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Investigating Neutron Spectra Changes in Deep Penetration Shielding Analyses

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Appendix E - UNIVERSITY HONORS PROGRAM
SENIOR PROJECT - APPROVAL

Name: Jamie Garvey

College: Engineering  Department: Nuclear Eng.

Faculty Mentor: Ron Pevey

PROJECT TITLE: Investigating Neutron Spectra Changes in Deep Penetration Shielding Analyses

I have reviewed this completed senior honors thesis with this student and certify that it is a project commensurate with honors level undergraduate research in this field.

Signed: (Signature)  Faculty Mentor

Date: MAY 2, 2015

General Assessment - please provide a short paragraph that highlights the most significant features of the project.

Comments (Optional):
General Assessment

The purpose of this research is to determine if asymptotic spectra exist in three common shielding materials: water, concrete, and lead. If such a spectrum can be identified, then a distance necessary for the spectrum to converge will also be identified. Neutron transport and multigroup diffusion theory were used to determine these spectra. Asymptotic spectra were identified for each material. The water spectrum was found to converge within 20 cm; the concrete spectrum in approximately 90 cm; the lead spectrum in 8 m.
Investigating Neutron Spectra Changes in Deep Penetration Shielding Analyses

Jamie Garvey

Faculty Mentor: Dr. Ron Pevey

May 2, 2005
Acknowledgements

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Abstract

The purpose of this research is to determine if asymptotic spectra exist in three common shielding materials: water, concrete, and lead. If such a spectrum can be identified, then a distance necessary for the spectrum to converge will also be identified. Neutron transport and multigroup diffusion theory were used to determine these spectra. Asymptotic spectra were identified for each material. The water spectrum was found to converge within 20 cm; the concrete spectrum in approximately 90 cm; the lead spectrum in 8 m.
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Introduction

This project investigates the behavior of the energy dependent neutron spectrum as a neutron penetrates into common shielding materials, specifically water, concrete, and lead. A neutron spectrum is the energy distribution of neutrons in the system under investigation. The asymptotic spectrum is the energy distribution expected after neutrons travel a sufficient distance in the shielding material. The goal of the project is twofold: to determine whether the asymptotic spectrum shape can be predicted from the material properties, and to determine how the neutrons approach the asymptotic spectrum as a function of distance. There are two main motivations for completing this research. First, if asymptotic spectra can be identified, it may be possible to reduce the number of energy groups used to model neutron flux in shielding applications. Second, the asymptotic neutron spectrum would provide a superior spectrum for albedo boundary conditions. In albedo boundary conditions, a large outside region (e.g. around a reactor or radiation shield) is replaced with a much faster mathematical boundary condition that assumes that a neutron leaving the reactor is partially reflected back with a new spectrum.

The crux of the project is based on two related theories in nuclear analysis: neutron transport and multigroup diffusion. The SCALE Shielding Analysis Sequence number 1 (SAS1) is based on neutron transport theory. The FORTRAN codes developed for this project are based on multigroup diffusion theory, in which the motion of neutrons is approximated by diffusion. This project will address the validity of the diffusion approximation in water, concrete, and lead by comparing flux determined through neutron transport in SAS1 and flux determined through the diffusion equation in the developed FORTRAN codes.
Theory

Determining the neutron flux in a shielding material requires accounting for the neutron motion in the material and neutron interactions with nuclei in the material. In this analysis, the neutron motion will be assumed to be at steady state; that is, the neutron distribution does not change with time. Before this neutron accounting can be accomplished, however, several core ideas must be defined, specifically neutron cross-sections and multigroup approximations.

Neutron cross-sections characterize the probability that a specific reaction will occur. These cross-sections depend on the reaction in question, the energy of the incident neutrons, and the material with which a neutron may interact. Two types of neutron cross-sections are used: microscopic and macroscopic. Microscopic cross-sections, $\sigma$, have units of cm$^2$ and can be thought of as the effective cross-sectional area presented by the target nucleus to the incident neutrons. Microscopic cross-sections give a constant of proportionality between reaction rate, $R$, and neutron beam intensity (that is, the number of neutrons that impinge on the target per unit area per second), $I$, and the number of target nuclei per unit area, $N_A$:

$$ R = \sigma I N_A $$

Microscopic cross-sections are developed by considering an extremely thin target. In this case, every target nucleus is exposed to the incident neutrons. In reality, targets are thicker and some nuclei are shielded from neutrons by those on the surface. The probability that a neutron will react with any nucleus in the target, then, is characterized by the product of the atomic number density of the target material and the microscopic cross-section of that material. This quantity is known as the macroscopic cross-section,
\( \Sigma \), which has units of inverse distance (cm\(^{-1}\)) and is also dependent on the interaction in question, neutron energy, and target material. It is important to note that the macroscopic cross-section of a heterogeneous material is the sum of the macroscopic cross-sections of each material constituent:

\[
\Sigma = \sum_i N_i \sigma_i
\]

Many concepts in nuclear theory, including neutron cross-sections, are energy dependent. However, it is difficult to determine neutron distributions and cross sections for continuous energies. For this reason, multigroup approximations are made. Energy is broken into discrete ranges over which properties are approximately constant (Figure 1). It is traditional to number these groups from high energy to low energy because of neutrons' tendency to lose energy, moving from a high energy group to a low energy group. With this discretization of energy, neutron microscopic cross-sections can be determined experimentally and tabulated for each energy range. This multigroup approach is utilized in SCALE sequences and in the developed FORTRAN codes.

\[\text{Figure 1: Multigroup Energy Discretization}\]

**Neutron Transport**

Neutron transport theory begins with the Boltzmann equation, formulated to describe dilute gases, which equates particle losses to particle sources in a given volume. Applying this same idea to neutrons gives rise to the neutron transport equation:

\[
\tilde{\Omega} \cdot \nabla \psi(\vec{r}, E, \tilde{\Omega}) + \Sigma_r(\vec{r}, E)\psi(\vec{r}, E, \tilde{\Omega}) = S(\vec{r}, E, \tilde{\Omega})
\]
where $\Sigma_t(\bar{r}, E)$ is the total macroscopic cross-section of the medium, $\psi(\bar{r}, E, \hat{\Omega})$ is the neutron flux, $\vec{\Omega} \cdot \nabla \psi(\bar{r}, E, \hat{\Omega})$ is the neutron loss due to leakage out of the volume, $\Sigma_t(\bar{r}, E)\psi(\bar{r}, E, \hat{\Omega})$ is the neutron loss due to collisions within the volume, and $S(\bar{r}, E, \hat{\Omega})$ is the neutron source within the volume. The neutron transport equation is a balance condition that equates losses due to leakage and collisions to neutron sources, at some point $\bar{r}$, energy $E$, and in direction $\hat{\Omega}$.

The neutron source term is specific to a material volume, neutron energy, and neutron direction of interest. It includes fixed sources within the volume of interest, neutrons entering the volume through the boundary, and neutrons with an initial energy, $E'$, and direction, $\hat{\Omega}'$, which undergo a scattering collision in the volume that changes the neutrons' energy and direction to those of interest.

The use of a one dimensional spherical model and multigroup approximation allows for significant simplification of the neutron transport equation. In a one-dimensional case, the neutron direction can be fully described by $\mu$, the cosine of the angle of neutron travel with a radius vector between the point and the center of the sphere, $\phi$ (Figure 2). With these changes in mind, the neutron transport equation reduces to:

$$\frac{\mu}{r^2} \frac{\partial (r^2 \phi_g)}{\partial r} + \frac{1}{r} \frac{\partial [(1 - \mu^2) \phi_g]}{\partial \mu} + \Sigma_t \phi_g = q_g + \sum_{g'} \Sigma_s (g' \rightarrow g) \phi_{g'}$$

where $g$ is the energy group of interest, $q$ is the fixed source term, and $\Sigma_s (g' \rightarrow g)$ is the scattering cross-section from some energy group $g'$ to the energy group of interest, $g$. 


Although the neutron transport equation is difficult to solve by hand, it is a fairly simple process for computer applications. The SCALE SAS1 sequence divides the region into a group of nodes and performs neutron transport calculations within each node. The specifics of the numerical methods used by the SAS1 sequence to solve the neutron transport equation in each node can be studied in the SCALE manual [Greene 2004].

**Multigroup Diffusion**

The neutron transport equation as described above can be simplified with further approximations. Diffusion is a process which describes the motion of gas particles; these particles move from areas of high particle concentration to areas of low particle concentration as described by Fick's Law, also called the diffusion approximation:

\[ J = -D \cdot \nabla \phi \]

where \( J \) is the particle current density and \( D \) is the diffusion coefficient. In many nuclear studies, the diffusion approximation is used to describe the motion of neutrons, so that it
is assumed that neutrons move from an area of higher neutron concentration to an area of lower neutron concentration. This leads to the multigroup diffusion equation:

\[- \nabla D_g \cdot \nabla \phi_g + \Sigma_{sg} \phi_g = \sum_{g'} \Sigma_{sg' \rightarrow g} \phi_{g'} + q_g \]

\[g=1, 2, \ldots, 27.\]

It can be shown through nuclear reactor analysis that the neutron diffusion coefficient, \(D\), is given by:

\[D = \frac{1}{3\Sigma_{\text{trg}}}\]

where \(\Sigma_{\text{trg}}\), the transport cross-section, is given by:

\[\Sigma_{\text{trg}} = \Sigma_r - \frac{2}{3A} \Sigma_s\]

where \(\Sigma_r\) is the total cross-section, \(\Sigma_s\) is the scattering cross-section, and \(A\) is the mass number. For the purposes of this research, the transport cross-section will be approximated by the total cross-section [Pevey 2004].

To further simplify the multigroup diffusion equation, the removal cross-section is introduced:

\[\Sigma_{\text{rg}} = \Sigma_g - \Sigma_{sg \rightarrow g} = \Sigma_{sg} + \sum_{g \neq g'} \Sigma_{sg' \rightarrow g} \]

The removal cross-section characterizes the probability that a neutron will undergo an event, either absorption or scatter, that will remove the neutron from energy group \(g\). Substituting the removal cross-section into the multigroup diffusion equation gives:

\[- \nabla D_g \cdot \nabla \phi_g + \Sigma_{\text{rg}} \phi_g = \sum_{g' \neq g} \Sigma_{sg' \rightarrow g} \phi_{g'} + q_g \]
This equation can be solved to determine the neutron flux for each group if the fixed source term is known. Unfortunately, while determining the asymptotic flux in a shielding material, the fixed source term is not known.

**Buckling Determination**

For a material without a source, $q_g$, there is no non-zero solution for the above equation, but an approximate solution can be found by inserting a buckling eigenvalue, $B^2$, into the equation to give:

$$- \nabla D_g \cdot \nabla \phi_g + \left( D_g B^2 + \sum_{Rg} \right) \phi_g = \sum_{g' \rightarrow g} \Sigma_{g' \rightarrow g} \phi_{g'}.$$

The value of buckling that makes the equation balance can be used to determine if a nuclear system is subcritical ($B^2 < 0$), critical ($B^2 = 0$), or supercritical ($B^2 > 0$). A critical system involves a self-sustaining chain reaction; that is, for every neutron that is absorbed by the system a neutron is produced, usually through fission. The shielding applications of interest to this research are subcritical, so $B^2$ should be negative.

**Methods**

Before any neutron flux analysis can be completed, the standard isotopic compositions must be established for the three shielding materials of interest. These compositions, shown in table 1, are tabulated in the SCALE manual [Petrie 2004]. These compositions are used in conjunction with the multigroup cross-section libraries in SCALE to determine macroscopic cross-sections within each shielding material.
Table 1: Standard Isotopic Compositions for Shielding Materials

<table>
<thead>
<tr>
<th>Element</th>
<th>Number Density (atoms/b*cm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water</td>
<td></td>
</tr>
<tr>
<td>Hydrogen</td>
<td>0.066</td>
</tr>
<tr>
<td>Oxygen</td>
<td>0.033</td>
</tr>
<tr>
<td>Concrete</td>
<td></td>
</tr>
<tr>
<td>Iron</td>
<td>0.000347</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>0.0137</td>
</tr>
<tr>
<td>Aluminum</td>
<td>0.00175</td>
</tr>
<tr>
<td>Calcium</td>
<td>0.00152</td>
</tr>
<tr>
<td>Oxygen</td>
<td>0.0461</td>
</tr>
<tr>
<td>Silicon</td>
<td>0.0166</td>
</tr>
<tr>
<td>Sodium</td>
<td>0.00175</td>
</tr>
<tr>
<td>Lead</td>
<td>0.00329</td>
</tr>
</tbody>
</table>

**SCALE SASI**

The asymptotic neutron spectrum in each material will be determined in two ways. The SCALE SASI sequence is used to determine the asymptotic spectrum through neutron transport analysis, with a 27 energy group cross-section library. The SCALE input deck (Appendix A, B, and C) includes a point source of high-energy neutrons of strength 1 neutron per second. A large sphere of a specific shielding material surrounds this point source. SCALE evaluates and outputs the neutron spectrum at several radial distances, as determined appropriate for each material. These spectra can be compared to each other in order to determine the asymptotic neutron spectrum in the material of interest.

**FORTRAN Code Developed for the Project: ASYMFLUX**

The FORTRAN code, ASYMFLUX, developed for this research use a 27 energy group multigroup diffusion as described above to determine the neutron flux in each
group at an effectively infinite distance from the high energy neutron source.

ASYMFLUX first utilizes a subroutine written by R. E. Pevey to extract neutron microscopic cross-section values from SCALE data files. These values are then combined with the appropriate number densities to determine the total, absorption, scatter, and removal macroscopic cross-sections.

Beginning with initial guesses for flux and buckling values, ASYMFLUX uses two iterations to determine the flux (figure 3). The inner iteration evaluates the multigroup diffusion equation to determine the group neutron flux for a given fixed source. The outer iteration determines the fixed source for a given group neutron flux. These iterations continue until the normalized neutron flux converges to 0.001% in each group.

The final outcome of this research is to determine an asymptotic neutron spectrum in each shielding material. Such spectra were established with ASYMFLUX for water, concrete, and lead. These spectra were compared to those determined in SCALE SAS1.
**Water**

The ASYMFLUX asymptotic neutron spectrum for water is tabulated (Appendix A) and plotted below (figure 4). The SCALE SAS1 neutron fluxes for seven radial distances from the monoenergetic source (5, 10, 15, 20, 25, 50, and 100 cm) are also tabulated in Appendix A. The asymptotic spectrum determined from this data is also plotted (figure 4). It can be seen from this data that the normalized neutron flux calculated with SCALE converges quickly to the spectrum found in ASYMFLUX. In fact, the flux spectra converge to 10% in each energy group within 20 cm from the neutron point source. It is important at this point to notice that the spectra calculated in SCALE SAS1 are more accurate estimations of the flux than that computed in ASYMFLUX. The strong convergence of these two sets of flux calculations shows that the diffusion approximation made in ASYMFLUX is a valid approximation in water.

![Asymptotic Water Neutron Flux Spectrum](image)

**Figure 4:** Asymptotic Spectra for Water determined by ASYMFLUX and SCALE
**Concrete**

The ASYMFLUX asymptotic neutron spectrum for concrete is tabulated (Appendix B) and plotted below (figure 5). The SCALE SAS1 neutron fluxes for seven radial distances from the monoenergetic source (25, 50, 75, 80, 90, 100 and 200 cm) are also tabulated in Appendix B, and the asymptotic spectrum from these calculations is shown below in figure 5. The SCALE spectra begin to converge at 90 cm from the point source.

It can be seen from the two plots below that while the flux shapes are similar, the magnitudes do not agree. This discrepancy indicates that the diffusion approximation is not a valid assumption for concrete, because while an asymptotic spectrum does exist, the diffusion approximation is not able to predict it.

![Asymptotic Concrete Neutron Flux Spectrum](image)

**Figure 5: Asymptotic Spectra for Concrete determined by ASYMFLUX and SCALE**

**Lead**

The ASYMFLUX asymptotic neutron spectrum for lead is tabulated (Appendix C) and plotted below (figure 6). The spectra calculated by SCALE at 100 cm intervals
from the point source from a minimum distance of 800 cm to a maximum distance of 1400 cm are shown in figure 7. It is clear that the lead spectrum is converging, but comparing the two figures below, it can be seen that the SCALE spectra are not converging to the spectrum determined by ASYMFLUX. Based on this observation, it is believed that the diffusion approximation is also not valid in lead. However, the neutron spectrum begins to converge approximately 800 cm from the point source.

![Asymptotic Lead Neutron Flux Spectrum](image)

Figure 6: Asymptotic Spectrum for Lead determined by ASYMFLUX
Conclusions

Asymptotic spectra were identified through SCALE SAS1 for water, concrete, and lead. The water spectrum was found to converge within 20 cm, and agreed well with the spectrum calculated in ASYMFLUX. This shows that the diffusion approximation is valid in water. The concrete spectrum began to converge in approximately 90 cm. This asymptotic spectrum did not agree with the spectrum found with ASYMFLUX, which indicates that the diffusion approximation is not valid in concrete. The lead spectrum began to converge in approximately 8 m. It was clear, though, that the SCALE spectra did not agree with the spectrum found with ASYMFLUX; this indicates that the diffusion approximation is also not valid in lead.
Future Work

The research presented here was limited by time constraints and project scope. The work only involved three shielding materials and one type of radiation source. Possible future research should include other shielding materials, different types of sources (i.e. gamma, alpha, and electron sources), and different source energies (low energy monoenergetic sources and multienergetic sources).
References


Appendix A: Water

SCALE input deck .................................................. 17
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`SCALE input deck`

```
=ss1
PARM=SIZE=999999

'*******************************
 Material Specifications *
'*******************************

Water Flux Spectrum
 Library Spatial Treatment
27N-18COUPLE INFHOMMEDIUM

'Material  Mixture  Density  Control
 h2o     1   1.0     END

END COMP
END
LAST

'*******************************
 GEOMETRY AND SOURCE *
'*******************************

Point source surrounded by water

'Geometry Type
 SPHERICAL

'Mixture  Dimension  #meshes  Source  Other_Mixture  Neutrons  Photons
 1    0.62035    10     -1     0    0.0     1.0     0
 1     5        200     0     1     0.0     1.0     0
 1     6        100     0     1     0.0     1.0     0
 1     10       100     0     1     0.0     1.0     0
 1     11       100     0     1     0.0     1.0     0
 1     15       100     0     1     0.0     1.0     0
 1     16       100     0     1     0.0     1.0     0
 1     20       100     0     1     0.0     1.0     0
 1     21       100     0     1     0.0     1.0     0
 1     25       100     0     1     0.0     1.0     0
 1     26       100     0     1     0.0     1.0     0
 1     50       96      0     1     0.0     1.0     0
 1     51        4      0     1     0.0     1.0     0
 1     100      196     0     1     0.0     1.0     0
 1     101        4     0     1     0.0     1.0     0

END ZONE

'*******************************
 * SOURCE SPECIFICATION (ENERGY DEPENDENCE) 1*
'*******************************

' Neutron Source Spectrum
 1 26z
' Photon source spectrum
18z

READ XSDOSE
END
END
```
ASYMFLUX Coding

** Program to determine the asymptotic spectrum for a high energy monoenergetic source using 27-group cross section library **

** q(27) source term for each group **

** flux(27) flux at each group for current iteration **

** flux_o(27) flux calculated at previous iteration **

** conv convergence factor at each iteration **

** S_r(27) macroscopic removal cross section for each group **

** sflux sum of flux for group1 times scattering from group1**

** conv convergence factor at each iteration **

** change placeholder for determining convergence criteria **

** S_s(27,27) macroscopic scattering cross section from group to **

** group **

** N(2) number density by isotope **

** D(27) diffusion coefficient by group **

** S_t(27) macroscopic total cross section for each group **

** normflux placeholder to normalize flux values **

** B2 buckling (<0 => subcritical) **

** B_num placeholder for evaluating B2 at each iteration **

** B_denom placeholder for evaluating B2 at each iteration **

** S_a(27) macroscopic absorption cross section for each group**

REAL q(27), flux(27), flux_o(27), conv, S_r(27), sflux,
*S_s(27,27), N(2), D(27), S_t(27), B2, B_num, B_denom, S_a(27), normflux,
*change

** Variables added by REP to read the micros **

**

** totalx(27,5) Total by group, isotope **

** scatx(27,27,5) Scattering by from group, to group, isotope **

** fissnux(27,5) nu*Fission by group, isotope **

** absorpx(27,5) Absorption by group, isotope **

**

real totalx(27,5), scatx(27,27,5), fissnux(27,5)
real absorpx(27,5)

** Read the micros **

**

** Materials: **

** 1 H-1 **

** 2 O-16 **

** 3 (Not used-available) **

** 4 (Not used-available) **

** 5 (Not used-available) **

**

call getxs('1001.dat', totalx(1,1), scatx(1,1,1), fissnux(1,1),
*absorpx(1,1))
call getxs('8016.dat', totalx(1,2), scatx(1,1,2), fissnux(1,2),

*absorpx(1,2))

******************************************************************************
** Add code to mix the micros into the macro **
******************************************************************************
N(1) = 0.066
N(2) = 0.033
DO l=1,27
  DO m=1,27
    S_s(m,l)=N(l)*scatx(m,1,l)+N(2)*scatx(m,1,2)
  ENDDO
ENDDO
DO p=1,27
  S_t(p)=N(1)*totalx(p,1)+N(2)*totalx(p,2)
ENDDO
DO a=1,27
  S_a(a)=N(1)*absorpx(a,1)+N(2)*absorpx(a,2)
ENDDO
******************************************************************************
** Add code to calculate removal cross sections, S_r **
******************************************************************************
DO h=1,27
  S_r(h)=S_a(h)
  DO e=1,27
    if(e.ne.h) then
      S_r(h)=S_r(h)+S_s(h,e)
    endif
  ENDDO
ENDDO
******************************************************************************
** Add code to calculate diffusion coefficient for each group, 1/(3SigmaT) **
******************************************************************************
DO f=1,27
  D(f)=1/(3*S_t(f))
ENDDO
******************************************************************************
** Put in the flux guess for first round **
******************************************************************************
data flux/27*1.0/
******************************************************************************
** Put in the B2 guess for first round **
******************************************************************************
B2=-0.002
conv=1.0
dowhile(conv.gt.0.0001)
  DO g=1,27
    
enddo
flux_o(g)=flux(g)
ENDDO

****************************************************************************
** Calculate the source from -D*B2*flux for each group **
**
****************************************************************************
DO r=1,27
    q(r)=-1.0*D(r)*B2*flux(r)
ENDDO

****************************************************************************
** Determine flux for given source term **
**
****************************************************************************
flux(l)=q(l)/s_r(l)
do i=2,27
    sflux=0.0
    do j=1,27
        if (i.ne.j) then
            sflux=sflux+s_s(j,i)*flux(j)
        endif
    enddo
    flux(i)=(q(i)+sflux)/s_r(i)
enddo

****************************************************************************
** Find the new guess of B2 from the flux **
**
****************************************************************************
B_num=0.0
DO b=1,27
    B_num=B_num+S_a(b)*flux(b)
ENDDO
B_denom=0.0
DO c=1,27
    B_denom=B_denom+D(c)*flux(c)
ENDDO
B2=-1.0*B_num/B_denom

****************************************************************************
** Normalize flux values **
**
****************************************************************************
normflux=0.0
DO w=1,27
    normflux=normflux+flux(w)
ENDDO
DO x=1,27
    flux(x)=flux(x)*27.0/normflux
ENDDO

****************************************************************************
** used convergence as maximum fractional flux change by group **
**
****************************************************************************
conv=0.0
DO y=1,27
   change=ABS(flux_o(y)-flux(y))/flux_o(y)
   if (conv.lt.change) then
      conv=change
   endif
ENDDO
Print *, 'FLUX SOURCE'
DO z=1,27
   PRINT *,flux(z) ,q(z)
ENDDO
PRINT *, 'conv = ',conv, ' B2 = ',B2
enddo
stop
end

C*****************************************************************************
C*****************************************************************************
subroutine getxs (filename, total, scat, fissnu, absorp)
character*(*)filename
character*1 a1
real total(27),scat(27,27),fissnu(27),absorp(27)
open(1,file=filename,form='formatted',status='old')
read(1,1(a1)) a1
read(1,1(a1)) a1
read(1,1(a1)) a1
read(1,1(a1)) a1
do i=1,27
   read(1,9010) total(i),fissnu(i),absorp(i)
9010 format(10x,e15.8,15x,e15.8,e15.8)
   absorp(i)=total(i)-absorp(i)
endo
read(1,1(a1)) a1
read(1,1(a1)) a1
read(1,1(a1)) a1
j2=0
10 if(j2.ne.27)then
   read(1,1(a1)) a1
   read(1,1(a1)) a1
   read(1,1(a1)) a1
   j1=j2+1
   j2=j1+4
   if(j2.gt.27)j2=27
   do i=1,27
      read(1,9020) (scat(j,i),j=j1,j2)
9020 format(11x,5e12.8)
endo
   go to 10
endif
   close(1)
   return
end
Results

Table 2: Water Spectrum calculated by ASYMFLUX

<table>
<thead>
<tr>
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</tr>
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<tbody>
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### Table 3: Water Spectra calculated by SCALE SAS1

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<td>total flux</td>
<td>norm flux</td>
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</tr>
</tbody>
</table>
Appendix B: Concrete

SCALE input deck ........................................... 25
ASYMFLUX coding .......................................... 26
Results ..................................................... 31
SCALE input deck

-sas1 PARM=SIZE=999999

********************************************************************************

Material Specifications

********************************************************************************

Concrete Flux Spectrum

Library Spatial Treatment
27N-18COUPLE INFHOMMEDIUM

'Material Mixture Density Control
REG-CONCRETE 1 1.0 END
END COMP
END
LAST

********************************************************************************

GEOMETRY AND SOURCE 1

********************************************************************************

Point source surrounded by concrete

'Geometry Type
SPHERICAL

'Mixture Dimension #meshes Source Other Mixture Neutrons Photons
1 0.62035 10 -1 0 0.0 1. 0
1 25 100 0
1 26 100 0
1 50 100 0
1 51 100 0
1 60 100 0
1 61 100 0
1 70 100 0
1 71 100 0
1 75 100 0
1 76 100 0
1 80 100 0
1 81 100 0
1 90 100 0
1 91 100 0
1 100 200 0
1 101 100 0
1 200 200 0
1 201 100 0

END ZONE

********************************************************************************

* SOURCE SPECIFICATION (ENERGY DEPENDENCE) 1*

********************************************************************************

Neutron Source Spectrum
1 26z

' Photon source spectrum
18z

********************************************************************************

READ XSDOSE
END
END
**ASYMFLUX coding**

**Program to determine the asymptotic spectrum for a high energy monoenergetic source using 27-group cross section library**

**q(27) source term for each group**
**flux(27) flux at each group for current iteration**
**flux_o(27) flux calculated at previous iteration**
**conv convergence factor at each iteration**
**S_r(27) macroscopic removal cross section for each group**
**Sflux sum of flux for group times scattering from group to group of interest**
**change placeholder for determining convergence criteria**
**S_s(27,27) macroscopic scattering cross section from group to group**
**N(7) number density by isotope**
**D(27) diffusion coefficient by group**
**S_t(27) macroscopic total cross section for each group**
**normflux placeholder to normalize flux values**
**B2 buckling (<0 => subcritical)**
**B_num placeholder for evaluating B2 at each iteration**
**B_denom placeholder for evaluating B2 at each iteration**
**S_a(27) macroscopic absorption cross section for each group**

REAL q(27), flux(27), flux_o(27), conv, S_r(27), Sflux,
*S_s(27,27), N(7), D(27), S_t(27), B2, B_num, B_denom, S_a(27), normflux,
*change

**Variables added by REP to read the micros**
**totalx(27,7) Total by group, isotope**
**scatx(27,27,7) Scattering by from group, to group, isotope**
**fissnux(27,7) nu*Fission by group, isotope**
**absorpx(27,7) Absorption by group, isotope**

**Materials:**
**H-1**
**O-16**
**Silicon**
**Calcium**
**Aluminum**
**Sodium**
**Iron**

**Read the micros**
call getxs('1001.dat', totalx(1,1), scatx(1,1,1), fissnux(1,1),
*absorpx(1,1))
call getxs('8016.dat', totalx(1,2), scatx(1,1,2), fissnux(1,2),
*absorpx(1,2))
call getxs('14000.dat', totalx(1,3), scatx(1,1,3), fissnux(1,3),
*absorpx(1,3))
call getxs('20000.dat', totalx(1,4), scatx(1,1,4), fissnux(1,4),
*absorpx(1,4))
call getxs('13027.dat', totalx(1,5), scatx(1,1,5), fissnux(1,5),
*absorpx(1,5))
call getxs('11023.dat', totalx(1,6), scatx(1,1,6), fissnux(1,6),
*absorpx(1,6))
call getxs('26000.dat', totalx(1,7), scatx(1,1,7), fissnux(1,7),
*absorpx(1,7))

***********************************************************************
**
** Add code to mix the micros into the macro
**
***********************************************************************

N (1) = 0.01374
N (2) = 0.04606
N (3) = 0.01662
N (4) = 0.001521
N (5) = 0.001746
N (6) = 0.001747
N (7) = 0.0003473
DO 1=1,27
DO m=1,27
SS(m,1)=N(1)*scatx(m,1,1)+N(2)*scatx(m,1,2)+N(3)*
* scatx(m,1,3)+N(4)*scatx(m,1,4)+N(5)*scatx(m,1,5)
* +N(6)*scatx(m,1,6)+N(7)*scatx(m,1,7)
ENDDO
ENDDO
DO p=1,27
ST(p)=N(1)*totalx(p,1)+N(2)*totalx(p,2)+N(3)*
* totalx(p,3)+N(4)*totalx(p,4)+N(5)*totalx(p,5)
* +N(6)*totalx(p,6)+N(7)*totalx(p,7)
ENDDO

DO a=1,27
SA(a)=N(1)*absorpx(a,1)+N(2)*absorpx(a,2)+N(3)*absorpx(a,3)
* +N(4)*absorpx(a,4)+N(5)*absorpx(a,5)+N(6)*absorpx(a,6)
* +N(7)*absorpx(a,7)
ENDDO

***********************************************************************
**
** Add code to calculate removal cross sections, S_r
**
***********************************************************************

DO h=1,27
S_r(h)=SA(h)
DO e=1,27
if(e.ne.h) then
  S_r(h)=S_r(h)+SS(h,e)
endif
ENDDO
ENDDO
ENDDO
** Add code to calculate diffusion coefficient for each group, **
** 1/(3\(\Sigma T\)) **

```
DO f=1,27
   D(f)=1/(3*S_t(f))
ENDDO

** Put in the flux guess for first round **
```
```
data flux/27*1.0/
```

** Put in the B2 guess for first round **
```
B2=-1.0
conv=1.0
dowhile(conv.gt.0.0001)
   DO g=1,27
      flux_o(g)=flux(g)
   ENDDO

** Calculate the source from \(-D\cdot B2\cdot \text{flux}\) for each group **
```
DO r=1,27
   q(r)=-1.0*D(r)*B2*flux(r)
ENDDO
```

** Determine flux for given source term **
```
flux(I)=q(I)/s_r(I)
do i=2,27
   sflux=0.0
   do j=1,27
      if (i.ne.j) then
         sflux=sflux+s_s(j,i)*flux(j)
      endif
   enddo
   flux(i)=(q(i)+sflux)/s_r(i)
endo

** Find the new guess of B2 from the flux **
```
B_num=0.0
DO b=1,27
   B_num=B_num+S_a(b)*flux(b)
ENDDO
B_denom=0.0
DO c=1,27
   B_denom=B_denom+D(c)*flux(c)
ENDDO
B2=-1.0*B_num/B_denom

**************************************************************************
** Normalize flux values **
**************************************************************************

normflux=0.0
DO w=1,27
   normflux=normflux+flux(w)
ENDDO
DO x=1,27
   flux(x)=flux(x)*27.0/normflux
ENDDO

**************************************************************************
** used convergence to maximum fractional flux change by group **
**************************************************************************

conv=0.0
DO y=1,27
   if (flux_o(y) .gt. 1.0e-10) then
      change=ABS(flux_o(y)-flux(y))/flux_o(y)
      if (conv.lt.change) then
         conv=change
      endif
   endif
ENDDO
Print *, 'FLUX'
DO z=1,27
   PRINT *, flux(z)
ENDDO
enddo
stop

**************************************************************************
C**********************************************************************

C**********************************************************************
subroutine getxs(filename,total,scat,fissnu,absorp)
character(*)filename
character*1 a1
real total(27),scat(27,27),fissnu(27),absorp(27)
open(1, file=filename, form='formatted', status='old')
read(1,(a1))a1
read(1,'(a1)')a1
read(1,'(a1)')a1
read(1,'(a1)')a1
read(1,'(a1)')a1
do i=1,27
   read(1,9010)total(i),fissnu(i),absorp(i)
9010   format(10x,e15.8,15x,e15.8,e15.8)
   absorp(i)=total(i)-absorp(i)
enddo
read(1,'(a1)')a1
read(1,'(a1)')a1
read(1,'(a1)')a1
j2=0
10 if(j2.ne.27)then
   read(1,'(a1)')a1
   read(1,'(a1)')a1
   read(1,'(a1)')a1
   j1=j2+1
   j2=j1+4
   if(j2.gt.27)j2=27
   do i=1,27
      read(1,9020)(scat(j,i),j=j1,j2)
   9020   format(11x,5e12.8)
   enddo
   go to 10
endif
close(1)
return
end
**Results**

Table 4: Concrete Spectrum calculated by ASYMFLUX

<table>
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<th>calc flux</th>
</tr>
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Appendix C: Lead

SCALE input deck ............................................ 34
ASYMFLUX coding .......................................... 35
Results ..................................................... 39
SCALE input deck

= SAS1   PARM-SIZE=999999

'**********************************************
'  Material Specifications  *
'**********************************************

Lead Flux Spectrum
' Library       Spatial Treatment
27N-18COUPLE   INFHOMMEDIUM
'
'Material     Mixture     Density     Control
Lead         1           1.0         END
END COMP
END
LAST

'**********************************************
' GEOMETRY AND SOURCE  *
'**********************************************

Point source surrounded by lead
' Geometry Type
SPHERICAL

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END ZONE

'* SOURCE SPECIFICATION (ENERGY DEPENDENCE) 1*

' Neutron Source Spectrum
1 26z
' Photon source spectrum
18z

'**********************************************

READ XSDOSE
END
END
**ASYMFLUX coding**

***
** Program to determine the asymptotic spectrum for a high energy monoenergetic source using 27-group cross section library
**
**
** q(27) source term for each group
** flux(27) flux at each group for current iteration
** flux_o(27) flux calculated at previous iteration
** conv convergence factor at each iteration
** S_r(27) macroscopic removal cross section for each group
** sflux sum of flux for group1 times scattering from group1**
** conv to group of interest
** change placeholder for determining convergence criteria
** S_s(27,27) macroscopic scattering cross section from group to group
**
** N number density by isotope
** D(27) diffusion coefficient by group
** S_t(27) macroscopic total cross section for each group
** normflux placeholder to normalize flux values
** B2 buckling (<0 => subcritical)
** B_num placeholder for evaluating B2 at each iteration
** B_denom placeholder for evaluating B2 at each iteration
** S_a(27) macroscopic absorption cross section for each group
***

* REAL q(27), flux(27), flux_o(27), conv, S_r(27), sflux,
  *S_s(27,27), N, D(27), S_t(27), B2, B_num, B_denom, S_a(27), normflux,
  *change
*

***
** Variables added by REP to read the micros
**
**
** totalx(27,5) Total by group, isotope
** scatx(27,27,5) Scattering by from group, to group, isotope
** fissnux(27,5) nu*Fission by group, isotope
** absorpx(27,5) Absorption by group, isotope
**
***

real totalx(27,5), scatx(27,27,5), fissnux(27,5)
real absorpx(27,5)

***
** Read the micros
**
**
** Materials:
**
** 1 Lead
**
**
**
**
**
**
**
**
**
**
**

call getxs('82000.dat', totalx(1,1), scatx(1,1,1), fissnux(1,1),
  *absorpx(1,1))
** Add code to mix the micros into the macro

```
N = 0.03298
DO l=1,27
   DO m=1,27
      S_s(m,l)=N*scatx(m,l,l)
   ENDDO
ENDDO
DO p=1,27
   S_t(p)=N*totalx(p,l)
ENDDO
DO a=1,27
   S_a(a)=N*absorpx(a,1)
ENDDO
```

** Add code to calculate removal cross sections, S_r

```
DO h=1,27
   S_r(h)=S_a(h)
DO e=1,27
   if(e.ne.h) then
      S_r(h)=S_r(h)+S_s(h,e)
   endif
ENDDO

```

** Add code to calculate diffusion coefficient for each group, 1/(3SigmaT)

```
DO f=1,27
   D(f)=1/(3*S_t(f))
ENDDO
```

Put in the flux guess for first round

```
data flux/27*1.0/
```

Put in the B2 guess for first round

```
B2=-0.002
conv=1.0
dowhile(conv.gt.0.0001)
   DO g=1,27
      flux_o(g)=flux(g)
   ENDDO
```

36
Calculate the source from \(-D \cdot B2 \cdot \text{flux}\) for each group

\[
\text{DO } r=1,27 \\
\quad q(r) = -1.0 \cdot D(r) \cdot B2 \cdot \text{flux}(r) \\
\text{ENDDO}
\]

Determine flux for given source term

\[
\text{flux}(l) = q(l) (1) \\
\text{do } i=2,27 \\
\quad s_{flux} = 0.0 \\
\text{do } j=1,27 \\
\quad \text{if (i.ne.j)} \\
\quad \quad s_{flux} = s_{flux} + s_s(j,i) \cdot \text{flux}(j) \\
\quad \text{endif} \\
\text{enddo} \\
\text{flux}(i) = (q(i) + s_{flux}) / s_r(i) \\
\text{enddo}
\]

Find the new guess of \(B2\) from the flux

\[
\text{B\_num} = 0.0 \\
\text{DO } b=1,27 \\
\quad \text{B\_num} = \text{B\_num} + S_a(b) \cdot \text{flux}(b) \\
\text{ENDDO} \\
\text{B\_denom} = 0.0 \\
\text{DO } c=1,27 \\
\quad \text{B\_denom} = \text{B\_denom} + D(c) \cdot \text{flux}(c) \\
\text{ENDDO} \\
\text{B2} = -1.0 \cdot \frac{\text{B\_num}}{\text{B\_denom}}
\]

Normalize flux values

\[
\text{normflux} = 0.0 \\
\text{DO } w=1,27 \\
\quad \text{normflux} = \text{normflux} + \text{flux}(w) \\
\text{ENDDO} \\
\text{DO } x=1,27 \\
\quad \text{flux}(x) = \text{flux}(x) \cdot 27.0 / \text{normflux} \\
\text{ENDDO}
\]

convergence is maximum fractional flux change by group

\[
\text{conv} = 0.0 \\
\text{DO } y=1,27 \\
\quad \text{if (flux_0(y) .gt. 1e-10)} \\
\quad \quad \text{then}
\]
change = \text{ABS}(\text{flux}_o(y) - \text{flux}(y))/\text{flux}_o(y)
if (\text{conv} .lt. \text{change}) then
conv = \text{change}
endif
endif
ENDDO
Print *, 'FLUX SOURCE'
DO z=1,27
PRINT *,\text{flux}(z),q(z)
ENDDO
PRINT *, 'conv = ', \text{conv}, ' B2 = ', B2
enddo
stop
end

C**********************************************************************
C**********************************************************************
C subroutine getxs(filename,total,scat,fissnu,absorp)
C**********************************************************************
C**********************************************************************
character(*)filename
character*1 al
real total(27),scat(27,27),fissnu(27),absorp(27)
open(1,file=filename,form='formatted',status='old')
read(1,'(a1)')al
read(1,'(a1)')al
read(1,'(a1)')al
read(1,'(a1)')al
do i=1,27
read(1,9010)total(i),fissnu(i),absorp(i)
9010 format(10x,e12.8)
else
enddo
read(1,'(a1)')al
read(1,'(a1)')al
read(1,'(a1)')al
j2=0
10 if(j2.ne.27)then
read(1,'(a1)')al
read(1,'(a1)')al
read(1,'(a1)')al
j1=j2+1
j2=j1+4
if(j2.gt.27)j2=27
do i=1,27
read(1,9020)(scat(j,i),j=j1,j2)
9020 format(11x,5e12.8)
endo
endo
enddo
end

C**********************************************************************
C**********************************************************************
C end subroutine getxs(filename,total,scat,fissnu,absorp)
C**********************************************************************
C**********************************************************************
Results

Table 6: Lead Spectrum calculated by ASYMFLUX

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