In order to solve optimization problems discussed in chapter 2, it is necessary to simulate the neutronic behaviour in a PHWR for any specified configuration and obtain important parameters such as effective multiplication factor and power distribution. The computational methods employed for this purpose are discussed in this chapter.

3.1. Introduction

The subject of reactor physics is an art of applying the suitable method for analyzing and performing the computations associated with the nuclear system. The reactor physics in a single statement can be described as the estimation of neutrons and their reaction rates with target nuclei. In reactor core calculation for all kind of reactors, we are mainly interested in determining reaction rates for individual reactions and leakage from the core. Strictly speaking, the neutron population and related quantities will have fluctuations. Usually our interest is to determine the average behavior. The average behavior of neutrons is rigorously described by the Boltzmann Transport equation. In transport theory, in the most general case, the directional flux $\Psi(r, \Omega, E, t)$ at position $r$, with energy $E$, in direction $\Omega$ at time $t$; is the unknown variable to be determined. In most practical cases, the equation has to be solved numerically. The independent variables have to be discretised. The energy variable is usually replaced by groups. The $r$ and $\Omega$ are also discretised in some way. The computational effort and memory requirements are prohibitively large for a numerical solution for 3-dimensional fine energy-group problems. The most common approach is to use transport theory for small repetitive structures (called lattices) occurring in the reactor in 2-D using fine energy group structure from which few group homogenized cross-sections for the full lattice are obtained. The full-core calculations are done in few energy groups using the homogenized cross-sections by the so-called “diffusion theory” which is an approximation to transport theory. In diffusion equation, the directional variable is absent and is much easier to solve than the transport equation.
In what follows, the time-dependent neutron transport equation is described. Thereafter, the static K-eigenvalue form is presented. Later, the simpler diffusion equation is presented. The levels at which transport and diffusion theories are used are explained.

### 3.2. Neutron Transport Equation

The transport theory was first proposed in 1800’s for kinetic theory of gases in the form of Boltzmann equation. The neutron transport equation is a simpler form in which non-linear collision term is absent. After the invention of chain-reacting nuclear reactors in 1940s, the neutron distributions were found in simple geometries using elegant approximations and analytic solutions. However, as computational power has increased, numerical approaches to neutron transport have become prevalent. The following assumptions are made in the derivation of the neutron transport equation [3]:

(i) Neutron is considered as a classical point particle. The De Broglie wave length of neutron is small compared to the inter-atomic distances between collisions. Hence, it can be adequately described by a point location and velocity.

(ii) Neutrons travel in straight line between two collisions: Neutrons have no charge, and therefore, long-range electrical and magnetic forces do not alter their straight-line trajectories.

(iii) Neutron - neutron collisions may be neglected: In nuclear reactors and radiation shields, the neutron densities are small compared with atomic densities and so neutron - neutron collisions can be neglected.

(iv) Collision may be considered instantaneous: After a collision, the emerging particles are emitted immediately for all practical purposes. The only exception is the fission reaction in which a small fraction of neutrons are being emitted by fission products. These delayed neutrons are incorporated as a separate term in the neutron transport equation.

(v) The material properties are assumed to be isotropic: This assumption is valid for reactor media.

(vi) The properties of the nuclei and the composition of materials under consideration are assumed to be known.

(vii) The expected or mean value of the particle density distribution is considered. Fluctuation about the mean is not considered.

Based on above assumptions, the neutron transport equation is derived by considering the rates at which neutrons of different energies moving in different directions enter and leave a small phase space element. The integro-differential form of the neutron transport equation can be written as:
\[
\frac{1}{v} \frac{\partial}{\partial t} \psi(r, \Omega, E, t) + \Omega \nabla \psi(r, \Omega, E, t) + \sum_s(r, E)\psi(r, \Omega, E, t) = q_f(r, \Omega, E, t) + q_d(r, \Omega, E, t) + S(r, \Omega, E, t)
\]  
(3.1)

where \(\psi(r, \Omega, E, t)\) is neutron flux at \(r\) having energy \(E\) and moving in direction \(\Omega\) at time \(t\). The fission source \(q_f(r, \Omega, E, t)\) denotes sum of prompt source \(q_p(r, \Omega, E, t)\) and delayed neutrons source \(q_d(r, \Omega, E, t)\). The rate at which prompt neutrons are produced can be expressed as

\[
q_p(r, \Omega, E, t) = \frac{1}{4\pi} \chi_p(r, E) (1 - \beta) \int dE' d\Omega' \nu \sum_f(r, E') \psi(r, \Omega', E', t)
\]  
(3.2)

The delayed neutrons arise from the decay of a variety of fission products. For neutron kinetics considerations these are usually divided into six groups, each with a characteristic decay constant \(\lambda_i\). The net yield \(\beta\) is summation over all six group-yields \(\beta_i\). If the concentration of the fission product precursors for any delayed group is \(C_i(r, t)\), then the rate at which delayed neutrons are produced can be expressed as

\[
q_d(r, \Omega, E, t) = \frac{1}{4\pi} \sum_i \chi_d^i(r, E) \lambda_i C_i(r, t)
\]  
(3.3)

The source of neutrons due to scattering with other nuclei can be expressed as

\[
q_s(r, \Omega, E, t) = \int dE' \int d\Omega' \sum_s(r, E' \rightarrow E, \Omega' \rightarrow \Omega) \psi(r, \Omega', E', t)
\]  
(3.4)

An additional equation is also required for each group precursor concentration for solving the neutron transport equation. The net rate of change in the precursor concentration is

\[
\frac{\partial}{\partial t} C_i(r, t) = \beta_i \int dE \nu \sum_f(r, E) \psi(r, E, t) - \lambda_i C_i(r, t)
\]  
(3.5)

The notations used to describe neutron transport equation are the following:

\(\psi(r, \Omega, E, t)\) : Neutron flux at location \((r)\) with energy \((E)\) along direction \((\Omega)\) at time \((t)\)

\(\Sigma_s(r, E)\) : Total macroscopic cross section at location \((r)\) for a neutron of energy \((E)\)

\(S(r, \Omega, E, t)\) : All neutron sources other than scattering and fission, i.e. external source

\(\Sigma(r, E' \rightarrow E, \Omega' \rightarrow \Omega)\) : Macroscopic differential scattering cross section, describing the transfer of neutrons with initial coordinates \((r, E', \Omega')\) to \((r, E, \Omega)\)
\[ \nu \sum_f(r, E) : \text{Fission production macroscopic cross section at location } (r) \text{ for neutron of energy } E \]

We are mainly concerned with steady state K-eigenvalue problem that can be written as

\[ \nabla \psi(r, \Omega, E) + \sum_i(r, E)\psi(r, \Omega, E) - q_s(r, \Omega, E) = \frac{1}{K} q'_{f}(r, \Omega, E) \]  

(3.6)

where

\[ q'_{f}(r, \Omega, E) = \frac{1}{4\pi} \chi_p(r, E) \int \int dE' d\Omega' \nu \sum_f(r, E')\psi(r, \Omega', E') \]  

(3.7)

Neutron balance is enforced by dividing fission source by K. There is no distinction between prompt and delayed neutron source.

The cross sections are the quantities which define the neutron interaction probabilities. The cross sections of each material are highly dependent on the energy of the incident neutron. At reasonably low energies of incident neutrons, cross sections are quite smooth in energy. However, as the energy increases, the cross sections are dominated by resonance peaks that result from unstable state of compound nucleus formed by the collision. In the off-resonance region, the variation in cross section shows $1/E^{1/2}$ or $1/v$ dependence. The deterministic neutron transport codes usually use appropriately generated multi-group cross section libraries.

The neutron transport equation is usually solved for finite region or space, in which cross-sections are known. There exist an infinite number of possible solutions of the neutron transport equation within any spatial region and hence, appropriate neutron angular density at the boundary of the region is needed to determine which of the solution corresponds to that physical problem. At the external boundary of a reactor, there are no incoming neutrons and free surface boundary conditions are used:

\[ \psi(r, \Omega, E) = 0 \quad \text{if} \quad n.\Omega < 0 \]  

(3.8)

where n is unit vector normal to external surface. If transport theory is used to simulate the repetitive lattice structure, reflective or white boundary condition is used.

### 3.3. Neutron Diffusion Equation

Because of its relative simplicity and range of applicability, the diffusion approximation to the Boltzmann neutron transport equation is widely used for reactor core simulation. Diffusion theory is sufficiently accurate to provide a quantitative understanding of many physics features of nuclear reactors and is, in fact, the workhorse computational method of nuclear reactor physics. The problem for which
very high accuracy is not required, or the calculation on large systems, in which the important regions are several neutron mean free paths in thickness, diffusion theory is used.

The angular flux and scattering function is expanded in terms of spherical harmonics. The term up to linearly anisotropic scattering are retained leading to the $P_1$ approximation. The $P_1$ approximation to the one-speed transport theory is equivalent to ordinary diffusion theory in a source free medium regardless of whether the scattering is isotropic or anisotropic. In multi-group theory, however, scattering from higher groups constitutes an anisotropic source and then diffusion theory and $P_1$ approximation are not equivalent.

The essential postulate of diffusion equation is Fick’s law, which assumes that the neutron current $J(r,E)$ is given by a diffusion coefficient $D(r,E)$ multiplied by the gradient of the flux; thus,

$$J(r,E) = -D(r,E) \frac{\partial \phi(r,E)}{\partial r} \quad (3.9)$$

The leakage term is $\nabla \cdot J(r,E)$ or $-\nabla D(r,E) \nabla \phi(r,E)$.

Three major approximations which lead to neutron diffusion equation are as follows [4]:

1. The first major approximation leading to diffusion theory is made that the flux is assumed to be sufficiently slowly varying in space.
2. The second major approximation that integral of in-scattering of neutrons from all energies to energy $E$ is equal to the integral of out-scattering of neutrons from energy $E$ to all other energies.
   When there is a weak absorber ($\Sigma_a \ll \Sigma_s$), these two quantities balance each other.
3. The third assumption that the neutrons are scattered isotropically.

The diffusion theory will not be valid near and inside an absorber like shut-off rod. It is also not accurate near external boundary of the reactor. However, usually the reactor is large-sized with a thick reflector. The flux is small at the periphery and it is a good approximation zero neutron flux as a boundary condition on the external surface.

The mathematical formulation of neutron diffusion theory is obtained by using the Fick’s law:

$$-\nabla D \nabla \phi(r,E) + \sum_s (r,E) \phi(r,E) = \int dE \sum_s (r,E \rightarrow E) \phi(r,E') + \frac{\chi(E)}{K} \int dE' \nu \sum_s (r,E') \phi(r,E') \quad (3.10)$$

The angular fluxes are collapsed as $\phi(r,E) = \int \psi(r,E,\Omega)d\Omega$
The (time-independent) multigroup neutron diffusion equations in K-eigenvalue form are a system of coupled elliptic partial differential equations of second order and can be written as follows:

\[-\nabla D_g (r) \nabla \phi_g (r) + \sum_{g \neq g}^r (r) \phi_g (r) - \sum_g \sum_{g \neq g} \phi_g (r) = \frac{1}{K} \sum_g \nu \sum_{g} (r) \phi_g (r) \quad g = 1, 2, 3, \ldots \tag{3.11}\]

The following group-dependent boundary conditions is used

\[D_g (r) \frac{\partial \phi_g (r)}{\partial n} + \alpha_g (r) \phi_g (r) = 0 \quad \text{where} \quad r \in \Gamma \tag{3.12}\]

Here \(g\) represents the energy group of the neutron and \(n\) is the normal outwardly directed to the boundary surface \(\Gamma\). The notations \(D_g (r), \Sigma_{g} (r), \nu \Sigma_{g} (r)\) represent diffusion coefficient, removal cross section and \(\nu\) times fission cross sections at location \(r\) respectively.

**3.2.1. Discretization of neutron diffusion equation**

The neutron diffusion equation is solved for practical problems using standard numerical analysis techniques such as finite-difference method. The continuous diffusion equation problem is converted to discrete representations by using meshes. The mesh centered finite difference approximation is used to convert the analytical diffusion equation to a system of linear coupled algebraic equations.

The two energy group analytical neutron diffusion equation can be written as

\[-\nabla D_1 (r) \nabla \phi_1 (r) + \sum_1^r (r) \phi_1 (r) = \frac{1}{K} [\nu \sum_1^r (r) \phi_1 (r) + \nu \sum_2^r (r) \phi_2 (r)] \tag{3.13}\]

\[-\nabla D_2 (r) \nabla \phi_2 (r) + \sum_2^r (r) \phi_2 (r) - \sum_2^{-1} (r) \phi_1 (r) = 0 \tag{3.14}\]

In the above equation the up scattering cross-section \(\Sigma_{2-1} (r)\) is assumed to be zero. In 3-D Cartesian geometry the mesh will be chosen such that the different lattice interfaces coincide with mesh surfaces while the mesh points are at centre of mesh volumes. It is called mesh centered finite difference scheme [5].

The integration is carried out over the mesh volume \(\Delta V_k\). The volume integration to the first term (leakage term) of diffusion equation transforms it into a surface integral owing to the divergence theorem.

\[\int -\nabla \cdot (D \nabla \phi) dV = \int -\nabla \cdot (D \nabla \phi) \cdot n dS = \int -D \frac{\partial \phi}{\partial n} dS = \sum_{j=1}^6 \int_{k_j} \Delta S_{kj} \]
Here, $J_{kj}$ are net currents from mesh volume $k$ to mesh volume $j$, averaged over their common surfaces $\Delta S_{kj}$. Replacing the volume averaged quantities by midpoint value of diffusion equation terms give

$$\sum_j J_{kj} \Delta S_{kj} + \sum_k \phi_k \Delta V_k = Q \Delta V_k$$  \hspace{1cm} (3.16)$$

Where, $Q$ represents the fission and scattering neutron source. If $\phi_{kj}$ is the redundant flux on the surface $\Delta S_{kj}$ and $J_{kj}$ the net current from $k$ to $j$, the new quantities can be defined using diffusion coefficient using mesh size i.e. $\Delta_x, \Delta_y, \Delta_z$ as:

$$d_x = \frac{D}{\Delta_x}; \quad \phi_{kj} = \frac{d_k \phi_k + d_j \phi_j}{d_k + d_j}; \quad d_{kj} = \frac{2d_k d_j}{d_k + d_j}; \quad J_{kj} = d_{kj}(\phi_k - \phi_j)$$ \hspace{1cm} (3.17)$$

The seven point discrete diffusion equation becomes

$$\sum_j \Delta S_{kj} d_{kj}(\phi_k - \phi_j) + \sum_k \phi_k \Delta V_k = Q \Delta V_k$$  \hspace{1cm} (3.18)$$

### 3.2.2. Solving neutron algebraic equation

The two energy group linear coupled algebraic neutron diffusion equation can be written as

$$\sum_j \Delta S_{kj} d_{kj}(\phi_{1,j} - \phi_{1,j}) + \sum_{1,k} \phi_{1,k} \Delta V_k = \frac{1}{K} \{v \sum_{1,k} \phi_{1,k} + v \sum_{2,k} \phi_{2,k}\} \Delta V_k$$ \hspace{1cm} (3.19)$$

$$\sum_j \Delta S_{kj} d_{kj}(\phi_{2,j} - \phi_{2,j}) + \sum_{2,k} \phi_{2,k} \Delta V_k - \sum_{1 \rightarrow 2,k} \phi_{1,k} \Delta V_k = 0$$ \hspace{1cm} (3.20)$$

For 3-D Cartesian geometry flux in each mesh point is directly related only to the flux in its six neighbors. If diffusion equation is solved for a system having $I_m \times J_m \times K_m$ meshes in $x$, $y$ and $z$ direction respectively, then the two energy group coupled algebraic neutron diffusion equation can be represented in matrix form as

$$M \phi = \frac{1}{K} F \phi$$ \hspace{1cm} (3.21)$$

The matrix $M$ represents capture, leakage and group-to-group transfers. The matrix $F$ is fission source operator. Both $M$ and $F$ are square matrices of dimension $\{2 \times I_m \times J_m \times K_m\}$ and $\phi$ is a vector with dimension $\{2 \times I_m \times J_m \times K_m\}$. Here, $K$ stands for eigenvalue. The above equation has a large number of eigenvalues $K_i$ and corresponding eigenfunctions $\phi_i$. All $K$ eigenvalues are real positive and they can be arranged as $K_1 > K_2 \geq K_3 ..$ etc. The largest value $K_1$ is the fundamental eigenvalue usually denoted by $K_{eff}$. 
The corresponding mode is the fundamental mode. One is usually interested in finding the fundamental mode. The most common method to obtain the fundamental mode is the power iteration method and it is implemented via the so-called inner and outer iterations as described below. Equation (3.21) can be written as,

\[ M^{-1}F \phi = K \phi \] (3.22)

Thus the problem is to find largest eigenvalue and corresponding eigenvector of \( M^{-1}F \). The basic idea in Power Iteration method is that if an arbitrary guess vector is repeatedly multiplied by \( M^{-1} F \) (and normalised), it will approach the fundamental eigenvector. In practice, the multiplication by \( M^{-1}F \) is implemented (without explicitly finding \( M^{-1}F \)) by carrying out certain inner and outer iterations [6]. One starts with a guess value for \( K \) and the fission source vector \( F \phi \) which are denoted by \( k^1 \) and \( F \phi^1 \). The superscript 1 indicates the outer iteration number. The successive outer iterations can be shown as:

\[ M \phi^{i+1} = \frac{1}{k^i} F \phi^i \] (3.23)

\[ K^{i+1} = K^i \frac{||F \phi^{i+1}||}{||F \phi^i||} \] (3.24)

The main task is to solve Eq.(3.23) to evaluate \( \phi^{i+1} \) (which equals \( M^{-1}F \phi^i / K^i \)). Usually, this is done by solving the problem group wise. Starting from the 1st energy group, an external fixed source problem is solved for each group. The fixed source consists of two types of contributions: one from fission source on R.H.S. of Eq.(3.23) and second from scattering of neutrons in other groups which is contained in matrix \( M \). Such an equation for group \( g \) can be written as:

\[ \nabla \cdot D_g \nabla \phi_g - \Sigma^R_g \phi_g = Q_g \] (3.25)

where \( Q_g \) is the external source. If \( n=2 \times 1m \times 1m \times K \), the CPU time required for a non-iterative method (i.e. direct methods) to solve Eq. (3.25) and find group fluxes scales in general as \( n^3 \). The direct methods like Gauss Elimination suffer from what is called fill-in (many zero elements becoming non-zeros). Hence, for large size system, iterative methods (like Gauss-Seidel iteration) offer better performance. For Gauss-Seidel iteration it is explained as follows:

Eq.(3.25) can be written in matrix form as:

\[ A \phi_g = Q_g \] (3.26)
A is a symmetric diagonally dominant matrix of order $Im \times Jm \times Km$. A is split into a diagonal, strictly lower triangular and strictly upper triangular parts giving:

$$(D - L - U) \phi_g = Q_g$$  \hspace{1cm} (3.27)

The Gauss-Seidel (or inner) iterations can be shown as:

$$(D - L) \phi^{i+1}_g = U\phi^i_g + Q_g$$  \hspace{1cm} (3.28)

where $j$ is iteration number. The convergence criterion for inner iterations is (for all energy groups separately):

$$\frac{|\phi^{i+1}_g - \phi^i_g|}{\phi^i_g} < \varepsilon 1$$  \hspace{1cm} (3.29)

It is possible to have over-relaxation in above iterations.

Eq.(3.28) is solved by using Gauss-Seidel iterations for all the groups. The convergence of the Jacobi method depends upon the spectral radius of $D^{-1}(L + U)$. The Gauss-Seidel method is an improvement over Jacobi method, where inverse of $(D - L)$ is considered. In case of upscattering, one may have to repeat these within-group calculations till group-to-group scattering sources converge. These calculations give the flux vector $\phi^{i+1}_g$ containing all group fluxes, which is solution of Eq.(3.21).

Using the computed $\phi^{i+1}_g$, the fission source vector $F\phi^{i+1}_g$ is computed and $K^{i+1}$ is evaluated by using Eq.(3.22). The outer iterations are continued till successive values of $K$ and fission source vector are close within a convergence criterion. Most of the well-established reactor physics codes are based on this method. The computer code ‘DOLP’ has been developed based on this approach. The power iteration method converges slowly if the dominance ration $K_2/K_1$ is close to unity.

The convergence criteria for multiplication factor $K$ can be written as:

$$\frac{|K^{i+1} - K^i|}{K^i} < \varepsilon 2$$  \hspace{1cm} (3.30)

In similar way the convergence criteria for fission source can also be written. Acceleration of the power iteration method and use of alternative efficient schemes has been an active field of research for a long time. One of the most popular acceleration schemes has been the Chebyshev acceleration scheme [7]. There exists another quite efficient approach based on Orthomin(1) algorithm [8] to solve the eigenvalue problem $M\phi = \lambda F\phi$. The residual vector $r = M\phi - \lambda F\phi$ is determined. The function $f(\phi) = (r, r)$ is minimized in Orthomin(1) algorithm. The algorithm used for chebyshev acceleration
and Orthomin(1) are shown in Fig.3.1 and Fig.3.2 respectively. A comparison of CPU time is made between power iteration, Chebyshev method and Orthomin(1) algorithm for a typical case. It is presented in Fig.3.3.

**Chebyshev Extrapolation**

In the two parameter Chebyshev method, the first $n^* (=3)$ iterations are carried out as simple power iterations. Subsequently parameters $\alpha$ and $\beta$ are computed and used to extrapolate the fission source vector as shown below.

Each outer-iteration fission source vector is extrapolated as

$$S^{(n^*+p)} = S^{(n^*+p-1)} + \alpha_p \left[ S^{(n^*+p)} - S^{(n^*+p-1)} \right] + \beta_p \left[ S^{(n^*+p-1)} - S^{(n^*+p-2)} \right]$$

Where, $S$ denotes the extrapolated vector. And $S$ denotes un-extrapolated vectors. The superscript of $S$ is outer iteration number. The parameters $\alpha$ and $\beta$ are given as

$$\alpha_p = \frac{1}{2 - d} - \frac{d^2 \alpha_{p-1}}{16}$$

$$\beta_p = \frac{(2 - d) \alpha_p}{2} - 1$$

$$\alpha_i = \frac{2}{2-d}; \quad \beta_i = 0.0; \quad d \text{ is dominance ratio and is estimated using latest source vectors.}$$

Figure 3.1: Chebyshev acceleration method

**Orthomin(1) algorithm to solve $Ax = \lambda Bx$**

1. Choose $x_0$
2. $\lambda_0 = \frac{(A_{x_0}, B_{x_0})}{(B_{x_0}, B_{x_0})}$
3. $r_0 = \lambda_0 B_{x_0} - Ax_0$
4. $s_0 = r_0$
5. For $i=0,1,2,\ldots$ until convergence, Do:
6. $\alpha_i = \frac{\{(r_i, A_{s_i}) - \tilde{\lambda}_i (r_i, B_{s_i})\}}{\{(A_{s_i}, A_{s_i}) - 2 \tilde{\lambda}_i (A_{s_i}, B_{s_i}) + \tilde{\lambda}_i^2 (B_{s_i}, B_{s_i})\}}$
7. $x_{i+1} = x_i + \alpha_i s_i$
8. $\tilde{\lambda}_{i+1} = \frac{(A_{x_{i+1}}, B_{x_{i+1}})}{(B_{x_{i+1}}, B_{x_{i+1}})}$
9. $r_{i+1} = \tilde{\lambda}_{i+1} B_{x_{i+1}} - A_{x_{i+1}}$
10. $\beta_i = \frac{-[\{(A_{x_i}, A_{s_i}) - \tilde{\lambda}_i (A_{x_i}, B_{s_i}) + (A_{s_i}, B_{x_i})\} + \tilde{\lambda}_i (B_{x_i}, B_{s_i})]}{\{(A_{s_i}, A_{s_i}) - 2 \tilde{\lambda}_i (A_{s_i}, B_{s_i}) + \tilde{\lambda}_i^2 (B_{s_i}, B_{s_i})\}}$
11. $s_{i+1} = r_{i+1} + \beta_i s_i$
12. End Do

Figure 3.2: Orthomin(1) algorithm
The comparison of CPU time among power iteration, Chebyshev acceleration method and Orthomin(1) algorithm indicated that Orthomin(1) algorithm is an efficient method to solve the K-eigenvalue problem.

### 3.3. Reactor Core Simulation

The relative geometric arrangement of fuel bundles, pressure tubes, coolant materials, calandria tubes, moderating material follows regular patterns inside the core. These patterns are referred to as lattices. At lattice level, the local flux varies strongly and resonance effect, interaction at boundaries of different materials etc are important. The Evaluated Nuclear Data File (ENDF/B-VI.8) collapsed in multi-group is used as the main source of nuclear cross sections of different materials. The lattice cell calculation is carried out to condense the vast amount of basic nuclear data relating to its constituent materials into a relatively small number of parameters that can be used subsequently during the full core simulation. Therefore, to cope with the complexity of the problem, full core simulation is broken down into smaller problems that are treated separately as lattice cell simulation and full core simulation. The lattice cell may be regarded as the smallest part of the reactor that has the properties of a self-sustaining chain reacting assembly. It is assumed that the complete reactor core is comprised of numerous unit
lattice cells. An important feature in reactor core analysis which is taken care in lattice calculation is that the cross-sections for typical heavy nuclides exhibit resonances. The flux drops substantially in the resonance energy range. Self shielding calculation is done to recover effective microscopic cross sections for a resonant reaction.

Two energy group homogeneous cross-sections are generated for a lattice by solving neutron transport equation. The computer code CLUB [9] is used for this purpose. The lattice geometrical details and ENDF/B-VI.8 cross section library serves as input and two energy group homogeneous lattice cross-sections are derived as output.

There are various reactivity devices in the core, which are located in between fuel channels. The presence of these devices, alter the 2 groups cross-section of the lattice cell. Thus a super cell calculation is required for the lattices, which are affected by the reactivity devices. This calculation is performed, by using the transport theory code BOXER [10]. This code gives the homogenized 2 group incremental cross-sections of the lattice cell affected by the particular reactivity device.

These two energy group homogeneous lattice cross sections are used in solving the neutron diffusion equation over full reactor core. Diffusion theory is a simple and less expensive scheme for modeling neutron transport. A computer code has been developed for this purpose. The differential equation has been discretised by finite-difference methods. Orthomin(1) algorithm is available for fast convergence. A flow chart diagram for reactor core simulation is presented in Fig.3.4.
Figure 3.4: Flow chart diagram for reactor core simulation