Laboratory Directed Research and Development on Disposal
of Plutonium Recovered from Weapons

John H. Pitts
Jor-Shan Choi

November 14, 1994

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

MASTER

DISCLAIMER

This document was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor the University of California nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial products, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or the University of California, and shall not be used for advertising or product endorsement purposes.

This report has been reproduced
directly from the best available copy.

Available to DOE and DOE contractors from the
Office of Scientific and Technical Information
P.O. Box 62, Oak Ridge, TN 37831
Prices available from (615) 576-8401, FTS 626-8401

Available to the public from the
National Technical Information Service
U.S. Department of Commerce
5285 Port Royal Rd.,
Springfield, VA 22161

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

FY1994 FINAL REPORT

LABORATORY DIRECTED RESEARCH AND DEVELOPMENT ON DISPOSAL OF PLUTONIUM RECOVERED FROM WEAPONS

by

JOHN H. PITTS and JOR-SHAN CHOI

November 14, 1994

SANT94-689JP

MASTER

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

72

TABLE OF CONTENTS

	Page
SUMMARY.....	3
ACCOMPLISHMENTS.....	4
LIBRARY OF RESOURCES.....	4
RAMONA-4B CODE.....	6
U.C. BERKELEY.....	7
LONG TERM CRITICALITY.....	8
DIFFERENCES IN THE U.S. AND RUSSIAN WEAPONS	
PLUTONIUM DISPOSITION OPTIONS.....	8
APPENDICES	
A. U. C. BERKELEY INTRA-UNIVERSITY TRANSFER	
AGREEMENT REPORT	
B. U. C. BERKELEY TECHNICAL REPORT	
C. DETAILS OF LONG-TERM CRITICALITY PROGRAM	

**FY1994 LDRD FINAL REPORT
ON
DISPOSAL OF PLUTONIUM RECOVERED FROM WEAPONS**

SUMMARY

1. Funding received for FY94: \$100,000
2. Tracking Code: 94-SR-060
3. Title: Disposal of Plutonium Recovered from Weapons
4. Principal Investigators: Jor-Shan Choi and John H. Pitts
5. This LDRD was conceived as a multi-year plan to study the use of mixed plutonium oxide-uranium oxide (MOX) fuel in existing nuclear reactors. Four areas of investigation were originally proposed: 1) study reactor physics including evaluation of control rod worth and power distribution during normal operation and transients; 2) evaluate accidents focusing upon the reduced control rod worth and reduced physical properties of PuO_2 ; 3) assess the safeguards required during fabrication and use of plutonium bearing fuel assemblies; and 4) study public acceptance issues associated with using material recovered from weapons to fuel a nuclear reactor.

First year accomplishments include the following:

We set up a library of resources on the disposition of plutonium and associated subjects. Included are the National Academy of Sciences study on Management and Disposition of Excess Weapons Plutonium, contractor reports for DOE's Phase II Plutonium Disposition Study, and numerous other documents.

We obtained a working version of the RAMONA-4B code from Brookhaven National Laboratory. It is operational on LLNL SUN workstations, and a test problem gives identical results to those produced at Brookhaven. This code was developed to simulate operations and reactivity transients in reactors such as a Simplified Boiling Water Reactor (SBWR). Future plans include using RAMONA-4B to evaluate reactor transients and potential accidents due to changes in reactivity when Pu-bearing fuel is used.

We initiated an Intra-University Transfer Agreement with the Department of Nuclear Engineering at U.C. Berkeley, to develop and validate advanced computational capabilities for MOX fueled Advanced Light Water Reactor (ALWR) assembly designs. Berkeley successfully coupled their GTRAN2 code, which calculates flux distribution and k_{eff} , with ORNL's SCALE4.2 depletion code system. The code package uses cross sections that are corrected for self shielding and resonance absorption. These codes now communicate with each other and act as a single package that can be universally applied to a variety of applications. Accurate calculation can be made on single pin geometries as well as the exact configurations present in fuel assemblies. We chose the ABB Combustion Engineering System 80+ reactor to model the effects of MOX fuel on criticality and control. Initial single pin geometry calculations were completed.

We studied the long-term criticality safety concerns when weapons Pu is disposed of in either a mined geologic repository or a deep bore hole. The higher fissile content in MOX spent fuel and/or in vitrified waste forms loaded with 3-7wt% of fissile Pu, affects criticality

safety. If ground water intrudes into the waste burying location, it could mix with the Pu or its decay daughter, uranium, to potentially form a critical system.

We initiated a preliminary study on the different approaches to disposition of weapons Pu by the U.S. and the Russians. In addition to the immobilization and deep hole options for Pu disposition, the U.S. DOE is also studying the use of existing (or evolutionary) thermal reactors for Pu disposition in a once-through fuel cycle. The Russians consider the use of fast reactors (BN-800) for the same purpose, except the fast reactors would probably be used with fuel reprocessing and recycling.

ACCOMPLISHMENTS

Library of Resources

Most research projects include an evaluation of related work. We accumulated a number of reports on Pu disposition during this study. Below is an annotated bibliography of these reports.

1. Omberg, Ronald P. and Walter, Carl E., "Disposition of Plutonium from Dismantled Nuclear Weapons: Fission Options and Comparisons", Lawrence Livermore National Laboratory Report UCRL-ID-113055, February 5, 1993.

The report summarizes and compares 14 fission options provided to the Fission Working Group Review Committee of the U.S. DOE Plutonium Disposition Task Force. Of these options, the committee concluded that the Advanced Light Water Reactor (ALWR) with an all MOX core and the Advanced Liquid Metal Reactor (ALMR) on the once-through cycle can best dispose of 50Mg of plutonium.

2. DOE, Idaho National Engineering Laboratory, "Weapons-Grade Plutonium Dispositioning", Report DOE/ID-10422, Volumes 1 through 4, June, 1993.

INEL provides an independent comparison of 12 reactor vendor options for plutonium dispositioning, evaluates the feasibility of non uranium-bearing plutonium fuel for LWRs, and gives a conceptual analysis of a reactor specifically designed to fission plutonium without producing electricity or tritium. If 90wt% or greater plutonium annihilation is required, INEL concludes that only 4 options are feasible: (1) an ALWR with plutonium-based ternary fuel, (2) a ALMR with plutonium-based fuel or (3) with MOX fuel, and (4) a Modular High Temperature Gas-Cooled Reactor (MHTGR) with plutonium-based fuel.

Plutonium fuels without uranium or thorium are desirable because production of additional plutonium is avoided, but these fuels result in reactors with positive temperature coefficients and reactor control problems. Rare-earth resonance absorbers such as gadolinium, erbium, and europium are attractive materials whose use can mitigate these control problems. INEL presents a reactor with low temperature, pressure, power density, and flow rate that efficiently destroys plutonium but produces no electricity and therefore sacrifices cost.

3. U.S. Department of Energy, Technical Review Committee, "Plutonium Disposition Report", Volumes 1 and 2, July 2, 1993

The Technical Review Committee concludes that fission reactors can effectively convert weapons-grade plutonium into forms undesirable for use in weapons. Three alternatives were considered: (1) a spiking alternative where plutonium is irradiated as quickly as possible to create a radiation barrier to diversion, (2) a spent fuel alternative where weapons-grade plutonium is converted as economically as possible into a form similar to commercial spent fuel, and (3) a destruction alternative where maximum destruction of the amount of plutonium is accomplished. The committee found that the spent fuel alternative is the most practical and economical.

4. Chow, Brian G. and Solomon, Kenneth A., "Limiting the Spread of Weapons-Usable Fissile Materials", Rand National Defense Research Institute, 1993

Five options are examined for dealing with weapons-grade plutonium: (1) use the plutonium as fuel in existing fast reactor demonstrators without reprocessing, (2) use it in LWRs with partial MOX fuel without reprocessing and (3) with all MOX fuel without reprocessing, (4) store the plutonium for 20 years or so, and (5) mix the plutonium with waste or spent fuel that is being prepared for final disposal. The least expensive option is (5) but repositories must be ready to accept this material.

5. U.S. Congress, Office of Technology Assessment, "Dismantling the Bomb and Managing the Nuclear Materials" U.S. Government Printing Office, Washington, DC, September, 1993

The report discusses the process for retiring weapons from active deployment in the military and returning the nuclear warheads to the facilities that manufactured them. Also discussed are the dismantlement of the warheads, subsequent handling of the parts, and storage, control, and ultimate disposition of key nuclear materials from the warheads.

6. National Academy of Sciences, Committee on International Security and Arms Control, "Management and Disposition of Excess Weapons Plutonium", Prepublication Copy, National Academy Press, 1994

Recommendations associated with plutonium disposition are (1) to fabricate and use the plutonium as fuel, without reprocessing, in existing or modified nuclear reactors, (2) vitrify the plutonium in combination with high-level radioactive waste, and (3) consider burial of excess plutonium in deep boreholes.

7. ABB Combustion Engineering, "DOE Plutonium Disposition Study--Screening Study for Evaluation of the Potential for System 80+ to Consume Excess Plutonium", Final Report, April 30, 1994

The report describes the System 80+ reactor in detail, which can be used with up to 100% MOX fuel. The MOX fuel consists of 6.7wt% PuO₂, 2.5wt% Er₂O₃, with the remainder UO₂. No recycling is suggested. Two reactors are needed to burn 50Mg of plutonium in 25 years.

8. General Atomics, "MHTGR Plutonium Consumption Study Phase II Final Report", Report GA/DOE-051-94, April 29, 1994

GA proposes using 600MW_e modules coupled to a direct cycle gas turbine power conversion system. Between 12 and 14 MHTGR modules are needed to burn 50Mg of plutonium in 25 years using a once-through cycle. Net thermal efficiency is 48%. Er₂O₃ is used as a burnable poison to enhance reactor control.

9. GE Nuclear Energy, "Study of Plutonium Disposition Using the GE Advanced Boiling Water Reactor (ABWR)", Report NEDO-32351, April 30, 1994

Two 1350MW_e ABWRs with up to 100% MOX fuel, are capable of burning 50Mg of plutonium in 22 years. The reactors use gadolinium burnable poison. The fuel elements are not recycled.

10. Westinghouse Electric Company, "Plutonium Disposition Study, Phase II Final Report", Report DOE/SF/19683--5, April 30, 1994

Westinghouse proposes four 600MW_e pressurized water reactors to burn 50Mg of plutonium. Criticality is maintained by varying the soluble boron concentration in the water coolant. The reactor, designated the PDR600, is an offshoot of the AP600 reactor.

11. GE Nuclear Energy, "Study of Plutonium Disposition Using Existing GE Advanced Boiling Water Reactors", Report NEDO-32361, June 1, 1994

Three 1155MW_e BWR-5 reactors, using up to 100% MOX fuel, can burn 50Mg of plutonium in 23 years. Gadolinium burnable poison is again used to enhance reactor control.

RAMONA-4B Code

Brookhaven's RAMONA-4B code simulates normal operation, reactivity transients, and instability issues in an SBWR. Neutron kinetics calculations in the reactor core, modeled in three dimensions, are coupled to multiple parallel-channel thermal hydraulics in the pressure vessel, recirculation loops, and steam lines. The thermal hydraulics uses a drift flux model with explicit integration. A number of improvements were incorporated from its predecessor, the RAMONA-3B code, including use with natural circulation channels and isolation condensers, flow dependent loss coefficients, balance of plant, boron circulation, and standby liquid control systems. Details of the code are found in Brookhaven's report NUREG/CR-3664, BNL-NUREG-51746, "A Description and Assessment of RAMONA-3B MOD.0 Cycle 4: A Computer Code with Three-Dimensional Neutron Kinetics for BWR System Transients" by W. Wulff et al., published in January, 1984. A manual for the RAMONA-4B code is being written at Brookhaven but has not been completed.

We obtained the code from Brookhaven, through a request to the NRC, for evaluation of potential control problems, reactor transients, and accidents caused by changes in reactivity when plutonium bearing fuel is used in BWRs. The code is now operational on LLNL's SUN workstations. A sample problem supplied by Brookhaven, gave identical results on LLNL computers. The license agreement signed in order to obtain the code restricts further distribution and does not permit use of

the code on foreign reactors. The contacts at Brookhaven is Alexander N. Mallen, (516) 282-2230 and U. S. (Kumar) Rohatgi, (516) 282-2475.

The code is complex and development of input files requires not only understanding of reactor analysis in general but also reactor neutronics and two-phase thermal hydraulics. A typical input takes several person-months to develop. We are presently evaluating if the effort necessary to develop inputs, understand the physics in the code, and make code changes as required for use with plutonium bearing fuel is within expected future budget allocations.

U.C. Berkeley

A \$20K Intra-University Transfer Agreement with U.C. Berkeley was consummated to model the effect of MOX fuel on reactor criticality and control. Principal investigators are Professors Jasmina Vujic and Ehud Greenspan of the Department of Nuclear Engineering. Berkeley's two-dimensional transport code, GTRAN2, was successfully coupled to ORNL's SCALE 4.2 modular code system that includes ORIGEN-S. The SCALE4.2 system provides cross sections corrected for resonance self shielding and resonance, and performs depletion calculations. These coupled codes now communicate with each other and act as a single code package, renamed GT-SCALE, that can be universally applied to a variety of applications. Accurate calculations can be made on single pin geometries as well as the exact configurations present in fuel assemblies.

GTRAN2 solves the multigroup steady-state neutron integral transport equation to determine the flux distribution in the reactor and k_{eff} . The code combines the geometric flexibility of Monte Carlo methodology with the computational efficiency of deterministic codes. Given macroscopic cross sections, the code solves an eigenvalue problem and gives the volumetric flux and incoming/outgoing current distributions. GTRAN2 also calculates the reaction rates. It performs an exact numerical integration to obtain collision, escape, and transmission probabilities for an assembly (or any region of interest). A modified combinatorial geometry processor is used to perform ray tracing, that permits detailed descriptions of complex and irregular assembly geometries. GTRAN2 is computationally efficient, using several orders of magnitude less computer time for the same accuracy obtained using the VIM Monte Carlo code.

The GT-SCALE code package has a number of unique features including the following:

1. a general two-dimensional geometry simulation capability that can accurately simulate fuel assemblies of any geometry, including hexagonal, square, and cluster assembly configurations,
2. ability to account for all heterogeneities within the fuel assembly to any degree of detail,
3. highly accurate and detailed space-dependent burnup calculations using the extensive data base available in SCALE4.2 with separate calculations for segments of the fuel (or burnable-poison) rods,
4. a multi-assembly simulation capability,
5. a comprehensive, continuously maintained data base as is provided by the SCALE4.2 code package,
6. flexibility in energy-group structuring due to the availability of a very fine structure multigroup master cross section library and the capability to collapse this library into any number of groups.

We chose the ABB Combustion Engineering System 80+ reactor to model the effects of MOX fuel on criticality and control. A SCALE4.2/GTRAN2 fuel-clad-moderator pin cell geometry for the System 80+ reactor, where the moderator has a square shaped outer boundary, was chosen as an initial test problem. Results were compared to those calculated using the SCALE4.2 system

alone, which only accepts an outer boundary that is circular. Values of k_{eff} were nearly identical (1.09459 vs. 1.0457 with MOX fuel and 0.99400 vs. 0.998267 with MOX fuel mixed with Erbium oxide). Reaction rate results were also in very close agreement. This test problem showed that for a pin cell geometry, the coupled SCALE4.2/GTRAN2 code package gave the same result as calculations with a well established and benchmarked code system (SCALE4.2). However, in the case of more complex geometries such as present in fuel assemblies, the SCALE4.2 system cannot give accurate results because it uses simplified modeling of the fuel assembly as a cylinder with one fuel zone. For fuel assembly geometries, particularly those with significant heterogeneity, the SCALE4.2/GTRAN2 coupled package gives much more accurate results due to the exact modeling of all geometrical details, and because the package has a space-dependent burnup capability.

It should be pointed out that GT-SCALE can be applied to accurately simulate (model) MOX fuel assemblies of any LWR design, as well as other reactor types. Details of this work can be found in Appendices A and B, which are U. C. Berkeley's intra-university transfer agreement report and a technical paper submitted for publication.

Long Term Criticality

The National Academy of Sciences Study (see our Library of Resources #6) has suggested that excess Pu could be disposed of by irradiation in nuclear reactors, or by immobilization into high-level waste glass followed by direct-disposal in a geologic repository, or by burying the Pu in 4-km-deep boreholes sealed with bentonite clay and concrete. All of these Pu-disposition options generate one or more final disposal waste-forms that require evaluation of long-term criticality safety.

Long term criticality safety concerns arise because the fissile contents (i.e. ^{239}Pu and its decay daughter ^{235}U) in these Pu-disposed waste-forms are higher than that in LWR spent UO_2 fuel. MOX spent fuel could contain 3 to 4 wt% of reactor-grade plutonium, compared to only 0.9wt% of Pu in the LWR spent UO_2 fuel. For the immobilization and the deep borehole options to be economically viable, a Pu content of 3 to 7wt% in the waste-forms would be needed. If these waste-forms were disposed of in a geological repository or a deep borehole, at some future long time (tens of thousand of years) when the waste-forms have deteriorated, intruding ground water could mix with the long-lived fissionable materials to form a critical system. If the critical system is self-sustaining, fission products produced could readily be available for dissolution and release to the accessible environment.

We are evaluating the long-term criticality safety associated with disposition of fissionable material in a geologic setting. Issues to be addressed include the identification of worst-case water-intrusion scenarios and waste-form geometries which present the most concern for long-term criticality safety. Suggestions for technical fixes will be included. Details of this program are found in Appendix C.

Differences in the U.S. and Russian Weapons Plutonium Disposition Options

The agreement between the United States and the Russian Federation at the end of the cold war to dismantle as many as 40,000 nuclear weapons will result in the accumulation of as much as 100 metric tonnes of excess weapons plutonium from both countries. This excess weapons Pu will need to be disposed of safely. As a result, both the U.S. and Russia have to seriously consider how they could safely store or dispose of large amounts of excess weapons plutonium.

But so far, neither country is anywhere close to reaching a consensus on the issue, and the problem of what to do with this excess fissile material remains a subject of speculation or debate. Jor-Shan Chui briefly summarized the similarities and differences of the intended approaches taken by both sides as follows.

Similarities:

The actual quantities of weapons plutonium in the stockpiles in the two countries are still classified. However, each side agrees that 50 metric tonnes of the weapons plutonium would be declared excess.

The predominant form of the excess weapons plutonium is metal from "pits". However, both countries have plutonium residues in various chemical forms (oxides, hydrides, nitrides, nitrates, etc.) and physical conditions (solid, scraps, chips, aqueous solution, etc.). It is this residual plutonium which presents the problem in worker's health and safety, and vulnerability for safeguards and security.

Both countries are required to store the weapons plutonium dismantled from nuclear weapons in interim storage facilities for an indefinite time period.

Neither country has a plutonium recycling program for civilian nuclear reactors. Neither has industrial-sized MOX fabrication facilities which could support a large-scale reactor-based plutonium disposition program.

Differences:

The disagreement between the two countries in weapons-plutonium disposition is that the U.S. regards the plutonium to have no value in the near future (may even have negative value for certain disposition options), while the Russian Federation considers the plutonium to have intrinsic energy value that could be exploited within a few decades.

In the U.S. the predominant viewpoint is to get rid of the excess weapons plutonium either by: (1) convert the plutonium metal pits into oxide, mix the plutonium oxide with uranium oxide into fabricated MOX fuel, and irradiate the fuel in existing, or modified thermal reactors; or (2) immobilize the weapons plutonium into vitrified glass or ceramic products with or without defense high-level wastes; or (3) dispose the weapons plutonium in deep boreholes 4 to 10 km deep and sealed with bentonite. The spent MOX fuel and the vitrified glass or ceramic would be disposed of in a geologic repository.

In the Russian Federation, the persistent viewpoint is to retain the excess fissile material for the eventual use for power generation in either breeder reactors or other, as yet undesigned, advanced reactors or accelerator concepts.

There is a sense of urgency on the U.S. side to disposition the weapons plutonium, however, the Russian do not seem to be in any hurry to dispose of their share. The U.S. approach to immobilize the Pu into waste form for direct-disposal, or to bury the Pu in deep holes would, most likely, not be acceptable to the Russians because they do not consider Pu as waste. Disposition of the Pu by irradiation in Russian's existing thermal reactors, RBMKs, is not desirable because of the additional safety problems induced by the use of Pu in a reactor already plagued with insufficient safety provisions. The Russian approach of using advanced breeder reactors or accelerators for disposition of weapons plutonium is deemed unacceptable to the U. S. because of the U.S. opposition to the use of reprocessing and recycling of special nuclear material in the advanced reactor/accelerator fuel cycle.

It appears that the U.S. has a more effective accountability and control systems on nuclear material than the Russian Federation, in light of the recent incidents involving theft and diversion of nuclear material from the Russian Federation.

Appendix A

U.C. Berkeley Intra-University
Transfer Agreement Report

by

Professors Jasmina L. Vujic and Ehud Greenspan
Department of Nuclear Engineering
University of California, Berkeley
Under Contract Number B283667

September 1994

UCBNE-NRP-942

Development and Validation of Advanced Computational Capability for MOX Fueled ALWR Assembly Designs

Final Report

by

**Jasmina L. Vujic and Ehud Greenspan
Department of Nuclear Engineering
University of California, Berkeley
Under Contract Number B283667**

Prepared for

**Dr. Jor-Shan Choi and Dr. John Pitts
Fission Energy and Systems Safety Program
Lawrence Livermore National Laboratory**

September 1994

TABLE OF CONTENTS

1.0	ABSTRACT.....	1
2.0	SUMMARY OF ACCOMPLISHMENTS.....	1
3.0	IMPORTANCE OF AN ACCURATE ANALYSIS AND DESIGN TOOL FOR MOX FUELED CORES	2
4.0	COMPONENTS OF THE NEW CODE SYSTEM.....	5
4.1	Selection of the Code Systems.....	5
4.2	The GTRAN2 Code System	6
4.3	The SCALE 4.2 Code Package.....	7
5.0	DESCRIPTION OF COMPUTATIONAL STRATEGY FOR GT-SCALE.....	9
5.1	The SAS2H Strategy	9
5.2	The GT-SCALE Strategy	10
5.3	Transport Corrected Cross Section Generation for GTRAN2.....	10
6.0	TESTING AND BENCHMARKING.....	13
6.1	Single Fuel Pin Test Problem: Description	13
6.2	System 80+ Control Rod Description	16
6.3	System 80+ Burnable Poison Rod Description.....	17
6.4	Assembly Test Case Based on System 80+ Design	18
7.0	UNIQUE FEATURES OF GT-SCALE	20
8.0	DISCUSSION	28
9.0	SUMMARY	28
	ACKNOWLEDGEMENTS	29
	REFERENCES	29
	APPENDIX A	31
	APPENDIX B	35

LIST OF TABLES

TABLE 1.	Results for Infinite Multiplication Factor	14
TABLE 2.	Comparison of Reaction Rates (normalized to one neutron absorption): UO ₂ -PuO ₂	15
TABLE 3.	Comparison of Reaction Rates (normalized to one neutron absorption): UO ₂ -PuO ₂ -Er ₂ O ₃	15
TABLE 4.	Three-Group Weighting Factors Calculated by COUPLE.....	15
TABLE 5.	Selected One-Group Cross Sections	16
TABLE 6.	Selected Nuclide Concentrations after 50 Days of Irradiation	16
TABLE 7.	Control Rod Lattice Cell Composition	17
TABLE 8.	Burnable Poison Rod Lattice Cell Composition	18
TABLE 9.	TASK DESCRIPTION AND MILESTONES	34

LIST OF FIGURES

FIGURE 1.	SCALE 4.2 System Components	8
FIGURE 2.	Geometrical Configurations Permitted in SCALE 4.2 with XSDRNPM-S	9
FIGURE 3.	Overall Strategy for Coupling SCALE 4.2 and GTRAN2 into GT-SCALE	11
FIGURE 4.	The Pin Cell Geometry for GTRAN2 and SCALE 4.2/CSASN	14
FIGURE 5.	Control Rod Lattice Cell	17
FIGURE 6.	Burnable Poison Rod Lattice Cell	18
FIGURE 7.	Exact Geometric Representation of the System 80+ Assembly Design for GT-SCALE	19
FIGURE 8.	GTRAN2 Unique Geometry Description Capability	20
FIGURE 9.	Normalized Fission Rate per Unit Energy (218-Group Library, No Er)	22
FIGURE 10.	Normalized Fission Rate (218-Group Library, No Er)	23
FIGURE 11.	Normalized Fission Rate per Unit Energy (27-Group Library)	25
FIGURE 12.	Fission Rate (27-Group Library, No Er)	26
FIGURE 13.	Fission Rate (27-Group Library, With Er)	27

PROJECT PARTICIPANTS

Professor Jasmina L. Vujic

Professor Ehud Greenspan

Steve Slater

Todd Postma

Greg Casher

Ibson Soares

1.0 ABSTRACT

The reactor route to the disposition of weapons grade plutonium could be accomplished by utilizing the existing LWRs or by developing new reactor concepts specifically designed for plutonium burning. Our study has been focused on the development of a computer code system which will enable to accurately study the influence of neutron spectrum in the Mixed Oxide (MOX) - UO_2 fueled cores (dependent on the particular design) on reactivity as well as on exposure dependent isotopic compositions. This code system is being developed by "marrying" two existing state-of-the-art methodologies - GTRAN2 and SCALE 4.2. The resulting code system, GT-SCALE, possesses several unique characteristics: exact 2D representation of a complete fuel assembly, while preserving the heterogeneity of each of its pin cells; flexibility in the energy group structure, the present upper limit being 218 groups; a comprehensive cross-section library and material data base; and accurate burnup calculations. The resulting GT-SCALE is expected to be very useful for a wide variety of applications, including the analysis of very heterogeneous UO_2 fueled LWR fuel assemblies; of hexagonal shaped fuel assemblies as of the Russian LWRs; of fuel assemblies for HTGRs; as well as for the analysis of criticality safety and for calculation of the source term of spent fuel.

2.0 SUMMARY OF ACCOMPLISHMENTS

We have proposed to combine and modify existing state-of-the-art methodologies employed in GTRAN2 and in SCALE 4.2 or EPRI-LWR code packages, to perform accurate (and computationally efficient) reference calculations with detailed representations of energy and two dimensional geometrical configurations for the MOX fueled assemblies. The scope of work and budget for Phase I, as well as the task description and milestones are included in Appendix A.

Regardless of the delays in the budget approval (the budget was approved starting June 16 instead of June 1), as well as the problems in implementation of the SCALE 4.2 code system on our Sun Unix network (the SCALE version obtained from ORNL was optimized for the IBM RISC workstations not for the Suns), we were able to accomplish most of what we proposed to do.

Step 1: Selection of the code systems. We have analyzed possible strategies of coupling GTRAN2 with the SCALE 4.2 system or with the EPRI's ARMP-02 system. The latest had certain advantages, because it was already developed and optimized for the LWR analysis and design. We were also more familiar with the EPRI's ARMP-02 system. However, the license that we received from EPRI limited the possible use of this system. In addition, we concluded that the SCALE 4.2 system had more accurate resonance and self-shielding calculations, larger, comprehensive, and continuously maintained nuclear and cross section data bases, flexibility in energy-group structuring, as well as more accurate and detailed burnup calculations. Thus, we decided to focus on developing strategy for the SCALE 4.2/GTRAN2 coupling.

Step 2: Development of the overall strategy for GTRAN2/SCALE 4.2 coupling. The SCALE 4.2 system was requested from Oak Ridge National Laboratory, and implemented on the Sun Unix workstation network at the Department of Nuclear Engineering. The SCALE 4.2

code system consists of large number of functional modules, data bases, and control modules, with many ways of combining them. Computational sequences of functional modules are automated, reducing the user's need to interact with the SCALE system. However, this feature of the SCALE system caused major difficulty for us, because many interface files and data libraries that system uses were "hidden". Thus, we spent considerable time in learning the details of how the SCALE system works, and what each module is supposed to do. Finally, we were able to develop an overall strategy for coupling SCALE 4.2/GTRAN2 into a new GT-SCALE system, by writing new interface codes and modifying SCALE 4.2 modules. The GT-SCALE code system is currently fully operational, although some additional work is needed to have it completely automated.

Step 3: GT-SCALE benchmarking. We decided to do extensive benchmarking at the pin cell level. The only part in the GT-SCALE system that deals with two-dimensional full assembly geometries is GTRAN2. The ability of GTRAN2 to accurately handle highly heterogeneous 2D assemblies of LWRs and HTGRs has been illustrated, by comparing against Monte Carlo calculations. The GTRAN2 vs. Monte-Carlo benchmark calculations are summarized in Appendix B. The other parts of GT-SCALE are to deal with a single pin cell (CSASN) or a single zone (COUPLE-ORIGEN). We developed two sets of pin cell test cases based on the CE System 80+ design: one with UO_2 - PuO_2 and the other one with UO_2 - PuO_2 - Er_2O_3 . The results obtained using the original SCALE 4.2/CSASN procedure and the GT-SCALE system were in excellent agreement. We also developed test cases including the System 80+ control rod and burnable poison rod.

Step 4: Preliminary analysis of System 80+ fuel assembly design with burnup calculations. Again, we decided to perform burnup calculation on a single fuel pin cell, in order to be able to compare GT-SCALE results with SCALE 4.2/SAS2H burnup calculations. We found an excellent agreement between the results, which gave us confidence in getting good GT-SCALE burnup results for full heterogeneous assembly test cases. We do have everything prepared and developed for the full assembly burnup calculations with GT-SCALE, and we will be performing this type of analysis in the near future.

3.0 IMPORTANCE OF AN ACCURATE ANALYSIS AND DESIGN TOOL FOR MOX FUELED CORES

The solution of the Boltzmann transport equation for the neutral particle distribution in a nuclear reactor remains one of the most computationally-intensive applications in engineering and science. A 3D transport analysis of the entire reactor core is still beyond the capability of current machines (and algorithms). A particularly difficult challenge is to be able to keep all geometrical details in large domains while preserving accurate mathematical models of the physical phenomena. Current and particularly future nuclear reactor designs show large heterogeneity effects due to complex configurations and require computational methodologies that can efficiently and accurately analyze and predict their behavior.

So far, the only computational methodology with these properties was Monte Carlo (MC). However, due to a probabilistic nature of Monte Carlo method, large number of particle histories is usually needed to reduce stochastic uncertainties. This is particularly the case when one requires

the detailed distribution of a dependent variable, such as spatial profiles of dose, flux, or power. If the cell size is small, the number of particle histories contributing to the dependent variable in that cell is also small, and, consequently, leads to an unacceptable increase in statistical uncertainty in the estimate of the dependent variable. So far, due to the above mentioned problems, Monte Carlo depletion calculations are not done. On the other hand, the deterministic methods available today (finite element, finite difference, Sn,...) suffer from the common problem - they cannot be easily and naturally extended from one- to two- or three-dimensional configurations without any change in the methodology. Similarly, it is not an easy transition to go from homogenized to complex heterogeneous configurations.

Generally speaking, MOX fueled LWR cores can be more heterogeneous than UO₂ fueled LWR cores. The extra heterogeneity of the MOX fueled cores is, usually, introduced in the fuel pin cell and in the assembly levels. This extra heterogeneity has important implications on the performance characteristics and, in particular, on safety related characteristics of the MOX fueled LWRs.

Consequently, it is of utmost importance to have neutronic design tools which are capable of accurate simulation of MOX fueled fuel assemblies. In the following we shall briefly review some of the unique features of MOX fueled assemblies which contribute to the enhanced heterogeneity and, hence, to the improved simulation capability.

1. Significant increase in the absorption (and fission) cross-sections.

The thermal XSEC of Pu-239 is, approximately, 50% higher than that of U-235. Moreover, the low energy resonance of Pu-239 extends well into the thermal energy range. These can lead to relatively steep flux gradients within the MOX fuel rod, and between adjacent uranium-oxide and MOX fuel rods.

2. Checker board core arrangement.

Most of the MOX containing LWR cores considered so far were to have MOX fuel loaded in 1/3 of the core, while the other 2/3 were to be fueled with uranium-oxide. The resulting "checker board" (or "color-set") core configuration will feature relatively strong flux gradients between adjacent assemblies loaded with the different fuel. Most of the conventional assembly codes can not take accurately into account this kind of interaction.

3. Extra use of bulk burnable poisons.

Many designs of MOX fueled LWR cores call for the incorporation of burnable poison in the MOX fuel pellets. For example, one of the Combustion Engineering core design for their system 80+ reactor¹ calls for the incorporation of 1.8 wt% erbium oxide in all the MOX fuel pellets. The erbium enables to load into LWR cores MOX fuel featuring higher plutonium concentrations than possible otherwise, without sacrificing the safety of such cores. For example, the erbium assures a negative moderator temperature coefficient of reactivity throughout the cycle, even when the soluble boron concentration in the water is high. The incorporation of erbium, along with an increase in the plutonium loading, increase the flux gradients. The ability to accurately predict the deple-

tion of the erbium and the burnup of the fuel in such assemblies is more computationally demanding than in present day LWRs.

4. Use of burnable poison coated cladding.

Some of the MOX fuel rods are designed to have a coating of a strong absorbing material, so as to aid conventional burnable poisons to compensate for the excess reactivity of the MOX fuel. For example, one of the designs² for the Westinghouse AP600 plutonium burner core calls for the use of coating made of zirconium diboride. Such a coating will increase the thermal flux gradient in MOX fueled rods, and thus contribute to the heterogeneity of the pin-cells and assemblies containing such rods.

5. Augmentation of the number of control elements.

Another consequence of the relatively large absorption cross-section of plutonium, of the relatively high loading of plutonium in the fuel, and of the relatively large amount of burnable poisons incorporated within the MOX loaded LWR cores is a reduction of the reactivity worth of a control rod. To compensate for this effect, many of the LWRs designed to burn plutonium call for an increase in the number of control elements. This contributes to an increase in the heterogeneity of the fuel assembly.

6. Introduction of water rods.

Certain PWRs aimed at burning plutonium are designed to have a higher moderator-to-fuel volume ratio than conventional PWRs; the extra moderation makes the neutron spectrum of the MOX fueled reactor similar to the spectrum of conventional PWRs which are fueled with uranium-oxide. In one of the French designs,³ for example, the enhanced moderation is to be obtained by replacing about 15% of the fuel rods in the assembly by "water rods". The water rods constitute small thermal flux "traps" which increase the thermal flux gradients within the fuel assembly and, hence, the assembly heterogeneity. Most of the assembly simulation codes can not accurately account for the effect of such water rods.

7. Use of non-fissionable resonance absorbers.

Some of the novel concepts for LWR cores for plutonium disposition call for the replacement of the major fertile isotopes (primarily, U-238) by a non-fissionable, non-fertile material (so as to eliminate the generation of additional plutonium in the LWR designed to dispose of plutonium). In the concept described in Ref. 4, for example, tungsten is proposed for the non-fuel material. Having strong absorbing resonances, the substitution of tungsten for U-238 can assure a negative doppler reactivity coefficient - a very important safety feature. The need to accurately simulate fuel rods containing strong resonance absorbers such as tungsten may require improved computational capability.

8. Going to higher burnups.

Certain designs of LWR cores for plutonium disposition call for higher fuel burnups than customary in contemporary LWRs. The higher the burnup, the more heterogeneous the assembly

becomes, and the more demanding is the accurate simulation of the neutronic behavior of the fuel assemblies.

9. Possible use of HTGRs.

High temperature gas cooled reactors are being considered as possible supplements to LWRs for plutonium disposition. In fact, the HTGRs offer a unique disposition possibility: achieving extremely high burnups (i.e., disposition of most of the plutonium) without the need for fuel reprocessing. The HTGR fuel assemblies have strong heterogeneities, and feature hexagonal cross-section area. These characteristics make the HTGR fuel assemblies very difficult to accurately simulate. The presently available simulation tools are unsatisfactory.

Most of the existing assembly-level code systems in use cannot accurately account for one or more of the above described heterogeneities. A large number of lattice physics codes homogenize pin cells for the assembly level calculations. Moreover, many of the assembly codes are set to simulate one assembly at a time, and cannot accurately account for the actual interface currents between assemblies of highly different compositions. Thus, we have proposed to develop an advanced methodology based on GTRAN2, a 2D general geometry transport theory code.⁵ A brief description of a new assembly code system under development, which is free of above mentioned deficiencies is given in the next Section.

4.0 COMPONENTS OF THE NEW CODE SYSTEM

4.1 Selection of the Code Systems

Two possible approaches have been analyzed: first, to combine GTRAN2 with the Oak Ridge National Laboratory SCALE 4.2 modular code system⁶ that includes ORIGEN-S for fuel depletion calculations, and second, to combine GTRAN2 with the Electric Power Research Institute LWR code package ARMP-02.⁷

In the SCALE calculation sequence, the one-dimensional discrete ordinates (Sn) transport code XSDRNPM-S is used to calculate averaged fuel cross sections that are applied in the ORIGEN-S isotope depletion code. Thus, the actual 2D geometry of fuel assemblies is modeled by a 1D geometry, which severely reduces the accuracy of the calculations, particularly in the case of MOX fuel. Approximations and restrictions imposed upon the SCALE package by the 1D geometry approximation can be removed by replacing the XSDRNPM-S module of SCALE, by the general geometry two-dimensional transport theory code GTRAN2, and adapting some functional and control modules of the SCALE depletion sequence. On the other hand, GTRAN2 gets access to the AMPX master library that includes more isotopes and reaction types than in most of the reactor physics codes. In addition, the SCALE depletion sequence greatly improves the accuracy of the decay chains and solves the burnup equations for the full isotopic matrix.

The EPRI LWR calculation sequence includes the CPM-2 code. This code is a multigroup two-dimensional transport theory code for burnup calculations of conventional LWR assemblies or simple pin cells. The nuclear data library contains microscopic cross sections in 69 energy groups. Effective resonance cross sections are calculated individually for each fuel pin. The trans-

port calculations are first done in simple pin-cell geometry (up to 4 spatial regions and 69 energy groups), using the collision probability method for 1D cylindrical geometry. As spatial detail is increased to the two-dimensional form, regions containing cylindrical geometries are spatially homogenized and the many-group cross sections are collapsed to few groups (maximum 12), using flux and volume weightings. The two-dimensional calculation is based on the simplified collision probability method for rectangular homogenized cells. As a result, the eigenvalue and flux distribution for geometrically and spectrally complex fuel assemblies (such as MOX fuel assemblies) is not accurate. In order to remove these restrictions and approximations, the 2D calculation in CPM-2 was planned to be replaced by the general geometry two-dimensional transport theory code GTRAN2.

However, the license that we received from EPRI limited the possible use of this system. In addition, we concluded that the SCALE 4.2 system had more accurate resonance and self-shielding calculations, larger, comprehensive and continuously maintained nuclear and cross section data bases, flexibility in energy-group structuring, as well as more accurate and detailed burnup calculations. Thus, we decided to focus on developing strategy for the SCALE 4.2/GTRAN2 coupling into a new code system, GT-SCALE

We have analyzed the following code systems to determine the overall computational methodology to be used for detailed assembly level depletion calculations:

4.2 The GTRAN2 Code System

GTRAN2⁸⁻¹² solves the multigroup steady-state neutron integral transport equation in arbitrary two-dimensional geometries that can be described by combinatorial geometry. The code combines the geometric flexibility of Monte Carlo methodology, with the computational efficiency of the deterministic codes. Given macroscopic cross sections, it solves an eigenvalue problem and gives the volumetric flux and incoming/outgoing current distributions. GTRAN2 also calculates the reaction rates and few group constants for nodal codes. GTRAN2 is based on the rigorous collision/transfer probability (CTP) method. It performs an exact numerical integration in order to obtain collision, escape, and transmission probabilities for an assembly (or any region of interest). A modified combinatorial geometry processor, is used to perform ray tracing. The use of combinatorial geometry permits a detailed description of complex and irregular assembly geometries in one, two, and three dimensions. The eigenvalue equations are derived assuming isotropic scattering (basic version of GTRAN2) or linearly anisotropic scattering. The double P_0 expansion of the angular flux on the outer assembly boundary is used. The final equations involve the volumetric flux and incoming/outgoing current distributions. This system of equations is solved by an iterative method.

Combinatorial geometry input for standard PWRs and BWRs is generated by a preprocessing code starting from the simple engineering-type input. Geometrical preprocessing is done ONLY ONCE, and the calculated geometric data are repeatedly used for all energies and burnup steps. VECTOR and PARALLEL processing is used to reduce CPU and wallclock times. GTRAN2 plots the fine mesh, edit region, and/or material layouts. It also generates 3D and/or contour plots of flux and power fine mesh distributions. A preprocessing code GIN is used for preparing a combinatorial geometry input data for GTRAN2. Also, GTRAN2 generates 3D and/or contour plots of flux and power fine mesh distributions.

GTRAN2 author, Jasmina Vujic, has recently been awarded a United States Patent (US Patent No. 5,267,278) for her novel methodology employed in this code. More details on the GTRAN2 transport methodology and benchmarking is given in Appendix B.

4.3 The SCALE 4.2 Code Package

The SCALE code system has been developed at Oak Ridge National Laboratory to perform standardized computer analysis for licensing evaluation. The system is widely used in the US and abroad by government contractors, private industry, and universities to perform:

- Problem-dependent multigroup cross section processing,
- Criticality safety analyses
- Shielding analyses,
- Heat transfer analyses, and
- Spent fuel and high-level waste characterization.

The SCALE system consists of functional modules, data base and control modules (Figure 1). Many sequences of functional modules are automated, reducing the user's need to interact with the SCALE system. These sequences perform the necessary cross-section preparation, and manipulation of functional modules (various computer codes) that are needed for particular calculations. The user needs to prepare a single set of input cards for the control module corresponding to particular sequence. The control module uses the input to derive additional parameters that the user does not need to know, and prepare the input for each of the functional modules in the sequence.

Functional Modules in the SCALE System. Only those functional modules considered to be part of the new system will be reviewed here:

NITAWL-S uses the Norheim Integral Technique to perform neutron cross-section processing in the resonance energy range. A fine energy group calculation of the slowing-down flux across each resonance is calculated with subsequent flux weighting of the resonance cross sections. The generated cross-sections will be problem-dependent.

BONAMI-S performs resonance shielding through the application of the Bondarenko shielding factor method. It is always used in conjunction with NITAWL-S, and produces a problem-dependent cross section master library for the SCALE system.

XSDRNPM-S is a one-dimensional discrete ordinates transport code for performing neutron or coupled neutron-gamma calculations. It prepares cell-averaged cross section and fluxes for subsequent one-dimensional criticality safety, radiation shielding and depletion calculations (in ORIGEN-S).

COUPLE is used to update ORIGEN-S libraries with flux-weighted cross sections provided by XSDRNPM-S. COUPLE uses multigroup fluxes from XSDRNPM-S to calculate THERM, RES, and FAST, the thermal spectral parameters used in ORIGEN-S.

ORIGEN-S is a part of the SCALE package and it is a zero-dimensional isotopic generation and depletion code. The code utilizes cross section libraries developed for a variety of particular reactor designs. The libraries include spectrum averaged three-group cross sections for heavy metals, fission products, and structural materials. Exposure dependent fission and radiative cross sections are included for a number of heavy metals. The system enables to update the cross sections used by ORIGEN-S to account for the spectrum variation with depletion.

Data Base in the SCALE System. The data base includes the cross-section libraries, a standard composition library, data libraries required by ORIGEN-S, and a thermal property library (Fig. 1). For our analysis we used the 27-group burnup library, as well as 218-group library.

Control Modules in the SCALE System. A variety of control modules have been developed within the SCALE system to automate and standardize various sequences. Two control modules were used in our calculation: CSASN and SAS2H.

FUNCTIONAL MODULES	DATA BASE	CONTROL MODULES
NTIAWL-S	218 GRP. ENDF/B-IV	CSAS1
BONAMI-S	27 GRP. ENDF/B-IV	CSAS2
ICE-S	123 GRP. GAM-THERMOS	CSAS4
COUPLE	16 GRP. HANSEN-ROACH	SAS1
KENO-IV	18 GRP. GAMMA	SAS2
KENO-V.a	27-18 GRP. COUPLED	SAS3
XSDRNP-S	22-18 GRP. COUPLED	SAS4
MORSE-SGC	STANDARD COMPOSITIONS	HTAS1
XSDOSE	ORIGEN-S DATA LIBRARIES	
ORIGEN-S	LLNL THERMAL PROPERTIES	
HEATING6	CRITICAL EXP. INPUT DATA	
JUNEBUG-II		
HEATPLOT		
REGPLOT		
PLORIGEN		
Available in SCALE-4:	INFORMATION PROCESSOR MARS GEOMETRY PACKAGE SUBROUTINE LIBRARY DRIVER	

FIGURE 1. SCALE 4.2 System Components

5.0 DESCRIPTION OF COMPUTATIONAL STRATEGY FOR GT-SCALE

5.1 The SAS2H Strategy

The control module SAS2H incorporated within the SCALE 4.2 system was originally set to perform depletion calculation in the following sequence: First, calculation is performed for a single fuel pin, assuming an infinite lattice of identical pins. BONAMI-S and NITAWL-II are run first to prepare problem-dependent cross sections through resonance self-shielding calculations. Then, XSDRNPM-S is called to perform 1-D discrete ordinates calculation for a pin cell and to prepare homogenized cell cross sections.

Secondly, the effect of water rods, burnable poison rods or control rods on the average assembly spectrum is estimated by re-applying XSDRNPM-S to a macro-cell, as illustrated in Figure 2. This different pin type is placed in the center of a large cylindricized assembly. A buffer region made of the homogenized pin cell generated in the first phase is placed around the central pin. The ratio of the volume of the buffer zone to the volume of the central cell is equal to the ratio of the number of regular fuel rods to the non-standard rods in the actual fuel assembly.

FIGURE 2. Geometrical Configurations Permitted in SCALE 4.2 with XSDRNPM-S

Thirdly, the above second step can be repeated to account for the effect of other non-standard rods on the assembly spectrum.

Finally, the representative assembly spectrum obtained with XSDRNPM-S is being used in COUPLE for generating effective one-group cross sections for the depletion calculations in ORIGEN-S. After a depletion step, the isotopic composition of the assembly is modified, and the sequence of calculation is repeated all over.

5.2 The GT-SCALE Strategy

In the SCALE 4.2 code system, the one-dimensional Sn code XSDRNPM-S is used for solving the transport equation. It can model fuel assemblies using only a highly simplified 1D representation. The GT-SCALE code system under development will eliminate this restriction. The strategy being developed for applying this code is as follows (See Fig. 3):

First, the code would call the CSASN control module, which seamlessly integrates the BONAMI-S and NITAWL-II modules to generate resonance self-shielded cross sections for a specified pin cell. These cross-sections are being read by XSDRNPM-S, which is set to solve the eigenvalue equation for the cylindricized pin cell and to generate zone-wise macroscopic cross sections for any specific number of groups (smaller or equal to the number of groups in the library). XSDRNPM-S was modified to generate transport-corrected cross-sections which are needed for the GTRAN2 calculations.

This CSASN/XSDRNPM-S procedure is performed for each pin cell in the fuel assembly. GT-SCALE then calls GTRAN2 to perform flux calculations on the entire assembly in one step while preserving all the heterogeneities and the 2D geometry. The GT-SCALE code then again starts a loop over each pin cell. An auxiliary routine reads the GTRAN2 output and writes a flux file for each of the pin cells in the fuel assembly. The COUPLE module then uses these fluxes to make the spectrum correction to the cross sections used for ORIGEN-S. After this, the ORIGEN-S code is used to calculate the burnup in the pin cells, looping over all of the pin cells one by one. The burnup step is completed by modifying the composition of each of the pin cells in the assembly.

5.3 Transport Corrected Cross Section Generation for GTRAN2

In order to evaluate volume-to-volume collision probabilities and escape probabilities in GTRAN2, the angular dependency of the volumetric sources must be known. The fission source does not usually depend on $\hat{\Omega}$, but the differential scattering cross sections in the scattering source depend on the cosine of the scattering angle between incoming and outgoing neutron directions, $\mu_0 = \hat{\Omega} \cdot \hat{\Omega}'$. If isotropic scattering is assumed, the volumetric sources do not depend on $\hat{\Omega}$ any more, and the evaluation of collision and escape probabilities is simplified. If linearly anisotropic scattering is assumed, the volumetric sources and fluxes could be expanded into spherical harmonics. In 2D, only three moments are present in the volumetric source expansion, as well as in the volumetric flux expansion. Consequently, instead of one collision probability matrix in the case of isotropic scattering, one needs to calculate 9 collision probability matrices relating different flux and source moments, which requires considerably more CPU time and memory. To remedy this, so-called transport correction is used, i.e., it is assumed that problems with linearly anisotropic scattering can be replaced by problems with isotropic scattering, provided that the total and scattering cross sections are reduced.¹²

The differential scattering cross section is usually expanded in Legendre polynomials, $P_l(\mu_0)$, where $\mu_0 = \hat{\Omega} \cdot \hat{\Omega}'$, is:

$$\Sigma_s(\mu_0, E \rightarrow E') = \sum_{l=0}^{\infty} \frac{2l+1}{4\pi} \Sigma_{sl}(E \rightarrow E') P_l(\mu_0). \quad (1)$$

FIGURE 3. Overall Strategy for Coupling SCALE 4.2 and GTRAN2 into GT-SCALE

where the angular components are defined as

$$\Sigma_{s1}(E \rightarrow E) = 2\pi \int_{-1}^1 d\mu_0 \Sigma_s(\mu_0, E \rightarrow E) P_1(\mu_0) .$$

The linearly anisotropic scattering approximation means that only the first two terms in Eq. (1) are considered, i.e.

$$\Sigma_s(\mu_0, E \rightarrow E) \approx \frac{1}{4\pi} [\Sigma_{s0}(E \rightarrow E) + 3\mu_0 \Sigma_{s1}(E \rightarrow E)] . \quad (2)$$

which after integration over E' gives

$$\begin{aligned} \Sigma_s(\mu_0, E) &\approx \frac{1}{4\pi} [\Sigma_{s0}(E) + 3\mu_0 \Pi_0(E) \Sigma_{s0}(E)] \\ &= \frac{1}{4\pi} [\Sigma_{s0}(E) + 3\mu_0 \Sigma_{s1}(E)] . \end{aligned} \quad (3)$$

where

$$\Pi_0(E) = \frac{2\pi \int \int d\mu_0 dE' \mu_0 \Sigma_s(\mu_0, E \rightarrow E')}{2\pi \int \int d\mu_0 dE' \Sigma_s(\mu_0, E \rightarrow E')} = \frac{\Sigma_{s1}(E)}{\Sigma_{s0}(E)} .$$

Usually, linearly anisotropic scattering is not treated explicitly in the integral transport methods. In fact, scattering is assumed to be isotropic, but the total and scattering cross sections are reduced (transport corrected) as follows:

$$\Sigma_{s,g' \rightarrow g}^{tr} = \begin{cases} \Sigma_{s0,g' \rightarrow g}, & g' \neq g \\ \Sigma_{s0,g' \rightarrow g} - \Pi_{0,g} \Sigma_{s0,g}, & \text{otherwise} \end{cases} \quad (4)$$

i.e., the diagonal of the P_0 scattering matrix is corrected, and the transport-corrected total cross section is given by

$$\Sigma_{t,g}^{tr} = \Sigma_{t,g} - \Pi_{0,g} \Sigma_{s0,g} .$$

From Eq. (78), by summing over g' , we get

$$\Sigma_{s,g}^{tr} = \sum_g \Sigma_{s0,g' \rightarrow g} - \Pi_{0,g} \Sigma_{s0,g} = \Sigma_{s0,g} - \Sigma_{s1,g} . \quad (5)$$

The stand-alone version of GTRAN2 reads macroscopic cross sections in card image format from logical unit 20. The following macroscopic cross sections are needed by GTRAN2 for each material/composition and each energy group:

- SA - macroscopic absorption cross section,
- SF - macroscopic fission cross sections,
- SNF - macroscopic nu fission cross section,

- ST - macroscopic total cross section, transport corrected,
- STOTSC- macroscopic total scattering cross section, transport corrected,
- SSC - P_0 macroscopic scattering cross section matrix, with transport corrected diagonal
- CHI - fraction of fission neutrons in each group.

In order to prepare cross sections for GTRAN2, several subroutines from XSDRNPM were modified. First, GTRAN2 needs macroscopic cross section for each region (for example: fuel, clad, and moderator), while XSDRNPM homogenizes each pin and calculates pin-averaged cross sections. Second, GTRAN2 needs transport corrected cross sections, as shown above. With the modifications in XSDRNPM, we were able to generate cross sections library needed for GTRAN2.

6.0 TESTING AND BENCHMARKING

In order to verify that our overall procedure, as well as the modifications of the SCALE functional modules, are correct, we developed two sets of test cases:

- Pin cell test cases: UO_2 - PuO_2 , and UO_2 - PuO_2 - Er_2O_3 .
- Assembly test case based on System 80+ design.

6.1 Single Fuel Pin Test Problem Description

In order to check the "front-end" interface between SCALE 4.2 and GTRAN2, we compared the results obtained using GT-SCALE with those calculated with SCALE 4.2/CSASN for a single pin cell test case based on the CE-System 80+ design for MOX fuel. The following parameters are used (the dimensions in SI units are calculated from the dimensions given in British units):^{1,13}

• Fuel outer diameter	$d_f = 0.97028$ cm
• Clad thickness	$t_{cl} = 0.0635$ cm
• Clad outer radius	$r_{cl} = 0.48514$ cm
• Pin cell pitch	$pcp = 1.28524$ cm
• Fuel composition	UO_2 - PuO_2 or UO_2 - PuO_2 - Er_2O_3
• Total Pu in Heavy Metal	6.75 w%(93.5% Pu-239, 6.5% Pu-240)
• Total U in Heavy Metal	93.25w% (99.8% U-238, 0.2% U-235)
• Total Er in MOX	1.6 w% of Er_2O_3 in MOX pellet.

The other parameters are: fuel temperature 980 K, clad temperature 615 K, moderator temperature 548.8 K, pressure $P = 2250$ psi, power density $P_d = 20$ W/g-fuel, boron concentration $B_c = 2450$ ppm. The 27-group SCALE burnup library was used for this tests.

We ran SCALE 4.2/CSASN requesting the following parameters for the transport calculations in XSDRNP-S: S_{16} quadrature set with P_3 approximation. In the case of GTRAN2, the pin cell was represented by three flat flux zones (Figure 4) in square lattice. The combinatorial ray tracing parameters for GTRAN2 were: 20 angles and 0.02 cm between parallel integration lines.

FIGURE 4. The Pin Cell Geometry for GTRAN2 and SCALE 4.2/CSASN

The results for the infinite multiplication factor, k , are presented in Table 1 for a couple of test cases; one with and the other without burnable poison. As can be seen, the results of the original SCALE 4.2 system and coupled SCALE4.2/GTRAN2 system are in excellent agreement.

TABLE 1. Results for Infinite Multiplication Factor

	UO_2 - PuO_2	UO_2 - PuO_2 - Er_2O_3
SCALE4.2/CSASN	1.09512	0.98911
GT-SCALE	1.09511	0.99201

In Tables 2 and 3 comparison between fission and absorption rates is given for both test cases. Again, we have a very good agreement.

We have also performed burnup calculation for the pin cell test cases defined above. Table 4 shows comparison of the SCALE 4.2/SAS2H and GT-SCALE results for the three-group weighting factors calculated by COUPLE and used for cross section preparation for ORIGEN-S.

TABLE 2. Comparison of Reaction Rates (normalized to one neutron absorption): $\text{UO}_2\text{-PuO}_2$

		Fission Rate	Absorption Rate
Region 1: Fuel	SCALE4.2/CSASN	3.80000-1	9.43670-1
	GT-SCALE	3.80902-1	9.42738-1
Region 2: Clad	SCALE4.2/CSASN	0	7.52031-3
	GT-SCALE	0	7.50547-3
Region 3: Moderator	SCALE4.2/CSASN	0	4.88107-2
	GT-SCALE	0	4.97530-2
Total	SCALE4.2/CSASN	3.80000-1	1.00000
	GT-SCALE	3.80902-1	1.00000

TABLE 3. Comparison of Reaction Rates (normalized to one neutron absorption): $\text{UO}_2\text{-PuO}_2\text{-Er}_2\text{O}_3$

		Fission Rate	Absorption Rate
Region 1: Fuel	SCALE4.2/CSASN	3.43162-1	9.48619-1
	GT-SCALE	3.44966-1	9.47600-1
Region 2: Clad	SCALE4.2/CSASN	0	7.39488-3
	GT-SCALE	0	7.39169-3
Region 3: Moderator	SCALE4.2/CSASN	0	4.39854-2
	GT-SCALE	0	4.50008-2
Total	SCALE4.2/CSASN	3.43162-1	1.00000
	GT-SCALE	3.44966-1	1.00000

TABLE 4. Three-Group Weighting Factors Calculated by COUPLE

Without Er	SCALE/SAS2H	GT-SCALE
therm	0.6320	0.6320
res	8.9575	8.8524
fast	64.6044	65.2212
With Er	SCALE/SAS2H	GT-SCALE
therm	0.6320	0.6320
res	10.4492	10.2794
fast	75.9313	76.1424

Selected one-group cross section prepared by COUPLE for ORIGEN-S are shown in Table 5. Table 6 shows comparison of the selected nuclide concentrations after 50 days of irradiation. It is observed that the neutron flux spectrum calculated with GTRAN2 is in excellent agreement with that calculated using XSDRNPM-S. Consequently, the effective one-group transmutation cross sections and burnup-dependent nuclide concentrations calculated using GT-SCALE are practically identical for a pin cell system, with those calculated by SCALE 4.2/SAS2H.

TABLE 5. Selected One-Group Cross Sections

Nuclide	SCALE4.2/ SAS2H	GT-SCALE
U236	4.47E-09	4.44E-09
U239	1.24E-10	1.23E-10
Pu241	6.54E-08	6.45E-08
Pu242	2.98E-12	2.94E-12

TABLE 6. Selected Nuclide Concentrations after 50 Days of Irradiation

Nuclide	SCALE4.2/ SAS2H	GT-SCALE
U235	1594.97	1571.67
U236	36.6644	36.9829
U238	17.4465	17.6519
Pu239	2079.68	2053.62
Pu240	109.062	109.531
Pu241	4193.73	4156.77
Pu242	86.4698	86.9469

6.2 System 80+ Control Rod Description

The values used in this report for the System 80+ control rod for a plutonium burning core are referenced from the Combustion Engineering report describing this core. These values were used in order to run SCALE 4.2/CSASN package.

The control rod is part of a lattice cell shown in Figure 5. The lattice cell contains three materials including the absorber material, the cladding, and the moderator. The absorber itself consists of B₄C. The clad is made from inconel and the moderator consists of water and boron.

The CSASN-type input consists of composition identifiers and lattice dimensions for the most part. It also specifies the cross-section library to be used. For this case, the 27BURNUPLIB is used which is a 27 energy group library. The lattice cell specification is used to describe the geometrical input. Table 7 lists the fuel compositions, densities (both atom and mass), and temperatures.

FIGURE 5. Control Rod Lattice Cell

TABLE 7. Control Rod Lattice Cell Composition

composition	atom density	mass density (g/cc)	Temp. (K)
B ₄ C		2.52	548.8
u-235	1.0E-20		548.8
incone1		8.30	548.8
H	2.612661E-2		548.8
O	2.607946E-2		548.8
B-10	2.291824E-5		548.8
B-11	9.224880E-5		548.8

6.3 System 80+ Burnable Poison Rod Description

The values used in this report for the System 80+ burnable poison rod for a plutonium burning core are referenced from the Combustion Engineering report describing this core. These values were used in order to run BONAMI/NITAWL/XSDRN from the SCALE package.

The burnable poison rod is part of a lattice cell shown in Figure 6. The lattice cell contains three materials including the absorber material, the cladding, and the moderator. The absorber itself consists of Al₂O₃-B₄C. The clad is made from zircalloy and the moderator consists of water and boron.

The lattice cell specification is used to describe the geometrical input. Table 8 lists the fuel compositions, densities (both atom and mass), and temperatures for this cell.

FIGURE 6. Burnable Poison Rod Lattice Cell

TABLE 8. Burnable Poison Rod Lattice Cell Composition

composition	atom density	mass density (g/cc)	Temp. (K)
(Al ₂ O ₃ -B ₄ C)		3.70	548.8
B ₄ C		3.70	548.8
u-235	1.0E-20		548.8
zircalloy	4.297468E-2		548.8
H	2.612661E-2		548.8
O	2.607946E-2		548.8
B-10	2.291824E-5		548.8
B-11	9.224880E-5		548.8

6.4 Assembly Test Case Based on System 80+ Design

The technical characteristics of the System 80+ fuel pin, control rod pin and burnable poison pin are given in Sections 6.1, 6.2, and 6.3, respectively. In this section we will describe the geometrical layout of the System 80+ fuel assembly needed for the full heterogeneous assembly calculations in GTRAN2. As can be seen in Figure 7, all design characteristics are represented without any homogenization or simplification. We used 1.28524 cm for the pin cell pitch, and 202.4888 cm for the fuel assembly pitch. The water gap between fuel assemblies is 0.52832 cm.

SYSTEM 80+ PWR FUEL ASSEMBLY

● --- Burnable Poison Rod

○ --- Fuel Rod

● --- Instrument Tube

○ --- Control Rod

FIGURE 7. Exact Geometric Representation of the System 80+ Assembly Design for GT-SCALE

Moderator is subdivided into rectangular (square) zones. If needed, each circular zone can be subdivided into additional concentric circles and/or azimuthal zones, as shown in Figure 8.

FIGURE 8. GTRAN2 Unique Geometry Description Capability

We have prepared both, the geometry input as well as the cross section libraries to run GT-SCALE for the full heterogeneous System 80+ assembly configuration as shown in Figure 7. This type of calculations will be performed in the near future.

7.0 UNIQUE FEATURES OF GT-SCALE

The fuel assembly code GT-SCALE incorporates a number of unique features of both the SCALE 4.2 code package and of the GTRAN2 transport equation solver. These unique features include the following:

- 1. A general two-dimensional geometry simulation capability.** The same code can be applied, as is, to accurately simulate fuel assemblies of any geometry, including hexagonal geometries (as of the Russian LWRs). The unique geometry description capability starts from the pin cell level. For example, Figure 8 illustrates how GTRAN2 can be used to investigate the validity of cylindricizing the pin cell needed for some calculations. The square shaped pin cell is azimuthally divided into 8 - 45° wide segments, each segment consisting of 3 zones: fuel, clad and moderator. GTRAN2 solution shows that the fission density in the fuel zone pertaining to the cell corner segments is larger than in the fuel zones pertaining to the flat faces of the cells by more than .5%

- 2. Ability to account for all heterogeneities within the fuel assembly, and to any degree of detail.** For example, not only can GT-SCALE discretely account for the fuel, clad and moderator regions pertaining to each of the pin cells within the assembly, but it can divide the rod to any number of concentric (or non-concentric) zones. This latter feature can be particularly important for accurate simulation of burnable poison rods, of control rods, and of fuel rods located near-by water rods or strong absorbing rods.

The description of the assembly geometry in GT-SCALE, as a whole, is to be done in, and only in the GTRAN2 part of this code system. The other parts are to deal with a single pin cell (CSASN) or a single zone (COUPLE-ORIGEN).

The ability of GTRAN2 to accurately handle highly heterogeneous 2D assemblies of LWRs and HTGRs has been illustrated, by comparing against Monte Carlo calculations. The GTRAN2 vs. Monte-Carlo benchmark calculations are summarized in Appendix B.

3. Highly accurate burnup calculations. This is due to the most extensive data base available in the SCALE-4.2 package, along with the accurate transmutation and radioactive decay chain modelling of ORIGEN-S.

4. Detailed space-dependent burnup calculations. In principle, GT-SCALE can perform separate burnup calculations for any segment of the fuel (or burnable-poison) rod. GTRAN2 is set to provide fluxes for.

5. Multi-assembly simulation capability. MAGGENTA,¹⁴ a MultiAssembly General Geometry Neutron Transport code, based in part on the existing GTRAN2 methodology, utilizes the p4 Parallel Programming System¹⁵ and networks of workstations or other supercomputers to solve large multi-assembly problems. This capability could be incorporated into GT-SCALE.

6. Comprehensive, continuously maintained data base - as provided by the SCALE 4.2 code package. For example, while working on the "marrying" between GTRAN2 and SCALE 4.2 we were informed¹⁶ that new neutron multigroup libraries for SCALE 4.2 have been released - a 284 group master library is to replace the present 218 group library, and a new 44 group library is to replace the present 27 group library. Both new libraries are based on ENDF/B-V.

7. Flexibility in energy-group structuring. This is due to the availability of a very fine structure master library and the capability built into GT-SCALE to collapse this library into any number of groups. This flexibility is particularly useful for accurate simulation of MOX fuel assemblies. For example, accurate simulation of plutonium bearing fuel assembly requires taking accurate account of the large low energy resonance of ²³⁹Pu which introduces a pronounced structure in the energy range between approximately 0.1 eV to 1.0 eV. The 218 master group library available to GT-SCALE provides 26 energy groups for this energy range! This is a higher resolution than necessary for accurate calculation of the thermal neutron spectrum and reaction rate in plutonium (and erbium, if used as burnable poison) bearing lattices.

As an illustration of the energy resolution available with GT-SCALE, we resolved the transport equation for the reference pin cell using the 218 group structure and the associated cross section library. Fig. 9 shows, for illustration, the fission rate per unit energy as a function of energy in the thermal energy range obtained from these calculations. Notice that the 0.3 eV resonance of ²³⁹Pu shows up as a hump on the high energy side of the slope of the thermal neutrons fission rate distribution. This distribution peaks around 0.05 eV. It should be realized that this seemingly small hump is responsible for a fission rate. This can be conveniently seen from Fig. 10, which presents the total fission rate for each of the groups (the total fission rate per unit energy given in Fig. 9, times the energy width).

FIGURE 9. Normalized Fission Rate per Unit Energy (218-Group Library, No Er)

FIGURE 10. Normalized Fission Rate (18-Group Library, No Er)

The fine energy resolution provided by the 218 group structure is apparent when comparing these results (Fig. 9) with those obtained for the same pin cell and computational tools and procedure with one exception: using the 27 group library (Fig. 11). It should be realized, through, that the infinite multiplication constant calculated with the 27 and 218 group libraries were very close.

We were also able to study the effect of erbium burnable poison on the neutron spectrum. Fig. 13 also shows the effect of including erbium burnable poison on the total fission rate for the reference pin cell, calculated using the 27 group library. Comparing Fig. 12 and 13 one can observe the effect of the large, low energy (approximately 0.5 eV) resonance of erbium - a significant reduction in the contribution of the 0.3 eV resonance of ^{239}Pu to the fission rate. The erbium also reduces the relative contribution of the lower energy thermal neutrons to the fission rate.

Relative to SCALE 4.2, GT-SCALE has one limitation - accounting for the anisotropy in the neutron distribution using transport corrected cross-sections (versus the $P_l - S_n$ transport approximation which can be handled by XSDRNPM-S; typical l and n values being 3 and 8). Nevertheless, as indicated in the comparison between the GTRAN2 and XSDRNPM-S results presented in Sec. 6, the transport approximation is accurate enough for the type of applications under consideration.

FIGURE 11. Normalized Fission Rate per Unit Energy (27-Group Library)

Fission Rates

MOX Fuel - no Erbium

FIGURE 12. Fission Rate (27-Group Library, No Er)

Fission Rates

MOX Fuel With Erbium

FIGURE 13. Fission Rate (27-Group Library, With Er)

8.0 DISCUSSION

Even though the direct incentive for the development of GT-SCALE was for the analysis of MOX fueled LWRs fuel assemblies, GT-SCALE is a general purpose code for LWR assembly analysis. Its detailed geometry description capability is expected to make GT-SCALE very attractive for the analysis of UO_2 fueled fuel assemblies the design of which is becoming more and more heterogeneous (for example; recent designs of fuel for BWRs may have as many as 10 different types of rods per assembly; the variation in rod composition will increase with burnup).

GT-SCALE will be also applicable to the analysis of LWR fuel assemblies of non-conventional geometries - such as the hexagonally shaped fuel assemblies of the Russian LWRs. In addition, it is expected that GT-SCALE will be applicable to the analysis of fuel assemblies for HTGRs and LMRs.

In the context of the application considered in the present report, we presented GT-SCALE as GTRAN2 aided by certain of the SCALE 4.2 package modules. However, from the viewpoint of the applications for which SCALE 4.2 was developed, GT-SCALE can be viewed as an upgrading of the capability of the SCALE 4.2 package. Specifically, by upgrading SCALE 4.2 by GTRAN2, it will be possible to more accurately calculate the criticality, and the source term of spent fuel (for transportation and storage facility design).

So far we have developed the "front-end" and "back-end" interfacing between GTRAN2 and the SAS2H sequence of SCALE 4.2 for a single pin cell. The next task will be to develop the "looping" capability, i.e., to go from the pin cell to the fuel assembly level calculations.

9.0 SUMMARY

We started the development of a new fuel assembly analysis code, referred to as GT-SCALE, by "marrying" GTRAN2 and the SAS2H sequence of the SCALE 4.2 code package. Similar approach was used in combining the capabilities of the SCALE depletion sequence and the lattice code WIMS.¹⁷ However, GT-SCALE is expected to enable a more accurate simulation of highly heterogeneous and MOX fueled LWR fuel assemblies than most of the existing assembly simulation codes. This is due to a combination of GT-SCALE's ability to solve the transport equation in as detailed a resolution in both the spatial and energy-dependent variables, along with its powerful burnup calculational capability. Specifically, GT-SCALE will be able to accurately simulate the evolution, with burnup, of the isotopic composition of each of the fuel pins in the assembly. Moreover, GT-SCALE will enable to simulate this composition variation with burnup for different cylindrical shells corresponding to a given (or any number of) fuel rods within the assembly. This capability can be particularly useful for the simulation of the effect of burnup on fuel or absorber rods which are subjected to strongly varying fluxes - such as for burnable poisons, particularly when using plutonium for the fuel.

In addition, the GT-SCALE code system will be more universal in its range of application than most of the existing assembly code systems. This is due to the general geometry description capability of GTRAN2 combined with the fine energy group structure of the master library of SCALE 4.2 and combined with the comprehensive burnup calculational capability (including

the corresponding nuclear data files) of SCALE 4.2 (via ORIGEN-S).

The preliminary benchmark calculations carried out give very good agreement between GTRAN2 and XSDRNP-S calculations of the neutron balance in a clean, MOX fueled pin-cell. The next step will be the development of the capability to simulate an entire fuel assembly with GT-SCALE.

Even though the development of GT-SCALE was initiated for the analysis of MOX fueled LWRs, GT-SCALE is expected to be very useful for a wide variety of other applications, including for criticality safety of spent fuel, and for accurate source term calculations for the design of shipping and storage casks for spent fuel.

ACKNOWLEDGEMENTS

This work was partly supported by Lawrence Livermore National Laboratory through Contract No. B283667. The authors would like to thank John Pitts and Jor-Shan Choi (LLNL) for providing the incentive and data for this work. In addition, the authors would like to thank the ORNL staff members L. Leal for his help with the SCALE 4.2 system, N. M. Greene for his help on the XSDRN code and O. W. Hermann for his help on the SCALE 4.2/SAS2H code system. This work would have been impossible without the help of our students: Steve Slater, Todd Postma, Greg Casher, and Ilson Soares.

REFERENCES

1. P.C. Rohr and U.N. Singh, "Physics and Safety Characteristics of the System 80+ TM Plutonium Burner," *Proc. 1994 Topical Mtg. on Advances in Reactor Physics*, Knoxville, TN, April 11-15, 1994
2. D. Biswas, R. Rathbun, S.Y. Lee and P. Rosenthal, "Neutronics and Safety Characteristics of a 100% MOX Fueled PWR Using Weapons Grade Plutonium," *ibid*
3. P. Barbrault, "A Plutonium-Fueled PWR 2000," *ibid*
4. G.S. Chang, "Physics Analysis of Tungsten in Weapons-Grade U/Pu Fuels for Light Water Weapons-Grade U/Pu Burning/Power Reactors," *ibid*
5. J. L. Vujic, "GTRAN2: An Advanced Transport Theory Code for Advanced Assembly Calculations," *Proc. of Joint International Conference on Mathematical Methods and Supercomputing in Nuclear Applications*, 19-23 April 1993, Karlsruhe, Germany, Vol.1, p.695 (1993).
6. SCALE 4.2, Modular Code System for Performing Standardized Computer Analysis for Licensing Evaluation, CCC-545, Oak Ridge National Laboratory, Oak Ridge, TN (December 1993).
7. EPSC Software Catalogue, EPRI (1993)

8. J. L. Vujic and R. N. Blomquist, "BWR Assembly Benchmark Solution by ANL General Geometry Transport Codes," *Proc. Int. Topl. Mtg. on Advances in Mathematics, Computations, and Reactor Physics*, Pittsburgh, PA, April 28 - May 2, 1991, Vol. 5, p. 30.1 11-1, American Nuclear Society (1991).
9. J. L. Vujic, "Validation of the GTRAN2 Transport Method for Complex Hexagonal Assembly Geometry," *Trans. Am. Nucl. Soc.*, **64**, p.523 (1991).
10. W. J. Wilson, J. L. Vujic, and A. G. Gu, "Parallel Multiple Assembly Calculations in GTRAN2/M," *Trans. Am. Nucl. Soc.*, **69**, p. 204 (1993).
11. S. M. Slater and J. L. Vujic, "P4 Parallelization of General Geometry Ray Tracing in Computational Physics," *Proc. of the conference on High Performance Computing '94*, La Jolla, April 11-15, 1994, pp. 175-180 (1994).
12. J. L. Vujic, "GTRAN2: A General Geometry Transport Theory Code in 2D," Volume 1: Theory and Numerics Manual, Draft, Argonne National Laboratory, August 1992.
13. "Plutonium Disposition Study: Technical Description," Combustion Engineering, Inc. Report (1994).
14. S. M. Slater and J. L. Vujic, "Multiassembly Collision Probability Calculations with MAGGENTA and P4," (A paper presented at this conference)
15. R. Butler and E. Lusk, "User's Guide to the p4 Programming System," Argonne National Laboratory, Argonne, IL., ANL-92/17 (1992).
16. RSIC Newsletter, No.358, September 1994.
17. P. F. A. de Leege, J. M. Li, and I. C. Gauld, "Linking WIMS with the SCALE Depletion Sequence," *Proc. of Joint International Conference on Mathematical Methods and Supercomputing in Nuclear Applications*, 19-23 April 1993, Karlsruhe, Germany, Vol.1, p.577 (1993).

APPENDIX A

Scope of Work

Phase I: June 1994 - September 1994

The following primary tasks have been proposed to be performed during this contract period (June - September 1994):

- Select the code system to be used as the basis for our method. The EPRI LWR option will require less time to completion. However, the option of coupling GTRAN2 with the SCALE 4.2 code system is also very attractive. In addition to its ability to simulate the MOX fueled cores, the resulting GTRAN2-SCALE code system will be very useful for calculating the source term for spent fuel from LWRs more accurately than what was possible so far.
- Develop the most efficient interface between GTRAN2 and the base code system to be selected.
- Benchmark the new GTRAN2-EPRI or GTRAN2-SCALE code system against published results (including burnup calculations) for a couple of MOX fueled PWRs - one using 1/3 MOX loading per fuel assembly, and the other using a colorset configuration.
- Preliminary analysis of some of the ALWR fuel assembly designs with the MOX fueled assemblies. Preliminary burnup calculation of plutonium-bearing fuel assemblies.

Proposed Research: Phase II: after September 1994

In the second phase (longer term proposal - after September 1994) the following tasks are planned, subject to funding availability and study progress:

- Evaluate the impact on reactor control and safety for locating plutonium-bearing fuel rods and assemblies in reactor cores.
- Provide assessments on the effectiveness of the control system for a plutonium-bearing fueled core, and quantify the important transients associated with such a reactor core.

TABLE 2. TASK DESCRIPTION AND MILESTONES

	Task Description	Duration	July			August			Sept.		
			10	20	31	10	20	31	10	20	30
1	Selection of the code system to be used as the basis for new methodology (ORNL's SCALE 4.2 or EPRI's ARMP-02).	2 weeks									
2	Analysis of the selected code system to determine the overall computational methodology to be used for detailed assembly level depletion calculations. It includes analysis of what modules will be used intact, what modules need to be modified, and what modules will be replaced by GTRAN2.	2 weeks									
3	Development of the most efficient interface between GTRAN2 and the selected base code system. Determination of the most appropriate format for the cross section library. Modification of the GTRAN2 input and output to interface with the cross section preparation and with the depletion modules.	5 weeks									
4	Selection and specification of benchmark problems: a) single pin-cell case, b) fuel assembly case.	1 week									
5	Comparison of the results of the new code package for a single fuel pin and a homogenized assembly with the results from the original code package.	2 weeks									
6	Comparison of the results of the new code package for a heterogeneous assembly with the benchmark. (If time permits)	3 weeks									
7	Report writing	3 weeks									

APPENDIX B

GTRAN2: An Advanced Transport Theory Code for Advanced Assembly Calculations

Jasmina L. Vujic¹
University of California
Department of Nuclear Engineering
Berkeley, CA

INTRODUCTION

Recent developments in both computer hardware and computer architecture (to name only few: rapid increase in speed and available memory, rapid decrease in price, vector and parallel processing) forced many scientists and engineers to rethink their approach to solving neutron transport problems. What was unthinkable only few years ago, is becoming an ordinary tool of today. Supercomputers, as somebody pointed out, are becoming the tools of imagination.

On the other hand, the design of modern thermal reactors requires a two-dimensional (possibly three-dimensional) lattice transport methods that can efficiently handle a variety of complex assembly geometries (square, hexagonal, ...) without any changes to the solution algorithm.

In developing GTRAN2, an advanced transport theory lattice code, we wanted to satisfy the requirements of nuclear industry to have a very accurate, computationally efficient, and geometry independent code. In addition, we took advantage of parallel and vector processing in order to reduce CPU and wall clock times, and allow the code to be used for global reactor calculations.

GTRAN2 TRANSPORT METHODOLOGY

GTRAN2 is a transport theory code that solves the multigroup steady-state integral transport equation in arbitrary two-dimensional geometries (Ref.1). The code is based on the rigorous collision/transfer probability (CTP) method. It performs an exact numerical integration in order to calculate the collision, escape, and transmission probability matrices for an assembly (or any region of interests). A modified combinatorial geometry processor is used to perform ray tracing. The use of combinatorial geometry permits an exact description of various assembly geometries in one-, two-, and three-dimensions.

Combinatorial geometry input for GTRAN2 is generated by a preprocessing code GIN (Ref. 2), starting from a Monte Carlo - type input. In the case of standard FWR or BWR assembly geometries, a simple engineering-type input is sufficient.

Given macroscopic cross sections, GTRAN2 solves an eigenvalue problem, and calculates the fine-mesh volumetric flux, incoming/outgoing current distributions, reaction rates and few group constants for nodal codes. The eigenvalue equations are derived assuming isotropic scattering (basic version of GTRAN2) or linearly anisotropic scattering. The double P_0 expansion of the angular flux on the outer assembly boundary is used. The system of equation is solved by the power iterative method for outer (fission source) iterations, the SOR method for inner iterations for the flux

1. Most of the work presented in this paper was done by the author while working at Argonne National Laboratory, Argonne, IL.

equations, and the direct method for the current equation.

GTRAN2 plots the fine mesh, edit region, and/or material layouts. In addition, GTRAN2 generates three-dimensional and/or contour plots of fine-mesh flux and power distributions.

The exact collision probability formalism is used in the GTRAN2 code (Vujic 1993) to solve the multigroup integral transport equation in general 2D geometries. Combinatorial geometry (CG) is used to describe complex and irregular configurations in one, two, or three dimensions. A modified CG processor is used to perform ray tracing needed for numerical calculation of the collision/transfer probability (CTP) matrices. Thus, GTRAN2 is a unique combination of the computational efficiency of the deterministic code and the geometric flexibility of Monte Carlo codes.

To obtain the discretized integral transport equations for two-dimensional geometry, the area A and boundary L are partitioned into N_f subareas (zones) and N_b subboundaries, respectively, such that

$$A = \sum_{i=1}^{N_f} A_i, \quad L = \sum_{\alpha=1}^{N_b} L_{\alpha},$$

and

$$A_i \bar{\Sigma}_{i,g,i} \Phi_{g,i} = \sum_j A_j Q_{g,i} P_g(A_i \leftarrow A_j) + \sum_{\alpha} L_{\alpha} J_{g,\alpha}^{in} P_g(A_i \leftarrow L_{\alpha})$$

$$L_{\alpha} J_{g,\alpha}^{out} = \sum_i A_i Q_{g,i} P_g(L_{\alpha} \leftarrow A_i) + \sum_{\alpha'} L_{\alpha'} J_{g,\alpha'}^{in} P_g(L_{\alpha} \leftarrow L_{\alpha'})$$

where g is the energy group index, and the neutron fluxes, sources and partial currents are spatially averaged over the corresponding volume and/or surface elements. In this case, $P_g(A_i \leftarrow A_j)$ is the first flight volume-to-volume collision probability that neutrons emitted uniformly and isotropically in A_j will have their next collision in A_i , whereas $P_g(A_i \leftarrow L_{\alpha})$ is the first flight surface-to-volume collision probability that neutrons entering through L_{α} uniformly and isotropically will have their next collision in A_i . Similarly, $P_g(L_{\alpha} \leftarrow A_i)$ is the first flight escape probability that neutrons emitted uniformly and isotropically in A_i will escape through L_{α} without having a collision, and $P_g(L_{\alpha} \leftarrow L_{\alpha'})$ is the transmission probability that neutrons entering through $L_{\alpha'}$ uniformly and isotropically will escape through L_{α} without having a collision. This system of equations can be presented in matrix form, as shown in Figure 1.

The collision, escape, and transmission probabilities are two-fold integrals that are numerically calculated. For example, the volume-to-volume collision probability is given by:

$$P_g(A_i \leftarrow A_j) = \frac{1}{A_i \bar{\Sigma}_{i,g,i}} \int_0^{2\pi} \int_{y_{min}(\varphi)}^{y_{max}(\varphi)} d\varphi \int_0^{\frac{d\varphi}{2\pi}} d\varphi' \zeta_g(A_i) \zeta_g(A_j) [Ki_3(\tau_{g,ir}) - Ki_3(\tau_{g,ir} + \tau_{g,i}) - Ki_3(\tau_{g,ir} + \tau_{g,i'}) - Ki_3(\tau_{g,ir} + \tau_{g,i'})]$$

where

$$\xi(Z) = \begin{cases} 1, & \text{if the track intersects region } Z \\ 0, & \text{otherwise} \end{cases}$$

$\tau_{g,i} = \tau_{g,i}(y')$ is the optical length across A_i in the direction of neutron motion at a distance y' above the x' -axis, and

$\tau_{g,ii'} = \tau_{g,ii'}(y')$ is the optical length between A_i and $A_{i'}$ in the direction of neutron motion.

In our approach, the calculation of the elements of CTP matrices is performed in two independent steps:

1. Geometrical Step (TPGEOM). The in-plane numerical integration is performed by covering the geometrical domain of interest (which is divided into flat flux zones) with a set of parallel integration lines at a number of discrete azimuthal angles. For each integration line, the following data are calculated: the intersections with the zone boundaries, the path length between the intersections, the total number of zones on the track, the zone, edit and material numbers, and the intersections with the outer boundary of the geometrical domain. The accuracy of collision/transfer probabilities can be increased by reducing the size of the flat flux zones, increasing the number of integration angles, and decreasing the distance between parallel integration lines. However, the CPU time increases rapidly with the increase in the accuracy of collision/transfer probabilities.
2. Numerical Integration Step (CTP). Given the geometric data and the total cross sections for all materials, the elements of the CTP matrices are calculated by numerical integration.

This approach has several advantages. By decoupling the geometric part from the calculation of the collision/transfer probability matrices, the geometric data, once precalculated, can be used for each energy group and time step.

VECTOR AND PARALLEL PROCESSING IN GTRAN2

In order to reduce CPU and wallclock times, GTRAN2 is optimized for vector and parallel processing on shared memory computing systems. In addition, the following has been accomplished by GTRAN2 optimization: a) supercomputer is more efficiently utilized, and b) GTRAN2 can be used for larger problems with more zones and/or energy groups.

GTRAN2 consists of three large modules: the ray tracing module (TPGEOM), the collision/transfer probability (CTP) module, and the solver (FLUJ). The first two modules are executed in parallel/vector mode, while the solver is executed in vector mode. We have chosen a coarse-grained (or subroutine-level) parallelism. In the ray tracing module, each processor performs ray tracing for a particular angle, while in the CTP module, each processor calculates all elements of the CTP matrices for a particular energy group (Figure 2).

If the domain of interest contains a large number of zones, the ray tracing can easily become the most time consuming part of GTRAN2. The advantage over some other methods (Monte Carlo, for example) is that the ray tracing needs to be done only once, and the calculated geometric data are repeatedly used for all energies and burnup steps. Also, the ray tracing in GTRAN2 is perfectly suited for parallel processing, i.e., each track is totally independent of all other tracks. In the calculation of the CTP matrices, the same geometric data are used for each energy group, thus, each parallel task is performing exactly the same calculations, and the load balancing for each processor is perfect. Figure 3 shows serial-to-parallel speedups for the calculation of the CTP matrices on the

The solver module is efficiently optimized for vector processing. The subroutines for inner iterations in both flux and current equations are running with the rate of up to 130 MFLOPS on the Cray X-MP.

Table 1 shows the CPU times for the BWR assembly benchmark problem No. 13 from the Argonne's Code Center Benchmark Problems Book (ANL-7416) on several mainframe computers and engineering workstations.

GTRAN2 RESULTS FOR SQUARE AND HEXAGONAL ASSEMBLY GEOMETRIES

In this paper we will be presenting the GTRAN2 results for two very different assembly geometries: a) a standard BWR assembly (8x8, with four different fuel rod enrichments and a water rod), and b) an MHTGR assembly (hexagonal graphite block with axial cylindrical channels for coolant flow or insertion of fuel compacts and absorber compacts). Due to a flat flux approximation in GTRAN2, large geometrical domains need to be subdivided into smaller zones. The meshing in GTRAN2 for the BWR assembly is shown in Figure 4, and for the MHTGR assembly in Figure 5. The calculations were done in 7 energy groups for the BWR assembly and 6 energy groups for the MHTGR assembly.

The reference solution for both assembly types is taken to be a Monte Carlo multigroup solution, performed by VIM (Ref. 3). We forsook the continuous energy computations in VIM for the multigroup treatment in order to use the same set of multigroup macroscopic cross sections in both GTRAN2 and VIM.

The k_{inf} results for the BWR assembly are shown in Table 2, and for the MHTGR assembly in Table 3. Summary of the GTRAN2 and VIM results for the average flux, fission and absorption rates is given in Table 3 (BWR) and Tables 4 and 5 (MHTGR). The GTRAN2 flux distributions and reaction rates are within one standard deviation of the corresponding VIM results.

For the BWR assembly, comparison of the GTRAN2 and VIM accuracy in flux distributions in fuel, cladding and moderator regions for one of the fast groups (2) is given in Figure 6, and for one of the thermal groups (5) in Figure 7. Figure 8 shows the 3D and contour plots of fine mesh flux distributions for energy groups 2 and 4, as generated by GTRAN2.

The relative differences in percent between the GTRAN2 and VIM results for fast and thermal flux in all zones are shown in Figure 9 for the MHTGR test case. Various background meshing is shown in Figure 10. Figure 11 shows the 3D and contour plots of fine mesh flux distributions for fast and thermal groups, as generated by GTRAN2.

CONCLUSIONS

The GTRAN2 results agree very well with the VIM Monte Carlo results for both square and hexagonal assembly geometries. In addition to its accuracy and geometrical flexibility, GTRAN2 is computationally very efficient: it needs several order of magnitude less CPU time than VIM, for about the same accuracy.

REFERENCES

1. J. L. Vujic, "GTRAN2: A General Geometry Transport Theory Code in 2D," *Proc. Int. Topl. Mtg. on Advances in Mathematics, Computations, and Reactor Physics*, Pittsburgh, PA, April 28- May 2, 1991, Vol. 5 , p. 30.4 1-1, American Nuclear Society (1991).
2. J. L. Vujic, Auxiliary Codes for GTRAN2," Inter-Laboratory Memo, Argonne National Laboratory (1992).
3. R. N. Blomquist, "VIM - A Continuous Neutronics and Photon Transport Code," *Proc. Topl. Meeting on Advances in Reactor Computations*, Salt Lake City, UT (1983).

Table 1. CPU Time (s) for BWR Assembly Benchmark: 361 zones, 20 angles, 0.1 cm step

	SPARC 1	SPARC 2	RS 530	HP 720	IBM 3090	HP 730	RS 530	Cray XMP
TPGEOM	139.23	57.47	50.32	20.06	45.74	22.29	29.24	30.85
CTP	26.56	10.58	7.92	3.84	4.06	3.41	4.86	2.56
FLU1	128.07	55.16	14.45	26.31	6.35	21.58	8.97	1.54
GTRAN2	293.85	123.21	72.59	60.21	56.35	47.75	43.07	35.75

Table 2. BWR Assembly Results

	VIM	GTRAN2
Number of Zones	195	1027
k_{eff}	1.31347 ± 0.00042 3.75x10 ⁶ histories	1.31626 (±0.2%)
CPU Time (s)	96.483 (Sun SPARC 2)	166 (Cray X-MP) 673 (IBM RS-350)

Table 4. MHTGR Assembly Results

	VIM	GTRAN2
Number of Zones	232	575
k_{eff}	1.15246 ± 0.00059 2.0x10 ⁶ histories	1.15251 (±0.004%)
CPU Time (s)	25 CPU days (Sun SPARC 1)	423 (IBM RS-350)

Table 3. Comparison of GTRAN2 and VIM Results for BWR Assembly

Group No.	Upper Energy (eV)	Average Flux			Fission Rate			Absorption Rate		
		VIM	GTRAN2	d(%) ^a	VIM	GTRAN2	d(%) ^a	VIM	GTRAN2	d(%) ^a
1	1.00+7	4.03433-2	4.02333-2	0.03	2.71273-3	2.70403-2	0.30	3.44724-2	3.43754-2	0.28
2	8.21+5	3.03944-2	3.03382-2	0.11	3.61559-3	3.61224-3	0.20	2.49763-2	2.48748-2	0.21
3	5.53+3	3.27836-2	3.27756-2	0.02	3.00300-2	3.00362-2	-0.02	1.74161-1	1.74192-1	-0.02
4	4.00+0	7.99106-3	7.99481-3	-0.03	1.21382-2	1.21488-2	-0.09	2.32266-2	2.32489-2	-0.09
5	6.25-1	1.49400-2	1.49084-2	0.21	9.67635-2	9.60724-2	0.06	1.53721-1	1.55448-1	0.18
6	1.40-1	1.70219-2	1.69852-2	0.22	1.71462-1	1.71660-1	-0.12	2.72435-1	2.72148-1	.10
7	3.80-2	1.07166-5	1.07287-2	-0.17	1.97313-1	1.98680-1	-0.69	3.12634-1	3.13752-1	-0.36
TOTAL		1.74182-1 ± 0.03%	1.74034	0.08	3.58451-1 ± 0.06%	3.59240-1	-0.27	9.99568-1 ± 0.04%	1.00004	-0.03

^a d(%) = (GTRAN2/VIM - 1) * 100

Table 5. Comparison of GTRAN2 and VIM Results for MHTGR Assembly

Group No.	Upper Energy (eV)	Absorption Rate in Fuel ^a				Fission Rate in Fuel ^a			
		VIM	d(%) ^b	GTRAN2	d(%) ^b	VIM	d(%) ^b	GTRAN2	d(%) ^b
1	1.00+7	9.09310-4	0.14	9.08618-4	0.08	6.92810-4	0.14	6.92319-4	-0.19
2	8.21+5	6.63410-2	0.09	6.63507-2	0.01	3.99770-2	0.09	3.99819-2	0.01
3	4.00+0	1.75560-2	0.16	1.74896-2	-0.38	1.38610-2	0.16	1.38112-2	-0.37
4	6.25-1	2.91470-2	0.18	2.99122-2	0.16	3.20440-2	0.18	3.30979-2	0.16
5	2.20-1	1.04580-1	0.19	1.04722-1	0.14	8.77930-2	0.19	8.79142-2	0.14
6	3.80-2	6.93120-2	0.30	6.93223-2	0.30	3.90810-2	0.30	3.91298-2	0.30
Fuel	1.00+7	8.48030-2	0.08	8.47489-2	-0.07	3.45340-2	0.08	3.44856-2	-0.09
Thermal	6.25-1	2.13740-1	0.17	2.14137-1	0.2	1.79900-1	0.17	1.80332-1	0.30
TOTAL		2.98350-1	0.12	2.98906-1	0.12	2.94330-1	0.13	2.94733-1	0.13

^a In 1/2 assembly. ^b VIM results are given with +/- standard deviation value.^c d(%) = (GTRAN2/VIM - 1) * 100.

Table 6. Comparison of GTRAN2 and VIM Results for MHTGR Assembly (Continued)

Group No.	Upper Energy (eV)	Average Flux in Graphite				Average Flux in Coolant ^a			
		VIM	d(%) ^b	GTRAN2	d(%) ^b	VIM	d(%) ^b	GTRAN2	d(%) ^b
1	1.00+7	3.63303-2	0.09	3.63492-2	0.03	3.96932-2	0.14	3.96036-2	0.23
2	8.21+5	2.37379-1	0.07	2.37896-1	0.04	2.36742-1	0.09	2.37398-1	0.28
3	4.00+0	2.90718-2	0.09	2.90206-2	-0.18	2.93966-2	0.16	2.92832-2	-0.39
4	6.25-1	1.92269-2	0.08	1.92278-2	0.00	1.92303-2	0.17	1.92633-2	0.07
5	2.20-1	2.96626-2	0.12	2.96337-2	-0.10	2.95312-2	0.19	2.95418-2	0.07
6	3.80-2	9.99703-3	0.19	9.94973-3	-0.47	9.64033-3	0.32	9.72916-3	0.30
Fuel	1.00+7	2.99200-1	0.06	2.99266-1	0.02	3.03834-1	0.08	3.06287-1	0.13
Thermal	6.25-1	5.88845-2	0.09	5.88102-2	-0.13	5.84518-2	0.13	5.85345-2	0.14
TOTAL		3.38087-1	0.03	3.38076-1	-0.00	3.64286-1	0.07	3.64820-1	0.15

^a In 1/2 assembly. ^b VIM results are given with +/- standard deviation value.^c d(%) = (GTRAN2/VIM - 1) * 100.

Figure 1. The T Matrix for Energy Group g

$$\begin{array}{c} N_r \\ N_b \end{array} \begin{array}{|c|c|} \hline & \\ \hline CP_t & SP_t \\ \hline EP_t & TP_t \\ \hline \end{array} \times \begin{array}{|c|} \hline q_t \\ \hline q_t \\ \hline \end{array} = \begin{array}{|c|} \hline r_t \\ \hline r_t \\ \hline \end{array}$$

Figure 2. Parallel Processing in GTRAN2

Figure 3. Serial-to-Parallel Speedups for the T Matrix Calculation

Figure 4. Meshing in VIM (a) and GTRAN2 (b) for BWR Assembly Calculations

Figure 5. Meshing in VIM (a) and GTRAN2 (b) for MHTGR Assembly Calculations

Figure 6. Accuracy in Zone Fluxes for GTRAN2 and VIM (BWR Assembly, Group 2 of 7)

0.33 0.30 0.24	1.01 0.96 0.54	s(%)	d(%)										
0.38 0.33 0.16	0.50 0.42 0.46	0.20 0.17 0.15	0.49 0.42 0.24										
0.30 0.22 0.24	0.23 0.27 0.23	0.32 0.34 0.20	0.42 0.22 0.44	0.29 0.29 0.22	0.48 0.39 0.36								
0.31 0.24 0.16	0.60 0.51 0.35	0.23 0.30 0.23	0.25 0.29 0.04	0.30 0.23 0.19	0.39 0.22 0.07	0.26 0.29 0.18	0.19 0.04 0.23	fuel cladding moderator					
0.34 0.30 0.19	0.02 -0.01 0.20	0.18 0.19 0.17	0.53 0.11 0.10	0.31 0.30 0.18	-0.07 -0.05 -0.15	0.32 0.28 0.21	-0.04 -0.37 -0.38	0.26 0.17 0.13	0.00 -0.23 -0.27	water rod			
0.16 0.26 0.19	0.16 0.42 0.23	0.14 0.23 0.13	0.53 0.40 0.22	0.26 0.21 0.23	-0.14 -0.08 -0.06	0.25 0.27 0.19	-0.75 -0.49 -0.35	0.28 0.32 0.20	0.15 0.23 -0.08	0.34 0.34 0.24	0.48 0.19 0.11		
0.23 0.24 0.16	0.57 0.28 0.09	0.26 0.17 0.23	0.24 0.07 0.05	0.30 0.28 0.25	0.14 0.05 0.00	0.17 0.22 0.20	0.00 0.03 -0.06	0.21 0.19 0.22	0.36 -0.03 -0.04	0.30 0.12 0.30	0.09 0.39 -0.06	0.33 0.41 0.28	0.38 0.39 0.06
0.26 0.36 0.27	0.55 0.01 0.14	0.34 0.41 0.30	-0.02 0.21 0.05	0.24 0.24 0.19	0.17 0.05 0.17	0.30 0.27 0.14	0.14 0.27 -0.01	0.34 0.31 0.21	0.26 0.31 0.21	0.23 0.27 0.27	0.30 0.02 0.19	0.50 0.47 0.39	0.38 0.03 -0.11
												0.43 0.43 0.36	-0.58 -0.60 -0.47

s(%) VIM standard deviation value.
d(%)=(GTRAN2/VIM-1)*100.

Average error:

VIM

0.266%

GTRAN2

0.234%

Figure 7. Accuracy in Zone Fluxes for GTRAN2 and VIM (BWR Assembly, Group 5 of 7)

0.45 0.54 0.44	0.75 1.20 1.25	s(%)	d(%)										
0.56 0.60 0.41	0.86 0.99 0.71	0.53 0.53 0.45	0.78 0.13 0.15										
0.41 0.54 0.36	0.47 0.45 0.73	0.58 0.57 0.37	-0.20 -0.46 -0.15	0.55 0.61 0.48	-0.73 -0.18 0.09								
0.47 0.64 0.33	1.58 1.01 1.42	0.51 0.48 0.35	0.32 -0.23 0.00	0.54 0.34 0.38	-0.95 -0.50 -0.49	0.60 0.63 0.47	-1.16 -1.18 -0.48	fuel cladding moderator					
0.46 0.38 0.29	0.27 0.13 0.75	0.62 0.63 0.28	-0.44 -0.66 -0.35	0.79 0.79 0.44	-0.81 0.00 -0.15	0.58 0.55 0.33	0.35 -0.50 -0.06	0.60 0.57 0.39	-0.24 -0.51 -0.84	water rod			
0.42 0.43 0.29	0.69 0.55 0.70	0.42 0.66 0.37	-0.10 -0.18 -0.39	0.67 0.61 0.44	-0.34 -0.57 -0.79	0.45 0.48 0.45	-0.04 -0.48 -0.71	0.39 0.46 0.33	-0.76 -1.39 -0.43	0.39 0.51 0.22	-0.44 -0.47 0.13		
0.35 0.47 0.35	0.59 0.84 0.65	0.51 0.60 0.40	0.53 -0.05 0.46	0.48 0.37 0.35	0.25 0.43 0.32	0.42 0.47 0.36	-1.03 -0.01 -0.25	0.52 0.52 0.27	-0.37 -0.69 -0.61	0.45 0.42 0.29	-0.19 -0.70 -0.50	0.57 0.39 0.40	0.38 -0.07 -0.01
0.49 0.58 0.49	1.19 1.44 1.12	0.53 0.48 0.39	0.64 0.58 0.98	0.49 0.58 0.34	1.37 1.31 0.92	0.42 0.27 0.18	0.44 0.69 0.73	0.52 0.48 0.33	0.06 -0.82 -0.37	0.48 0.61 0.41	-0.43 -0.31 0.01	0.55 0.56 0.44	0.26 0.26 0.32
												0.65 0.67 0.49	1.41 1.43 1.57

s(%) VIM standard deviation value.
d(%)=(GTRAN2/VIM-1)*100.

Average error:

VIM

0.459%

GTRAN2

0.581%

Figure 9. GTRAN2 Accuracy in Zone Fluxes for MHTGR Assembly

GTRAN2 / VIM RESULTS
FAST FLUX (G: TRIANG MESH 5752, V: 2 MIL HIST)
AV. STAT ERR (VIM) = 0.17(%) AV. REL. ERR (GTRAN2) = 0.12(%)
AV. ERROR = 1.29 (SIGMA)

GRAPHITE: VIM = 0.06%, GTRAN2 = 0.02%, DIFFERENCE = 0.40 SIGMA

○ 0.0 TO 0.25 (%) ⊕ 0.75 TO 1.0 (%)
⊙ 0.25 TO 0.5 (%) ⊗ 1.0 TO 1.25 (%)
⊗ 0.5 TO 0.75 (%) ● ABOVE 1.25 (%)

GTRAN2 / VIM RESULTS
THERMAL FLUX (G: TRIANG MESH 5752, V: 2 MIL HIST)
AV. STAT ERR (VIM) = 0.33(%) AV. REL. ERR (GTRAN2) = 0.30(%)
AV. ERROR = 0.81 (SIGMA)

GRAPHITE: VIM = 0.03%, GTRAN2 = 0.13%, DIFFERENCE = 1.44 SIGMA

○ 0.0 TO 0.25 (%) ⊕ 0.75 TO 1.0 (%)
⊙ 0.25 TO 0.5 (%) ⊗ 1.0 TO 1.25 (%)
⊗ 0.5 TO 0.75 (%) ● ABOVE 1.25 (%)

Figure 10. Background Meshing Generated by GIN

GTRAN2 - MHTGR
BACKGROUND MESHING
GRAPHITE MOTIVE : EQUILATERAL TRIANGLES

3 TRIANGLES ON A FACE
ZONES TOTAL : 362

GTRAN2 - MHTGR
BACKGROUND MESHING
GRAPHITE MOTIVE : EQUILATERAL TRIANGLES

10 TRIANGLES ON A FACE
ZONES TOTAL : 730

Figure 8. 3D and Contour Plots of Fine Mesh Flux Distributions - BWR Assembly

GTRAN2: FLUX DISTRIBUTION IN BWR ASSEMBLY
CASE: 994 SOURCE: 10 ANGLES: 0.1 CM STEP
ENERGY GROUP 7 OF 9

GTRAN2: FLUX DISTRIBUTION IN BWR ASSEMBLY
CASE: 994 SOURCE: 10 ANGLES: 0.1 CM STEP
ENERGY GROUP 8 OF 9

Figure 11. 3D and Contour Plots of Fine Mesh Flux Distributions - MHTGR Assembly

GTRAN2: FLUX DISTRIBUTION IN MHTGR ASSEMBLY
CASE: 975 SOURCE: 30 ANGLES: 0.1 CM STEP
ENERGY GROUP FAST

GTRAN2: FLUX DISTRIBUTION IN MHTGR ASSEMBLY
CASE: 975 SOURCE: 30 ANGLES: 0.1 CM STEP
ENERGY GROUP THERMAL

Appendix B

Technical Report entitled

"Development of Coupled SCALE4.2/GTRAN2
Computational Capability for Advanced MOX
Fueled Assembly Designs"

by

Jasmina Vujic et al.
Department of Nuclear Engineering
University of California, Berkeley

Submitted for presentation and publication

to

International Conference on Mathematics,
Computations, Reactor Physics and Environmental Analysis
ANS Topical Meeting
Portland, Oregon

April 30 - May 4, 1995

*Conference paper
submitted and accepted
separately.*

Appendix C

Exposition entitled

"Long-Term Criticality Safety Concerns
Associated with Weapons Plutonium Disposition"

by

J.S. Choi
Lawrence Livermore National Laboratory

1994

LONG-TERM CRITICALITY SAFETY CONCERNS ASSOCIATED WITH WEAPONS-PLUTONIUM DISPOSITION

J. S. Choi
Lawrence Livermore National Laboratory

Abstract

A substantial inventory of excess plutonium would result from ongoing and planned dismantlement of the U.S. and Russian nuclear weapons. This excess plutonium, as suggested by the study¹ conducted by the U. S. National Academy of Sciences (NAS), could be dispositioned by irradiation in nuclear reactors, or immobilization into high-level waste glass, followed by direct-disposal in geologic repository. Another option mentioned by the NAS study is to bury the plutonium in 4-km-deep boreholes sealed with bentonite clay and concrete. Virtually, all these plutonium-disposition options would generate one or more final disposal waste-forms which would require the evaluation for long-term criticality safety.

The long-term criticality safety concerns arise because the fissile contents (i.e., Pu-239 and its decay daughter U-235) in these Pu-dispositioned waste-forms are higher than that in a LWR spent UO₂ fuel. MOx spent fuel could contain 3 to 4 wt% of reactor-grade plutonium, compared to only 0.9 wt% of plutonium in the LWR spent UO₂ fuel. For the immobilization and the deep borehole options to be economically viable, a plutonium content of 3 to 7 wt% in the waste-forms would be required². If these waste-forms were disposed of in a geologic repository or boreholes, in some future time (tens of thousand of years) when the waste forms were deteriorated by the intruding groundwater, the water could mix with the long-lived fissionable materials to form into a critical system. If the critical system is self-sustaining, fission products produced could readily be available for dissolution and release out to the accessible environment and adversely affecting public health and safety.

This study is to evaluate the long-term criticality safety concerns associated with disposition of fissionable material in a geologic setting. Issues to be addressed include the identification of worst-case water-intrusion scenario and waste-form geometries which present the most concern for long-term criticality safety; and suggestions of technical fixes for such concerns.

References:

- (1) National Academy of Sciences, Committee on International Security and Arms Control, "Management and Disposition of Excess Weapons Plutonium," National Academy Press, 1994.
- (2) Bette Hileman, "U.S. and Russia Face Urgent Decisions on Weapons Plutonium," Chemical & Engineering News, June 13, 1994.

LONG-TERM CRITICALITY SAFETY CONCERNS ASSOCIATED WITH WEAPONS-PLUTONIUM DISPOSITION

J. S. Choi
Lawrence Livermore National Laboratory

I. Introduction

A substantial inventory of excess plutonium would result from ongoing and planned dismantlement of the U.S. and Russian nuclear weapons. This excess plutonium, as suggested by the study¹ conducted by the U. S. National Academy of Sciences (NAS), could be dispositioned in two realistic options: (1) by fabricating the weapons-plutonium into fuel, and irradiating the plutonium-bearing fuel in nuclear reactors, and (2) by immobilizing the weapon-plutonium into high-level waste glass or ceramic. Waste-forms generated in these options, MOx spent fuel in Option 1 and vitrified glass or ceramics in Option 2, would be directly disposed of in a geologic repository. Another possible option mentioned by the NAS study is to bury the plutonium in 4-km-deep boreholes sealed with bentonite clay and concrete. Virtually, all these plutonium-disposition options would generate one or more waste-forms which would require the evaluation for long-term criticality safety.

II. Concerns for long-term criticality safety

The long-term criticality safety concerns arise because the fissile contents (i.e., Pu-239 and its decay daughter U-235) in these Pu-dispositioned waste-forms are significant (i.e., the content could amount to several tens or hundreds of possible critical masses and configurations). MOx spent fuel could contain 3 to 4 wt% of reactor-grade plutonium, compared to only 0.9 wt% of plutonium in the commercial LWR spent UO₂ fuel. For the immobilization and the deep borehole options to be economically viable, a plutonium content of 3 to 7 wt% in the waste-forms would be required². If these waste-forms were disposed of in a geologic repository or boreholes, in some future time (tens of thousand of years) when the waste forms were deteriorated by the intruding groundwater, the water could mix with the long-lived fissionable materials to form into a critical system. If the critical system is self-sustaining, fission products produced could readily be available for dissolution and release out to the accessible environment and adversely affecting public health and safety. The consequences of the long-term criticality safety issue could also lead to concerns in regulatory assessment, and could possibly impact the program schedule for operation of the repository.

III. Waste-package disposal program

The current DOE repository program is managed by the Office of Civilian Radioactive Wastes Management, OCRWM. A potential geologic repository being investigated by the program is located in Yucca Mountain, Nevada. If the site is characterized to be acceptable for disposing high-level radioactive wastes, the spent-fuel from commercial reactors, the small quantities of vitrified HLW glass from West-Valley Processing Plant, and the vitrified defense HLW glass from Defense-Waste Processing Facility (DWPF) in Savannah River Site (SRS), would be disposed of in this first geologic repository. The Site Characterization Report (SCP) for Yucca Mountain described a spent fuel waste package, capable for holding 3 PWR, or 6 BWR spent-fuel assemblies, could be emplaced in a vertical hole within the emplacement drift. Such a vertical hole would also

Figure 1. Yucca Mountain Project reference spent fuel container

DWPF FILLED CANISTER

MATERIAL:	304L SS
EMPTY WEIGHT:	1,100 LB
NET WEIGHT:	3,700 LB
WEIGHT OF RADIONUCLIDES:	56 LB
ACTIVITY:	176,000 Ci
DECAY HEAT:	470 W
DOSE RATE(AT SURFACE)	5,500 RAD/HR
CONTAMINATION:	< 10 ⁻⁴ μ Ci/cm ²

Figure 2. DWPF Waste-glass canister

accommodate a single canister of vitrified waste glass. Figures 1 and 2 shows the dimensions and internal configurations of the vertical-emplacement container for spent-fuel and vitrified glass, respectively.

OCRWM is also considering the usage of a multiple-purpose-container (MPC) for storage, transportation and final disposal of commercial LWR spent UO₂ fuel and DWPF vitrified waste glass. A MPC could hold up to 21 PWR spent-fuel assemblies, or four vitrified glass containers (as depicted in Figures 3 and 4). Such MPCs would be emplaced horizontally in an emplacement drift, with proper spacing to account for the thermal heat effects. Figure 5 gives the graphical presentation of the MPC emplacement method.

IV. Quantities of fissile material in waste-package

Table 1 depicts the amount of plutonium in different waste-types and packages. As plutonium-239 decays (with half-life of 24,400 years), as function of disposal time, into its decay daughter U-235, also a fissile material, the potential for a criticality incident occurring may have been lessened somewhat because of the lesser reactivity potential with U-235. Nevertheless, the concern for long-term criticality safety with U-235 (with half life of 700 million years) remains, if ground water could intrude into the waste emplacement location and form into a critical system with U-235.

V. Waste-package degradation scenarios

Hundreds of thousands years after the emplacement of waste packages in the geologic repository, it is assumed, for the purpose of simplistic illustration with a glass waste package, that water could intrude into the emplacement location by means of a wet-drip water contact model. Groundwater dripped from the cold surfaces of the shield-plug (for vertical emplacement) or the inner wall of the horizontal drift (for MPC emplacement without backfill) and impinging on the waste canister could degrade the canister at the point of contact and result in water entering the waste canister, as shown in Figures 6 & 7 for waste packages in vertical and MPC emplacement, respectively. As water filled up the void space inside the canister, it would dissolve and leach away the soluble ingredients in the waste form, leaving behind those insoluble elements, such as plutonium. The resulting system with plutonium mixed in groundwater inside the waste canister could reach to a configuration and fissile contents such that a sustaining criticality could be possible.

VI. Criticality concern for a water-reflected plutonium-water system

Figure 8 shows the spherical critical volume as a function of plutonium density for a plutonium-water system fully reflected by water. This curve was generated by using known critical experimental data and analytical methods. It is used here to simulate the plutonium-groundwater mixture surrounded by the host rock. When constant-fissile-mass curves were drawn and shown in the same figure, it is indicated that for a spherical system of homogeneous Pu-water solution, fully reflected, only 0.5 kg would be subcritical for all Pu concentrations and volumes. For any other Pu quantities, it would be subcritical only for certain combinations of volumes and Pu concentration. For 16 kg of weapons plutonium in the homogeneous mixture, it would be always critical except for the Pu concentration lower than 0.007 g/cc. Since the waste package could contain many times the critical mass, there is a concern for a criticality incident if formation for such a fissile aqueous system is possible.

VII. Suggestions for technical solution to the criticality concern

To prevent a long-term criticality incident in a geologic setting, it is proposed here to mix into the plutonium-bearing waste packages with neutron absorbers. The presence of

Figure 4. MPC Package for vitrified waste glass

Figure 5 MPC Emplacement

Table 1:

Amount of plutonium in:

Waste Type:	Unit loading:		Waste package emplacement:	
	<u>wt%</u>	<u>kg</u>	<u>vertical(kg)</u>	<u>drift/MPC(kg)</u>
UO2 spent fuel	0.9	4	12	84
MOx spent fuel	4	18	54	378
glass	2 - 5	34 - 84	34 - 84	136 - 336
ceramic	25	?	?	?

Figure 6. The Wet-Drip Water Contact Mode *for vertical emplacement*

Figure 7. Wet-Dry Water Contact mode for MPC

SPHERICAL CRITICAL VOLUME (L)

Figure 8. Critical volumes of homogeneous water-moderated plutonium spheres.

neutron absorbing material in the homogenous fissile-aqueous system would significant reduce the possibility of a criticality. Possible neutron absorbing materials are: Boron (with isotope B-10), Gadolinium, Erbium (with isotope Er-167), Dysprosium, Hafnium, etc. The selected neutron poison should possess similar geo-chemical characteristics, such as solubility, leachability, and chemical stability, as plutonium. This is because the neutron absorber should not be easier dissolved and leached away from the waste-package than plutonium. The selection criteria for the proper neutron absorbing material, as well as their quantities which would be sufficient to prevent a long-term criticality from happening with a plutonium (or a U-235) system, are currently being explored.

VIII. Conclusion

This study presented a concern for long-term criticality safety associated with the disposition of weapons-plutonium in a geologic repository. It described the scenario which could lead to such a criticality condition, including the fissile-material quantities, the worst-case configuration for a degraded waste-package, and the resulting consequence of releasing fission products generated in the criticality incident. It also suggested a possible technical fix to the problem, which is the inclusion of neutron absorbing material in the making of the waste-form. The presence of neutron poison in the aqueous fissile solution would stifle the nuclear chain reactions, and subsequently reduce the possibility of a criticality. However, the selection of the proper neutron poison, the amount, as well as the method of doping the absorber into the plutonium-bearing waste form, would require further feasibility study to assure that the long-term criticality safety concern could be technically resolved.