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Nuclear Criticality Analyses of Separations Processes for the Transmutation Fuel Cycle: Quaterly Report

William Culbreth
University of Nevada, Las Vegas, william.culbreth@unlv.edu

Pang Tao
University of Nevada, Las Vegas, pang@physics.unlv.edu

Quarterly Report
AAA/UNLV University Participation Program

Title:

Nuclear Criticality Analyses of Separations Processes for the Transmutation Fuel Cycle
2362-254-504L

Principal Investigators:

William Culbreth, Ph.D.
Department of Mechanical Engineering
University of Nevada, Las Vegas
4505 Maryland Parkway, Las Vegas, NV 89154-4027
(702) 895-3426, culbreti@clark.nscee.edu
FAX: (702) 895-3936
http://culbreth.me.unlv.edu

Tao Pang, Ph.D.
Department of Physics, 4002
University of Nevada, Las Vegas
(702) 895-4454
FAX: (702) 895-0804
pang@nevada.edu

Collaborators:

George Vandegrift, Ph.D.
Senior Chemist, Group Leader
Separation Science and Technology
Chemical Technology Division
Argonne National Laboratory
(630) 252-4513
FAX: (630) 972-4513
Vandergrift@cmt.anl.gov

James Laidler, Ph.D.
Director, Chemical Technology Division
Argonne National Laboratory
(630) 252-4479
FAX: (630) 252-5528
Laidler@cmt.anl.gov

Denis Beller, Ph.D.
UNLV/ATW University Liaison
Harry Reid Center for Environmental Studies
4505 Maryland Parkway, Las Vegas, NV 89154-4009
(702) 895-2023, beller@lanl.gov, FAX: (702) 895-3094

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Contents

1. Project Description

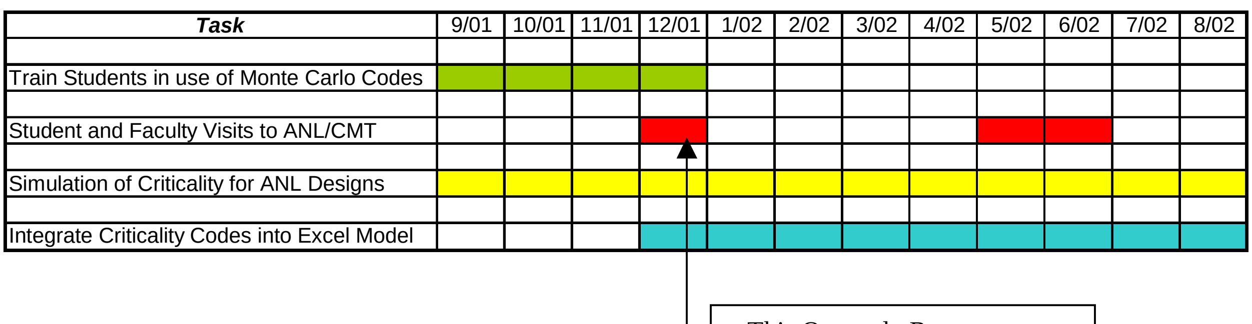
The success of the ATW program will rely upon the ability of radiochemists to separate spent nuclear fuel into uranium, fission products, and transuranic wastes. The Chemical Technology Division at the Argonne National Laboratory is actively involved in the development of pyrochemical separation technology that minimizes the usage of strong acids with the subsequent problems involved in disposing of the acidic residue.

Small scale experiments are being validated at ANL to separate spent fuel, but they must be scaled up to accommodate the large amount of commercial spent fuel that must be treated. As the volume of waste to be treated is increased, there is a higher probability that fissionable isotopes of plutonium, americium, and curium can accumulate and form a critical mass. Criticality events can be avoided by ensuring that the effective neutron multiplication factor, k_{eff}, remains below a safe level. NRC regulations normally allow an upper value of 0.95 for k_{eff}. This parameter can be computed for any combination of fuel and geometry using Monte Carlo neutron transport codes. SCALE 4.4a from the Oak Ridge National Laboratory and MCNP4C2 from the Los Alamos National Laboratory are two codes that are regularly used to assess criticality.

In this project, students at the University of Nevada were trained in the use of KENO and SCALE 4.4a to assist Dr. Laidler and his team at ANL in criticality safety assessments.

2. Review of Tasks

The proposed tasks for this project are listed in the timetable shown below:



This Quarterly Report covers progress to this point.

During the first quarter of the work, the tasks included training students in the use of Monte Carlo codes used in radiation transport studies and the assessment of neutron multiplication factors for specific problems outlined by ANL-East through Drs. Laidler and Vandegrift.

The proposal also included objectives for the first year of work on this project, as listed below. The work conducted in the first quarter of the project was in partial completion of these objectives.

- Train UNLV students in the use of SCALE and/or MCNP for the assessment of nuclear criticality.

- Assess neutron multiplication factor, k_{eff}, for geometries and material concentrations as defined by the collaborating team from ANL-CMT for the ATW project.

- Provide software, extrapolation tables, or other methods to incorporate criticality estimates into the existing ANL Excel model of the pyrochemical treatment process to be used for ATW.

3. Progress in the First Quarter

- Student Training

The students presented their progress in oral and poster presentations at the 2001 Winter Annual Conference of the American Nuclear Society in Reno, Nevada. Students were trained by Dr. Culbreth in the use of KENO and SCALE 4.4a. The students employed on the project included:

- Jason Viggato – doctoral student in mechanical engineering.
- Elizabeth Bakker – senior in mechanical engineering.
- Daniel Lowe – sophomore in mechanical engineering
- Maurice Moore – part-time masters student in mechanical engineering.

All of the students also assisted on another AAA project involving radiation transport calculations for neutron spallation target studies at LANSCE. During the first quarter of both projects, students were taught to use KENO in preparation for their work in radiation transport and criticality.

<u>American Nuclear Society Conference</u>

Mr. Viggato, Mr. Lowe, Ms. Bakker, and Dr. Culbreth attended the American Nuclear Society Conference in November 2001 held in Reno, Nevada. Each student presented a paper on their work on the AAA project. Their work was also presented in poster form. Each student's paper discussed both this project and their initial work on the AAA Radiation Transport project. Copies of two of the papers are included with this report as Appendix C and D.

In September, 2001, Dr. Culbreth was invited to give a departmental seminar on the AAA project. A copy of his presentation is included as Appendix B.

<u>Computational Resources</u>

The students working on the project have been trained in the use of SCALE 4.4a, a Monte Carlo simulation code that simulates the scattering and absorption of neutrons in nuclear fuel. Students began their training with simple problems using KENO IV and are now involved in preparing CSPAN input files. Danny Lowe and Elizabeth Bakker are also involved in writing BASIC programs that automate the process of preparing CSAS and KENO-VI input.

Several computers have been ordered to allow the students to complete their calculations. Two 1.8 GHz Gateway computers with 512 MB of memory have been ordered. The students are using computers in Dr. Culbreth's office until the additional computers arrive.

- Visits to Laboratory Sites

The students met Dr. Laidler at the American Nuclear Society meeting in late November. In mid-December, W. Culbreth, D. Lowe, and E. Bakker traveled to Chicago to meeting with Dr. Laidler's staff at the Argonne National Laboratory. The visit helped us understand the geometry of the equipment used in fuel separation along with the possible scenarios that can lead to possible criticality events. The complexity of working with radioactive and fissionable substances through gloveboxes also helped in our understanding of the process.

- Simulation of Criticality for ANL Designs

Criticality assessments were completed using SCALE 4.4a based on mixtures of process salts, fission products, and actinides as specified by Drs. Laidler and Vandergrift. The mixture is to be placed in a cylindrical steel container and excessive quantities of transuranic wastes in the mixture can lead to criticality safety problems. The results of the criticality assessments were submitted as a report to Argonne titled: "Assessment of Criticality Safety for Cylindrical Containers to be Used In the Processing of Spent Fuel.". A copy is enclosed as Appendix A.

- Integrate Criticality Codes into Excel Model

The results included an Excel program that could be used to predict the value of k-effective for a shielded cylinder containing a combination of process salts, actinides, and fission products. The composition of material, as well as the geometry of the cylinder, can be changed in the spreadsheet and an assessment of the criticality safety is completed by the Excel program. The program incorporates the uncertainty reported from SCALE 4.4a to determine whether k-effective < 0.95 for any combination of fuel and geometry.

4. Work Scheduled for Second Quarter

During the second quarter of the project, the students will travel to the Argonne National Laboratory to meet with Dr. Laidler and his staff. There are two criticality problems that we are preparing to analyze.

The first problem involves an assessment of the maximum mass of transuranic material that can be safely accumulated in a pyrochemical cell as shown in figure 1. Spent fuel, as shown in the figure, is dissolved in process salt at a high temperature. The uranium has been depleted by fission and will remain subcritical. Concentrations of plutonium, americium, and curium in the transuranic wastes collecting about the second electrode can form a critical mass. We plan to use SCALE 4.4a to assess the safety of the pyrochemical cell as transuranics are accumulated.

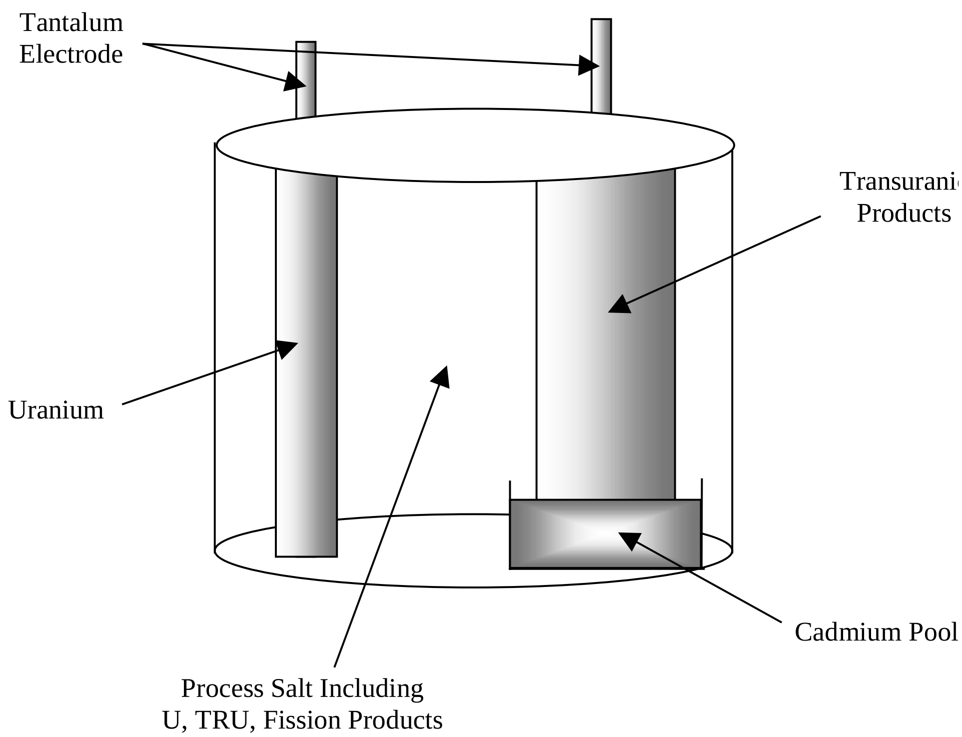


Figure 1 Example of a Pyrochemical Cell Used to Separate Transuranics from Uranium and Fission Products

A second problem to be analyzed involves criticality in separated quantities of curium. Curium is a fissionable actinide and its separation from other transuranic wastes simplifies further treatment of spent fuel. We plan to conduct SCALE 4.4a analyses of curium to assess what quantities will result in a critical mass.

Appendix A

Report to ANL

Assessment of Criticality Safety for Cylindrical Containers to be Used In the Processing of Spent Fuel

Report

UNLV

Assessment of Criticality Safety for Cylindrical Containers to be Used In the Processing of Spent Fuel

October 28, 2001

Bill Culbreth
Daniel Lowe
Jason Viggato

Department of Mechanical Engineering
Box 4027
University of Nevada
Las Vegas, NV 89154-4027
Phone: (702) 895-3426
FAX: (702) 895-3936
Culbreti@clark.nscee.edu
http://culbreth.me.unlv.edu

Introduction

The UREX process separates uranium from transuranic wastes (TRU) and fission products (FP). Nuclear reactors require *fissile* isotopes that will absorb neutrons and break apart into smaller nuclei while releasing a large amount of energy as well as multiple neutrons. Fissile isotopes in spent fuel include not only ^{235}U, but also ^{239}Pu, ^{241}Pu, and several isotopes of americium (Am) and curium (Cm).

TRU contains the actinides with atomic numbers greater than that of uranium. This includes Pu, Np, Am, and Cm. When TRU is separated from uranium, the TRU still poses a significant risk of sustaining a chain reaction. This is quantified through the effective neutron multiplication factor, k_{eff}.

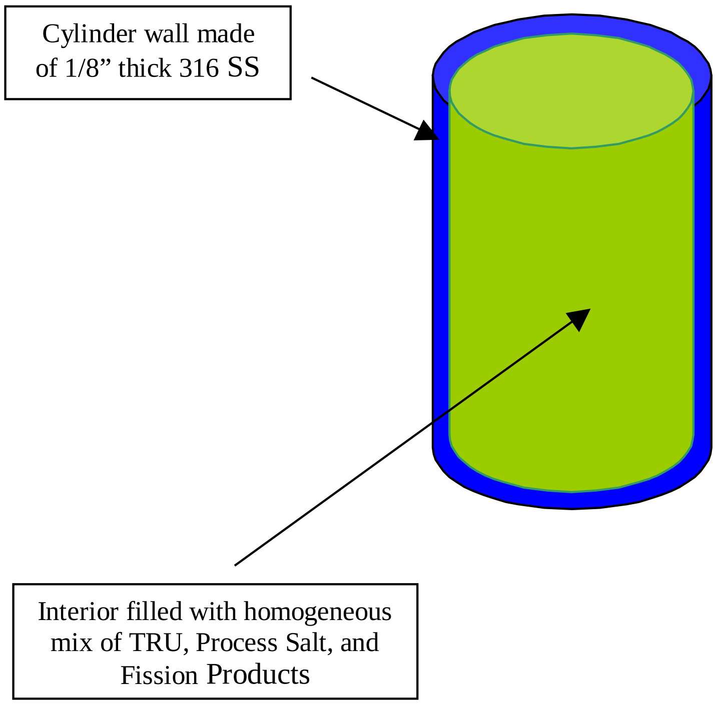


Figure 1 Cylindrical Problem with TRU, Process Salt, and Fission Products

$k_{eff} < 1$, subcritical
$k_{eff} = 1$, critical
$k_{eff} > 1$, supercritical

To prevent TRU from becoming critical (sustaining a chain reaction), k_{eff} must be maintained at a value of less than 1. The presence of neutron poisons (Sm, Xe, B, Hf, Cd, etc.) will decrease k_{eff}. Neutron poisons are found in fission products. The presence of neutron moderators (H, C, Be) or materials that reflect neutrons will enhance k_{eff}.

To assess k_{eff}, Monte Carlo simulation codes are used. The concentration of TRU, process salts, and fission products along with the geometry of the mixture and surrounding reflective material are inputs to these codes.

Geometry to be Analyzed

To begin k_{eff} studies of reprocessing material, CMT identified a sample problem based on the geometry shown in figure 1. The cylindrical container is 75 cm high and 50 cm in diameter. The ratio of D/H, %TRU, and %FP were to be varied.

Analysis

SCALE 4.4a, a neutron transport code developed by the Oak Ridge National Laboratory, was used for these studies. Microsoft Basic programs were used to prepare SCALE input files and to process the results. A schematic of the analysis is shown in figure 2.

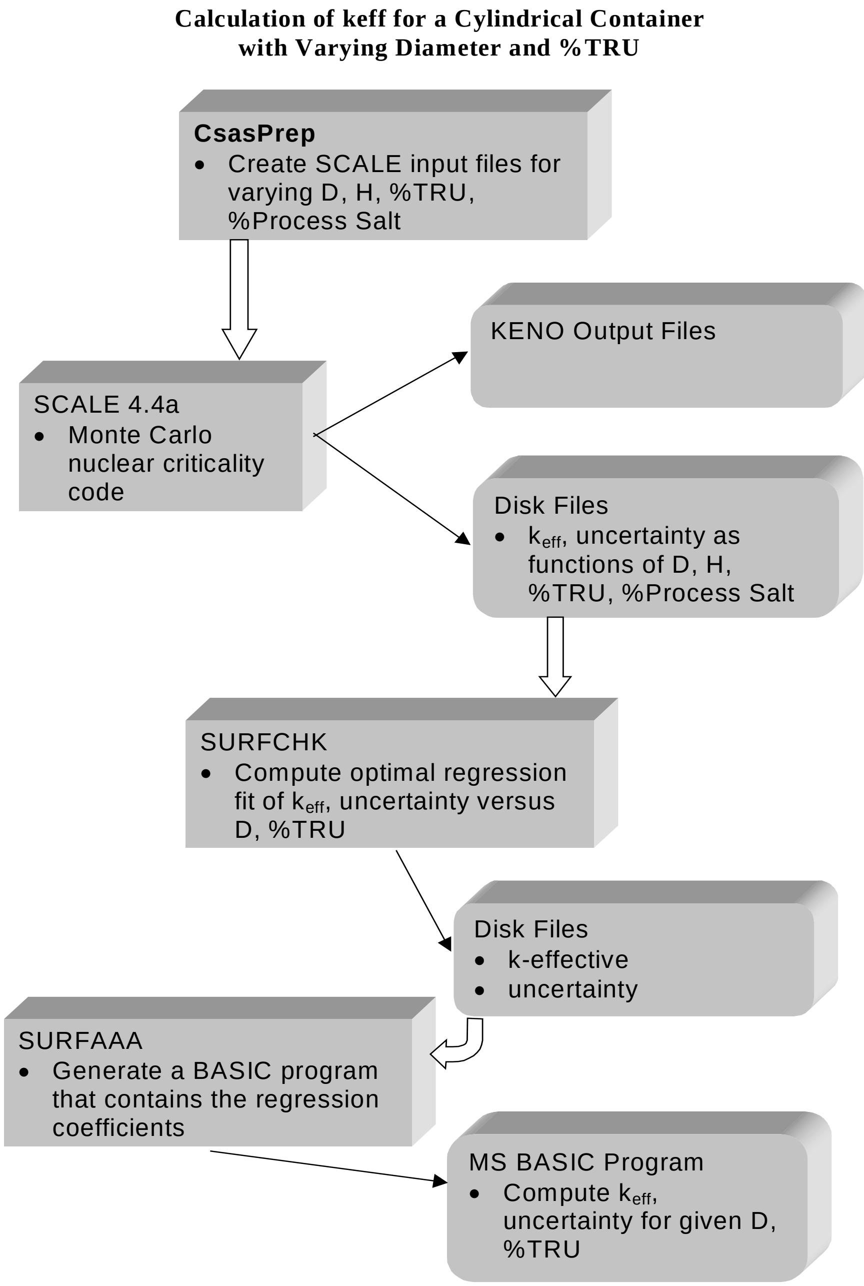


Figure 2 Schematic of the Computer Processing used in the Analysis of k-effective

The program CSASPREP generated the SCALE input files. These files contained the "reactor" geometry and the number densities of TRU, fission products, and process salts within the mixture. Since regression fits were used, a large number of SCALE runs were made. CSASPREP automatically generated each file, called the SCALE software through a DOS command, and collected the values of keff and its uncertainty from the SCALE output files. A separate disk file containing the container diameter, height, %TRU, and % process salt was automatically written by the program. Sample results are shown in Appendix A.

The cylinder diameter and the % TRU were varied by the program. Cylinder volume was assumed constant and height was automatically calculated as diameter was varied. For these initial results, no fission products were assumed to exist within the mixture. The percentage of process salts within the mixture was computed from the % TRU.

A two-dimensional regression fit of the data was made to calculate keff(D, %TRU). The optimal order of the fit was determined using program SURFCHK. The actual fit was accomplished using SURFAAA. Results are shown in figure 3 as a contour plot and in figure 4 as a surface plot.

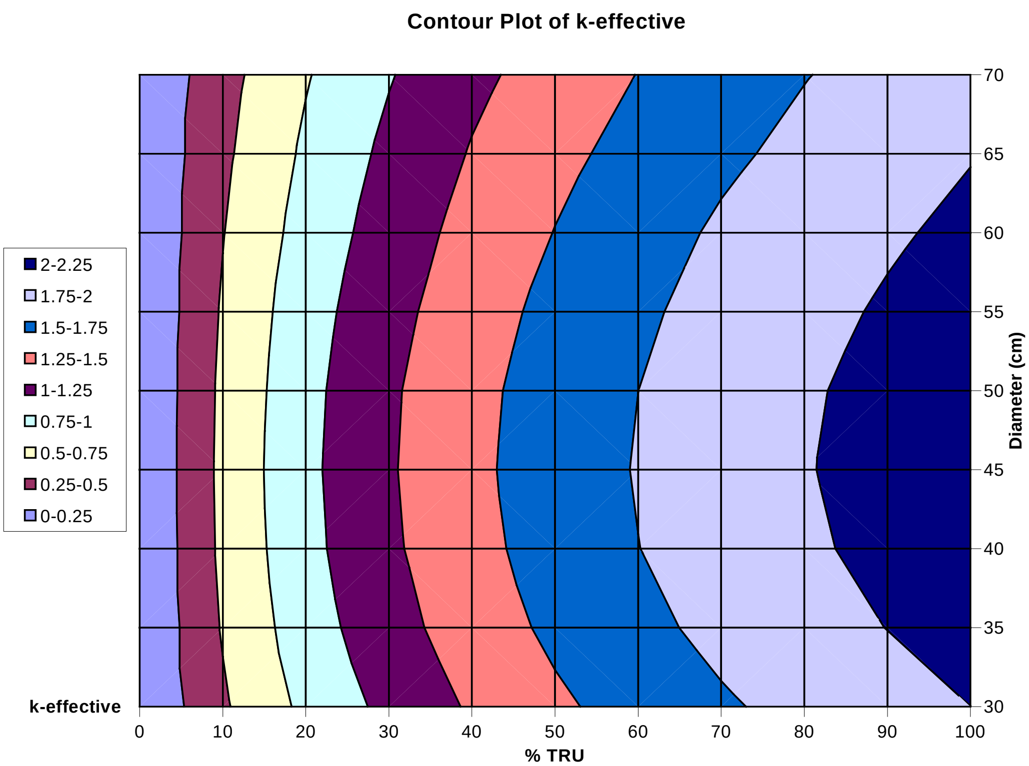


Figure 3 Contour Plot of the Effective Neutron Multiplication Factor As a function of Cylinder Diameter and % TRU in the Mixture

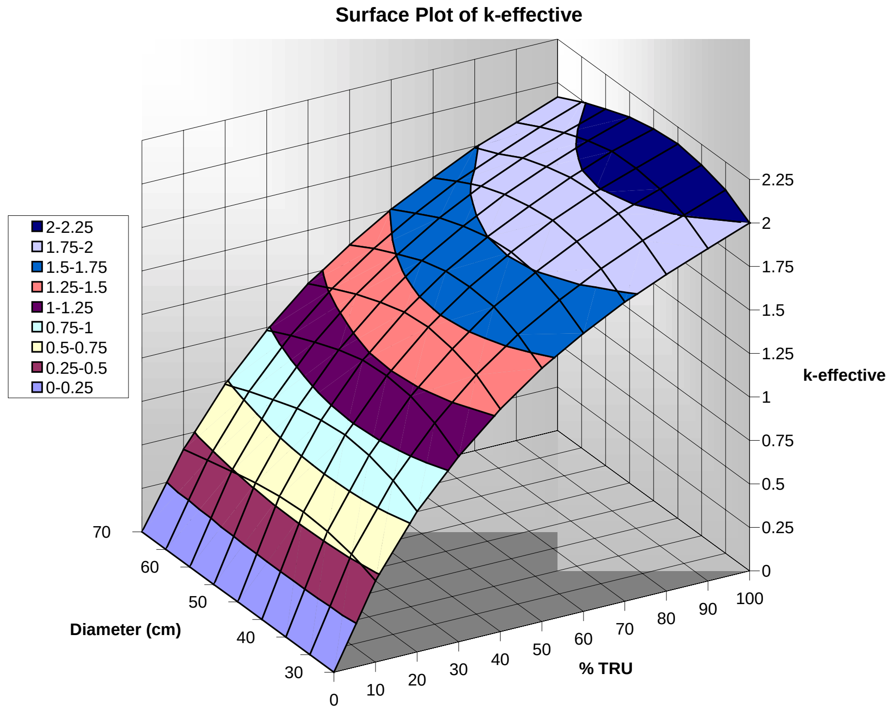


Figure 4 Surface Plot of k-effective as a Function of %TRU and Cylinder Diameter

To ensure criticality safety, the value of k_{eff} must be less than 1. Although SCALE 4.4a is approved by the Nuclear Regulatory Commission (NRC) for use in designing nuclear power plants, the NRC requires a margin of safety of 5% in assessing k_{eff}. The SCALE code also generates a statistical uncertainty. To maintain safe operation:

$$k_{eff} < 0.95 \text{ - statistical uncertainty}$$

During a recent visit by J. Laidler and G. Vandergrift to UNLV, we learned that the AMUSE code was written in Microsoft EXCEL to allow both MAC and PC users to run the code. We followed this trend and also prepared an EXCEL code to assess criticality safety for the cylindrical geometry containing TRU and process salt. The program is titled ***cylinder-criticality.xls*** and it is attached with this report. A sample screen from the program is shown in figure 5.

The EXCEL program receives, as input, the cylinder diameter and the percentage of TRU in the mixture within the cylinder. The effective neutron multiplication factor is computed from the curve fit coefficients and the resulting value is compared with the safety limit:

$$k_{eff} < 0.95 \text{ - statistical uncertainty - maximum error of the curve fit}$$

Calculation of k-effective for a Cylindrical Container with TRU and Process Salt

Bill Culbreth
University of Nevada, Las Vegas

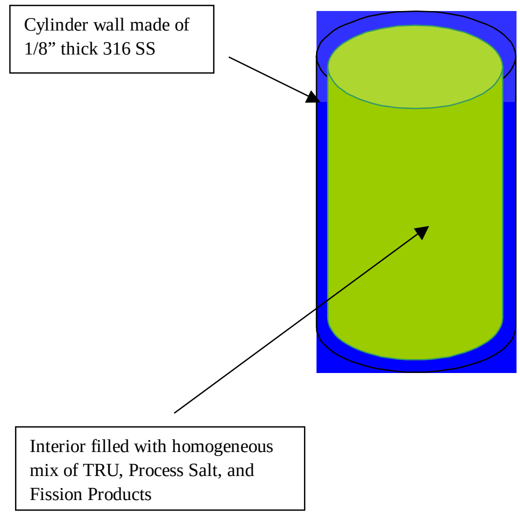
This program calculates the effective neutron multiplication factor, k-effective, for a cylindrical container with a 1/8 inch thick wall made from 316 SS. The mixture inside the container is assumed to be composed of TRU with Process Salt. The nominal diameter may be varied, and the height will be computed to preserve the original container volume. SCALE 4.4a was used to generate the results. A least-squares regression fit o fthe data was used to estimate k-effective as a function of cylinder diameter and %TRU.

A. Input

Please change the two values included below to recalculate the value of k-effective:

Enter the Cylinder Diameter (cm):	50
Enter the percent (%) TRU:	40

Nominal Volume (cm^3) is:	147262.15
The Resulting Container Height (cm) is:	75



B. Results

k-eff:	**1.403**
Standard Error:	3.05E-002
Maximum Error:	5.82E-002

Maximum KENO Uncertainty:	0.0031	
Maximum Possible Value of k-eff:	1.464	
Limit of k-eff for Safety:	0.95	
Is this Safe from a Criticality Event?	SAFE	**UNSAFE**

C. Calculations

Order	Coefficient	I	J	
0	-9.78E-002	0	0	-0.09783378
1	0.6884337	0	1	0.27537349
2	-0.0522729	0	2	-0.00836366
3	0.6726148	1	0	0.48043915
4	2.8150107	1	1	0.80428877
5	-2.1761193	1	2	-0.24869935
6	-0.507453	2	0	-0.25890461
7	-2.0879773	2	1	-0.42611782
8	1.6187672	2	2	0.13214426
			Sum:	0.65232646
			k-eff:	1.40289329

Figure 5 Microsoft Excel Program *Cylinder-Criticality.xls* Used to Assess Criticality Safety

The resulting value of k_{eff} is used to determine whether the mixture and geometry is safe or unsafe.

Conclusions

An attached EXCEL program assesses the criticality safety of a cylindrical vessel containing both TRU and process salts. The program represents the results of a series of SCALE 4.4a runs that have been fit to a regression curve.

The SCALE neutron libraries contain the cross-sections of all of the radioisotopes contained within TRU, the process salts, and fission products as identified by CMT. We are working on a general curvefit in three independent variables to model the cylindrical geometry where % fission product can also be varied. We would appreciate additional geometries to model. Would also like feedback on the best way to present the criticality results to CMT.

Appendix A
Sample SCALE 4.4a Results

Diameter	Height	TRU	Process Salt	k-effective	uncertainty
(cm)	(cm)	(percent)	(percent)		
30	208.3333	10	90	0.4673	0.0009
30	208.3333	20	80	0.8078	0.0016
30	208.3333	30	70	1.0652	0.0017
30	208.3333	40	60	1.2796	0.0018
30	208.3333	50	50	1.4569	0.0022
30	208.3333	60	40	1.5989	0.0026
30	208.3333	70	30	1.7203	0.0027
30	208.3333	80	20	1.8205	0.0025
30	208.3333	90	10	1.913	0.0022
30	208.3333	100	0	1.9995	0.0025
35	153.0612	10	90	0.5191	0.001
35	153.0612	20	80	0.8847	0.0016
35	153.0612	30	70	1.1566	0.0023
35	153.0612	40	60	1.3748	0.0023
35	153.0612	50	50	1.5494	0.0022
35	153.0612	60	40	1.6897	0.0026
35	153.0612	70	30	1.8116	0.0025
35	153.0612	80	20	1.9154	0.0029
35	153.0612	90	10	2.0032	0.0025
35	153.0612	100	0	2.0876	0.0023
40	117.1875	10	90	0.5495	0.001
40	117.1875	20	80	0.9283	0.0016
40	117.1875	30	70	1.2097	0.002
40	117.1875	40	60	1.4246	0.0025
40	117.1875	50	50	1.6074	0.0021
40	117.1875	60	40	1.7468	0.0026
40	117.1875	70	30	1.866	0.0024
40	117.1875	80	20	1.9689	0.0024
40	117.1875	90	10	2.0521	0.0026
40	117.1875	100	0	2.1307	0.0027
45	92.59259	10	90	0.559	0.0009
45	92.59259	20	80	0.9441	0.0015
45	92.59259	30	70	1.226	0.0024
45	92.59259	40	60	1.4481	0.0026
45	92.59259	50	50	1.6217	0.0024
45	92.59259	60	40	1.7639	0.0021
45	92.59259	70	30	1.8872	0.0026
45	92.59259	80	20	1.988	0.0025
45	92.59259	90	10	2.0706	0.0026
45	92.59259	100	0	2.1506	0.0024
50	75	10	90	0.5501	0.001
50	75	20	80	0.929	0.0016
50	75	30	70	1.2148	0.0017

50	75	40	60	1.4344	0.0023
50	75	50	50	1.611	0.0021
50	75	60	40	1.7497	0.0026
50	75	70	30	1.8676	0.0023
50	75	80	20	1.9739	0.0022
50	75	90	10	2.0662	0.0025
50	75	100	0	2.1375	0.0026
55	61.98347	10	90	0.526	0.0011
55	61.98347	20	80	0.8961	0.0016
55	61.98347	30	70	1.1735	0.0019
55	61.98347	40	60	1.3894	0.0023
55	61.98347	50	50	1.5701	0.0023
55	61.98347	60	40	1.7111	0.0024
55	61.98347	70	30	1.8341	0.0023
55	61.98347	80	20	1.9359	0.0031
55	61.98347	90	10	2.0254	0.0026
55	61.98347	100	0	2.104	0.0024
60	52.08333	10	90	0.4909	0.0011
60	52.08333	20	80	0.8451	0.0018
60	52.08333	30	70	1.1172	0.0018
60	52.08333	40	60	1.3334	0.0019
60	52.08333	50	50	1.5057	0.0026
60	52.08333	60	40	1.657	0.0026
60	52.08333	70	30	1.7813	0.0026
60	52.08333	80	20	1.8839	0.0024
60	52.08333	90	10	1.9723	0.0022
60	52.08333	100	0	2.0487	0.0031
65	44.3787	10	90	0.4546	0.001
65	44.3787	20	80	0.7908	0.0015
65	44.3787	30	70	1.0554	0.0017
65	44.3787	40	60	1.2663	0.0023
65	44.3787	50	50	1.4375	0.002
65	44.3787	60	40	1.5819	0.0021
65	44.3787	70	30	1.7077	0.0021
65	44.3787	80	20	1.8082	0.0025
65	44.3787	90	10	1.9039	0.0023
65	44.3787	100	0	1.9899	0.0026
70	38.2653	10	90	0.4161	0.0008
70	38.2653	20	80	0.7316	0.0014
70	38.2653	30	70	0.9838	0.0018
70	38.2653	40	60	1.1925	0.0019
70	38.2653	50	50	1.3578	0.0019
70	38.2653	60	40	1.5053	0.0028
70	38.2653	70	30	1.6263	0.002
70	38.2653	80	20	1.7412	0.0026
70	38.2653	90	10	1.829	0.0025
70	38.2653	100	0	1.9178	0.0025

Appendix B

Powerpoint Presentation

“Nuclear Criticality Analyses of Separations Processes for the Transmutation Fuel Cycle“

Department of Mechanical Engineering Seminar

Slide 1

Nuclear Criticality Analyses of Separations Processes for the Transmutation Fuel Cycle

September 26, 2001

Bill Culbreth
Department of Mechanical Engineering
Tao Pang
Department of Physics
University of Nevada, Las Vegas

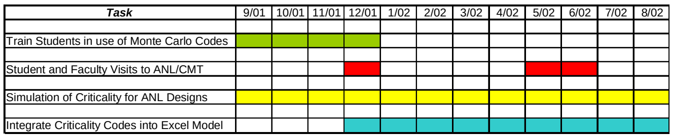
Slide 2

Research Objectives and Goals

- Train UNLV students in the use of SCALE and/or MCNP for the assessment of nuclear criticality.
- Assess neutron multiplication factors, k_{eff}, for geometries and material concentrations as defined by the collaborating team from ANL-CMT for the ATW project.
- Provide software, extrapolation tables, or other methods to incorporate criticality estimates into the existing ANL Excel model of the pyrochemical treatment process to be used for ATW.

Slide 3

Schedule



Slide 4

Project Initiation

- Review of the literature and standards on criticality safety during fuel separation and processing of actinides.
- Schedule visits for UNLV students and faculty to ANL-East to acquire information on the separation process, to review the steps in the process that may lead to criticality problems, and to learn the use of the CMT Excel program used to simulate the separation process.

Slide 5

Initial Tasks from CMT

- SCALE 4.4/KENO VI input files will be prepared based on the isotopic composition of the transuranic material (TRU), the fission products (FP), and the molten process salt (PS).
- Conduct parametric studies of k_{eff} as a function of the process vessel aspect ratio and the ratio of (TRU + FP) to process salt.

Slide 6

Initial Tasks II

- Compute the variation of k_{eff} with fission product concentration in the process mixture.
- Compute the effect of the key neutron absorbers within the fission products on k_{eff}. Report the results of the criticality runs through tables and curvefits of k_{eff}.
- Work with the ANL-CMT scientists to provide additional criticality data as required for their work on the separation processes for ATW.

Slide 7

Initial Tasks III

- EXCEL or Visual Basic Programs: ANL-CMT has developed a Microsoft Excel program to model the separation processes. UNLV will work with ANL-CMT to incorporate criticality safety predictions into their Excel code. Excel or Visual Basic programs will be written to spawn KENO or MCNP runs based on the process mix and the vessel geometry and composition. The KENO or MCNP runs will return k_{eff} to the Excel simulation to ensure that the geometry and composition are allowable.

Slide 8

Students

- Jason Viggato
  - Doctoral Student in Mechanical Engineering
  - M.S. at UNLV in porous media flow
  - Dissertation work on criticality simulations in natural uranium reactor sites in Gabon, Africa
  - Preparing CSAS Input Files within SCALE 4.4a for Criticality Simulations

Slide 9

Students II

- Danny Lowe
  - Undergraduate Student in Mechanical Engineering
  - Worked with W. Culbreth on Liquid Nitrogen Engines for Cars
  - Learning KENO V and conducting simulations

Slide 10

Students III

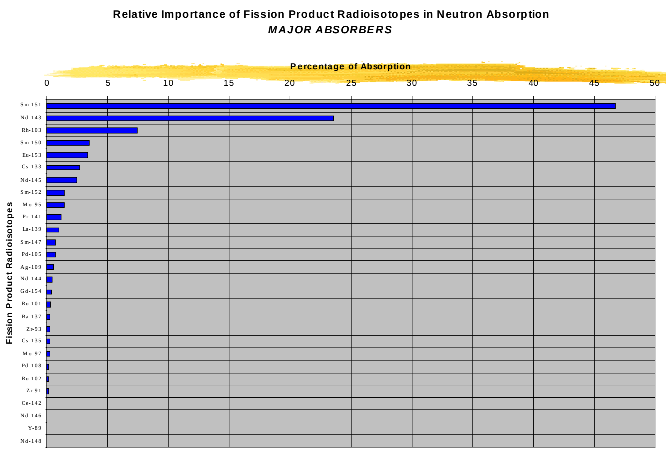
- Elizabeth Bakker
  - Undergraduate Student in Mechanical Engineering
  - Summer Internship with Bechtel, Nevada at the Nevada Test Site
  - Learning KENO V and Running Simulations

Slide 11

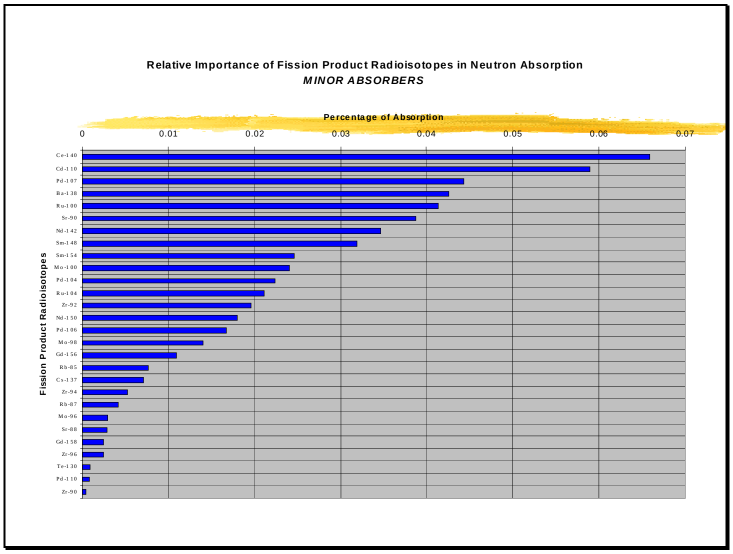
Progress to Date

- KENO V
  - Students are being trained in its usage
  - Students are writing BASIC programs to automate k_{eff} simulations
- SCALE 4.4a
- MS Visual Basic
- Student Workstations
  - 1.8 GHz Intel computers with 512 MB RAM

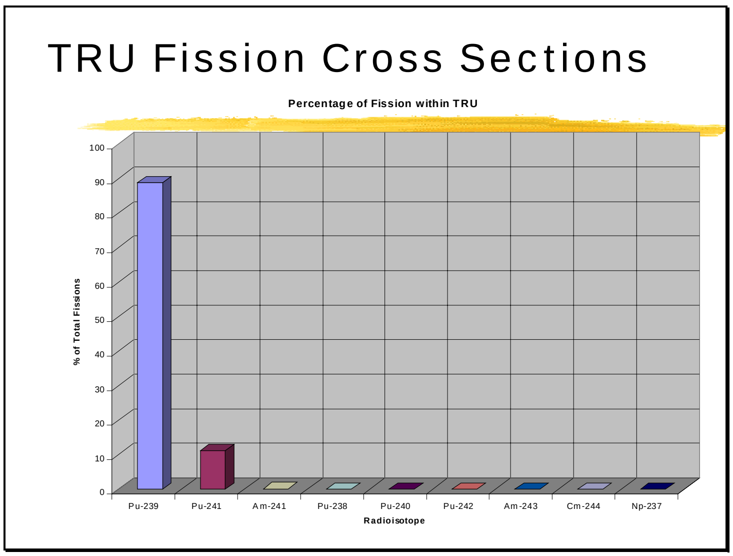
Slide 12



Slide 13

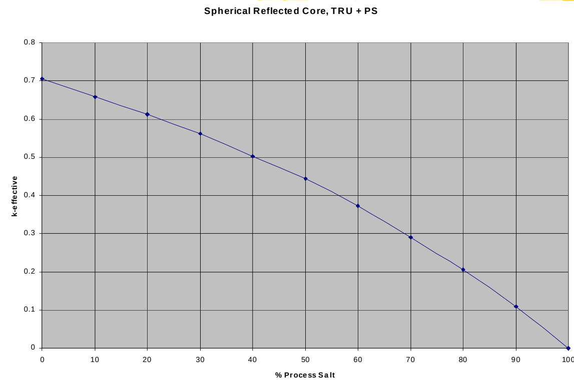


Slide 14



Slide 15

Parametric Calculations of k_{eff}



Slide 16

Parametric Calculations of k_{eff}

- Values of k_{eff} are calculated as a function of cylinder radius, height, %TRU, %FP, and %PS
- KENO V is used for initial calculations with a limited selection of radioisotopes
- Results are plotted on contour and surface plots
- Regression fits provide k_{eff}(r,h,%TRU,%FP,%PS)

Slide 17

Next Step

- Provide initial results to CMT
- Use the extended cross section libraries available in SCALE 4.4a
  - All requested TRU, FP, and PS radioisotopes are available in the SCALE cross section libraries.
- Schedule visits to Argonne to learn CMT EXCEL program

Slide 18

Conclusion

- Students trained in AAA problems
- Computation of k_{eff} for fuel separations processes can become an automatic part of process design

Appendix C

Student Presentation
at the Fall 2001 Conference of the
American Nuclear Society in
Reno, Nevada

"Criticality Assessment of Transuranic Waste Containers produced in the Electrometallurgical Treatment of High-level Radioactive Waste"

Slide 1

Criticality Assessment of Transuranic Waste Containers produced in the Electrometallurgical Treatment of High-level Radioactive Waste

By:
Jason Viggato, M.S.E.
Research Assistant and Ph.D. Candidate
Department of Mechanical Engineering
University of Nevada, Las Vegas

American Nuclear Society Conference- Reno
November 10, 2001

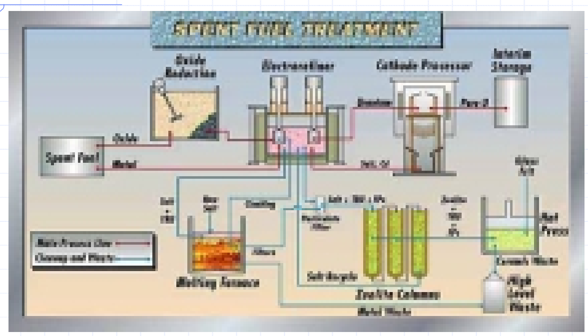
Slide 2

Introduction

Argonne National Laboratory's (ANL) Chemical Division has recently developed an electrometallurgical treatment process for high-level radioactive waste. In this process, an electro refining technique is used to separate uranium, inert materials, and fissionable materials including transuranic (TRU) elements from spent nuclear fuels.

Slide 3

Spent Fuel Treatment Cycle



Picture from ANL web page

Slide 4

Introduction (Continued)

After the entire treatment process, uranium and transuranic wastes such as plutonium, americium, and curium are placed in a cylindrical container. A sustained chain reaction inside waste containers is possible if the critical mass of fissionable material is present. The effective neutron multiplication factor, k_{eff}, will be determined for each of the given geometries and then will be checked against acceptable criticality values.

Slide 5

Waste Package Canister

Picture from ANL web page

Slide 6

Criticality

- *Critical* describes a chain reaction that is maintained at a constant rate per unit time.
- *Sub-critical* is a chain reaction in which the rate of fissioning is decreasing.
- *Super-critical* is a reaction in which the rate of fissioning is increasing.
- An atomic bomb would be an example of a super-super-critical reaction.

Slide 7

The Steady-State Reactor Core

- Thermal reactor cores contain fast neutrons resulting from fission. These fast neutrons slow to thermal energies when they collide with moderator nuclei. Some fast neutrons are absorbed by fissionable nuclei, producing further fissions and new generations of neutrons.
- The ratio of the number in the new generation to the number in the old generation is known as the *neutron multiplication factor*.

Slide 8

The Steady-State Reactor Core (continued)

- In a core of infinite length, k_∞ is the infinite multiplication factor and is defined as:

$$k_\infty = \frac{n'}{n}$$

- In an actual reactor, the diffusion of neutrons is from the center toward the boundaries, where they may leak out of or be lost to subsequent fissions. The effective multiplication factor is then multiplied by the non-leakage probability.

$$k_{eff} = k_\infty \cdot P_{NL}$$

The Steady-State Reactor Core (continued)

- For an infinite core, k_∞ is:

$$k_\infty = \varepsilon p f \eta$$

Where ε is the fast fission factor, p is the resonance escape probability, f is the thermal utilization factor and η is the reproduction factor.

Slide 10

The Steady-State Reactor Core (continued)

- A value of $k_\infty < 1$ is said to be *sub-critical*.
- A value of $k_\infty = 1$ is said to be *critical*.
- A value of $k_\infty > 1$ is said to be *super-critical*.

Slide 11

Criticality Assessment of Waste Packages

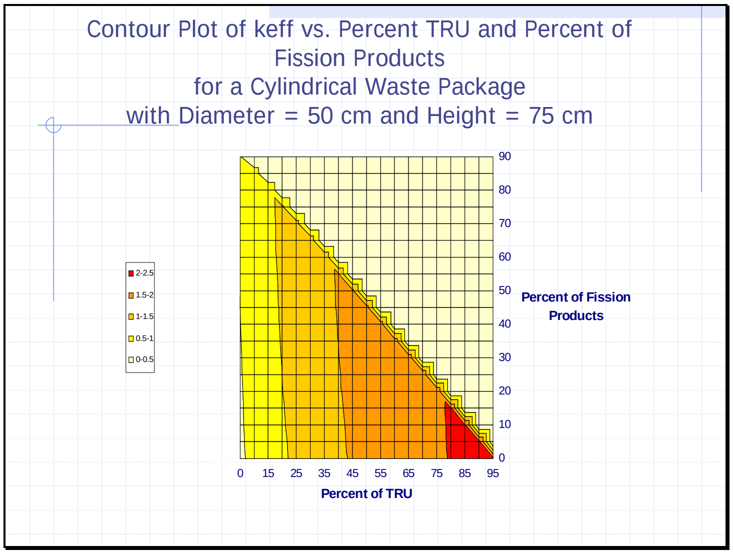
- The neutron multiplication factor, k_{eff} for various cylindrical geometries(i.e.. Sizes) are determined though computational methods.
- Values for k_{eff} are then checked and determined to be either safe or unsafe.
- A five percent factor of safety is added in addition to the uncertainties of the Scale 4.4a Code.
- Thus any $k_{eff} < 0.95$ is considered *safe*, and any $k_{eff} > 0.95$ is *unsafe*.

Slide 12

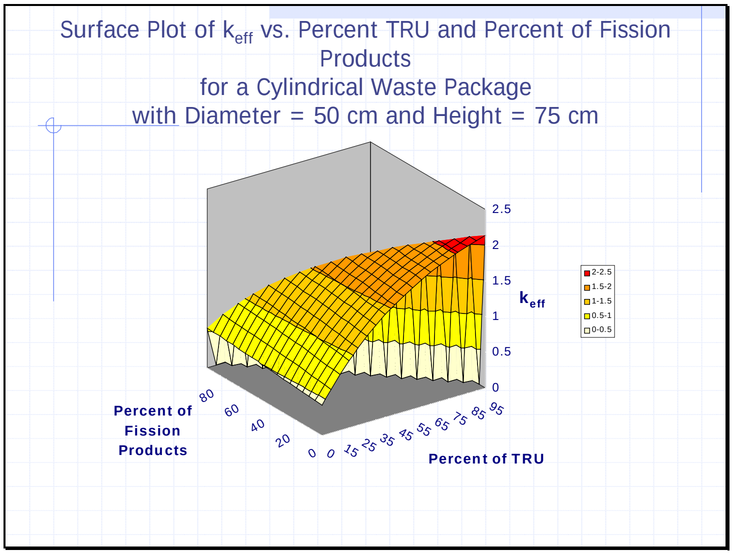
Method of the Neutron Multiplication Factor Calculation

- Create Scale 4.4a Monte-Carlo Criticality Code input files with varying Diameters, Heights and percentages of TRU and Process Salts through use of the CsasPrep Module.
- Run KENO module of Scale to calculate k_{eff} .
- Send k_{eff} and uncertainty values into into SURFCHK to compute the optimal regression fit.
- Input regression data in to SURFAAA to generate BASIC Program that contains regression coefficients.
- Run MS BASIC to compute k_{eff} and uncertainty for given Diameter and percent TRU.

Slide 13

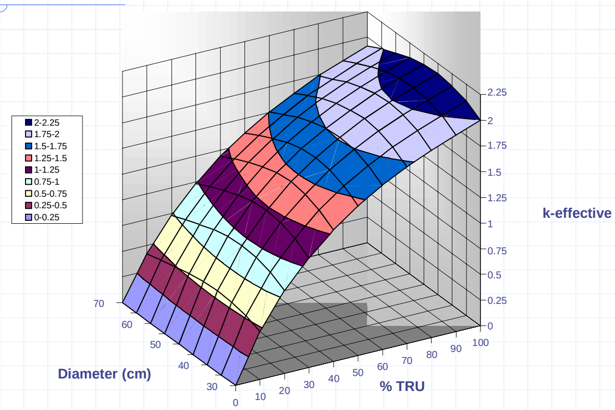


Slide 14



Slide 15

Surface Plot of k_{eff} for a Cylinder with varying Diameter and Percent TRU



Slide 16

Conclusion

- Preliminary results indicate that an increased percentage of TRU in canisters of both varied and constant diameters results in an increased value in neutron multiplication factor.
- The graphs of initial computer test cases indicate safe values of k_{eff} result mostly below 20 % TRU concentration.
- Further cases need to be carried out to acquire a more exact percentage of TRU that may be placed in a canister and that produce safe k_{eff} values.

Appendix D

Student Presentation
at the Fall 2001 Conference of the
American Nuclear Society in
Reno, Nevada

"Nuclear Criticality Analysis of Fissionable Material
in the Material Separation Stage for
Accelerated Transmutation of Nuclear Waste"

Slide 1

Nuclear Criticality Analysis of Fissionable Material in the Material Separation Stage for Accelerated Transmutation of Nuclear Waste

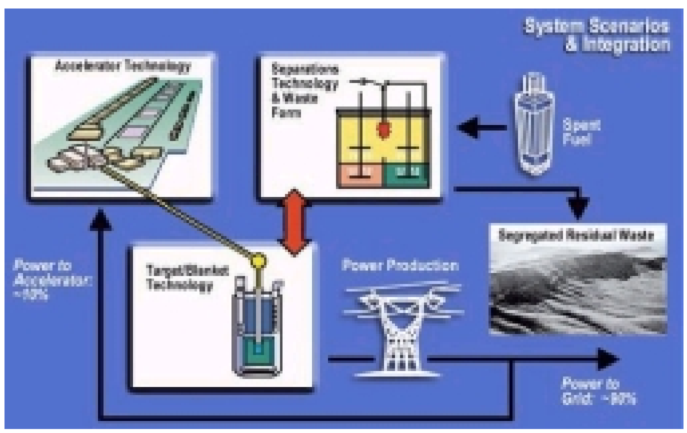
November 9, 2001

Daniel R. Lowe
Department of Mechanical Engineering
University of Nevada Las Vegas

Dr. William Culbreth
Department of Mechanical Engineering

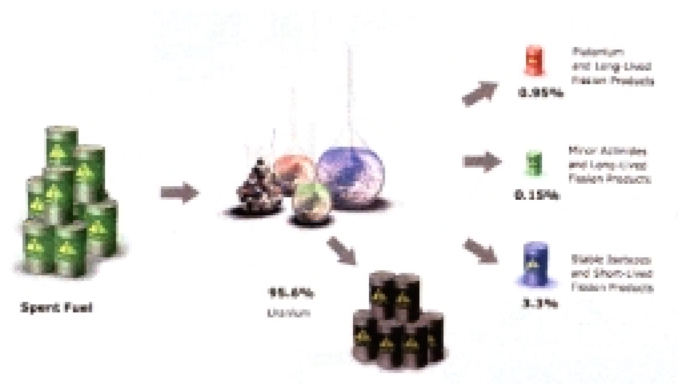
Slide 2

Accelerated Transmutation Waste Cycle



Slide 3

Materials Separation Cycle



Slide 4

Objectives and Goals

- Assess neutron multiplication factors, k_{eff}, for geometries and material concentrations as defined by the collaborating team from ANL-CMT for the AAA project.
- Provide fully automated computer software in order to compute criticality estimates to be used in the AAA's existing software packages.

Slide 5

What is CSAS 4/SCALE/MCNP?

CSAS 4/SCALE 4

- Standardized Computer Analyses for Licensing Evaluation dedicated to applications related to nuclear fuel facilities.

MCNP

- MCNP is a general-purpose Monte Carlo N-Particle code that can be used for neutron, photon, electron, or coupled neutron/photon/electron transport

Slide 6

What is KENO Va4?

- Extension of the KENO V Monte Carlo criticality program and was developed for use in the SCALE system.
- Primary purpose is to determine k-effective.
- Other calculated quantities include lifetime and generation time, energy-dependent leakages, energy- and region-dependent absorptions, fissions, fluxes, and fission densities.

Slide 7

Initial Tasks I

- Literature review of KENO Va4 for criticality calculations.
- Run KENO Va4 with sample data containing elementary mixtures, variables, and geometries to ensure proper use of the program.
- Curve-fit data to ensure curve-fitting techniques are adequate.

Slide 8

Initial Tasks II

- Create a fully automated QBasic program that will take certain parameters governed by AWT and calculate k_{eff} for those parameters.
- Modify an existing 2 dimension, 10^{th} order curvefit program to a 4 dimension, 4^{th} order program.

Slide 9

QBasic Program Layout

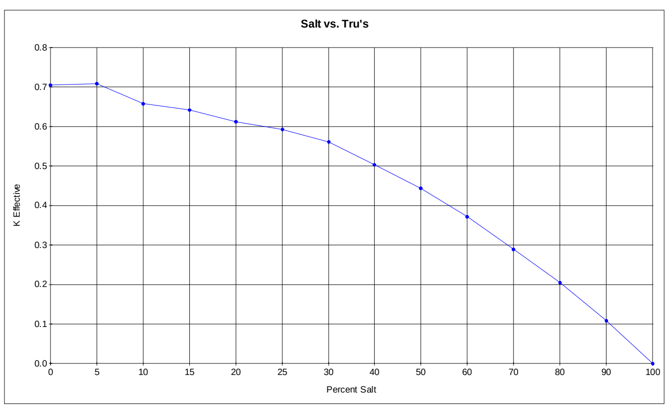
- Currently a 4 variable input program, which includes height and radius of nuclear core, percent TRU's, and percent Process Salts.
- Theoretically 5 variables (the 5th being Fissionable Products) but can be deduced from the fact that

  100% - %TRU's - %PS = %Fission Products

- Calculates k_{eff} for these 4 variables.
- Output in form of Qbasic/DOS that shows coefficients of the best surface fit.

Slide 10

Change in the Effective Neutron Multiplication Factor as a Function of TRU and Process Salt Concentrations



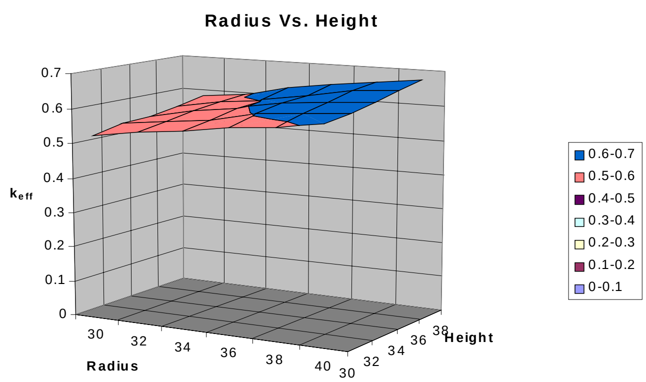
Slide 11

Surface/Curve Fit Program Outline

- Modifications to a two variable curve fit program were done in order to incorporate a four variable data set.
- With increased dimensions, the amount of data points also increases.
- Amount of needed data points in a 2 dimensional plot is 25, whereas in 4 dimensions the number is 625.

Slide 12

Change in Effective Neutron Multiplication Factor for a Cylindrical Container



Slide 13

Current Status

- Debugging surface fit program.

- Assessing needed geometries and materials for critical mass calculations on cathode separation.

- Writing VBasic Script code for ANL use.

- Converting from KENO V input to SCALE input.

- Integrating SCALE input, Qbasic programs, and Excel to perform specialized tasks.

Slide 14

Conclusions

- Sufficient in KENO V/SCALE programming code to complete current task.
- Automation program initiated and tested, but further code needs to be developed.
- Surface fit program modified for 4 dimensional, 4th order fits.

Slide 15

Future Tasks I

- Convert from KENO Va4 input to CSAS/MCNP input.
  - Complete library of isotopes
  - Complex geometry parameters allowed
- Create user friendly interface (web page) with governed input parameters to calculate and display k_{eff}.
- Assess and calculate k_{eff} for fissionable mass on the cylindrical cathode during separation of Plutonium from the TRU's and process salt mixture.

Slide 16

Future Tasks II

- Tour of Argonne National Lab - East to observe material separation process in order to determine correct geometries, materials, etc. and/or possible criticality problems.
- Further training in MCNP languages (MCNPX, KENOVI).

Slide 17

Acknowledgments

- Funding for this project has been provided by the UNLV AAA University Participation Program

- For information, (graduate research oppertunities), please contact Dr. Tony Hechanova at hechanova@nevada.edu
- http://hrcweb.nevada.edu/rsatg/atw/AAAhome.html