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Summary

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Inverse Depletion/Decay Analysis Using the SCALE Code System

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INTRODUCTION

The inverse depletion/decay problem is an important element of nuclear forensics—the identification of the origin and history of nuclear material. The standard depletion/decay problem is to predict nuclide inventories given basic irradiation conditions such as reactor type, power level, enrichment, irradiation time, and decay time; nuclide inventories are then calculated using codes such as ORIGEN/ARP.[1] An inverse problem arises if a set of nuclide inventories is known, and it is desirable to predict various depletion/decay parameters that would have resulted in such a nuclide distribution. The code INDEPTH (INverse DEPLEtion THEory) was developed to do this task and has been tested on several simple problems.

DESCRIPTION OF THE METHODOLOGY

The procedure used in this work involves nonlinear least-squares regression using an algorithm outlined by Fletcher.[2] The process requires repeated runs of the ORIGEN/ARP sequence, each of which yields a set of nuclide inventories. The squared error residual is calculated using these computed inventories and the set of inventories from the known values (i.e., from isotopic assay measurements). The algorithm uses a gradient search technique (a combination of the Gauss-Newton and BFGS quasi-Newton approaches) [2] to obtain progressively better parameter estimates, terminating when the sum of the squared error is at or near its minimum. Since ORIGEN/ARP calculations typically take a few seconds, thousands of depletion calculations can be performed in a reasonable amount of time on a modern personal computer.

TEST RESULTS

A test case was constructed by running a simple depletion/decay sequence using the values in the second column of Table I. The inventories of the 38 most plentiful actinides and fission products were stored and used as “data.” The reactor parameters were known and constitute the “exact” solution to the inverse problem (shown in Column 1). Using the nuclide inventories as input, the INDEPTH routine was applied using various initial guesses (values different from the exact solution) for the parameters to be estimated (power, irradiation time, decay time, enrichment); the code was then run to find the optimal choice of the parameters. Three example cases are shown in Table I. In each case, fuel enrichment and decay time are optimized, together with a third parameter used to describe burnup. Example 1 (Columns 3 and 4) comprises a case in which the power level is optimized, while the irradiation time is held constant at its known optimal value. Example 2 (Columns 5 and 6) illustrates a case in which the power level is constant, but the irradiation time is optimized. As seen in the table, both cases result in parameters near the known exact solutions.

Using the particular set (i.e., the 38 most plentiful set) of input nuclides in these examples, it was not possible to properly isolate the individual effects of the power level as opposed to irradiation time in the calculation of burnup, which is typically the independent variable used for fuel exposure. However, a different choice of input nuclides might allow all four parameters to be estimated. A preliminary evaluation was conducted, and a different set of 35 nuclides was selected, some of which were a part of the original nuclide set. This set was used to produce the results for Example 3 in Table I. Using the revised nuclide set, the INDEPTH code was able to successfully estimate all four parameters.

TABLE I. Reactor Parameter Estimation Using Actinide and Fission Product Nuclides.

Parameter	Exact Solution	Example 1		Example 2		Example 3	
		Initial	Final	Initial	Final	Initial	Final
Power (MW/MTU)	35	50	34.85	—	—	30	35.004
Irrad. time (d)	100	—	—	140	99.4	140	99.984
Decay time (d)	365.24	50	368.1	50	357	900	365.17
Enrichment (%)	2	3	1.89	2	1.9	3	2.0006

To provide further validation, the INDEPTH tool was used with measured isotopic data from actual spent fuel assemblies.[3–5] The measured fission product and actinide inventories representing available measured values were not chosen with predictive capability in mind; in some cases, as few as ten nuclides were involved. Therefore, these cases resemble Examples 1 and 2 in Table I in that only total burnup is able to be calculated. The results are shown in Table II, which shows that prediction is generally quite good, even though there is some level of error in both the nuclide inventories and the “actual” parameter values.

The Trino reactor case has an extended intermediate downtime. It can be seen that the code is not currently able to differentiate between intermediate and ending downtimes because it assumes only full-power operation to the target burnup values. Additional capabilities are needed in this area, along with identification of specific nuclides that are sensitive to this activity.

SUMMARY

A method for potential use in nuclear forensics has been developed and tested in this work. The results for both a numerical example and an actual test case have been demonstrated. Further studies are planned to make the procedure more efficient, as well as a sensitivity study to assess the nuclides to be used for predictive purposes.

TABLE II. Prediction of Actual Reactor Fuel Assembly Parameters.

Reactor (Assembly)	Burnup (GWd/MTU)		Decay time (d)		Enrichment (%)	
	Actual	Predicted	Actual	Predicted	Actual	Predicted
Calvert Cliffs (D047)	37.1	34.1	1870	1851	3.04	2.96
Calvert Cliffs (BT03)	46.5	43.5	2447	2832	2.45	2.30
Gosgen (GU3)	52.4	53.0	NA ^a	1332	4.10	4.27
Mihama-3 (87C03)	31.4	28.7	1825	1863	3.24	3.21
Trino (ESL7)	24.5	26.2	10(ext.) ^b	584	3.13	3.35
Turkey Point (D04/RG10)	31.3	30.3	927	1273	2.56	2.52
TMI-1 (D1A2)	55.7	52.6	1711	1563	4.00	4.47
Takahama (SF96-4)	28.9	29.5	0	15.6	2.63	2.90
Takahama (SF97-4)	47.0	46.8	0	1	4.11	4.16

^a Value not currently known.

^b This case had an extended intermediate downtime that affected the results.

REFERENCES

1. *SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluations*, Version 5, ORNL/TM-2005/39, Vols. I-III, April 2005. Available from Radiation Safety Information Computational Center at Oak Ridge National Laboratory as CCC-725.
2. R. FLETCHER, *Practical Methods of Optimization*, Wiley-Interscience, Inc., New York (1987).
3. C. E. SANDERS, I. GAULD, *Isotopic Analysis of High-Burnup PWR Spent-Fuel Samples from the Takahama-3 Reactor*, NUREG/CR-6798 (ORNL/TM-2001/259), Oak Ridge National Laboratory (January 2003).
4. O. W. HERMANN, S. M. BOWMAN, M. C. BRADY, C. V. PARKS, *Validation of SCALE System for PWR Spent Fuel Isotopic Composition Analysis*, ORNL/TM-12667, Oak Ridge National Laboratory (March 1995).
5. M. D. DEHART, O. W. HERMANN, *An Extension of the Validation of SCALE (SAS2H) Isotopic Predictions for PWR Spent Fuel*, ORNL/TM-13317, Oak Ridge National Laboratory (September 1996).