AAEC/E620

AUSTRALIAN ATOMIC ENERGY COMMISSION RESEARCH ESTABLISHMENT

LUCAS HEIGHTS RESEARCH LABORATORIES

ICPP — A COLLISION PROBABILITY MODULE FOR THE AUS NEUTRONICS CODE SYSTEM

by

G.S. ROBINSON

OCTOBER 1985

AUSTRALIAN ATOMIC ENERGY COMMISSION RESEARCH ESTABLISHMENT LUCAS HEIGHTS RESEARCH LABORATORIES

ICPP - A COLLISION PROBABILITY MODULE FOR THE AUS NEUTRONICS CODE SYSTEM

by

G.S. ROBINSON

ABSTRACT

The isotropic collision probability program (ICPP) is a module of the AUS neutronics code system which calculates first flight collision probabilities for neutrons in one-dimensional geometries and in clusters of rods. Neutron sources, including scattering, are assumed to be isotropic and to be spatially flat within each mesh interval. The module solves the multigroup collision probability equations for eigenvalue or fixed source problems.

National Library of Australia card number and ISBN 0 642 59815 0
The following descriptors have been selected from the INIS Thesaurus to describe the subject content of this report for information retrieval purposes. For further details please refer to IAEA-INIS-12 (INIS: Manual for Indexing) and IAEA-INIS-13 (INIS: Thesaurus) published in Vienna by the International Atomic Energy Agency.
NEUTRONS; COLLISIONS; PROBABILITY; FUEL RODS; CYLINDERS; REFLECTION; BOUNDARY CONDITIONS; MATHEMATICAL MODELS; MULTIGROUP THEORY; I CODES; FUEL ELEMENT CLUSTERS; ISOTROPY

CONTENTS

1.	INTRODUCTION	1
	BRIEF DESCRIPTION OF COLLISION PROBABILITY ROUTINES 2.1 PROB1 - Free Slab Routine 2.2 PROB2 - Reflected Slab Routine 2.3 PROB3 - Periodic Slab Routine 2.4 PROB4 - Free Spherical Routine 2.5 PROB5 - White Reflected Spherical Routine 2.6 PROB6 - Free Cylinder Routine Using Numerical Integration 2.7 PROB7 - White Reflected Cylinder Routine (Numeric) 2.8 PROB8 and PROB9 - Approximate Cylinder Routines 2.9 PROB10 - Cylinder With Mirror Reflection 2.10 PROB11 - Cylinder With Square Reflective Boundary 2.11 PROB12 - Cylinder With Hexagonal Reflective Boundary 2.12 PROB13 - Rod Cluster Numerical Routine	1 1 1 1 1 2 2 2 2 2 2 2 2 2 2 2 2
	 2.13 PROB15 - Rod Cluster Semi-numerical Routine 2.14 PROB19 - Rod Cluster Approximate Routine 2.15 PROB108 and PROB109 - Approximate Cylinder Routines 	2 2 3
3.	INPUT DESCRIPTION 3.1 General 3.2 Input Block 1 3.3 Input Block 2 3.4 Input Block 3 3.5 Input Block 4 3.6 Input Block 5 3.7 Input Block 6	3 3 3 3 3 4 5
4.	REFERENCES	5

1. INTRODUCTION

The AUS neutronics code system [Robinson 1975] was developed for fission reactor neutronics calculations and recently has been extended to fusion blanket studies [Robinson 1984]. The isotropic collision probability program (ICPP) is a general purpose collision probability module for one-dimensional geometries and for the rod clusters typical of pressure tube reactors. It may be used within the AUS system either for few-region cell calculations suitable for group condensation or for many-region calculations after group collapsing. The collision probability approach is most suited to few-region calculations but also is preferable to S_N methods for detailed calculations in slab cells and clusters.

The ICPP module calculates first flight collision probabilities with the usual assumptions that neutron sources, including those due to scattering, are isotropic and spatially flat within each mesh interval. The module also solves the multigroup collision probability equations for eigenvalue or fixed source problems. Where the source gradient is large, ICPP requires many more mesh intervals than a corresponding S_N calculation.

The module includes a variety of collision probability routines which vary from very fast approximate routines through normal routines to slow routines most suited to few-group check calculations. Details of the methods used in the various routines and the accuracy obtained have been given by Doherty [1969a, 1969c, 1970] and Robinson [1979]. These reports include intercomparisons of the various routines for a number of simple cells and standard clusters. The method of solution for the multigroup collision probability equations has been given by Doherty [1969b]. The present report is restricted to an outline of the various routines and a description of input to ICPP.

2. BRIEF DESCRIPTION OF COLLISION PROBABILITY ROUTINES

A selection from the set of collision probability routines in ICPP may be made indirectly, as described in section 3, or by referring to a particular routine by number. Each of the routines has been given a name of the form PROBn, where n is an integer associated with each routine.

2.1 PROB1 - Free Slab Routine

In this routine, a boundary condition of zero incoming angular flux is imposed on both left and right boundaries. Collision probabilities are simple E₃ exponential functions so the routine is very fast. With only limited application of collision probabilities to free boundary problems, a routine with reflected and free boundaries has not been included. Void regions must be omitted when using this routine. Further details are given by Doherty [1969a].

2.2 PROB2 - Reflected Slab Routine

A reflective boundary condition is imposed at both left and right boundaries. Collision probabilities are evaluated by Gaussian quadrature in μ the cosine of the angle between the neutron direction and the direction normal to the slab. Void regions must be omitted. Further details are given by Doherty [1969a].

2.3 PROB3 - Periodic Slab Routine

The system of slabs repeats from left to right and is taken to be infinite. Again, the collision probabilities are obtained by Gaussian quadrature in μ and void regions must be omitted. Further details are given by Doherty [1969a].

2.4 PROB4 - Free Spherical Routine

To evaluate the collision probabilities, only neutron paths normal to a reference radial direction need be considered. The integration over r within each mesh interval is performed using Gaussian quadrature. Further details are given by Doherty [1969c].

2.5 PROB5 - White Reflected Spherical Routine

This routine uses the collision probabilities evaluated tor a free boundary condition on the sphere (PROB4) together with a surface/volume reciprocity relation to include the white reflective boundary condition. The routine is intended to be used for an array of spheres with a constant spacing or for dispersed fuel particles.

2.6 PROB6 - Free Cylinder Routine Using Numerical Integration

In this routine, the probabilities are evaluated by considering the projection of the neutron paths in the x-y plane. Only paths normal to a reference radial direction need be considered. The integration over the z direction cosine is performed analytically using K_{i3} Bickley functions. The integration over r within each mesh interval is performed by Gaussian quadrature. Further details are given by Doherty [1969a].

2.7 PROB7 - White Reflected Cylinder Routine (Numeric)

This routine uses the collision probabilities evaluated for a free boundary condition on the cylinder (PROB6) together with a surface/volume reciprocity relation to include the white reflective boundary condition.

2.8 PROB8 and PROB9 - Approximate Cylinder Routines

The PROB8 routine is used for cylinders with a free boundary condition and the PROB9 routine for cylinders with a reflective boundary. These routines use an approximate method given by Robinson [1979] and based on the work of Bonalumi [1961, 1965].

The method allows the outer boundary to be either circular or polygonal. A white reflective boundary condition may be applied on an outer circular boundary. For a reflective polygonal boundary, the boundary condition is restricted to a two-region system, which is formed by volume smearing the actual geometry as specified by the user. Normally, the inner region is fuel and the outer region is smeared cladding and coolant. These routines are very fast and suitable for few-region, many-group calculations to provide condensation spectra.

2.9 PROB10 - Cylinder With Mirror Reflection

Double Gaussian integration is required in this routine. One integration is over the r mesh, as in the PROB6 routine, the other is over the z direction cosine, which can no longer be performed analytically. The routine is slow and used only for check calculations. Further details are given by Doherty [1969a].

2.10 PROB11 - Cylinder With Square Reflective Boundary

This routine uses a double Gaussian integration. As in the PROB6 routine, projections of neutron paths normal to a radial direction are considered. One integration is over the r mesh, with the integration over the z direction cosine being in terms of the K_{i3} function. The second integration is over the angle between the radial direction and a reference side of the square. The routine is slow and used only for check calculations. Further details are given by Doherty [1969a].

2.11 PROB12 - Cylinder With Hexagonal Reflective Boundary

This routine is similar to the PROB11 routine, but a non-orthogonal co-ordinate set is used to relocate neutrons after reflection. The routine is slow and used only for check calculations.

2.12 PROB13 - Rod Cluster Numerical Routine

This routine integrates numerically over the entire cluster cell which is taken to have a white reflecting outer boundary condition. The integration is performed by laying out a set of parallel lines in the x-y plane at a number of discrete angular orientations to a reference diameter of the cluster. The integration along each line is performed using K_{i3} functions for the integration over the z direction cosine. This routine is slow and used for few-group calculations. Further details are given by Doherty [1970].

2.13 PROB15 - Rod Cluster Semi-numerical Routine

This routine is similar to PROB13 but the numerical integration is applied only to the inner annuli of the cluster. An approximate method of the Bonalumi type is applied to the outer annuli. The numerical integration is used for one more annulus than the number which contain rods. This routine is slow and used for few-group calculations. Further details are given by Doherty [1970].

2.14 PROB19 - Rod Cluster Approximate Routine

This is an approximate routine for clusters with a white reflective outer boundary condition. The collision probabilities are formed by a synthesis of collision probabilities for an average pincell in each ring of rods and collision probabilities for the entire cell with smeared cross sections. The pincell and smeared-cell collision probabilities are calculated by the method used in PROB8 and PROB9. This routine is fast

and suitable for most applications. Further details are given by Robinson [1979].

2.15 PROB108 and PROB109 - Approximate Cylinder Routines

PROB108 and PROB109 are another pair of approximate routines for a cylinder and are similar to the pair PROB8 and PROB9 but are based on an earlier model of Bonalumi [1901]. The PROBS and PROB9 routines are preferred because they provide for polygonal as well as circular boundaries. PROB108 is used for a free boundary and PROB109 for a circular white reflecting boundary. The method of these routines is used for the outer annuli in PROB15. Further details are given by Doherty [1969a].

3. INPUT DESCRIPTION

3.1 General

The input data on FORTRAN unit 1 consist of card images which are read using the SCAN free input routine [Bennett & Pollard 1967]. The input is in the form of keywords, which are given in upper case in the following description, followed where necessary by an appropriate string of numeric data. The data are supplied in blocks; all data required for one block should have been supplied before any are given for a succeeding block.

The input routine first attempts to read from three AUS data pools: geometry data from FORTRAN unit 13; cross-section data from FORTRAN unit 14; and a FLUXB data pool from FORTRAN unit 11. Any data obtained from these data pools are modified if the appropriate input data are supplied. The FLUXB data pool may be used as a flux guess. Output AUS data pools are written on the same FORTRAN units as those which may be used for input.

Default values for all input data items are available. Therefore, no input data at all (i.e. an empty data set) may be given if geometry and cross-section data pools are available and the standard options are suitable.

3.2 Input Block 1

This block consists simply of a card image which is used as a title. It must be given if any other input data are supplied.

3.3 Input Block 2

The user may enter any of the following:

NP(i)=n or

NP(i-j)=n where i.j.n are integers with $0 < i < j \le 36$ and $n \ge 0$, is used to alter default values of the triggers NP(1) to NP(36) which control printing. Printing is suppressed for trigger values greater than zero. The trigger NP(i) refers to cross sections (i=2), fission spectra (i=3), fixed source (i=4), geometry (i=6), flux guess (i=7), calculated fluxes (i=35), collision probabilities (i=36). The default is NP(1-36)=1.

followed by a real number is used to specify the tolerance on the eigenvalue, or the activations (normally absorptions) in a source calculation. The default is 0.0001.

NGAUSS followed by an integer specifies the order of Gaussian integration (default 16).

LINES followed by an integer specifies the number of lines per annulus for PROB13 or PROB15.

NANGLES followed by an integer specifies the number of angles for PROB13 or PROB15. The integration is over the range 0 to 2π and the number of angles should be neither a divisor of, nor be divisible by, the number of rods on any ring of the cluster.

3.4 Input Block 3

The data supplied in this block either specify the complete geometry of the system or are used to modify the data obtained from the AUS geometry data pool.

JOM followed by an integer specifies geometry type. The integer has the values 0 for plane, 1 for cylinder and 2 for sphere. The default is 1.

IBR

followed by an integer specifies the right hand boundary condition. The integer has the values 0 for free. 1 for mirror reflective. 2 for periodic and 3 for white reflective. The default is 3 for curved boundaries, otherwise 1.

SQUARE and

HEXAGON specify the shape of the outer boundary in cylindrical geometry if numerical routines are used. The shape is circular by default.

BOUND

followed by a real and an integer specifies the boundary for the approximate cylinder routine. The real (normally an integer) specifies the number of sides of a polygonal boundary. The integer specifies the number of inner annuli to be included in the first region of a two-region system constructed in applying a reflective boundary condition, or is zero for a free boundary. The default is a circular white reflecting boundary.

BONALUMI

and

NUMERICAL specify whether approximate or numerical methods are to be used for cylinders and clusters. The default is BONALUMI.

IPROB followed by an integer specifies the collision probability routine directly by number rather than indirectly with the preceding entries.

NDIV followed by an integer specifies whether, in the PROB13 routine, coolant annuli are used to subdivide the rods. The default is no such subdivision. The integer gives the number of radial subdivisions of a rod which are to be further subdivided by coolant annuli.

NI followed by an integer specifies the number of mesh intervals. This entry should be followed by a mesh interval specification:

R followed by (NI+1) reals giving the mesh interval positions; or

DR followed by NI reals giving the mesh interval spacings. R(1)=0 is implied when using DR and must be specified when using R. R(i+1)=R(i)+DR(i).

MNI followed by NI integers specifies the material numbers for each mesh interval, or the materials may be specified by zones using the three entries:

NZ followed by an integer to specify the number of zones;

MZI followed by NI integers giving the zone number for each interval; and

MNZ followed by NZ integers giving the material number for each zone.

The following entries specify the rods in cluster geometry. The rods are taken to be arranged on a number of rings.

RODSUB n,j,(dr(i),i=1,j),(mat(i),i=1,j)

where n is the number of the ring, numbered from the centre outward,

j is the number of radial subdivisions of a rod in this ring, dr(i) specifies the mesh interval spacings of the subdivision, and mat(i) specifies the material number in each subdivision.

ARRAY n,nrod,prod,grod

where n is as for RODSUB.

nrod is the number of rods in this ring.

prod is the radius of the circle on which the rod centres lie, and

qrod is the angular displacement of one rod from a reference diameter of the cluster. The rods are taken to be equally spaced around the ring. The parameter qrod may be given in radians or degrees.

3.5 Input Block 4

Data in this block consist of directives which stop the writing of AUS data pools. The default option is to write the data pools. This may be altered using any of

NOWGM NOWXS NOWFL

for geometry, cross-section and flux data pools respectively.

3.6 Input Block 5

This block is given only if all cross sections are to be entered in the input stream. Partial modification of the data from the AUS data poo! is not supported. The cross sections are entered as one block following a single keyword.

NG

ng.((1ps(i,n),1v(i,n),act(i,n),nuf(i,n),(grp(j,i,n),j=1,1v(i,n)), i=1,ng),n=1,nmat),(chi(i),i=1,ng) where ng is the number of groups.

lps is the position of the self-scatter cross section in the vector grp.

ly is the length of the vector grp.

act is the activation cross section, normally absorption,

nuf is the fission emission cross section.

grp is a vector giving the absorption cross section followed by the outscatters from the group, nmat is the largest material number referred to in the geometry description, and chi is the fission spectrum which is used for all materials. (A material dependent spectrum is supported when cross sections are obtained from an AUS data pool.) A single zero value

should be entered if a fission spectrum is not needed.

3.7 Input Block 6

The code performs an eigenvalue (k_{eff}) calculation unless it is directed to perform a calculation with a fixed volume source. The source calculation is performed if a source is entered using

QV

ngs.((qv(i,j),i=1,nreg),j=1,ngs) where ngs is the number of groups with a fixed source, qv(i,j) is the source in interval i for group j, and nreg is the number of spatial intervals.

The end of the input data is signalled by including the keyword END

Only one case may be done each time the module is executed.

4. REFERENCES

Bennett, N.W., Pollard, J.P. [1967] - SCAN - a free input subroutine for the IBM360. AAEC/TM399.

Bonalumi, R.A. [1961] - Neutron first collision probabilities in reactor physics. Energ. Nucl. (Milan), 8:326.

Bonalumi, R.A. [1965] - Systematic approximations in neutron first collision probabilities. *Energ. Nucl.* (Milan), 12:1.

Doherty, G. [1969a] - Some methods of calculating first flight collision probabilities in slab and cylindrical lattices. AAEC/TM489.

Doherty, G. [1969b] - Solution of the multigroup collision probability equations. AAEC/E197.

Doherty, G. [1969c] - Solution of some problems by collision probability methods. AAEC/E199.

Doherty, G. [1970] - Collision probability calculations in cluster geometry. AAEC/E205.

Robinson, G.S. [1975] - AUS - the Australian modular scheme for reactor neutronics computations. AAEC/E369.

Robinson, G.S. [1979] - Approximate first collision probabilities for neutrons in cylindrical and cluster lattices. AAEC/E465.

Robinson, G.S. [1984] - Extension of the AUS reactor neutronics system for application to fusion blanket neutronics. AAEC/E583.