MY model with impurities)

- chn2*.* - batch, input, and output files for ACHAIN run to generate parent-daughter-process chain information for structures in MY model (with full set of impurities)
 *** This run generates two chain libraries - a full library and a filtered library (only the filtered library named chn2part.lib is used here).
- mat2.* - files for ACTMAT run to generate initial nuclide densities for MY model (with impurities) [needs chn2part.lib library file]
- act2.* - files for ACTIV run that uses 229 isotopes in

the nuclide vector with 636 parent-daughter-process relationships (includes impurities) [needs chn2part.lib & mat2.lib] (this run contains a full power burn to 7300 days and a 1200 day shutdown run - same as act1)

For convenience in getting all these data on a single diskette, the files in each of the above directories have been compressed into *.zip files with the name of the directory as the primary file name (ie. src1.zip, xslib.zip, etc.).

When restoring, the files should be uncompressed into a directory structure similar to that indicated here.

Disk #2

This disk contains a variety of material associated with the release of Version 2 of the ACTXS code and the generation of the ACTXS47.LIB activation library which is fully compatible with the BUGLE-96 library. This activation library is designed for use with the ACTIV space and energy dependent activation analysis package (with the BUGLE96-DORT combination for computing the multigroup fluxes). Version 2 of ACXTS only involves minor changes relative to Version 1.

A description of the procedure for the generation of a suitable activation library is available in the report "Development of Activation Libraries for Use with the ACTIV Code." This readme file identifies the files that were used in the development of the ACTXS47.LIB library. The organization and description of the files given here correspond to the discussion in the above report.

The ACTXS and ANXSEC codes were developed locally at UMass-Lowell. All the other routines needed for the generation of ACTXS47.LIB were obtained from the SCALE4.3 package.

SRC2 directory

actxs.f - source code for ACTXS Ver. 2
 anxsec.f - source code for ANXSEC Ver. 1
 sfidas.f - source code for FIDAS input processor and associated routines (needed for above codes)

Note: This version of FIDAS is different from previous versions. This version is a collection of several routines from the SCALE 4.3 package (some with slight modifications). The only noticeable differences from the user viewpoint are:

1. all output from FIDAS is in upper case (it will accept both upper and lower case input and convert it all to upper case)
2. a single quote in column 1 denotes a comment card (the / no longer works)

This version appears to work on both the PC and the UNIX workstation. The previous version, yfidas.f, had problems on the PC.

XSLIB directory

actxs47.lib - 47n group activation library compatible with BUGLE96

DATALIB directory (under ACTXS)

xsectpho - ORIGEN nuclear data libraries
 end6dec - ORIGEN decay libraries

Note: Both these files are available in the SCALE4.3 package. They are included here as a convenience.

GRP47A directory (under ACTXS) (Phase I library development)
 vb6_47g.bat - DOS batch file for generation of the Phase I activation library
 *.in - MALOCS, NITAWL, ALPO, and ANXSEC input files for this run
 vb6_47g.out - output file for this case
 vb6_47g.lib - the Phase I library (binary ANISN format)
 datadir - file needed by SCALE system to locate data directories

GRP47B directory (under ACTXS) (Phase II library development)
 actxs47.bat - DOS batch file for generation of the Phase II activation library
 actxs47.in - ACTXS input file for this run
 actxs47.out - output file for this case
 actxs47.lib - the Phase II library (ascii ANISN format)

Note: actxs47.lib is also stored separately in the main XSLIB directory

PWRSPEC directory (under ACTXS) (Generate concrete weighting spectrum)
 pwrwlib.bat - DOS batch file for generation of a working library for subsequent 1-D fine group XSDRN calculations of a typical PWR model
 xsdpwr1.bat - DOS batch file to run XSDRN case consistent with BUGLE93
 xsdpwr2.bat - DOS batch file to run XSDRN case consistent with BUGLE96
 *.in - input files for above cases (see listing of BAT files)
 *.out - output files for above cases (see listing of BAT files)
 datadir - file needed by SCALE system to locate data directories
 *.dat - various stages in editing the concrete spectrum from the XSDRN output files

Note: wtg199g1.dat contains the BUGLE93 concrete weight function (directly from the BUGLE93 report - this is almost identical with the solution from the xsdpwr1 case)

wtg199g2.dat contains the BUGLE96 concrete weight function (generated as part of this work). This is the spectrum used to generate the ACTXS47.LIB file for use with BUGLE96 data.

For convenience in getting all these data on a single diskette, most of the files in the above directories have been compressed into *.zip files with the name of the directory as the primary file name (i.e. grp47a.zip, grp47b.zip, etc.). When restoring, the files should be uncompressed into a directory structure roughly similar to that indicated here.

Disk #3

This disk contains much of material associated with the JPDR benchmark calculations that were used to help validate the DORT-ACTIV system. The latest calculations used the BUGLE-96 shielding library and recently developed ACTXS47.LIB activation library (derived from VITAMIN-B6). The Case D model used here had a 155x201 mesh grid and it used a full S16 quadrature everywhere (this is an enhanced model relative to previously reported work).

A description of the complete model development and a detailed presentation of the key results from the Case D JPDR computations are in the report "Summary Results for the JPDR Activation Analysis Benchmark Using VITAMIN-B6 and BUGLE96 Data." This readme file identifies some of the files that were used in the benchmark calculations and in the post processing and plotting of the results (used Matlab to do most of the plotting). The description

of the files given here correspond to the discussion in the above report.

JPDRSRC directory (Generate fixed source for JPDR Case D DORT model)

- jpdrsrcd.m - Matlab file to develop the fixed source for the JPDR Case D DORT model
- wattsp.m - Matlab file to determine the fission source spectrum (used by jpdrsrcd.m)

CASED directory (GIP/DORT/PROCESS/ACTIV runs for JPDR Case D model)

- gcs47.* - GIP related files for JPDR materials
- dcs47d.* - DORT related files for JPDR Case D model
- pcs47d.* - PROCESS related files for JPDR Case D model
- respf04.g47 - response file for use in PROCESS (selects broad group fluxes)
- jpdrchn.lib - chain library (generated by hand with only major production paths included - as specified for benchmark)
- jpdrmat.* - ACTMAT related files for JPDR Case D model
- acs47d.* - ACTIV related files for JPDR Case D model

RESULTSD directory (processing of primary results for benchmark report)

- bgrpflx.dat - portion of ACTIV output containing space dependent broad group fluxes
- *.xs - portion of ACTIV output containing space dependent broad group cross sections for selected reactions
- pcs47d.ip - portion of PROCESS output with selected first dimension reaction profiles (broad group fluxes)
- pcs47d.jp - portion of PROCESS output with selected second dimension reaction profiles (broad group fluxes)
- pflx47d.m - Matlab file to read specific data from a PROCESS output file and plot selected radial and axial response profiles (uses pcs47d.ip and pcs47d.jp)
- pltxsd.m - Matlab file to read the broad group cross sections from ACTIV and plot the radial and axial profiles of the 1-g effective cross for selected reactions (uses co59ng.xs, fe54ng.xs, and fe54np.xs)
- pltrrd.m - Matlab file to read the broad group fluxes and cross sections from ACTIV and plot the radial and axial reaction rate profiles (uses bgrpflx.dat and the *.xs files)
- compd47.m - Matlab program used to compare ACTIV results with the experimental data listed in the JPDR report (the space dependent activities are extracted from the ACTIV output and copied directly into this file - thus this file has all the raw computed results and the original experimental data)

For convenience in getting all these data on a single diskette, most of the files in the above directories have been compressed into *.zip files with the name of the directory as the primary file name (i.e. jpdrsrc.zip, etc.). When restoring, the files should be uncompressed into a directory structure roughly similar to that indicated here.