THE DOT-III MULTIGROUP TWO-DIMENSIONAL DISCRETE ORDINATES
CODE WITH ANISOTROPIC SCATTERING†

Code Developed by:

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The DOT-III computer program solves the energy and angular dependent Boltzmann equation with general anisotropic scattering for rectangular, polar, or cylindrical geometries. Principal applications are to neutron and/or gamma-ray transport problems in either forward or adjoint mode. Both homogeneous and external source problems can be solved and searches on multiplication factor, time absorption, nuclide concentration, and zone thickness are available. However, the code is particularly designed and suited to the solution of deep penetration radiation transport problems.

The discrete ordinates, or Carlson's S_n , method is utilized to solve the Boltzmann equation. A good account of the historical development and application of this method is included by Mynatt *et al.* in a description of the development and verification of two-dimensional transport theory for radiation shielding applications.¹ Briefly, the discrete ordinates method involves the solution of difference equations derived in a term-wise manner by integrating the analytic form of the Boltzmann equation over a five-dimensional finite cell defined in terms of location, direction, and energy phase space variables. Supplementary difference equations are required to obtain a solution to the flux. These equations relate the average flux for a cell with each pair of associated cell face fluxes. The equations should provide a good approximation to the true variation and at the same time be easily and quickly solved on the computer. Two forms of the supplementary equations which have been utilized in earlier versions of DOT are "diamond difference" and "step function" equations.

The cross sections required by DOT-III are of the multigroup, P_n , expansion type generated by codes such as AMPX, which is described in Mrs. Maskewitz's paper. The utilization of this type of multigroup cross-section data allows the solution of coupled neutron and secondary gamma-ray transport problems with anisotropic scattering.

Various versions of DOT and related computer programs have been developed over the years and several have been placed at RSIC. Some examples of

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various applications of the program are found in references 2 through 7. See Appendices A, B, and C for detailed abstracts describing some of the existing versions of the DOT program.

The DOT-III program incorporates some features and also includes considerable improvements to these versions of DOT. These features are designed to improve the calculational ability and simplify the utilization of the code. Some of these are as follows:

1. An analytic first collision source can be calculated internally and used.
2. Weighted difference mode is available by option or when linear gives negative flux values.
3. Multiple zones of convergence can be specified.
4. Iterative space dependent scaling improved (logic and speed).
5. Sources can be specified on an internal boundary.
6. Flux output for restarting a subsequent calculation is written as each group is processed and incomplete output can be used to restart a problem.
7. Angular flux can be output along either radial or axial boundaries, internal or external, and used as source in a subsequent problem.
8. Flux and group organized cross section input can be copied to allow reuse.
9. For coupled neutron and gamma-ray runs, outer iterations can be limited to neutron groups.
10. Flux guesses can be synthesized from one-dimensional calculations.
11. Input flux guesses can be made using results from other calculations with different P_k , S_n , or number of groups.
12. Scattering expansion order can be specified for each group.
13. Short list I/ϕ is utilized, improving speed significantly.
14. Timing routines give breakdown of time consumption in major sections of the program.
15. Angular flux output can be obtained from single outer iteration problems.
16. Free field FIDØ input simplifies data preparation.
17. Multiple problems can be run.

18. User assignment of logical units is checked for errors.
19. Diffusion theory is available.
20. The amount of printed output can be selected to suite the user's need.

References

1. F. R. Mynatt, F. J. Muckenthaler, and P. N. Stevens, "Development of Two-Dimensional Discrete Ordinates Transport Theory for Radiation for Shielding," CTC-INF-952 (AD-692168) (August 1969).
2. F. R. Mynatt, "A User's Manual for DOT," K-1694 (1967).
3. R. G. Soltesz, R. K. Disney, and G. Collier, "Users Manual for DOT IIW Discrete Ordinates Transport Computer Code," WANL-TME-1982 (1969); see also WANL-TME-1982 (Revision A) (1970).
4. D. Lindetrom, "Technical Report and User's Manual DASH-FORTRAN-IV Void Tracing and S_n -Monte Carlo Bridging Code," SRT-TRM01-W393-4C (May 1970).
5. D. G. Lindstrom and J. H. Price, "Coupled Discrete Ordinates - Monte Carlo Technique and Applications to NERVA," AGC-NRO 1373 (1969).
6. P. A. Read, W. E. Selph, and R. J. Cerbone, "Duct Code Manual," GULF-RT-10654 (April 1971).
7. R. Protsik and E. G. Leff, "User's Manual for DOT2DB: A Two-Dimensional Multigroup Discrete Ordinates Transport/Diffusion Code with Anisotropic Scattering," GEAP-13537 (September 1969).

Appendix A

RSIC CODE PACKAGE CCC-89

1. NAME AND TITLE OF CODE

DOT: Multigroup Two-Dimensional Discrete Ordinates Transport Code with Anisotropic Scattering.

DOT was first available in 1966. The DOT-II version was made available in 1969.

2. CONTRIBUTORS

Computing Technology Center and the Oak Ridge National Laboratory Neutron Physics Division, Union Carbide Corporation, Nuclear Division, Oak Ridge, Tennessee.

Atomics International, Canoga Park, California.

U. S. Air Force Weapons Laboratory, Kirtland Air Force Base, New Mexico.

3. CODING LANGUAGE AND COMPUTER

FORTRAN IV; IBM 7090, IBM 360/75, and CDC 6600.

4. NATURE OF PROBLEM SOLVED

DOT is a general purpose program which solves the linear, energy-dependent, Boltzmann transport equation for two-dimensional r-z, x-y, and r- θ geometries. The basic form of the solution is the quantity $\bar{\phi}(r_i, z_j, E_g, \Omega_d) \Delta E_g = \phi_{ijgd}$, the flux, averaged in the spatial interval surrounding r_i, z_j , integrated over the energy group g, and averaged in the solid segment surrounding Ω_d .

5. METHOD OF SOLUTION

The gradient or convection term in the Boltzmann equation is approximated by a finite difference technique known as discrete ordinates - Carlson's S_n method. The inscatter integral is approximated by expanding the differential cross-section in a Legendre series which allows the integral to be computed by quadrature. DOT will solve forward or adjoint, homogeneous or inhomogeneous problems. The inhomogeneous problems may have a

volume distributed source or a specified angular flux at the right or top boundaries; fissions may be included for a subcritical system. Homogeneous (eigenvalued) problems will determine the following: (1) static multiplication factor, " k ", (2) time absorption, "Rossia", (3) concentration for a specified k , (4) zone thickness for a specified k .

The primary differences between DDK and DOT are given in the following:

- a. general anisotropic scattering is allowed,
- b. boundary sources may be treated by specifying the angular flux at the right or top boundaries,
- c. angular fluxes may be printed or written on binary tape,
- d. the pass B scaling for problems with reflected right or top boundaries has been removed,
- e. if specified, a pointwise inner iteration flux convergence criteria is used instead of the integral test,
- f. the integral inner iteration convergence criteria specifies that the average absolute pointwise flux error be less than epsilon,
- g. input data is processed by the FIDO routine used in DTF-II and ANISN, and
- h. if the linear difference equations produce a negative flux, the flux is recalculated using the step function difference equations. This technique, which inhibits oscillation due to extrapolation, is optional.

6. RESTRICTIONS OR LIMITATIONS

Problem size is limited by machine size.

7. TYPICAL RUNNING TIME

No statistics have been accumulated by RSIC as to typical running time.

Estimated running time on the IBM 7090 for the two packaged sample problems: 16 minutes.

8. COMPUTER HARDWARE REQUIREMENTS

Standard equipment is used on either computer, and a maximum of 7 tapes or direct access devices in addition to I-O is utilized.

9. COMPUTER SOFTWARE REQUIREMENTS

CCC-89A: The code is operable on the IBM 7090/7094 IBSYS Operating System using IBJOB Processor.

CCC-89B: The code is operable on the IBM 360/75 Operating System using G Compiler.

CCC-89C The code is operable on the IBM 360/75 Operating System using OS-360 Fortran H Compiler.

CCC-89D: The code is operable on the CDC-6600.

Any non-standard library routines used are included in the affected code package.

10. REFERENCES

F. R. Mynatt, "A User's Manual for DOT," K-1694 (January 1967).

F. R. Mynatt, "Development of Two-Dimensional Discrete Ordinates Transport Theory for Radiation Shielding," to be published in Nucl. Sci. Eng. (1969).

11. CONTENTS OF CODE PACKAGE

The package contains the following items:

- a. the referenced document,
- b. a reel of magnetic tape on which is written in separate files: the source card decks and BCD input and output listing from a sample problem.

12. HOW TO OBTAIN PACKAGE

Inquiries or requests for the code package may be mailed to

CODES COORDINATOR
Radiation Shielding Information Center
Oak Ridge National Laboratory
Post Office Box X
Oak Ridge, Tennessee 37830

or telephoned to

Area Code 615; 483-8611, extension 3-6944, or to

FTS xx-615-483-6944.

Persons requesting the code package should send a reel of magnetic tape to the above address.

13. DATE OF ABSTRACT

May 1969.

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LaboratoryAppendix B
RSIC Code Package CCC-89GWANL-TME-1982
(Revision A)

COMPUTER CODE SYNOPSIS

1. Name: DOT-IIW⁽¹⁾
2. Computer: The code is designed for CDC-6600 and IBM 360/75 computers.
3. Nature of Physical Problem Solved: DOT-IIW solves the two-dimensional, energy dependent, linear Boltzmann transport equation with general anisotropic scattering for x , y ; r , z ; and r , θ geometries in one of two approximations (discrete ordinates - S_n and diffusion. DOT solves forward or adjoint, homogeneous or inhomogeneous problems. The inhomogeneous problems may have a fixed volume distributed source, or in discrete ordinates, a specified angular dependent boundary source at the right or top boundaries; fissions may be included for a subcritical system with fixed source. Vacuum, reflective and periodic boundary conditions may be specified for both approximations. White or albedo boundary conditions can be specified in a discrete ordinates - S_n solution. Time absorption calculations, concentration searches, or zone thickness searches are also solved. Cross sections may be input from a library tape and/or from cards. Asymmetric or symmetric quadrature calculations in discrete ordinates - S_n may be performed. The code includes a choice of Gaussian Iteration, Successive Overrelaxation, Space Point Scaling, or Chebyshev Acceleration to achieve a flux solution on inner iterations in the discrete ordinates method and Successive Overrelaxation to achieve a flux solution in the diffusion method. Group dependent scaling techniques are used in the multigroup solution to accelerate convergence of forward or adjoint calculations containing upscatter, fissions, and/or fixed sources. Detailed system and zone balance tables are provided.
4. Method of Solution: The discrete ordinates or Carlson's S_n method using a diamond, step, weighted or mixed difference solution technique or a diffusion solution technique⁽⁸⁾ is employed. The method is applicable to both neutron and gamma ray transport problems. The discrete ordinates solution in the code will approach the exact solution of the Boltzmann equation with increasing orders of approximation as the space, angle, and energy mesh approaches differential size.

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(Revision A)

5. **Restrictions on the Complexity of the Problem:** The DOT-IIW computer code utilizes variable dimensioning to facilitate dynamic core data storage allocation at execution time. Because of the variable dimensioning technique, on any given data array, no size restriction is imposed; only a size restriction on the length of the sum of all arrays is imposed. The amount of core data storage for a given problem may be exactly computed as indicated in the documentation. The total amount of core storage for a given problem may then be specified at execution time, if desired.
6. **Typical Running Time:** Two versions of the DOT-IIW code are available. The all-FORTRAN IV version of the code computes approximately 4500 angular fluxes per second in the discrete ordinates solution and 1500 scalar fluxes per second in the diffusion solution. The FORTRAN IV plus COMPASS Assembly Language version of the code computes approximately 9100 angular fluxes per second in the discrete ordinates solution on the CDC-6600 computer. Both versions compute identical discrete ordinates results.
7. **Unusual Features of the Program:** The code employs a general anisotropic scattering capability, variable dimensioning, and the concentration of the bulk of the discrete ordinates solution computations in one subroutine which is available in assembly language in one of the supplied versions of the code.
8. **Related and Auxiliary Programs:** Cross sections may be supplied by the GAMB1T⁽³⁾ or GAMLEG⁽⁴⁾ codes. Fixed distributed neutron or photon sources as well as energy deposition may be calculated with the NAGS⁽⁵⁾ code. Isoflux or isodose rate plots may be obtained with the FLUXPLT⁽⁶⁾ code. Coupling of discrete ordinates solutions through external voids may be done using the MAP⁽⁷⁾ code.
9. **Status:** The code is in production use at WANL with additional development effort being devoted to extend its flexibility and usefulness. Users at WANL load the code from a disk or tape with control cards followed by the user's input data.

WANL-TME-1982
(Revision A)

10. References:
1. R. G. Soltesz, R. K. Disney, and G. Collier, WANL-TME-1982, "User's Manual for the DOT-IIW Discrete Ordinates Transport Computer Code," December 1969.
  2. F. R. Mynatt, F. J. Muckenthaler, and P. N. Stevens, CTC-INF-952, "Development of Two-Dimensional Discrete Ordinates Transport Theory for Radiation Shielding," August 1969.
  3. G. Collier and G. Gibson, WANL-TME-1752, "GAMBIT Program," April 1968.
  4. K. D. Lathrop, LA-3268, "GAMLEG--A FORTRAN Code to Produce Multigroup Cross Sections for Photon Transport Calculations," April 1965.
  5. WANL-PR(LL)-010, "Synthesis of Computational Methods for the Design and Analysis of Radiation Shields for Nuclear Rocket Systems," Volume 7, June 1967.
  6. L. L. Moran and R. G. Soltesz, WANL-TME-1813, "FLUXPLT, A FORTRAN IV Program to Plot Isoflux Lines Based on the Scalar Flux Calculated by the DOT Program," June 21, 1968.
  7. R. G. Soltesz and R. K. Disney, "Two-Dimensional Transport Techniques," to be published.
  8. W. W. Little, Jr. and R. W. Hardie, BNWL-831, Revision 1, "2DB User's Manual -- Revision 1," August 1969.
11. Machine Requirements: The DOT-IIW code is in production at WANL on 65K and 131K CDC-6600 computers. The source program required 30K decimal locations; the remaining locations are used for problem data storage. Up to seven tape or disk devices are required in addition to input and output disks.
12. Programming Languages Used: Two versions of the DOT-IIW code are available. The first version is written in standard, ASA FORTRAN IV. The second version is identical to the first with the exception of Subroutine GRIND, which is written in COMPASS assembly language. The second version runs approximately a factor of two faster than the all-FORTRAN version.

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(Revision A)

13. Operating System or Monitor Under Which Program is Executed: The DOT-IIW code is operational under the CDC-6600 SCOPE 3.2 Monitor System or the IBM 360 Release 18 Monitor System.
14. Other Programming or Operating Information or Restrictions: None.
15. Name and Establishment of Authors:

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S. L. Zeigler, and G. C. Collier
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Appendix C

RSIC CODE PACKAGE CCC-151

1. NAME AND TITLE OF CODE

DOT2DB: Two-Dimensional Multigroup Discrete Ordinates
Transport/Diffusion Code with Anisotropic Scat-
tering.

DOT2DB is a conglomerate of the diffusion subroutines of the
BNWL computer code 2DB and the ORNL transport code DOT (CCC-89).

2. CONTRIBUTORS

General Electric Company, (BRD), Sunnyvale, California.
Battelle Northwest Laboratory, Richland, Washington.
Oak Ridge National Laboratory, Oak Ridge, Tennessee.

3. CODING LANGUAGE AND COMPUTER

FORTRAN IV; GE-635.

4. NATURE OF PROBLEM SOLVED

DOT2DB solves both the multigroup discrete ordinates transport theory and the multigroup diffusion theory equations in two dimensions. Anisotropic scattering of any order Legendre expansion is allowed in the transport theory option. Anisotropic scattering in the diffusion theory option is treated with the "transport" approximation, using the P_1 scattering matrix, when provided, to calculate the transport cross sections. Options include solutions in (x,y), (r,z), (r, θ), and, in the diffusion theory option, triangular geometries. Both direct and adjoint fluxes may be computed for fixed volume-distributed source, multiplication constant iteration, time absorption iteration, concentration search, zone thickness search, and fixed boundary source problems. In addition to the fixed boundary source problem, options include vacuum, reflection, periodic and white boundary conditions. Cross sections may be entered from cards or from tape in the DTF format.

Activities for any material in the system may be output by interval (optional) and zone. Other output includes the interval fluxes and sources and a reaction summary table for each zone and for the system.

5. METHOD OF SOLUTION

DOT2DB has three iteration levels. The innermost iteration level computes the spatial flux distribution within an energy group. Convergence at this level may be accelerated by extrapolation of the scalar flux (and, in the transport theory option, the flux moments) by an input factor. The second iteration level computes the energy spectrum of the flux and the multiplication constant or time absorption eigenvalues. Convergence at this level may be accelerated by extrapolation of the fission source distribution by an input factor. The outermost iteration level searches for the material concentration or zone thickness eigenvalues of the problem.

6. RESTRICTIONS OR LIMITATIONS

Variable dimensioned arrays are used exclusively within the program. Hence, the only problem size restriction is dictated by the amount of available computer memory.

7. TYPICAL RUNNING TIME

Running time varies widely, depending on the problem size and the options chosen. An S_6 , one group, 10×10 spatial mesh, multiplication constant iteration problem required 212 seconds of computer processor time. The same problem in diffusion theory required 13 seconds.

8. COMPUTER HARDWARE REQUIREMENTS

The code is designed for the GE-635 computer and can be made to run in various memory sizes due to its variable dimensioning. The

code when operating at 45K handles a majority of desired problem sizes.

Seven scratch files are required and optionally one file tape. Each scratch file consists of approximately 80,000 to 100,000 words. Two output files are used (06,33), requiring the use of a printer.

9. COMPUTER SOFTWARE REQUIREMENTS

DOT2DB runs under the GECOS-III operating system which precludes any operator intervention. The code requires segmentation (chaining - linking). It operates under time surveillance with the following subroutines which are written in GMAP, the GE-635 assembly language.

CLOCK - Returns current processor time in seconds.

MYTIME - Returns user time limits in hundredths of an hour.

LIMRIN - When run time is exceeded, this GE routine will allow the user to obtain five more minutes of processor time.

10. REFERENCES

R. Protsik, "User's Manual for DOT2DB: A Two-Dimensional Multi-group Discrete Ordinates Transport/Diffusion Code with Anisotropic Scattering," GEAP-13537 (September 1969).

W. W. Little, Jr., and R. W. Hardie, "2DB, A Two-Dimensional Diffusion Burnup Code for Fast Reactor Analysis," BNWL-640 (January 1968).

W. W. Little, Jr., and R. W. Hardie, "2DB User's Manual," BNWL-831 (July 1968).

W. W. Little, Jr., and R. W. Hardie, "2DB User's Manual - Revision 1," BNWL-831 Rev. 1 (February 1969).

F. R. Mynatt, "A User's Manual for DOT - A Two-Dimensional Discrete Ordinates Transport Code with Anisotropic Scattering," K-1694 (January 1967).

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13. DATE OF ABSTRACT

February 1972.