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**SNEX: Semianalytic Solution of the One-Dimensional
Discrete Ordinates (S_n) Transport Equations with
Diamond Differenced Angular Fluxes**

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SNEX: Semianalytic Solution of the One-Dimensional Discrete Ordinates (S_n) Transport Equations with Diamond Differenced Angular Fluxes

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SNEX: SEMIANALYTIC SOLUTION OF THE ONE-DIMENSIONAL
DISCRETE ORDINATES (S_n) TRANSPORT EQUATIONS WITH DIAMOND
DIFFERENCED ANGULAR FLUXES

by

B. R. Wienke

ABSTRACT

SNEX is a code which exactly solves the spatial single group, one-dimensional (plane, cylinder, sphere) discrete ordinates transport equations with diamond approximation for the angular fluxes. Its purposes are to provide a standard for comparisons of spatial differencing schemes as well as an exact numerical solution to the discrete ordinates equations in one-dimensional geometries. Full solutions are generated by numerically integrating the inhomogeneous source terms and adding them to the homogeneous (analytic) solutions in the standard fashion. Simple relationships between angular quadratures permit application of the method to plane, cylindrical and spherical geometries. Analysis is confined to isotropic scattering. Simple theory and methodology are presented and discussed. A code listing and sample problems are also included.

I. INTRODUCTION

Typically, multigroup discrete ordinates codes solve the transport equations by using finite difference or finite element techniques on compatible meshes. As the meshes are refined, solutions converge to the exact values. An alternative, exact (but more time consuming) approach consists in solving the transport equations numerically by formal inversion of differential operators. Such procedure also has the advantage that exact solutions are generated independently of mesh size for given convergence criteria. In the following, we describe and detail SNEX, a transport equation solver which can be used to provide exact

numerical solutions to the linear transport equation in one dimensional plane, cylindrical and spherical geometrics.

SNEX solves the single group transport equation with isotropic scattering for specified left and right boundary conditions. It is structured closely to ONETRAN¹ as far as input/output formats. Coarse and fine meshes are defined with material zones specified on the coarse mesh. External sources of any functional form are admissible. Both the standard diamond and step starting schemes are options. Iteration on the scattering source is controlled by a convergence parameter computed from the difference in successive scalar flux estimates. To stabilize scattering iteration cycles, weighted averages of flux iterates may be employed. The code is structured for arbitrary S_n order, depending, of course, on available core storage (which scales roughly as the fine mesh size times the S_n order). All angular quadrature data, such as directions cosines, weights and angular coefficients, are read into the code directly. Output consists of pointwise angular and scalar fluxes computed on the fine mesh, as well as a listing of all input parameters and options. The solution algorithm requires numerical integration of an inhomogeneous source term (composed of external, scattering and angular edge components) and is effected with an adaptive Newton-Cotes (7-point) routine².

SNEX serves to provide an exact numerical solution to the monoenergetic discrete ordinates equations and a standard for comparison of differencing schemes.

II. TRANSPORT EQUATION, DISCRETE ORDINATES APPROXIMATION AND PHENOMENOLOGY

The time independent transport (linear) equation is written in the monoenergetic case,

$$\vec{\nabla} \cdot \vec{\Omega} \psi + \sigma \psi = \int d\Omega' \sigma_s \psi' + q \quad (1)$$

where ψ is the particle flux (density times speed), σ, σ_s are the total, scattering cross sections, $\vec{\Omega}, \vec{\Omega}'$ are unit vectors in the directions of particle travel and q is the external source of particles. The streaming operator, $\vec{\nabla} \cdot \vec{\Omega}$, takes the explicit form in the one dimensional geometries,

$$\begin{aligned}
\vec{\nabla} \cdot \vec{\Omega} \psi &= \mu \frac{\partial}{\partial x} \psi && \text{(plane)} \\
&= \frac{\mu}{\rho} \frac{\partial}{\partial \rho} (\rho \psi) - \frac{1}{\rho} \frac{\partial}{\partial \phi} (\eta \psi) && \text{(cylinder)} \\
&= \frac{\mu}{r^2} \frac{\partial}{\partial r} (r^2 \psi) + \frac{1}{\rho} \frac{\partial}{\partial \mu} (1 - \mu^2) \psi, && \text{(sphere)}
\end{aligned} \tag{2}$$

where μ is the angle between the position vector (in the three systems) and the direction of travel. The direction cosines satisfy,

$$\mu^2 + \eta^2 + \xi^2 = 1 \tag{3}$$

and,

$$\tan \phi = \frac{\eta}{\mu} . \tag{4}$$

The discrete ordinates approximation assume that the value of the angular flux, or ordinate, is determined at sets of discrete directions, $\Omega_m = (\mu_m, \eta_m, \xi_m)$ with $m = 1, 2, 3, \dots M$. The corresponding angular flux is denoted generally by,

$$\psi_m(\vec{r}) = \psi(\vec{r}, \Omega_m) , \tag{5}$$

and angular integrals and moments involving ψ_m are evaluated with quadrature weights, w_m , such that

$$\int \psi(\vec{r}, \vec{\Omega}) d\Omega = 4\pi \sum_{i=1}^M w_m \psi_m(\vec{r}) \tag{6}$$

for,

$$\sum_{i=1}^M w_m = 1 \quad (7)$$

Differencing of the angular variable is based upon the diamond approximation³ between edge, $\psi_{m\pm 1/2}$, and cell centered, ψ_m , fluxes,

$$2\psi_m = \psi_{m+1/2} + \psi_{m-1/2}, \quad (8)$$

which yields a simple recursion relationship for the edge (entering) flux in the m^{th} angular cell,

$$\psi_{m-1/2} = 2\psi_{m-1} - 2\psi_{m-2} + \dots \mp 2\psi_1 \pm \psi_{1/2} \quad (9)$$

The angular differenced form of the transport equation in each of the three geometries is written,

$$\mu_m \frac{\partial \psi_m}{\partial x} + \sigma \psi_m = S_m \quad (\text{plane})$$

$$\mu_m \frac{\partial}{\partial \rho} (\rho \psi_m) + (\alpha_{m+1/2} \psi_{m+1/2} - \alpha_{m-1/2} \psi_{m-1/2}) w_m^{-1} + \rho \sigma \psi_m = \rho S_m \quad (\text{cylinder})$$

$$\mu_m \frac{\partial}{\partial r} (r^2 \psi_m) + (\alpha_{m+1/2} \psi_{m+1/2} - \alpha_{m-1/2} \psi_{m-1/2}) w_m^{-1} r + r^2 \sigma \psi_m = r^2 S_m \quad (\text{sphere}) \quad (10)$$

with $\alpha_{m\pm 1/2}$ sets of angular coefficients satisfying,

$$\alpha_{m+1/2} = \alpha_{m-1/2} = 0 \quad (\text{plane})$$

$$\alpha_{m+1/2} - \alpha_{m-1/2} = -w_m \mu_m \quad (\text{cylinder})$$

$$\alpha_{m+1/2} - \alpha_{m-1/2} = -2w_m \mu_m \quad (\text{sphere})$$

$$\alpha_{1/2} = \alpha_{M+1/2} = 0, \quad (\text{all geometries}) \quad (11)$$

and S_m the sum of external and scattering sources,

$$S_m = q_m + \sum_{n=1}^M w_m \sigma_s (\mu_n \rightarrow \mu_m) \psi_n \quad (12)$$

Using Eqs. (8) and (11), we can rewrite Eqs. (10) into the simple general form,

$$\mu_m q \frac{\partial \psi_m}{\partial q} + \mu_m \gamma_m \psi_m + q \sigma \psi_m = q S_m + \mu_m \gamma_m \psi_{m-1/2} \quad (13)$$

where in the various geometries,

$$q = x$$

$$\gamma_m = 0, \quad (\text{plane})$$

$$q = \rho$$

$$\gamma_m = (\alpha_{m+1/2} + \alpha_{m-1/2}) (w_m \mu_m)^{-1} \quad (\text{cylinder})$$

$$q=r$$

$$\gamma_m = (\alpha_{m+1/2} + \alpha_{m-1/2}) (w_m \mu_m)^{-1}, \quad (\text{sphere}) \quad (14)$$

and the $\alpha_{m\pm 1/2}$ still satisfy Eq. (11).

Equation (13) is easily inverted, with the result,

$$\psi_m = \psi_m^0 e^{\frac{-\sigma(q-q_0)}{\mu_m}} \left(\frac{q}{q_0} \right)^{-\gamma_m}$$

$$+ e^{\frac{-\sigma q}{\mu_m}} q^{-\gamma_m} \int_{q_0}^q dq' e^{\frac{\sigma q'}{\mu_m}} q'^{\gamma_m} \left[\frac{S_m}{\mu_m} + \frac{\gamma_m \psi_{m-1/2}}{q'} \right], \quad (15)$$

for ψ_m^0 the boundary angular flux at $q=q_0$. The content of Eq. (15) is straightforward. The first term on the right hand side is the homogeneous solution and the second term is the inhomogeneous integral. The pseudosource angular flux term, $\psi_{m-1/2}$, appearing in Eq. (15) is generated recursively from lower order solutions by means of Eq. (9). SNEX solves Eq. (15) by numerically integrating the source terms and adding them to the homogeneous solutions. If scattering is present, iteration takes place on the scattering term, Eq. (12), subject to satisfaction of the convergence criterion for the scalar flux.

The angular parameters α_m , w_m , μ_m are user specified. Typically in S_n applications, the quadrature sets $\{\mu_m, w_m\}$ are chosen to be Gaussian and the α_m are generated recursively from Eqs. (11) in the three geometries. The coefficients γ_m are automatically computed by SNEX.

III. METHODOLOGY

Equation (15) is evaluated numerically once boundary conditions and starting direction options are specified. Space/angle sweeps start at the right boundary for specified incoming boundary fluxes ($\mu_m < 0$) and proceed to the left boundary for specified incoming boundary fluxes ($\mu_m > 0$) and then return to the right boundary. Directions are angularly coupled through Eq. (9). In addition to boundary values, the value of $\psi_{1/2}$ must be specified to "start" the calculation. In cylindrical and spherical geometry, $\psi_{1/2}$ corresponds to the angular flux at $\mu = -1$, $\eta = 0$. Examination of Eqs. (2) reveals that $\psi_{1/2}$ then satisfies the slab-like equation in all three geometries,

$$- \frac{\partial \psi_{1/2}}{\partial q} + \sigma \psi_{1/2} = S_{1/2} \quad (16)$$

which can be simply integrated for constant source $S_{1/2}$. Alternatively, one might make the step approximation,

$$\psi_{1/2} = \psi_1, \quad (17)$$

in which case the angular coupling is somewhat simplified in higher orders. Both options are available in SNEX. In the case of pure absorbing regions, the computation is completed after one space/angle sweep. If scattering is present, the scattering source, Eq. (12), is updated with the new angular flux iterate at the end of each space/angle sweep until convergence is met, or the iteration limit is exceeded.

The integral over the angular flux $\psi_{m+1/2}$ on the right hand side of Eq. (15) could be generated numerically from a corresponding lower order, $\ell \leq m-1$, equation of the same functional form. Thus, each angular flux term of order $\ell \leq m-1$, appearing on the right hand side of Eq. (15) would be the result of ℓ -dimensional nested integrations. Such procedure would be extremely time consuming and prone to divergence, particularly if negative fluxes occur either at cell edges or in the integrand. Early investigations⁴ have demonstrated the occurrence of negative fluxes (due to the angular diamond approximation) for highly localized sources in absorbing regions. To avoid this situation, the effective source fluxes, $\psi_{m+1/2}$, appearing in Eq. (15) were approximated as piecewise linear functions on the fine mesh. That is, for given m in Eq. (15), each lower order flux term, $\ell \leq m-1$ computed earlier, is linearly interpolated across the mesh cell. As the mesh size decreases, the solutions converge to the exact result. For this reason, the overall approach in cylindrical and spherical geometries ($\gamma_m \neq 0$) is termed semianalytic.

IV. INPUT AND CODE PARAMETERS

Input to SNEX consists of the following parameters and arrays:

```

ANAME - title
      A - Sn order (arbitrary)
      ICT - coarse mesh intervals (arbitrary)
      IACC - acceleration parameter (100-0)
      IGEOM - geometry (1-plane, 2-cylinder, 3-sphere)
      IBL - left boundary condition (0-specified
           flux, 1-reflective)

```

IBR - right boundary condition (0-specified
 flux)
 IL - iteration limit (arbitrary)
 ISTEP - starting direction option (0-slab
 exact, 1-step)
 CS(A) - direction cosines
 W(A) - weights
 B(A+1) - angular coefficients
 X(ICT+1) - coarse mesh
 IIT(ICT) - fine mesh intervals/coarse mesh
 SG(ICT) - total cross sections/coarse mesh
 ST(ICT) - scattering cross sections/coarse mesh
 Q(ICT) - external source/coarse mesh
 FB(1,A/2) - left boundary flux,
 FB(IFT+1,A/2) - right boundary flux

with IFT the number of fine mesh points. Additionally the following parameters and arrays are employed in SNEX:

Z(IFT+1) - fine mesh points
 DX(ICT) - fine mesh interval widths/coarse mesh
 FB(IFT+1,A+1) - angular flux
 SF(IFT+1) - scalar flux
 PB(IFT+1,A+1) - previous iterate angular flux
 CV - convergence parameter
 IN - iteration count
 RIACC - acceleration parameter (IACC/100).

In present form, A+1, IFT+1 are set at 17 and 301 in array statements, while ICT is set to 10. The user is free to change these parameters to suit his needs. The left boundary flux FB(1,A/2) for outgoing directions is only read if IGEOM = 1 (plane). Otherwise, in curved (cylinder, sphere) geometries (IGEOM = 2,3), a reflective boundary condition is assigned at the origin (left boundary). The acceleration parameter IACC is used to fractionally weight presently computed values of the angular flux with the previous flux iterates. The weighting parameter used on the k^{th} flux iterate is RIACC = IACC/100 while the

parameter RIACCM = 1.-RIACC is used on the (k-1)th flux iterate. In most applications, successive flux iterations monotonically approach the convergence criterion and one uses IACC = 100. In oscillatory situations, further mesh refinement and/or taking IACC<100 will aid convergence. If ISTEP=0 is chosen as the starting direction option, $\psi_1 = \psi_{1/2}$, yielding a slab solution for ψ_1 , as seen from Eq. (13). If ISTEP = 1, $\psi_1 \neq \psi_{1/2}$, and the slab equation for $\psi_{1/2}$ provides the starting point for space/angle sweeps.

The origin is a singular point in curved geometries, as seen from Eq. (13) or (15). Integrations over the origin diverge (overflow). In these cases, the origin is automatically set to 1×10^{-6} for computational simplicity.

The data are read into SNEX in the following order and formats:

ANAME(10)	10A8
A, ICT, IACC, IGEOM, IBL, IBR, ISTEP	10(I7,1x)
CS(A)	5(E14.8,2x)
W(A)	5(E14.8,2x)
B(A)	5(E14.8,2x)
X(ICT)	5(E14.8,2x)
IIT(ICT)	10(I7,1x)
SG(ICT)	10(F7.2,1x)
ST(ICT)	10(F7.2,1x)
Q(ICT)	10(F7.2,1x)
FB(1,A/2)	5(E14.8,2x)
FB(IFTP,A/2)	5(E14.8,2x).

V. SAMPLE PROBLEM

As a sample problem, we consider a scattering/absorbing sphere (IGEOM=3) 1 mean free path (mfp) thick with uniform $\sigma_s / \sigma_t = .5$. An isotropic source is placed in a localized slice of thickness .00002 mfp at unit distance from the origin. Reflective boundary conditions are automatically assigned at the left boundary and the incoming right boundary flux is taken to be zero. An S_4 angular quadrature (Gaussian) is assigned and the slab starting direction option is used (ISTOP=0). The acceleration parameter is set to maximum value (IACC=100) and the iteration limit to 30 (IL=30). The sphere is coarse meshed into 3 regions of approximately .1 mfp (fine mesh) intervals.

The input file for the above sample problem is given below.

```

ABSORBER/SCATTERER SOURCE TEST PROBLEM
  4      3      100      3      1      0      30      0
-.36113630E+00  -.33998100E+00  .33998100E+00  .36113630E+00
.17392700E+00  .32607200E+00  .32607200E+00  .17392700E+00
.00000000E+00  .29955000E+00  .52126700E+00  .29955000E+00  .00000000E+00
.10000000E-05  .99000000E-02  .10100000E-01  .10000000E+02
  1      1      10
  .10      .10      .10
  0.05      0.05      0.05
  0.00      1.00      0.00
  0.00      1.00      0.00
  0.00      1.00      0.00
  0.00      1.00      0.00
.00000000E+00  .00000000E+00

```

The corresponding output is listed below. Entries are self-explanatory. Angular and scalar fluxes are given. For a given order A, there are A+1 angular fluxes printed, with the (A+1)st entry the starting direction flux, $\psi_{1/2}$. The last two (unlabeled), numbers are the iteration count (IN) and acceleration parameter (RIACC).

```

ABSORBER/SCATTERER SOURCE TEST PROBLEM

  4 ORDER
  3 INTERVALS
 100 ACCELERATION
  3 PLANE/CYLINDER/SPHERE
  1 LEFT BDY/SPECIFIED/REFLECTIVE
  0 RIGHT BDY/SPECIFIED
  30 ITERATION LIMIT
  0 STARTING/STEP

COARSE MESH
.10000000E-05  .99000000E-02  .10100000E-01  .10000000E+02
  FINE MESH

  1      1      10
.10000000E-05  .99000000E-02  .10100000E-01  .10090900E+01  .20080800E+01
.30070700E+01  .40360600E+01  .50050500E+01  .60040400E+01  .70030300E+01
.80020200E+01  .90010100E+01  .10000000E+02
  CROSS SECTIONS

  .10      .10      .10
  .05      .05      .05
  SOURCE

  0.00      1.00      0.00
  0.00      1.00      0.00
  0.00      1.00      0.00
  0.00      1.00      0.00
  QUADRATURE ( GAMMA/BETA/COSINE /WEIGHT )

.17222743E+01  .25172876E+01  .25172876E+01  .17222743E+01
0.             .29955000E+00  .52126700E+00  .29955000E+00  0.
-.36113630E+00  -.33998100E+00  .33998100E+00  .36113630E+00
.17392700E+00  .32607200E+00  .32607200E+00  .17392700E+00

```

LEFT/RIGHT BOUNDARY FLUXES

0.	3.				
		POSITION	ANGULAR FLUX		
		.100000E-05	.224181E-03	.224182E-03	.224181E-03
			.224181E-03		
		.990000E-02	.255937E-03	.589812E-03	.812321E-03
			.224199E-03		
		.101000E-01	.243263E-04	.245563E-04	.130919E-02
			.241952E-04		
		.100909E+01	.782970E-05	.104182E-04	.166968E-04
			.709065E-05		
		.200808E+01	.284647E-05	.381839E-05	.799981E-05
			.262568E-05		
		.300707E+01	.150957E-05	.204510E-05	.407675E-05
			.139514E-05		
		.400606E+01	.911333E-06	.125765E-05	.252053E-05
			.841656E-06		
		.500505E+01	.581500E-06	.824681E-06	.169865E-05
			.534350E-06		
		.600404E+01	.375995E-06	.555322E-06	.119909E-05
			.342760E-06		
		.700303E+01	.235725E-06	.372099E-06	.867638E-05
			.213554E-06		
		.800202E+01	.136243E-06	.235955E-06	.631622E-06
			.121278E-06		
		.900101E+01	.599907E-07	.120848E-06	.449721E-06
			.525233E-07		
		.100000E+02	0.	0.	.285307E-06
			0.		.471160E-05
		POSITION	SCALAR FLUX		
		.10000000E-05	.22418071E-03		
		.99000000E-02	.59964694E-03		
		.10100000E-01	.58418792E-03		
		.10090900E+01	.15570912E-03		
		.20080800E+01	.39703920E-04		
		.30070700E+01	.17238235E-04		
		.40060600E+01	.93261853E-05		
		.50050500E+01	.56802532E-05		
		.60040400E+01	.37192616E-05		
		.70030300E+01	.25518983E-05		
		.80020200E+01	.18033086E-05		
		.90010100E+01	.12911359E-05		
		.10000000E+02	.91250462E-06		

9 1.000000

VI. CODE LISTING

The present code listing of SNEEX used on the CDC 7600 under the Livermore Time Sharing System (LTSS) is listed below. All reads and writes to unit 59 are commands to a terminal. Units 5 and 6 are the standard input and output devices.

LASL Identification No. LP-1066.

```

PROGRAM SNEK (INPUT,OUTPUT,TTY,TAPE5=INPUT,TAPE6=OUTPUT,TAPE59=TTY
1 )
COMMON /QNC7OUT/ HDWFA7, VALU7
COMMON Z(301), SG(10), FB(301,17), CS(16), G(16), SR(300,16), ST(1
1 0)
COMMON PB(301,17), d(16), K, M, KC, AH, ISTEP
DIMENSION SF(301), ANAME(10)
DIMENSION X(11), DX(10), IIT(10), Q(10,16), B(17), KG(300)
INTEGER A, AP, AH, AHP
C READ DATA
READ (5,280) (ANAME(I),I=1,10)
CV=1.E-4
TMAX=1.0
READ (5,290) A,ICT,IACC,IGEOM,IBL,IBR,IL,ISTEP
AH=A/2
AP=A+1
AHP=AH+1
RIACC=IACC
RIACC=RIACC/100.
RIACCM=1.-RIACC
READ (5,390) (CS(I),I=1,A)
READ (5,390) (d(I),I=1,A)
READ (5,390) (B(I),I=1,AP)
ICTP=ICT+1
READ (5,390) (X(I),I=1,ICTP)
IF (X(1).EQ.0.00.AND.IGEOM.NE.1) X(1)=1.E-6
READ (5,290) (IIT(I),I=1,ICT)
READ (5,270) (SG(I),I=1,ICT)
READ (5,270) (ST(I),I=1,ICT)
DO 10 N=1,A
10 READ (5,270) (Q(I,N),I=1,ICT)
C FORM MESH-MATERIAL REGIONS
IFT=0
DO 20 I=1,A
20 G(I)=(B(I)+B(I+1))/d(I)
DO 30 I=1,ICT
FT=IIT(I)
IFT=IFT+IIT(I)
30 DX(I)=(X(I+1)-X(I))/FT
IFTP=IFT+1
READ (5,390) (FB(IFTP,I),I=1,A4)
FB(IFTP,AP)=FB(IFTP,1)
IF (IGEOM.EQ.2.OR.IGEOM.EQ.3) IBL=1
IF (IBL.EQ.1) GO TO 40
READ (5,390) (FB(1,I),I=AHP,A)
FB(1,AP)=FB(1,1)
40 CONTINUE
DO 50 I=1,IFTP
DO 50 J=1,A
50 PB(I,J)=0.00
L=0
DO 70 I=1,ICT
IT=IIT(I)
DO 70 J=1,IT
L=L+1
DO 60 N=1,A
60 SR(L,N)=Q(I,N)
KG(L)=I
70 Z(L)=X(I)+(J-1)*DX(I)
Z(IFTP)=X(ICTP)
C WRITE DATA
WRITE (6,290) (ANAME(I),I=1,10)
WRITE (6,410)

```

```

WRITE (6,380) A,ICT,IACC,IGEDM,IBL,IBR,IL,ISTEP
WRITE (6,300)
WRITE (6,390) (X(I),I=1,ICTP)
WRITE (6,310)
WRITE (6,290) (IIT(I),I=1,ICT)
WRITE (6,390) (Z(I),I=1,IFTP)
WRITE (6,320)
WRITE (6,270) (SG(I),I=1,ICT)
WRITE (6,270) (ST(I),I=1,ICT)
WRITE (6,330)
DO 80 N=1,A
80 WRITE (6,270) (Q(I,N),I=1,ICT)
WRITE (6,340)
WRITE (6,390) (G(I),I=1,A)
WRITE (6,390) (B(I),I=1,AP)
WRITE (6,390) (CS(I),I=1,A)
WRITE (6,390) (W(I),I=1,A)
WRITE (6,370)
IF (IBL.EQ.0) WRITE (6,390) (FB(1,I),I=AMP,A)
WRITE (6,390) (FB(IFTP,I),I=1,AH)
WRITE (59,280) (ANAME(I),I=1,10)
WRITE (59,410)
WRITE (59,380) A,ICT,IACC,IGEDM,IBL,IBR,IL,ISTEP
WRITE (59,300)
WRITE (59,390) (X(I),I=1,ICTP)
WRITE (59,310)
WRITE (59,290) (IIT(I),I=1,ICT)
WRITE (59,390) (Z(I),I=1,IFTP)
WRITE (59,320)
WRITE (59,270) (SG(I),I=1,ICT)
WRITE (59,270) (ST(I),I=1,ICT)
CH=0.00
DO 90 I=1,ICT
90 IF (ST(I).NE.0.00) CH=ST(I)
WRITE (59,330)
DO 100 N=1,A
100 WRITE (59,270) (Q(I,N),I=1,ICT)
WRITE (59,340)
WRITE (59,390) (G(I),I=1,A)
WRITE (59,390) (B(I),I=1,AP)
WRITE (59,390) (CS(I),I=1,A)
WRITE (59,390) (W(I),I=1,A)
C      SPACE/ANGLE SWEEPS
IN=0
110 CONTINUE
IN=IN+1
WRITE (59,420) IN,TMAX
KC=1
DO 120 I=1,IFT
K=IFT-I+1
Y=Z(K)
M=KG(K)
FB(K,AP)=S1(Y)
120 CONTINUE
DO 140 I=1,IFT
K=IFT-I+1
Y=Z(K)
M=KG(K)
DO 130 J=1,AH
KC=J
FB(K,J)=FF(Y)
IF (J.EQ.1.AND.ISTEP.EQ.1) FB(K,1)=S1(Y)
130 CONTINUE

```



```

140 CONTINUE
   IF (IBL.NE.1) GO TO 160
   DO 150 I=AHP,A
150 FB(1,I)=FB(1,A-I+1)
160 CONTINUE
   DO 180 I=1,IFT
   K=I
   Y=Z(K+1)
   M=KS(K)
   DO 170 J=AHP,A
   KC=J
170 FB(K+1,J)=FF(Y)
180 CONTINUE
   IF (CH.EQ.0.00) GO TO 220
C   CONVERGENCE TEST
   TMAX=CV
   DO 200 I=1,IFTP
   TP=0.0
   TF=0.0
   DO 190 J=1,A
   TP=TP+PB(I,J)*d(J)
   TF=TF+FB(I,J)*d(J)
190 CONTINUE
   CMAX=ABS((TP-TF)/TF)
   IF (CMAX.GT.TMAX) TMAX=CMAX
200 CONTINUE
   IF (TMAX.LE.CV) GO TO 220
   DO 210 I=1,IFTP
   DO 210 J=1,A
210 PB(I,J)=FB(I,J)*RIACC+PB(I,J)*RIACCM
   IF (IN.GT.IL) GO TO 220
   GO TO 110
220 CONTINUE
C   WRITE OUTPUT
   WRITE (59,410)
   DO 240 I=1,IFTP
   SF(I)=0.0
   DO 230 J=1,A
230 SF(I)=SF(I)+FB(I,J)*d(J)
240 CONTINUE
   WRITE (6,350)
   DO 250 I=1,IFTP
250 WRITE (6,400) (Z(I),(FB(I,K),K=1,AP))
   WRITE (6,360)
   DO 260 I=1,IFTP
260 WRITE (6,390) (Z(I),SF(I))
   WRITE (6,410)
   WRITE (6,420) IN,RIACC
   STOP
C
270 FORMAT (10(F7.2,1X))
280 FORMAT (10A8)
290 FORMAT (10(I7,1X))
300 FORMAT (1X,4X,11HCJARSE MESH/)
310 FORMAT (1X,4X,94FINE MESH/)
320 FORMAT (1X,4X,14HCROSS SECTIONS/)
330 FORMAT (1X,4X,54SOURCE/)
340 FORMAT (1X,4X,36HQUADRATURE(GAMMA/BETA/COSINE/WEIGHT)/)
350 FORMAT (/2X,8HPOSITION,7X,12HANGULAR FLUX)
360 FORMAT (/1X,9HPOSITION,8X,11HSCALAR FLUX)
370 FORMAT (1X,4X,26HLEFT/RIGHT BOUNDARY FLUXES/)
380 FORMAT (1X,4X,I3,6H ORDER/5X,I3,10H INTERVALS/5X,I3,13H ACCELERATI
   ON/5X,I3,22H PLANE/CYLINDER/SPHERE/5X,I3,30H LEFT BDY/SPECIFIED/RE

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2 FLECTIVE/5X,I3,20H RIGHT BODY/SPECIFIED/5X,I3,16H ITERATION LIMIT/5
3 X,I3,14H STARTING/STEP//)
390 FORMAT (5(E14.8,2X))
400 FORMAT (1X,E12.6,3X,4(E12.6,1X)/15X,4(E12.6,1X)/16X,4(E12.5,1X)/16
1 X,5(E12.6,1X))
410 FORMAT (/)
420 FORMAT (1X,I6,2X,F10.6)
END
FUNCTION QNC7 (FOF,Y1,Y2,FERR,MXEVALS,KJUN7)
C      ADAPTIVE NEWTON-COTES INTEGRATION ROUTINE
INTEGER DELTEV
COMMON /QNC7OUT/ HDWFA7, VALU7
DIMENSION FOT(20), F1T(20), F2T(20), F3T(20), F4T(20), F5T(20),
1 F6T(20), F(13), W(4), LEG(20), DXT(20), XMT(20), ART(20), EPST(20
2 ), ESTT(20), SUM1(20)
DATA W /4.8809523809523809524E-02,2.57142857142857142857E-01,3.214
1 2857142857142857E-02,3.23809523809523809524E-01/
DATA TWLTH /0.033333333333333333/
KINDCR=+1
MAXEV=MXEVALS
DELTEV=MXEVALS
LMAX=20
A=Y1
B=Y2
EPS=FERR
DA=B-A
AREA=1.
EST=1.
L=0
H2=DA*TWLTH
DO 10 I=1,13,2
PT=A+H2*(I-1)
F(I)=FOF(PT)
10 CONTINUE
KJUN7=7
20 DX=0.5*DA
H2=DA*TWLTH
XM=A+DX
DO 30 I=2,12,2
PT=A+H2*(I-1)
F(I)=FOF(PT)
30 CONTINUE
QNC7=0.
KJUN7=KJUN7+6
IF (KJUN7.GT.MAXEV) GO TO 100
40 ESTL=(W(1)*(F(1)+F(7))+W(2)*(F(2)+F(6))+W(3)*(F(3)+F(5))+W(4)*F(4)
1 )*DX
ESTR=(W(1)*(F(7)+F(13))+W(2)*(F(8)+F(12))+W(3)*(F(9)+F(11))+W(4)*F
1 (10))*DX
AREA=AREA-ABS(EST)+ABS(ESTL)+ABS(ESTR)
SUM4=ESTL+ESTR
IF (ABS(EST-SUM4)-EPS*AREA) 50,50,60
50 IF (EST-1.) 80,60,80
60 IF (L-LMAX) 70,80,80
70 L=L+1
LEG(L)=2
FOT(L)=F(7)
F1T(L)=F(8)
F2T(L)=F(9)
F3T(L)=F(10)
F4T(L)=F(11)
F5T(L)=F(12)
F6T(L)=F(13)

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```

DXT(L)=DX
XMT(L)=XM
ART(L)=AREA
EPST(L)=EPS/1.4
ESTT(L)=ESTR
DA=DX
F(13)=F(7)
F(11)=F(6)
F(9)=F(5)
F(7)=F(4)
F(5)=F(3)
F(3)=F(2)
EST=ESTL
EPS=EPST(L)
GO TO 20
80 IF (LEG(L)-2) 140,90,90
90 SUM1(L)=SUM
LEG(L)=1
A=XMT(L)
DA=DXT(L)
F(1)=F0T(L)
F(3)=F1T(L)
F(5)=F2T(L)
F(7)=F3T(L)
F(9)=F4T(L)
F(11)=F5T(L)
F(13)=F6T(L)
AREA=ART(L)
EST=ESTT(L)
EPS=EPST(L)
GO TO 20
100 CONTINUE
IF (KINDCR.EQ.+1) GO TO 120
110 DELTEV=0.5*DELTEV
MAXEV=MAXEV+DELTEV
LMAX=10.*(Y2-A)/(Y2-Y1)+1.
KINDCR=-1
GO TO 40
120 VALU7=A
VALU7=0.0
IL=L
130 IF (IL.LT.1) GO TO 110
IF (LEG(IL).EQ.1) VALU7=VALU7+SUM1(IL)
IL=IL-1
GO TO 130
140 SUM=SUM1(L)+SUM
L=L-1
IF (L.LT.1) GO TO 150
GO TO 80
150 QNC7=SUM
KOUN7=ISIGN(KOUN7,KINDCR)
RETURN
END
FUNCTION R1 (Y)
C SLAB SOLUTION INTEGRAND
COMMON Z(301), SG(10), FB(301,17), CS(16), G(16), SR(300,16), ST(1
1 0)
COMMON PB(301,17), W(16), K, M, KC, AH, ISTEP
EXTERNAL SFUN, SSS
INTEGER AH
YB=Z(K+1)
SB=SG(M)
CB=-1.0

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IF (ISTEP.EQ.1) CB=CS(1)
SS=SFUN(Y)+SSS(Y)
R1=EXP(SB*Y/CB)*SS/CB
RETURN
END
FUNCTION S1 (Y)
C      SLAB SOLUTION STARTING DIRECTION
COMMON Z(301), SG(10), FB(301,17), CS(16), G(16), SR(300,16), ST(1
1 0)
COMMON PB(301,17), W(16), K, M, KC, AH, ISTEP
EXTERNAL QNC7, R1
INTEGER AH
KP=2*AH+1
YB=Z(K+1)
SB=SG(M)
CB=-1.0
IF (ISTEP.EQ.1) CB=CS(1)
F=F3(K+1,KP)
S1=F*EXP(-SB*(Y-YB)/CB)+EXP(-SB*Y/CB)*QNC7(R1,Y,YB,1.E-4,500,KOUN7
1 )*(-1.)
RETURN
END
FUNCTION QQ (Y)
C      INHOMOGENEJUS TOTAL SOURCE INTEGRAND
COMMON Z(301), SG(10), FB(301,17), CS(15), G(15), SR(300,15), ST(1
1 0)
COMMON PB(301,17), W(16), K, M, KC, AH, ISTEP
EXTERNAL RR, SSS, SFUN
INTEGER AH
SB=SG(M)
CB=CS(KC)
GB=G(KC)
SS=SFUN(Y)+SSS(Y)
QQ=Y**((GB/CB)*EXP(SB*Y/CB))*((SS/CB+GB/(CB*Y))*RR(Y))
RETURN
END
FUNCTION FF (Y)
C      INHOMOGENEJUS TOTAL SOURCE INTEGRAL
COMMON Z(301), SG(10), FB(301,17), CS(16), G(16), SR(300,16), ST(1
1 0)
COMMON PB(301,17), W(16), K, M, KC, AH, ISTEP
EXTERNAL QQ, QNC7
INTEGER AH
CB=CS(KC)
GB=G(KC)
SB=SG(M)
IF (KC.GT.AH) GJ TJ 10
F=FB(K+1,KC)
YB=Z(K+1)
FF=F*EXP(-SB*(Y-YB)/CB)*(YB/Y)**((GB/CB)+EXP(-SB*Y/CB)*Y**(-GB/CB)
1 *QNC7(QQ,Y,YB,1.E-4,500,KJUN7)*(-1.)
GO TO 20
10 F=FB(K,KC)
YB=Z(K)
FF=F*EXP(-SB*(Y-YB)/CB)*(YB/Y)**((GB/CB)+EXP(-SB*Y/CB)*Y**(-GB/CB)
1 *QNC7(QQ,YB,Y,1.E-4,500,KJUN7)
20 CONTINUE
RETURN
END
FUNCTION RR (Y)
C      LINEAR INTERPOLATION OF PSEUDOSOURCE EDGE FLUX
COMMON Z(301), SG(10), FB(301,17), CS(16), G(16), SR(300,16), ST(1
1 0)

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COMMON PB(301,17), W(16), K, M, KC, AH, ISTEP
INTEGER AH
DIMENSION R(17)
DO 20 KK=1,KC
KT=KK-1
IF (KK.EQ.1) KT=2*AH+1
IF (KC.GT.AH) GO TO 10
YB=Z(K+1)
R(KK)=(FB(K,KT)-FB(K+1,KT))/(Z(K)-Z(K+1))*(Y-YB)+FB(K+1,KT)
GO TO 20
10 YB=Z(K)
R(KK)=(FB(K+1,KT)-FB(K,KT))/(Z(K+1)-Z(K))*(Y-YB)+FB(K,KT)
20 CONTINUE
TOT=0.00
IC=1
DO 30 I=1,KC
IC=IC+1
J=KC-I+1
WT=2.0
IF (J.EQ.1) WT=1.0
SN=(-1)**IC
30 TOT=TOT+SN*WT*R(J)
RR=TOT
RETURN
END
FUNCTION SSS (Y)
C SCATTERING SOURCE FUNCTION
COMMON Z(301), SG(10), FB(301,17), CS(16), G(16), SR(300,16), ST(1
1 0)
COMMON PB(301,17), W(16), K, M, KC, AH, ISTEP
INTEGER AH
IF (ST(M).EQ.0.00) RETURN
A=0.00
NN=2*AH
DO 20 J=1,NN
IF (KC.GT.AH) GO TO 10
YB=Z(K+1)
AB=(PB(K,J)-PB(K+1,J))/(Z(K)-Z(K+1))*(Y-YB)+PB(K+1,J)
A=A+ST(M)*W(J)*AB
GO TO 20
10 YB=Z(K)
AB=(PB(K+1,J)-PB(K,J))/(Z(K+1)-Z(K))*(Y-YB)+PB(K,J)
A=A+ST(M)*W(J)*AB
20 CONTINUE
SSS=A
RETURN
END
FUNCTION SFUN (Y)
C EXTERNAL SOURCE FUNCTION
COMMON Z(301), SG(10), FB(301,17), CS(16), G(16), SR(300,16), ST(1
1 0)
COMMON PB(301,17), W(16), K, M, KC, AH, ISTEP
INTEGER AH
SFUN=SR(K,KC)
RETURN
END

```

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APPENDIX A.

DIFFERENCE SCHEMES AND INVERSION OF THE ONE DIMENSIONAL TRANSPORT EQUATION

As described in the foregoing, SNEX formally inverts the discrete ordinates equations with diamond approximation in angular variable by numerically integrating the inhomogeneous term. Partitioning the spatial domain into $i = 1, 2, 3, \dots, I$, with cell boundaries at $q_{i+1/2}$

$$q_{i-1/2} \leq q_i \leq q_{i+1/2}$$

$$\Delta = q_{i+1/2} - q_{i-1/2} \tag{A-1}$$

in the i^{th} cell, the general solution can be written in the standard representation

$$\psi_{i,m}(q) = \psi_{i-1/2,m} e^{\frac{-\sigma(q-q_{i-1/2})}{\mu_m}} \left(\frac{q}{q_{i-1/2}} \right)^{-\gamma_m}$$

$$+ e^{\frac{-\sigma q}{\mu_m} q^{-\gamma_m}} \int_{q_{i-1/2}}^q dq' e^{\frac{r q'}{\mu_m} q'} \gamma_m \left[\frac{S_{i,m}}{\mu_m} + \frac{\gamma_m \psi_{i,m-1/2}}{q'} \right] \quad (\text{A-2})$$

with i denoting the cell and $i-1/2$ the cell edge (left). The form of Eq. (A-2) suggests bases for differencing schemes.

In plane geometry, $\gamma_m = 0$, and Eq. (A-1) reduces to

$$\psi_{i,m} = \psi_{i-1/2,m} e^{\frac{-\sigma(x-x_{i-1/2})}{\mu_m}} + e^{\frac{-\sigma x}{\mu_m}} \int_{x_{i-1/2}}^x dx' e^{\frac{\sigma x'}{\mu_m}} \frac{S_{i,m}}{\mu_m} \quad (\text{A-3})$$

For $S_{i,m}$ a polynomial in x' , the integrand in Eq. (A-3) can always be directly inverted. Cases for $S_{i,m}$ a constant and linear function from the basis for the recently developed and investigated characteristic method⁵ in slabs, an extremely accurate and efficient scheme.

Angular coupling ($\gamma_m \neq 0$) in curvilinear geometries modifies the basic exponential scheme in plane geometry by powers of q^{γ_m} . In cylindrical and spherical geometries, a basic difference scheme of the form,

$$\psi_{i,m}(q) = \psi_{i-1/2,m} e^{\frac{-\sigma(q-q_{i-1/2})}{\mu_m}} \left(\frac{q}{q_{i-1/2}} \right)^{-\gamma_m} + T_{i,m}(q_{i-1/2}, q) \quad (\text{A-4})$$

is advocated, where $T_{i,m}$ represents the inhomogeneous source,

$$T_{i,m}(q_{i-1/2}, q) = e^{\frac{-\sigma q}{\mu_m} q^{-\gamma_m}} \int_{q_{i-1/2}}^q dq' e^{\frac{\sigma q'}{\mu_m} q'} \gamma_m$$

$$\left[\frac{S_{i,m}}{\mu_m} + \frac{\gamma_m \psi_{i,m-1/2}}{q'} \right] \quad (A-5)$$

Some general comments about $T_{i,m}$ are obvious from Eq. (A-5). If γ_m is integer, a simple polynomial representation for $S_{i,m}$ and $\psi_{i,m-1/2}$ (in q') could permit direct integration of Eq. (A-5). At best, all integrals could be obtained. At worst, one functional integration, or table lookup of the exponential integral,

$$\int_{q_{i-1/2}}^q dq' \frac{e^{-\frac{\sigma q'}{\mu_m}}}{q'} = \left[E_1(\sigma q_{i-1/2}/\mu_m) - E_1(\sigma q/\mu_m) \right], \quad (A-6)$$

would be required. A constant or linear representation for $S_{i,m}$ and $\psi_{i,m-1/2}$, is used in slabs, might then extend slab methodology directly to cylinders and spheres (and would recover slab results for $\gamma_m = 0$). The total source term for γ_m integer and $S_{i,m}$, $\psi_{i,m-1/2}$ L^{th} order polynomials is written symbolically,

$$T_{i,m}(q_{i-1/2}, q) = e^{-\frac{\sigma q}{\mu_m}} q^{-\gamma_m} \sum_{\ell=0}^L a_{m,\ell} \int_{q_{i-1/2}}^q dq' e^{\frac{\sigma q'}{m}} q'^{\gamma_m + \ell} \quad (A-7)$$

with $a_{m,\ell}$ appropriate constants from Eq. (A-5). Unfortunately, except for the S_2 case, γ_m is not generally integer with Gaussian quadrature sets.

If one works on a very fine mesh, such that,

$$\frac{\sigma \Delta q}{\mu_m} \ll 1, \quad (A-8)$$

in the exponential term, then a Taylor series expansion could be employed to facilitate the reduction,

$$T_{i,m}(q_{i-1/2}, q) \cong q^{-\gamma_m} \int_{q_{i-1/2}}^q dq' q'^{\gamma_m} \left[1 - \frac{\sigma(q-q')}{\mu_m} + \frac{\sigma^2(q-q')^2}{2\mu_m^2} - \dots \right] \times \left[\frac{S_{i,m}}{\mu_m} + \frac{\gamma_m \psi_{i,m-1/2}}{q'} \right] \quad (\text{A-9})$$

Again, a polynomial representation for $S_{i,m}$, $\psi_{i,m-1/2}$ permits direct evaluation. As reported earlier⁵, the expansion to first order in $(q-q')$ was used near the spherical origin to check SNEX.

As both $q_{i-1/2}$, $q \rightarrow \infty$, one has $q' \rightarrow \infty$ and Eq. (A-5) approaches the expression,

$$T_{i,m}(q_{i-1/2}, q) \cong e^{-\frac{\sigma q}{\mu_m}} \int_{q_{i-1/2}}^q dq' e^{\frac{\sigma q'}{\mu_m}} \frac{S_{i,m}}{\mu_m}, \quad (\text{A-10})$$

which is the usual slab result. This result is of course required by the transport. Eq. (1) when $q \rightarrow \infty$ in cylindrical and spherical geometries.

Apart from the various situations described above, an explicit differenced source term based upon integration of $T_{i,m}$ is difficult excepting for some possibly complicated hybrid representations of the external scattering and diamond edge flux sources. However, some simpler approaches can be made.

Removing q'^{γ_m} from inside the integrand and replacing it with $q_i^{\gamma_m}$ on the outside of Eq. (A-5) yields,

$$T_{i,m}(q_{i-1/2}, q) \cong e^{-\frac{\sigma q}{\mu_m}} \left(\frac{q}{q_i} \right)^{-\gamma_m} \int_{q_{i-1/2}}^q dq' e^{\frac{\sigma q'}{\mu_m}}$$

$$\left[\frac{S_{i,m}}{\mu_m} + \frac{\gamma_m \psi_{i,m-1/2}}{q'} \right] \quad (\text{A-11})$$

which is slab-like, except for the additional term involving $\psi_{i,m-1/2}$. The factor q_i scales the integrand and might be the cell center coordinate, or some other appropriately averaged quantity. If we express $S_{i,m}$ and $\psi_{i,m-1/2}$ as linear functionals in the i^{th} cell,

$$\begin{aligned} S_{i,m} &= S_{i,m}^0 + S_{i,m}^1 q' \\ \psi_{i,m-1/2} &= \psi_{i,m-1/2}^0 + \psi_{i,m-1/2}^1 q', \end{aligned} \quad (\text{A-12})$$

with the superscripted quantities constant, and take $q = q_{i+1/2}$, we can write Eq. (A-11) in differenced form,

$$\begin{aligned} T_{i,m}(q_{i-1/2}, q_{i+1/2}) &= \left(\frac{q_{i+1/2}}{q_i} \right)^{-\gamma_m} \left\{ \frac{S_{i,m}^0}{\sigma} \left(1 - e^{\frac{-\sigma \Delta q}{\mu_m}} \right) \right. \\ &\quad \left. + \frac{S_{i,m}^1}{\sigma} \left(q_{i+1/2} - q_{i-1/2} e^{\frac{-\sigma \Delta q}{\mu_m}} \right) \right. \\ &\quad \left. - \frac{S_{i,m}^1 \mu_m}{\sigma^2} \left(1 - e^{\frac{-\sigma \Delta q}{\mu_m}} \right) \right\} \end{aligned}$$

$$\begin{aligned}
& + \psi_{i,m-1/2}^0 \gamma_m e^{\frac{-\sigma q_{i+1/2}}{\mu_m}} \left[E_1(\sigma q_{i-1/2}/\mu_m) \right. \\
& \qquad \qquad \qquad \left. - E_1(\sigma q_{i+1/2}/\mu_m) \right] \\
& + \frac{1}{\sigma} \psi_{i,m-1/2}^{\mu} \gamma_m \left(1 - e^{\frac{-\sigma \Delta q}{\mu_m}} \right) \Bigg\}, \tag{A-13}
\end{aligned}$$

for,

$$\Delta q = q_{i+1/2} - q_{i-1/2}$$

$$2q_i = q_{i+1/2} + q_{i-1/2} \tag{A-14}$$

Since, from Eq. (A-4)

$$\psi_{i,m}(q) \sim e^{\frac{-\sigma(q-q_{i-1/2})}{\mu_m} - \gamma_m q} \tag{A-15}$$

it is tempting to assume a similar exponential representation for $\psi_{i,m-1/2}$ in $T_{i,m}$, (in contrast to the linear expression of Eq. (A-12)). We take,

$$\psi_{i,m-1/2}(q') \sim \psi_{i,m-1/2}^3 e^{\frac{-\sigma q'}{\mu_m} - \gamma_m q'} \tag{A-16}$$

and $\psi_{i,m-1/2}^3$ some appropriately determined constant in the cell. Using the linear source of Eq. (A-12) and the exponential diamond edge flux of Eq. (A-16), another difference scheme is suggested. Inserting Eqs. (26), (A-14) and (30), (A-16) into Eq. (A-5) yields,

$$\begin{aligned}
T_{i,m}(q_{i-1/2}, q_{i+1/2}) &\cong \left(\frac{q_{i+1/2}}{q_i} \right)^{-\gamma_m} \left\{ \frac{S_{i,m}^0}{\sigma} \left(1 - e^{-\frac{\sigma \Delta q}{\mu_m}} \right) \right. \\
&+ \frac{S_{i,m}^1}{\sigma} \left(q_{i+1/2} - q_{i-1/2} e^{-\frac{\sigma \Delta q}{\mu_m}} \right) \\
&\left. - \frac{S_{i,m}^1 \mu_m}{\sigma^2} \left(1 - e^{-\frac{\sigma \Delta q}{\mu_m}} \right) \right\} \\
&+ \psi_{i,m-1/2}^3 \gamma_m e^{-\frac{\sigma q_{i+1/2}}{\mu_m}} q_{i+1/2}^{-\gamma_m} \ln \left(\frac{q_{i+1/2}}{q_{i-1/2}} \right) \quad (A-17)
\end{aligned}$$

which is simpler than Eq. (A-13) and exhibits the property that the term involving $\psi_{i,m-1/2}^3$ approaches zero as q gets large.

The basic differencing scheme suggested by Eq. (A-2) is exponential with modification of powers of $q^{-\gamma_m}$,

$$\psi_{i,m}(q) = \psi_{i-1/2,m} e^{-\frac{\sigma(q-q_{i-1/2})}{\mu_m}} \left(\frac{q}{q_{i-1/2}} \right)^{\gamma_m}, \quad (A-18)$$

while the diamond scheme relates cell centered and edge fluxes only,

$$2 \psi_{i,m}(q_i) = \psi_{i-1/2,m} + \psi_{i+1/2,m}, \quad (A-19)$$

and the linear discontinuous scheme assumes a Lagrangian representation,

$$\psi_{i,m}(q) = \frac{1}{\Delta q} \left[\psi_{i-1/2,m}(q_{i+1/2} - q) + \psi_{i+1/2,m}(q - q_{i-1/2}) \right] \quad (A-20)$$

Expanding Eq. (A-18) in Taylor series gives the result,

$$\psi_{i,m}(q) \sim \psi_{i-1/2,m} \left\{ 1 - \left(\frac{\sigma}{\mu_m} + \frac{\gamma_m}{q_{i-1/2}} \right) (q - q_{i-1/2}) \right. \\ \left. + \frac{1}{2} \left[\left(\frac{\sigma}{\mu_m} \right)^2 + \frac{\gamma_m(\gamma_{m+1})}{q_{i-1/2}^2} \right. \right. \\ \left. \left. + \frac{\sigma\gamma_m}{\mu_m q_{i-1/2}} \right] (q - q_{i-1/2})^2 + \dots \right\} \quad (A-21)$$

Substituting the expansion Eq. (A-21) into the diamond Eq. (A-19) yields the identity relationship thru first order. Substituting Eq. (A-21) into Lagrangian Eq. (A-20) yields the identity relationship in zeroth order for $q \neq q_i$ and first order at $q = q_i$.

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051-075	5.25	176-200	9.00	301-325	11.75	426-450	14.00	551-575	16.25
076-100	6.00	201-225	9.25	326-350	12.00	451-475	14.50	576-600	16.50
101-125	6.50	226-250	9.50	351-375	12.50	476-500	15.00	601-up	

Note: Add \$2.50 for each additional 100-page increment from 601 pages up.