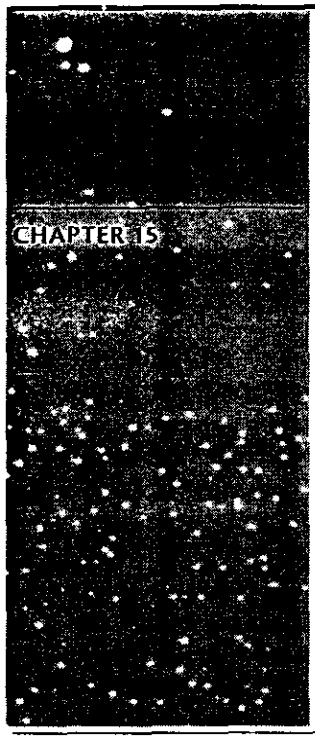


Mesh Centered Finite Differences

IT IS NOT POSSIBLE TO SOLVE EXACTLY the space-time kinetics equations at each point of space and time. Approximate methods must be resorted to. Even simple methods based on space and time separation, such as point kinetics method, requires the solution of a spatial problem. This spatial solution can only be obtained by discretisation techniques like finite differences, such as those of chapter 8, *Elementary Numerical Methods in Reactor Statics*, page 79.

It is necessary to perform such a discretisation for the space-time kinetics equations. The approach we take is to proceed with spatial discretisation first, and to keep the time derivatives out of the problem. We get the so-called semi-discrete form of the space-time kinetics equations. The study of different time integration schemes is then easier, and they

will be covered in chapter 16, *Time Integration of the Space Time Kinetics Equations*, page 187.

We choose to derive here the Mesh Centered Finite Differences, because it is a widely used method throughout the nuclear industry. However the approach we take in the derivation is based on modern nodal theory; extending the method to the analytic nodal method for example could be done quite easily with this derivation.

Geometry and Notation

The first step is a partition of the reactor core in a number of contiguous rectangular parallelepipeds in cartesian geometries, as discussed in chapter 6, *Spatial Mesh Considerations*, page 49. The nuclear properties do not vary spatially within a node, but they are allowed to vary with time.

A coordinate system origin is chosen, from which the boundaries of each region or node can be located. The mesh widths are obtained by taking the differences in the coordinates between these boundaries. This is shown on Figure 9, "Coordinate System", page 163.

The parallelepiped (i,j,k) is thus the one for which:

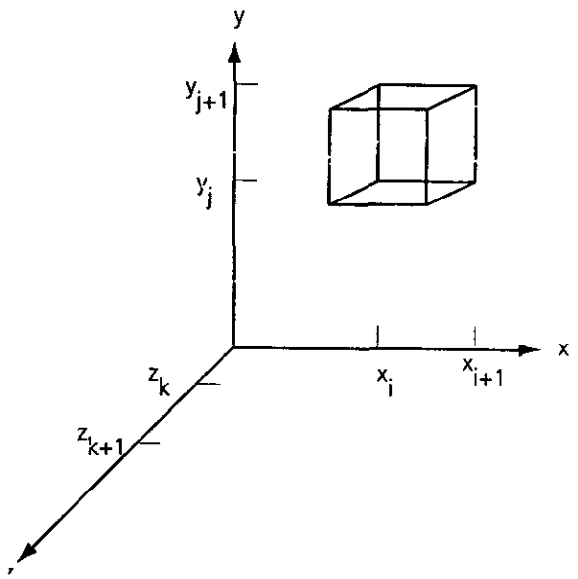
- the x coordinates go from x_i to x_{i+1}
- the y coordinates go from y_j to y_{j+1}
- the z coordinates go from z_k to z_{k+1}

The widths of the parallelepiped (i,j,k) are thus

- in x: $h_i^x \equiv x_{i+1} - x_i$
- in y: $h_j^y \equiv y_{j+1} - y_j$
- in z: $h_k^z \equiv z_{k+1} - z_k$

The volume of parallelepiped (i,j,k) is then $V_{ijk} = h_i^x \cdot h_j^y \cdot h_k^z$.

FIGURE 9. Coordinate System



Spatial Discretisation

Once the mesh has been chosen, the next step is a spatial integration of the space-time kinetics equations on each parallelepipeds, whose nuclear properties are spatially constant.

We apply the operator

$$\int_{x_i}^{x_{i+1}} dx \quad \int_{y_j}^{y_{j+1}} dy \quad \int_{z_k}^{z_{k+1}} dz$$

to the diffusion equations (20), including the delayed precursor equations. The average flux in such a region is

$$[\bar{\phi}]_{ijk} = \frac{1}{h_x^i h_y^j h_z^k} \int_{x_i}^{x_{i+1}} dx \quad \int_{y_j}^{y_{j+1}} dy \quad \int_{z_k}^{z_{k+1}} dz[\phi(x, y, z, t)]$$

and that of the average delayed neutron precursor concentration of family d

$$\bar{C}_{e,ijk} = \frac{1}{h_x^i h_y^j h_z^k} \int_{x_i}^{x_{i+1}} dx \quad \int_{y_j}^{y_{j+1}} dy \quad \int_{z_k}^{z_{k+1}} dz C_e(x, y, z, t)$$

This is like applying the theorem of Gauss to replace the space integral of the divergence of the neutron current by surface integrals. We get for the flux equations,

$$
\begin{aligned}
&[v]^{-1}_{ijk}\frac{\partial}{\partial t}[\bar{\phi}]_{ijk}V_{ijk} \\
&= -([\bar{J}(x_{i+1})]_{x,jk} - [\bar{J}(x_i)]_{x,jk})h^j_y h^k_z \\
&\quad -([\bar{J}(y_{j+1})]_{y,ik} - [\bar{J}(y_j)]_{y,ik})h^i_x h^k_z \\
&\quad -([\bar{J}(z_{k+1})]_{z,ij} - [\bar{J}(z_k)]_{z,ij})h^i_x h^j_y \qquad \text{(EQ 95)} \\
&- [\Sigma]_{ijk}[\bar{\phi}]_{ijk}V_{ijk} + (1-\beta)[\chi^p][\nu\Sigma_f]^T_{ijk}[\bar{\phi}]_{ijk}V_{ijk} \\
&\quad + \sum_{e=1}^{D}[\chi^d_e]\lambda_e\bar{C}_e V_{ijk}
\end{aligned}
$$

and for the delayed neutron precursors,

$$
\frac{\partial}{\partial t}\bar{C}_{e,ijk}V_{ijk} = \beta_e[\nu\Sigma_f]^T_{ijk}[\bar{\phi}]_{ijk}V_{ijk} - \lambda_e\bar{C}_{e,ijk}V_{ijk} \qquad \text{(EQ 96)}
$$

We used the following the definitions for the average surface currents

$$
[\bar{J}(x_i)]_{x,jk} \equiv \frac{1}{h^j_y h^k_z}\int_{y_j}^{y_{j+1}} dy \int_{z_k}^{z_{k+1}} dz[J_x(x_i, y, z, t)]
$$

$$
[\bar{J}(x_{i+1})]_{x,jk} \equiv \frac{1}{h^j_y h^k_z}\int_{y_j}^{y_{j+1}} dy \int_{z_k}^{z_{k+1}} dz[J_x(x_{i+1}, y, z, t)]
$$

$$
[\bar{J}(y_j)]_{y,ik} \equiv \frac{1}{h^i_x h^k_z}\int_{x_i}^{x_{i+1}} dx \int_{z_k}^{z_{k+1}} dz[J_y(x, y_j, z, t)]
$$

$$
[\bar{J}(y_{j+1})]_{y,ik} \equiv \frac{1}{h^i_x h^k_z}\int_{x_i}^{x_{i+1}} dx \int_{z_k}^{z_{k+1}} dz[J_y(x, y_{j+1}, z, t)]
$$

$$[\bar{J}(z_k)]_{z,ij} \equiv \frac{1}{h_x^i h_y^j}\int_{x_i}^{x_{i+1}} dx \int_{y_j}^{y_{j+1}} dy[J_z(x, y, z_k, t)]$$

$$[\bar{J}(z_{k+1})]_{z,ij} \equiv \frac{1}{h_x^i h_y^j}\int_{x_i}^{x_{i+1}} dx \int_{y_j}^{y_{j+1}} dy[J_z(x, y, z_{k+1}, t)]$$

The precursor equations (96) do not present any immediate problems, given that the average fluxes and the nuclear properties of node (i,j,k) would be known.

However, the equations for the average fluxes (95) do present a difficulty. Even though these equations represent the exact neutron balance in node (i,j,k), they bring up the average currents over the six surfaces of the node. But we do not have the relationship between these average currents and the average fluxes. The discretisation technique will generate the sought relationships, which are approximations only, and which are a characterization of the method. We could then eliminate the surface currents from (95) and get a system which would involve only the average fluxes and average delayed precursor concentrations of the nodes.

A One-Dimensional System Within a Node

In order to eliminate any confusion with regards to the interpretation of the various terms appearing in the finite difference formulation, we adopt a rather complex approach in the derivation of the coupling coefficients. It follows very closely the much more difficult derivation of many of the modern nodal methods.

The first step is to integrate the space time kinetics equations over two directions at a time. This will generate a system of equations in one dimension. The solution to this system will then provide surface currents in terms of the average fluxes of neighboring nodes. By repeating this process for each of the three directions, it will be possible to eliminate from (95) all the surface currents by average fluxes. We illustrate this approach in the x direction.

Flux Equation

Let us integrate the space-time kinetics equations over the y and z directions inside node (i,j,k). This means applying the operator

$$\frac{1}{h_y^j h_z^k}\int_{y_j}^{y_{j+1}} dy \int_{z_k}^{z_{k+1}} dz$$

to these two equations. We get for the fluxes,

$$
\begin{aligned}
[v]^{-1}\frac{1}{h_y^j h_z^k}\frac{\partial}{\partial t}\left\{\int_{y_j}^{y_{j+1}}dy \quad \int_{z_k}^{z_{k+1}}dz[\phi(x,y,z,t)] \quad \right\} \\
= -\frac{1}{h_y^j h_z^k}\int_{y_j}^{y_{j+1}}dy \quad \int_{z_k}^{z_{k+1}}dz\frac{\partial}{\partial x}[J_x(x,y,z,t)] \\
-\frac{1}{h_y^j h_z^k}\int_{y_j}^{y_{j+1}}dy \quad \int_{z_k}^{z_{k+1}}dz\frac{\partial}{\partial y}[J_y(x,y,z,t)] \\
-\frac{1}{h_y^j h_z^k}\int_{y_j}^{y_{j+1}}dy \quad \int_{z_k}^{z_{k+1}}dz\frac{\partial}{\partial z}[J_z(x,y,z,t)] \qquad \text{(EQ 97)} \\
-[\Sigma]_{ijk}\frac{1}{h_y^j h_z^k}\int_{y_j}^{y_{j+1}}dy \quad \int_{z_k}^{z_{k+1}}dz[\phi(x,y,z,t)] \\
+(1-\beta)[\chi^p][\nu\Sigma_f]_{ijk}^T\frac{1}{h_y^j h_z^k}\int_{y_j}^{y_{j+1}}dy \quad \int_{z_k}^{z_{k+1}}dz[\phi(x,y,z,t)] \\
+\sum_{e=1}^{D}[\chi_e^d]\lambda_e\frac{1}{h_y^j h_z^k}\int_{y_j}^{y_{j+1}}dy \quad \int_{z_k}^{z_{k+1}}dzC_e(x,y,z,t)
\end{aligned}
$$

and for the precursors,

$$
\begin{aligned}
\frac{1}{h_y^j h_z^k}\frac{\partial}{\partial t}\int_{y_j}^{y_{j+1}}dy \quad \int_{z_k}^{z_{k+1}}dzC_e(x,y,z,t) \\
= \beta_e\frac{1}{h_y^j h_z^k}[\nu\Sigma_f]_{ijk}^T\int_{y_j}^{y_{j+1}}dy \quad \int_{z_k}^{z_{k+1}}dz[\phi(x,y,z,t)] \qquad \text{(EQ 98)} \\
-\lambda_e\frac{1}{h_y^j h_z^k}\int_{y_j}^{y_{j+1}}dy \quad \int_{z_k}^{z_{k+1}}dzC_e(x,y,z,t)
\end{aligned}
$$

In order to simplify these expressions, we have to define the following quantities:

- the transverse integrated flux,

$$[\phi(x, t)]_{ijk} \equiv \frac{1}{h_y^j h_z^k}\int_{y_j}^{y_{j+1}} dy \int_{z_k}^{z_{k+1}} dz[\phi(x, y, z, t)]$$

- the transverse integrated precursor,

$$C_e(x, t)_{ijk} \equiv \frac{1}{h_y^j h_z^k}\int_{y_j}^{y_{j+1}} dy \quad \int_{z_k}^{z_{k+1}} dz C_e(x, y, z, t)$$

- the transverse integrated x directed current

$$[J_x(x, t)]_{ijk} \equiv \frac{1}{h_y^j h_z^k}\int_{y_j}^{y_{j+1}} dy \quad \int_{z_k}^{z_{k+1}} dz[J_x(x, y, z, t)]$$

- the transverse x directed leakage along the y direction,

$$[\mathcal{S}_y(x, t)]_{ijk} \equiv \frac{1}{h_y^j h_z^k}\int_{z_k}^{z_{k+1}} dz([J_y(x, y_{j+1}, z, t)] - [J_y(x, y_j, z, t)])$$

- the transverse x directed leakage along the z direction,

$$[\mathcal{S}_z(x, t)]_{ijk} \equiv \frac{1}{h_y^j h_z^k}\int_{y_j}^{y_{j+1}} dy([J_z(x, y, z_{k+1}, t)] - [J_y(x, y, z_k, t)])$$

- the total x directed transverse leakage

$$[\mathbb{S}_x(x, t)]_{ijk} \equiv [\mathcal{S}_y(x, t)]_{ijk} + [\mathcal{S}_z(x, t)]_{ijk}$$

Let us note that

$$[\bar{\phi}]_{ijk} = \frac{1}{h_x^i}\int_{x_i}^{x_{i+1}} dx[\phi(x, y, z, t)]$$

$$[\bar{J}(x_i)]_{x, jk} = [J_x(x, t)]_{ijk}\Big|_{x = x_i}$$

$$[\bar{J}(x_{i+1})]_{x, jk} = [J_x(x, t)]_{ijk}\Big|_{x = x_{i+1}}$$

which are three of the quantities that appear in the nodal balance equation.

With all these definitions, the transverse flux equation (97)becomes simply

$$[v]^{-1}\frac{\partial}{\partial t}[\phi(x, t)]_{ijk} = -\frac{\partial}{\partial x}[J_x(x, t)]_{ijk} - [\mathbb{S}_x(x, t)]_{ijk}$$
$$-[\Sigma]_{ijk}[\phi(x, t)]_{ijk} + (1 - \beta)[\chi^p][\nu\Sigma_f]^T_{ijk}[\phi(x, t)]_{ijk} \quad \text{(EQ 99)}$$
$$+ \sum_{e=1}^{D}[\chi_e^d]\lambda_e C_e(x, t)_{ijk}$$

while the transverse precursor equations (98) becomes

$$\frac{\partial}{\partial t}C_e(x, t)_{ijk} = \beta_e[\nu\Sigma_f]^T_{ijk}[\phi(x, t)]_{ijk} - \lambda_e C_e(x, t)_{ijk} \quad \text{(EQ 100)}$$

In order to further simplify the underlying algebra, we eliminate the time derivatives by introducing the exponential transform of the flux

$$\frac{\partial}{\partial t}[\phi(x,t)]_{ijk} = [\omega^p]_{ijk}[\phi(x,t)]_{ijk}$$

and of the precursors,

$$\frac{\partial}{\partial t}C_e(x,t)_{ijk} = [\omega_e^d]_{ijk}C_e(x,t)_{ijk}$$

This permits the transformation of the precursor equations (100),

$$C_e(x,t)_{ijk} = \frac{\beta_e[\nu\Sigma_f]^T_{ijk}[\phi(x,t)]_{ijk}}{[\omega_e^d]_{ijk} + \lambda_e}$$

and the transverse integrated flux equation (99) becomes

$$[v]^{-1}[\omega^p]_{ijk}[\phi(x,t)]_{ijk} = -\frac{\partial}{\partial x}[J_x(x,t)]_{ijk} - [\mathbb{S}_x(x,t)]_{ijk}$$
$$-[\Sigma]_{ijk}[\phi(x,t)]_{ijk} + (1-\beta)[\chi^p][\nu\Sigma_f]^T_{ijk}[\phi(x,t)]_{ijk}$$
$$+ \sum_{e=1}^{D}[\chi_e^d]\lambda_e\frac{\beta_e[\nu\Sigma_f]^T_{ijk}[\phi(x,t)]_{ijk}}{[\omega_e^d]_{ijk} + \lambda_e}$$

We now use the matrix definitions that we have introduced in chapter 5, *Matrix Form of the Equations*, page 45, to write this last equation in the much simpler form

$$\frac{\partial}{\partial x}[J_x(x,t)]_{ijk} + [\Sigma']_{ijk}[\phi(x,t)]_{ijk} = -[\mathbb{S}_x(x,t)]_{ijk} \quad \text{(EQ 101)}$$

The matrix $[\Sigma']$ is defined in the following way

$$[\Sigma']_{ijk} = [\Sigma]_{ijk} - (1-\beta)[\chi^p][\nu\Sigma_f]^T_{ijk}$$
$$- \sum_{e=1}^{D} [\chi_e^d]\lambda_e \frac{\beta_e}{[\omega_e^d]_{ijk} + \lambda_e}[\nu\Sigma_f]^T_{ijk} + \mathrm{Diag}([v]^{-1}[\omega^p]_{ijk}) \quad \text{(EQ 102)}$$

Equation for the Currents

We still have in equation (101), a mixture of fluxes and currents. We need an extra relationship between these variables. Fick's law will provide it.

Let us integrate Fick's law over the two y and z directions in node (i,j,k).

$$\frac{1}{h_y^j h_z^k}\int_{y_j}^{y_{j+1}} dy \int_{z_k}^{z_{k+1}} dz[J_x(x,y,z,t)]_{ijk} =$$
$$-\frac{1}{h_y^j h_z^k}\int_{y_j}^{y_{j+1}} dy \int_{z_k}^{z_{k+1}} dz[D]_{ijk}\frac{\partial}{\partial x}[\phi(x,y,z,t)]_{ijk}$$

which gives

$$[J_x(x,t)]_{ijk} = -[D]_{ijk}\frac{\partial}{\partial x}[\phi(x,t)]_{ijk} \quad \text{(EQ 103)}$$

in terms of the variables defined in the previous section.

Final Form of the 1-D System

We regroup here the one-dimensional equations (101) and (103) slightly re-arranged,

$$\frac{\partial}{\partial x}[\phi(x,t)]_{ijk} + [D]^{-1}_{ijk}[J_x(x,t)]_{ijk} = 0$$

$$\frac{\partial}{\partial x}[J_x(x,t)]_{ijk} + [\Sigma']_{ijk}[\phi(x,t)]_{ijk} = -[\mathbb{S}_x(x,t)]_{ijk}$$

We can put all this in a single matrix system, by defining the following vectors and matrix:

$$\left[\psi(x,t)\right]_{ijk} \equiv \begin{bmatrix} \left[\phi(x,t)\right]_{ijk} \\ \left[J_x(x,t)\right]_{ijk} \end{bmatrix} \quad \text{(EQ 104)}$$

$$\left[\mathbb{L}_x(x,t)\right]_{ijk} \equiv \begin{bmatrix} [0] \\ -\left[\mathbb{S}_x(x,t)\right]_{ijk} \end{bmatrix} \quad \text{(EQ 105)}$$

$$\left[N\right]_{ijk} = \begin{bmatrix} [0] & [D]^{-1}_{ijk} \\ [\Sigma']_{ijk} & [0] \end{bmatrix} \quad \text{(EQ 106)}$$

We can then write in a very compact form the flux and current equations,

$$\frac{\partial}{\partial x}\left[\psi(x,t)\right]_{ijk} + \left[N\right]_{ijk}\left[\psi(x,t)\right]_{ijk} = \left[\mathbb{L}_x(x,t)\right]_{ijk} \qquad \text{(EQ 107)}$$

Finite Difference Approximation

This last equation, together with identical counterparts in the y and z directions, constitute the starting point of many modern nodal methods. We limit ourselves here to the derivation of mesh centered finite differences, which are, in effect, the nodal method of lowest order.

Transverse Leakages

First, let us note that (107) is a non-homogeneous linear equation system, because of the transverse leakage term. The formally exact solution of (107) will then be made from the general solution of the homogeneous system, plus a contribution from a particular solution of the heterogeneous system.

This non-homogeneous part can the be viewed has a perturbation acting on the homogeneous solution. The first hypothesis leading to finite differences is to completely neglect this perturbation. This is the same as supposing that the transverse leakages $\left[\mathbb{L}_x(x,t)\right]$ are essentially zero. This may seem questionable, but detailed calculations provided by nodal methods show that these transverse leakages are quite small compared to the fluxes. Their effect are more important in regions where the fluxes are highly non-separable, like in corners near the fuel reflector areas for example. Furthermore, the zero transverse leakage approximation is compatible with the other hypotheses leading to the

mesh centered finite differences, particularly with the truncation of the matrix exponentials, which is the subject of the next section.

Solution of the Homogeneous System

The homogeneous version of (107) is

$$\frac{\partial}{\partial x}\left[\psi(x, t)\right]_{ijk} + \left[N\right]_{ijk}\left[\psi(x, t)\right]_{ijk} = \left[0\right]$$

and the solution of this can be written formally as

$$\left[\psi(x, t)\right]_{ijk} = \exp(-\left[N\right]_{ijk}x)\left[A\right]$$

where the $\left[A\right]$ vector is arbitrary, and depends on the initial values that we use for $\left[\psi(x, t)\right]_{ijk}$.

If we choose for initial value of $\left[\psi(x, t)\right]_{ijk}$ the value it has at $x = x_i$, we will have

$$\left[\psi(x_i, t)\right]_{ijk} = \exp(-\left[N\right]_{ijk}x_i)\left[A\right]$$

and then

$$\left[A\right] = \exp(\left[N\right]_{ijk}x_i)\left[\psi(x_i, t)\right]_{ijk}$$

so that

$$\left[\psi(x, t)\right]_{ijk} = \exp(-\left[N\right]_{ijk}(x - x_i))\left[\psi(x_i, t)\right]_{ijk} \qquad \text{(EQ 108)}$$

If, on the other hand, we choose as initial value of the flux on the other side of the node, $\left[\psi(x, t)\right]_{ijk}$ has for value at $x = x_{i+1}$, we will have

$$\left[\psi(x_{i+1}, t)\right]_{ijk} = \exp(-\left[N\right]_{ijk} x_{i+1})\left[A\right]$$

and then

$$\left[A\right] = \exp(\left[N\right]_{ijk} x_{i+1})\left[\psi(x_{i+1}, t)\right]_{ijk}$$

so that

$$\left[\psi(x, t)\right]_{ijk} = \exp(\left[N\right]_{ijk}(x_{i+1} - x))\left[\psi(x_{i+1}, t)\right]_{ijk} \quad \text{(EQ 109)}$$

Exponential Matrix Expansion

The fundamental hypothesis leading to the mesh centered finite difference approximation is that the matrix exponential found (108) and (109) can be truncated to low order terms in their expansions. In other words,

$$\left[\psi(x, t)\right]_{ijk} \approx \left\{\left[I\right] - \left[N\right]_{ijk}(x - x_i)\right\}\left[\psi(x_i, t)\right]_{ijk} \quad \text{(EQ 110)}$$

and

$$\left[\psi(x, t)\right]_{ijk} \approx \left\{\left[I\right] + \left[N\right]_{ijk}(x_{i+1} - x)\right\}\left[\psi(x_{i+1}, t)\right]_{ijk} \quad \text{(EQ 111)}$$

Note that these expansions imply a linear variation of the fluxes and the currents within each of the (i,j,k) nodes. This is a good indication that the finite differences are not a solution of the true diffusion equations. Locally, we have linear variations which do not represent the true intra-node shapes of the fluxes and the currents. We can only hope that the diffusion equations are better approximated when only the node averaged quantities are involved.

Relationship Between Average Fluxes and Currents

As we have seen previously, the problem that we have to solve is the determination of a relationship between the nodal average fluxes and the average currents over the surfaces that bound the node. The finite difference approximation gives rise to such a relationship.

To get the relationship, we integrate (110)and (111) over the x direction, and divide by the width h_x^i of node (i,j,k).

Integration with $\psi(x_i)$

We find, after integration,

$$\left[\bar{\psi}(t)\right]_{ijk} = \left\{\left[I\right] - \frac{h_x^i}{2}\left[N\right]_{ijk}\right\}\left[\psi(x_i, t)\right]_{ijk}$$

But the vector $\left[\bar{\psi}(t)\right]_{ijk}$ is made from fluxes and currents. Let us write the first portion of this vector, the flux portion. We have

$$\left[\bar{\psi}(t)\right]_{1,ijk} = \left[I\right]\left[\psi(x_i, t)\right]_{1,ijk} - \frac{h_x^i}{2}\left[N\right]_{11,ijk}\left[\psi(x_i, t)\right]_{1,ijk} - \frac{h_x^i}{2}\left[N\right]_{12,ijk}\left[\psi(x_i, t)\right]_{2,ijk}$$

Thus,

$$\left[\bar{\phi}\right]_{ijk} = \left[\phi(x_i, t)\right]_{ijk} - \frac{h_x^i}{2}\left[N\right]_{12,ijk}\left[J_x(x_i, t)\right]_{ijk}$$

but by the definition of the matrix $\left[N\right]$, equation (106),

$$\left[\bar{\phi}\right]_{ijk} = \left[\phi(x_i, t)\right]_{ijk} - \frac{h_x^i}{2}\left[D\right]_{ijk}^{-1}\left[J_x(x_i, t)\right]_{ijk} \qquad \text{(EQ 112)}$$

We see that the finite difference approximation does not involve the $\left[\Sigma'\right]$ matrix. This makes the method particularly simple, since we do not have to take into account the exponential transforms in the coupling coefficients. The mesh centered finite differences do not take into account the kinetic distortion terms.

Integration with $\psi(x_{i+1})$

We have, after integration,

$$\left[\bar{\psi}(t)\right]_{ijk} = \left\{\left[I\right] + \frac{h_x^i}{2}\left[N\right]_{ijk}\right\}\left[\psi(x_{i+1}, t)\right]_{ijk}$$

Once again, the vector is made of both fluxes and currents. Writing the first portion of the vector gives

$$\left[\bar{\psi}(t)\right]_{1,ijk} = \left[I\right]\left[\psi(x_i,t)\right]_{1,ijk} + \frac{h_x^i}{2}\left[N\right]_{11,ijk}\left[\psi(x_{i+1},t)\right]_{1,ijk} + \frac{h_x^i}{2}\left[N\right]_{12,ijk}\left[\psi(x_{i+1},t)\right]_{2,ijk}$$

Thus,

$$\left[\bar{\phi}\right]_{ijk} = \left[\phi(x_{i+1},t)\right]_{ijk} + \frac{h_x^i}{2}\left[D\right]_{ijk}^{-1}\left[J_x(x_{i+1},t)\right]_{ijk}$$

We rewrite this last expression for node (i-1,j,k), and we have

$$\left[\bar{\phi}\right]_{i-1jk} = \left[\phi(x_i,t)\right]_{ijk} + \frac{h_x^{i-1}}{2}\left[D\right]_{i-1jk}^{-1}\left[J_x(x_i,t)\right]_{i-1jk} \quad \text{(EQ 113)}$$

Relationship Between Average Fluxes and Currents

We now take the difference between (112) and (113). We find

$$\left[\bar{\phi}\right]_{ijk} - \left[\bar{\phi}\right]_{i-1jk} = \left[\phi(x_i,t)\right]_{ijk} - \left[\phi(x_j,t)\right]_{ijk} - \frac{h_x^i}{2}\left[D\right]_{ijk}^{-1}\left[J_x(x_i,t)\right]_{ijk} + \frac{h_x^{i-1}}{2}\left[D\right]_{i-1jk}^{-1}\left[J_x(x_i,t)\right]_{i-1jk}$$

By the continuity of the flux, the first two terms in this equation annihilate each other. By the current continuity, the two currents are the same. Thus, we get

$$\left[\bar{\phi}\right]_{ijk} - \left[\bar{\phi}\right]_{i-1jk} = -\left(\frac{h_x^i}{2}\left[D\right]_{ijk}^{-1} + \frac{h_x^{i-1}}{2}\left[D\right]_{i-1jk}^{-1}\right)\left[J_x(x_i,t)\right]_{ijk}$$

and finally

$$\left[J_x(x_i, t)\right]_{ijk} = \left(\frac{h_x^i}{2}\left[D\right]_{ijk}^{-1} + \frac{h_x^{i-1}}{2}\left[D\right]_{i-1jk}^{-1}\right)^{-1}\left(\left[\bar{\phi}\right]_{ijk} - \left[\bar{\phi}\right]_{i-1jk}\right)$$

which at last gives us the sought relationship between the average surface currents and the average fluxes of the two nodes surrounding the interfaces.

An identical calculation performed on node (i+1,j,k) would give the expression

$$\left[J_x(x_{i+1}, t)\right]_{ijk} = \left(\frac{h_x^{i+1}}{2}\left[D\right]_{ij+1k}^{-1} + \frac{h_x^i}{2}\left[D\right]_{ijk}^{-1}\right)^{-1}\left(\left[\bar{\phi}\right]_{i+1jk} - \left[\bar{\phi}\right]_{ijk}\right)$$

Coupling Coefficients

In the preceding section, we have found a relationship between the node average fluxes and currents in the x direction. Similar calculations could be made in the other two directions, which would give rise to the following relationships:

X Direction

$$\left[J_x(x_i, t)\right]_{ijk} = \left[\frac{h_x^i}{2}\left[D\right]_{ijk}^{-1} + \frac{h_x^{i-1}}{2}\left[D\right]_{i-1jk}^{-1}\right]^{-1}\left(\left[\bar{\phi}\right]_{ijk} - \left[\bar{\phi}\right]_{i-1jk}\right)$$

and

$$\left[J_x(x_{i+1}, t)\right]_{ijk} = \left[\frac{h_x^{i+1}}{2}\left[D\right]_{i+1jk}^{-1} + \frac{h_x^i}{2}\left[D\right]_{ijk}^{-1}\right]^{-1}\left(\left[\bar{\phi}\right]_{i+1jk} - \left[\bar{\phi}\right]_{ijk}\right)$$

Y Direction

$$\left[J_y(y_j, t)\right]_{ijk} = \left[\frac{h_y^j}{2}\left[D\right]_{ijk}^{-1} + \frac{h_y^{j-1}}{2}\left[D\right]_{ij-1k}^{-1}\right]^{-1}\left(\left[\bar{\phi}\right]_{ijk} - \left[\bar{\phi}\right]_{ij-1k}\right)$$

and

$$\left[J_y(y_{j+1}, t)\right]_{ijk} = \left[\frac{h_y^{j+1}}{2}\left[D\right]_{ij+1k}^{-1} + \frac{h_y^j}{2}\left[D\right]_{ijk}^{-1}\right]^{-1}\left(\left[\bar{\phi}\right]_{ij+1k} - \left[\bar{\phi}\right]_{ijk}\right)$$

Z Direction

$$\left[J_z(z_k, t)\right]_{ijk} = \left[\frac{h_z^k}{2}\left[D\right]_{ijk}^{-1} + \frac{h_z^{k-1}}{2}\left[D\right]_{ijk-1}^{-1}\right]^{-1}\left(\left[\bar{\phi}\right]_{ijk} - \left[\bar{\phi}\right]_{ijk-1}\right)$$

and

$$\left[J_z(z_{k+1}, t)\right]_{ijk} = \left[\frac{h_z^{k+1}}{2}\left[D\right]_{ijk+1}^{-1} + \frac{h_z^k}{2}\left[D\right]_{ijk}^{-1}\right]^{-1}\left(\left[\bar{\phi}\right]_{ijk+1} - \left[\bar{\phi}\right]_{ijk}\right)$$

Flux Equation

Finally, we substitute these expressions in the nodal balance equation (95), to get

$$
\begin{aligned}
\left[v\right]^{-1}_{ijk}\frac{\partial}{\partial t}\left[\bar{\phi}\right]_{ijk}V_{ijk} \;=\; & h^j_y h^k_z\left[\frac{h^{i+1}_x}{2}\left[D\right]^{-1}_{i+1jk}+\frac{h^i_x}{2}\left[D\right]^{-1}_{ijk}\right]^{-1}\left[\bar{\phi}\right]_{i+1jk}\\
& + h^j_y h^k_z\left[\frac{h^i_x}{2}\left[D\right]^{-1}_{ijk}+\frac{h^{i-1}_x}{2}\left[D\right]^{-1}_{i-1jk}\right]^{-1}\left[\bar{\phi}\right]_{i-1jk}\\
& + h^i_x h^k_z\left[\frac{h^{j+1}_y}{2}\left[D\right]^{-1}_{ij+1k}+\frac{h^j_y}{2}\left[D\right]^{-1}_{ijk}\right]^{-1}\left[\bar{\phi}\right]_{ij+1k}\\
& + h^i_x h^k_z\left[\frac{h^j_y}{2}\left[D\right]^{-1}_{ijk}+\frac{h^{j-1}_y}{2}\left[D\right]^{-1}_{ij-1k}\right]^{-1}\left[\bar{\phi}\right]_{ij-1k}\\
& + h^i_x h^j_y\left[\frac{h^{k+1}_z}{2}\left[D\right]^{-1}_{ijk+1}+\frac{h^k_z}{2}\left[D\right]^{-1}_{ijk}\right]^{-1}\left[\bar{\phi}\right]_{ijk+1}+\\
& \left\{\begin{array}{l}
-h^j_y h^k_z\left[\frac{h^{i+1}_x}{2}\left[D\right]^{-1}_{i+1jk}+\frac{h^i_x}{2}\left[D\right]^{-1}_{ijk}\right]^{-1}\\
-h^j_y h^k_z\left[\frac{h^i_x}{2}\left[D\right]^{-1}_{ijk}+\frac{h^{i-1}_x}{2}\left[D\right]^{-1}_{i-1jk}\right]^{-1}\\
-h^i_x h^k_z\left[\frac{h^{j+1}_y}{2}\left[D\right]^{-1}_{ij+1k}+\frac{h^j_y}{2}\left[D\right]^{-1}_{ijk}\right]^{-1}\\
-h^i_x h^k_z\left[\frac{h^j_y}{2}\left[D\right]^{-1}_{ijk}+\frac{h^{j-1}_y}{2}\left[D\right]^{-1}_{ij-1k}\right]^{-1}\\
-h^i_x h^j_y\left[\frac{h^{k+1}_z}{2}\left[D\right]^{-1}_{ijk+1}+\frac{h^k_z}{2}\left[D\right]^{-1}_{ijk}\right]^{-1}\\
-h^i_x h^j_y\left[\frac{h^k_z}{2}\left[D\right]^{-1}_{ijk}+\frac{h^{k-1}_z}{2}\left[D\right]^{-1}_{ijk-1}\right]^{-1}
\end{array}\right\}\left[\bar{\phi}\right]_{ijk}\\
& -\left[\Sigma\right]_{ijk}\left[\bar{\phi}\right]_{ijk}V_{ijk}+(1-\beta)\left[\chi^p\right]\left[\nu\Sigma_f\right]^T_{ijk}\left[\bar{\phi}\right]_{ijk}V_{ijk}+\sum_{e=1}^{D}\left[\chi^d_e\right]\lambda_e\bar{C}_eV_{ijk}
\end{aligned}
\qquad \text{(EQ 114)}
$$

Precursor Equations

The precursor equations is given by equation (96),

$$\frac{\partial}{\partial t}\bar{C}_{e,ijk}V_{ijk} = \beta_e[\nu\Sigma_f]^T_{ijk}[\bar{\phi}]_{ijk}V_{ijk} - \lambda_e\bar{C}_{e,ijk}V_{ijk} \qquad \text{(EQ 115)}$$

Boundary Conditions

When a node (i,j,k) encompasses a boundary surface, the expression for the coupling coefficient will be different from those of centrally located nodes. First, we set the coupling to quantities that are outside the domain to 0. We then have to find expressions that relate surface currents to the node average fluxes. We must go back to equations (112) and (113) and to substitute the desired relationship between the fluxes and currents, for example by using albedos. The resulting expression is the substituted in the nodal balance equation of node (i,j,k). The case of zero current is even easier to take care of, since we only have to substitute $J = 0$ on the appropriate surface, which can be done directly in the nodal balance equation.

Matrix Formulation

We can now express the system of equations for the average fluxes (114) and for the average precursor concentrations (115) in matrix form.We use the following numbering scheme: the fluxes are numbered according to the position index first, and according to group

index second. We thus have G blocks of N (=I × J × K) elements each. We also include D blocks of N precursor values. Therefore, we define a vector containing the following components:

$$[\psi] = \begin{bmatrix} [\Phi_1] \\ [\Phi_2] \\ \cdot \\ [\Phi_G] \\ [C_1] \\ [C_2] \\ \cdot \\ [C_D] \end{bmatrix}$$

The semi-discrete system of the space-time kinetics equations is then written

$$\frac{\partial}{\partial t}[\psi] = [H][\psi] \qquad \text{(EQ 116)}$$

where the inverse of the diagonal matrix containing the volumes divided by the velocities for the flux part and ones for the precursor parts has multiplied the matrix containing the coupling coeffi-

cients.The resulting matrix has the structure illustrated Figure 10, "H-Matrix Structure", page 185.

FIGURE 10. **H-Matrix Structure**