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

Dr. John R. White
Chemical and Nuclear Engineering Department
University of Massachusetts Lowell

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Final Report for Project No. 05-07741

Development of the ACTIV Code

Dr. John R. White
Chemical and Nuclear Engineering Department
University of Massachusetts Lowell

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Introduction

This report summarizes and organizes the final deliverables for Project No. 05-07741. This project, supported by Yankee Atomic Electric Company, focussed on upgrading and documenting the ACTIV code system for release and use at Yankee Atomic. The ACTIV system includes a series of four computer codes that provides unique capability to perform detailed neutron activation studies in the excore regions of nuclear systems. This new analysis capability is essential for making informed decisions concerning the feasibility of various decommissioning scenarios.

The ACTIV system allows fully coupled space-energy neutron activation calculations in the structural components surrounding the core of large power reactors (including the baffle, shroud, thermal shield, vessel structure, and any biological shield materials present in the system). These components, upon exposure to a neutron field over long periods of time, become activated with both short and long-lived radioactive isotopes. Upon shutdown, these activation products tend to decay, but depending on the original activity level and the isotopic distribution within the material, it could take hundreds or thousands of years before the materials no longer present a hazard. The ability to accurately quantify the induced activity in these materials is critical for identifying the waste classification for the various excore structures and for making decisions for their safe handling and long-term disposal.

Multigroup transport calculations are usually employed to determine the neutron flux distribution in the excore regions. This capability is well established, and a reasonable level of confidence has been achieved in regions extending radially through the vessel and axially to the top and bottom regions just outside the core (with less confidence as one moves further from the active core region). ACTIV takes advantage of this capability by performing space-dependent activation calculations using multigroup activation cross sections with the same multigroup structure that is employed in the transport calculations. In this way, one can make full use of all the detailed space-energy neutron flux information available from the transport calculations, and minimize (or eliminate) the additional uncertainty that is usually introduced in simple zero-dimensional analyses (the usual ORIGEN treatment, for example).

The original version of ACTIV was developed in the summer of 1994 at UMass-Lowell as an unfunded research project. Involvement with an IAEA-organized international benchmark exercise to address the adequacy of data and methods for excore neutron activation analysis quickly proved the utility of the ACTIV methodology, and the good agreement with some measurements from the Japan Power Demonstration Reactor (JPDR) decommissioning program validated the basic procedures and implementation details. However, the early ACTIV work was focused on base code capability and not on the development and documentation of a general activation analysis tool for production use outside UMass-Lowell. The goal of the current project was to formalize all the early ACTIV work and to enhance and integrate the previous capability into a series of production-oriented analysis tools – with appropriate documentation and validation.

Summary of Work Accomplished

The original proposal for this project identified four areas of focus, as follows:

1. Full testing, validation, and documentation of the methods utilized.
2. Documentation relative to the operation and integration of the various modules.
3. Expand functionality and usefulness of the codes.
4. Package and release the codes and full documentation for use at Yankee Atomic.

Each of these items has been addressed as part of the current project and a summary of the work accomplished for each task is given below and a more detailed overview is presented in the attached appendices. The appendices are structured as nearly independent reports for ease of use and for future updating (as needed).

Full testing, validation, and documentation of the methods utilized: The weakest part of the ACTIV system when this project was started was the obvious lack of documentation. This summary report and the attached appendices resolve this deficiency. In particular, a User Guide (Appendix II) has been written that overviews the methods implemented within the ACTIV system and defines all the notation needed to properly interpret the input instructions. In addition, separate documents are available that detail the development of a 47-group activation library based on VITAMIN-B6 and report upon the latest validation results for the JPDR benchmark calculations performed using the new activation library and the BUGLE-96 shielding library (see Appendix III and Appendix IV, respectively). The validation efforts, for example, show good agreement with the JPDR measurements for most points within the reactor vessel (C/E values are within a ±30% range around unity for most experimental points).

One item that still needs further work here is related to the detailed calculations deep within the ACTIV code. In particular, some further testing and enhancements to the matrix exponential solution algorithm (which uses a truncated Taylor series expansion) are probably needed to increase the range of applicability and to improve convergence and efficiency. One obvious change that should improve the numerical stability is the use of a double precision version of the core calculational algorithms. This development activity was planned as part of the current project but other code improvements were given higher priority (and we simply ran out of time).

Documentation relative to the operation and integration of the various modules: The report "User Guide and Sample Problems for the ACTIV Code System" addresses and resolves the goals for this task. In addition to supplying code input documentation, this report (Appendix II) also gives some hints and general guidance for the proper and efficient use of the codes. A series of three sample problems is also discussed briefly, and these illustrate a variety of code options and the proper integration of the individual modules to perform a complete activation analysis. This sample problem sequence is quite simple (uses a simple 1-D model of the Maine Yankee system), but it demonstrates a lot of capability within easy-to-follow examples (shows the use of ACHAIN, ACTMAT, and ACTIV and the coupling and interaction among the various modules). The reader is also referred to the readme file listed in Appendix I (with file name VER2.RME) that briefly identifies, among other things, the various files used for the sample problems.

Expand functionality and usefulness of the codes: This task received a lot of emphasis during the project period, adding functional capability and additional edit as needed to meet the needs of the ongoing Connecticut Yankee (CY) decommissioning project at Yankee Atomic. In particular, all the codes were modified to fix a variety of bugs found during initial testing and to include a consistent set of internal documentation so that the code logic could be followed and easily maintained in future upgrades. Several additional edit options were added (especially to the ACTIV code) and the interface files that link the codes (actlib, chnlib, and matlib) were modified for easier readability and modification by the user (if needed). The most important new features include a filter option in ACHAIN that only selects the parent-daughter-process triplets that eventually lead to a specified set of activation products, and a restart capability in ACTIV that allows one to continue a previous computation using an updated flux file and possibly some other minor changes – but be careful here because the continuation calculation must be essentially identical in most respects (same nuclide vector, mesh layout, nontrivial activation points, etc.). In all, the new versions of the codes represent a significant improvement over previous capability and the codes are now suitable for routine activation analysis studies.

As with any code development effort, there is always additional capability that could enhance the functionality of the overall system. Practical time and funding limitations, however, usually restrict implementation of only the highest priority items. A new gamma source capability, for example, was originally planned as part of the current project, but other developments and testing took precedence over this item. However, this is still considered a potentially significant enhancement. In many practical applications, surface dose measurements will probably be available. Since lots of uncertainty, especially associated with impurity content, is expected, these measurements should be useful for normalizing the ACTIV results. However, at present, the link between the calculated specific activities and an estimate of surface dose is missing. This requires accessing a library of discrete decay photon line data, converting it to multigroup format, and finally generating a multigroup gamma source from the isotope dependent activities to drive a subsequent transport calculation to determine dose at the measured locations. Since ACTIV can compute pointwise activities, one should be able to generate a pointwise decay gamma source and do a rigorous dose rate calculation. With normalization to a few measurements, this can then produce very accurate activity profiles and/or dose rate distributions for a variety of configurations (and also at various time points).

Other potential enhancements to the overall system include:

1. Further testing and enhancements to the matrix exponential solution algorithm (see above).
2. The development of a new activation library that includes more isotopes (the current library based on VITAMIN-B6 is lacking in several important isotopes, some of which are needed for waste classification). A new energy group structure with more thermal groups may also be appropriate.
3. The ability to deal with 3-D flux distribution information (formal coupling of the Rθ and RZ flux results for the ongoing CY activation analyses would have made the activation results easier to manipulate and understand).

4. The capability to visualize many of the space and time dependent quantities computed by ACTIV (densities, activities, scaling factors, etc.). ACTIV could, for example, be modified to write a data file with full space and time dependent information. Then, an auxiliary code could be written to interactively plot a variety of desired quantities for the isotopes of interest.
5. Additional edit and analysis capability. For example, the fractional contribution edit in ACTIV is now based on the activity level. This is useful because it clearly identifies which isotopes are the dominant contributors. If the gamma source capability is implemented (see above), one could optionally rank the isotopes relative to their contribution to the total gamma source (or to actual dose if an approximate source–to-dose conversion factor was available). This capability would allow a different, potentially useful, perspective in terms of what isotopes are most important.

   Another useful edit might be an actual waste classification map by zone (or even mesh) for the important system components. With the detailed activities available for all the important classification isotopes, this capability would be a relatively straightforward, but useful, edit option for the user. This could be provided for several different decay intervals after final shutdown to evaluate the various decommissioning scenarios that are available (and their sensitivity to the shutdown time prior to transport and final disposal).
6. Additional verification testing. At present, the very important, but limited, database of measured data from the JPDR decommissioning project has been used to validate the current codes. Clearly more benchmark data are needed for greater confidence in the overall calculational capability and in ACTIV's ability to predict the induced activity in a variety of locations in the system (especially in regions far away from the active core). Some data from the Rowe decommissioning effort and some experimental data from the CY project could potentially be useful in this activity.
7. Etc. (there are lots of other possibilities here …)

Package and release the codes and full documentation for use at Yankee Atomic: This task simply formalized the final deliverables for this project, and the current report, supporting appendices, and source code and sample problems on the accompanying diskettes complete this item. Appendix I discusses the contents of the distribution disks in more detail. Under this contract with the UMass-Lowell Research Foundation, Yankee Atomic has been given unlimited rights to use and modify the ACTIV sequence of codes (Version 2) as needed, but the codes and associated data libraries shall not be distributed or sold to companies outside of Yankee.

Summary

The completion of the four tasks itemized above formally represent the end of Project No. 05-07741. This work has brought the ACTIV code system for detailed space-energy activation analysis to a production-ready state and it has significantly enhanced the overall functionality of the code system. As always, additional improvements could be made (some possibilities are described above), but the current version of the codes (Version 2) represent a fully functional capability that is somewhat unique in the industry. It is relatively easy to use and it represents a more accurate and more rigorous approach for addressing the long term activation of excore structural components. It should prove to be very useful for addressing a variety of decommissioning scenarios and options.