Theoretical developments and studies in the reactor physics of accelerator driven systems

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I, hereby declare that the investigation presented in the thesis has been carried out by me. Whenever contributions of others are involved, every efforts is made to indicate this clearly with due reference to the literature and acknowledge of collaborative research and discussions. The work is original and has not been submitted earlier as a whole or in part for a degree / diploma at this or any other Institution / University.

K.P.Singh

DECLARATION

I, hereby declare that the corrections suggested by the examiners have been incorporated in the thesis.

Dr. S.B. Degweker

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Dedicated to my father

for his love, endless support and encouragement

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CONTENTS

SYNOPSIS

There is increasing worldwide concern on account of the growing stockpile of high level radioactive waste produced in nuclear reactors which constitutes a potential threat to future generations due to its long lived radio toxicity. Accelerator driven sub-critical systems (ADSs) [Nifenecker, et al., 2001] have caught the attention of scientific community worldwide in recent years as a possible solution to the problem of nuclear waste. It is believed that ADSs can transmute radioactive waste faster and safer than conventional nuclear reactors and also produce useful energy. Indian interest in ADSs is primarily related to their application to large scale utilization of thorium.

Due to their sub-critical mode of operation, ADSs must be fed continuously with neutrons from an external source. In most proposed ADSs (Rubia, C., 1995; Abderahim A.H., 2005) the source neutrons are produced by the spallation process, wherein a high energy (typically about 1 GeV) proton beam interacts with a heavy target. Though the idea of using high power proton accelerators (~1 GeV, 300 mA) to drive a sub-critical blanket for breeding fissile material or for waste transmutation is quite old (Bowman et al., 1992; Venneri et al., 1993), there has been a renewed interest in ADSs after the proposal of C. Rubbia (1995) based on accelerators with relatively modest power (~ 1 GeV, 10 mA).

This has led to the setting up of R&D programs for ADS development in several countries (Abderrahim, 2001; Kapoor, 2001; Mukaiyama et al., 2001; Gohar Y. and Smith D.L., 2010) including India. Development of high power accelerators, and suitable targets and coupling these with the sub-critical reactor are the main focus areas of these efforts. On the reactor front, the R&D effort is mainly geared towards development of accurate simulation tools, nuclear data and

experiments oriented towards understanding the physics of accelerator driven sub-critical reactors (which is quite different from that of critical reactors) and methods for determining the degree of sub-criticality.

Several experiments devoted to reactivity monitoring of ADS have been carried out around the world. The major important subcritical experiments have been done at YALINA (Carl-Magnus Persson et al., 2005) and MUSE (Soule et al., 2004). In MUSE, a large number of reactivity measurement methods applicable in zero or low power systems, such as the Feynman-alpha and the Rossi-alpha methods, and pulsed neutron source methods were investigated. Different techniques showed that the interpretation of the kinetic behavior of subcritical systems with the aim of reactivity determination requires at least to some extent the inputs from theoretical calculations.

In India, the main R&D activities are related to development of accelerator technologies leading to construction of a high energy high current accelerator. A major effort is also directed towards target and window technologies. The Reactor related R&D effort includes basic research activities in the area of the sub-critical reactor physics, development of new computer codes and nuclear data for analysis of ADSs, conceptual design studies of ADSs for thorium utilization and experimental program for understanding the physics of ADSs and for developing methods for measuring and monitoring the sub-criticality of ADS.

A considerable amount of theoretical work (Pazsit and Yamane, 1998; Pazsit et al., 2005; Degweker, 2000, 2003) has been carried out for understanding reactor noise in ADSs and its application to measurement of the degree of sub-criticality. Many physics experiments are

proposed (Rasheed et al., 2010) in PURNIMA sub-critical facility and one of the aims of the proposed experiments would be to verify the theory and interpret the results in terms of the theory. The system planned is a natural U sub-critical assembly moderated by water or high density polyethylene and driven by a D-D or D-T neutron generator. The maximum K_{eff} of the assemblies is expected to be about 0.9.

In the present thesis we discuss theoretical work aimed at developing computer codes for analysis of sub-critical systems including design and interpretation of experiments described above. Placement of detectors at suitable locations to minimize modal effects in pulse neutron and noise experiments is very important (Rugama et al., 2002). For getting the idea of suitable locations, we have developed new methods to evaluate time eigenvalues of neutron diffusion equation and zeros of alpha modes are possible locations of detectors. We have also developed space time kinetics computer code for the analysis of neutron flux evolution in pulse neutron experiments and also for the analysis of any reactivity initiated transient in ADS. A transport theory based analogue Monte Carlo method has also been developed (Singh and Degweker, to be submitted for publication) for simulating the noise experiments planned at BARC.

The thesis is organized in seven chapters as elaborated below.

Chapter 1 is a brief introduction to the ADS concept. The concept of ADS and its evolution over the years is discussed. A survey of the theoretical and experimental studies on such systems is presented.

In chapter 2, we begin our discussion with a brief discussion of numerical methods in reactor physics such as the Monte Carlo method, and those based on solving the linear Boltzmann

transport equation which is the governing equation for neutron transport and its multiplication in a reactor and to obtain the neutron distribution in energy, angle and space variables. We also discuss an approximate form of the transport equation viz., the diffusion equation which is the equation we are concerned with in this thesis. The power distribution in a nuclear reactor core is usually obtained by solving λ-eigenvalue problem for the multi-group neutron diffusion equations for critical systems and a source problem for sub-critical systems (ADSs). While in general the highest λ-eigenvalue (which is the K_{eff} of the system) and the corresponding eigenfunction are enough for estimation of core reactivity and power distribution, there are situations in which other eigenvalues and eigenfunctions are also required. There are yet other situations which require solution of another type of eigenvalue problem commonly referred to as the alpha-eigenvalue problem.

We present a literature survey of the research on methods for solving the diffusion equation using the finite difference method, to obtain fundamental and higher eigenvalues and eigenfunctions corresponding to both types of eigenvalue problems mentioned above. We also present a survey of various Monte Carlo approaches available in literature for simulating pulsed neutron and noise methods for experimental determination of the degree of sub-criticality of accelerator driven subcritical reactors.

In chapter 3, we focus on the determination of the alpha modes (time-eigenvalues) using our experience with the calculation of the 3-D λ-modes (Verdu et al., 1994). In alpha eigenvalue problem (Bell and Glasstone, 1970; Lathouwers, 2003), the eigenvalue α appears in the form of a (positive or negative) 1/v absorber. The α-modes are important in developing modal neutron kinetics where these modes form the expansion bases for neutron flux under perturbation. They

are also important in the context of monitoring reactivity of ADS and also for identification of suitable detector locations in pulse neutron experiments. Here we present some numerical schemes developed by us for the evaluation of alpha modes of diffusion equation.

Two new methods (Singh and Degweker, 2009) of obtaining dominant prompt alpha modes (sometimes referred to as time eigenfunctions) of the multigroup neutron diffusion equation are discussed. In the first of these, we initially compute the dominant K-eigenfunctions and K-eigenvalues (denoted by λ_1, λ_2, λ_3 …etc; λ_1 being equal to the K_{eff}) for the given nuclear reactor model, by method based on sub space iteration (SSI) technique (Modak and Jain, 1996; Modak and Gupta, 2007; Doring et al., 1993), which is an improved version of power iteration method. Subsequently, a uniformly distributed (positive or negative) 1/v absorber of sufficient concentration is added so as to make a particular eigenvalue λ_i equal to unity. This gives i^{th} alpha mode. This procedure is repeated to find all the required alpha-modes. In the second method, we solve the alpha-eigenvalue problem directly by SSI method. This is clearly possible for a sub-critical reactor for which the dominant alpha-eigenvalues are also the largest in magnitude as required by the SSI method. Here, the procedure is made applicable even to a super-critical reactor by making the reactor model sub-critical by the addition of a 1/v absorber. Results of these calculations for a 3-D two group PHWR test-case are given. These results are validated against the results as obtained by a different approach based on Orthomin algorithm (Modak & Gupta, 2006). The direct method based on the sub-space iteration strategy is found to be a simple and reliable for obtaining any number of alpha modes. Also comments have been made on the relationship between fundamental α and k-eigenvalues.

In the eigenvalue problems discussed in chapter 3, we have assumed that all neutrons are prompt. In chapter 4, we focus on neutron diffusion equation with prompt and delayed neutrons. For complete description of a pulsed neutron experiment, delayed neutrons should be taken into account (Singh and Degweker, 2011) in defining the eigenvalue problem. Substituting an exponential time dependence of the flux (as in the case of the alpha modes) results in the "delayed-alpha" eigenvalue problem, (also referred to as natural modes). Corresponding to each alpha-mode there is one prompt mode and six delayed modes. An expansion in these modes is more appropriate for describing transients in which delayed neutron effects are to be included. In this chapter, we extend the numerical schemes of our previous chapter for the evaluation of alpha- modes of diffusion equation including delayed neutrons. There have been a few studies for obtaining (Hoogenboom, 2002) alpha-modes with the inclusion of delayed neutrons. These evaluations have been limited to only fundamental modes. In this chapter we have the proposed method to evaluate higher alpha modes.

It has been known for quite some time that space –dependent calculations of reactor transients are required in certain situations in order to accurately predict the power behavior and the spatial distribution of neutron flux. This is more so in the case of sub-critical reactors where the flux distribution departs rather strongly from the fundamental mode flux distribution.

In chapter 5, we describe the development of a three dimensional space time kinetics code [KINFIN] which solves the few group time dependent diffusion equation with delayed neutrons. The spatial discretisation is done using the finite difference method in which the space can be divided into rectangular meshes. A centre mesh finite differencing method is used for the spatial derivatives. The time integration is carried out using the backward Euler scheme. Thermal

hydraulic feedback effects can be taken into account (Singh et al., to be submitted for publication). For sub-critical systems, kinetics problems in the presence of a source can be solved. Validation of KINFIN by comparison of the results with existing 3-Dimensional PHWR and LWR benchmarks (Judd and Roubin, 1981) also form a part of this chapter.

Finally we describe the modification of KINFIN to calculate the time dependent adjoint functions in the presence of an external source [which in the adjoint calculation is a detector cross section]. Modified code can calculate the backward functions $G_{z_1}(\mathbf{r},\mathbf{\Omega},E,t;1,1)$, $G_{z_2}(\mathbf{r},\mathbf{\Omega},E,t;1,1)$ or $G_z(\mathbf{r},\mathbf{\Omega},E,t;1)$ and the forward function $\varphi(\mathbf{r},\mathbf{\Omega},E,t)$ which are required to evaluate the various integrals to compute the Rossi alpha and the Feynman Y, functions respectively.

As a part of the planning of experiments in the Purnima sub-critical facility, Rana et.al (2013) have carried out simulations of the proposed noise experiments using a Monte Carlo based neutron diffusion code developed for this purpose. These simulations have provided valuable information about the feasibility of the proposed experiments and the kind of accuracy that can be expected from such measurements. However, a more realistic description of the experiments will be provided by transport theory based analog Monte Carlo (Máté Szieberth and Gergely Klujber 2010). In chapter 6 we discuss the development of such a code (Singh and Degweker, to be submitted for publication) specifically intended for simulating the noise based experiments such as Rossi-alpha and Feynman-alpha. The code is based on the delta neutron tracking method (also called Woodcock and Coleman method) which results in fast and relatively simple handling of complex geometries. The code has been validated with a few K-eff and noise benchmark

problems. In this chapter we have given the results of simulation of the proposed ADS noise experiments at the PURNIMA facility obtained using our code.

Chapter 7 gives a brief summary of the results presented in the thesis and the main conclusions drawn.

The thesis describes the development of new methods for solving alpha-eigenvalue problems in multi-group diffusion theory with and without delayed neutrons to obtain fundamental and higher modes and computer codes developed based on these methods. It also describes the development of other codes which will be useful in simulating transients in ADSs, and for simulating various experiments planned for measurement of the degree of sub-criticality in ADS by pulsed neutron and noise methods.

An attempt was made to calculate higher prompt and delayed modes using the sub-space iteration methods but was not very successful. This is due to the fact that with the inclusion of delayed neutrons in the diffusion equation and elimination of the precursor variables, the eigenvalue problem is no longer linear. It would be interesting to develop a method for computing higher prompt and delayed modes which do not suffer from these difficulties.

In the analogue Monte Carlo code for simulating various experiments, we have simplified our problem by treating the energy variable by the method of groups and by assuming isotropic scattering. Further work in this direction would be to develop a code capable of continuous energy treatment with anisotropic scattering.

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LIST OF FIGURES

LIST OF TABLES

NOMENCLATURE

List of symbols

φ^*	Source importance factor
K_s	Subcritical multiplication factor
K_{eff}	Subcritical multiplication factor
ρ	Reactivity
v or V	Neutral particle speed
V	Variance
$\phi(\underline{r}, E, \underline{\Omega}, t)$	Angular flux
$\underline{\Omega}$	Unit vector in direction of particle motion
$\underline{r}$	Particle coordinates location in space
E	Particle energy
t	Time
S_{ext}	External independent particle source
Σ_t	Macroscopic total cross section
Σ_s	Macroscopic scattering cross section
χ	Fission spectrum
Σ_f	Macroscopic fission cross section
Σ_r	Macroscopic removal cross section

ν	Average number of fission neutrons produced per fission
Σ_{tr}	Macroscopic transport cross section
J	Neutron current density
$<\mu>$	The average cosine of the scattering angle in a neutron scattering collision
C_i	Time-dependent precursor concentrations
D	Diffusion coefficient
α	Time-eigenvalues
β	Delayed neutron fraction
Λ	Prompt neutron generation time
$p(r,\Omega,E,t;n_1,n_2)$	Probability of the number of detections n_1 and n_1 in two intervals length Δt_1 and Δt_2 around the times t_1 and t_2 $(t_2 > t_1)$ due to a neutron injected at (r,Ω,E,t)
$G(r,\Omega,E,t;z_1,z_2)$	Probability generating function (PGF)

Acronyms

ADI	Alternating Direction Implicit
ADS	Accelerator Driven Sub-critical System
CPSD	Cross Power Spectral Density
ENDF	Evaluated Nuclear Data File
FP	Fission Product
HLW	High Level Waste (HLW)
IAEA	International Atomic Energy Agency

IEA	International Energy Agency
ILW	Intermediate Level Waste
IQS	Improved Quasi Static
LLW	Low Level Waste
LMW	Langenbuch-Maurer-Werner
LWR	Light Water Reactor
MC	Monte Carlo
PDF	Probability Density Function
PHWR	Pressurised Heavy Water Reactor
PGF	Probability Generating Function
TRU	Transuranic

CHAPTER 1

Overview on Accelerator Driven Sub-critical System (ADS)

Meeting the rapid increase in global energy demand is a major challenge to the world community. According to the IEA, the global demand for energy (IEA, 2011) will grow more than 33% by 2035. This large expansion cannot be met by the limited fossil fuel reserves alone. Moreover there are concerns of emission of green house gases due to burning of fossil fuels resulting in global warming and climate change (IAEA, 2011). Nuclear power can make an important contribution in reducing greenhouse gases while delivering energy in increasingly large quantities required for global economic development. This has resulted in a revival of interest in nuclear energy. But production of nuclear energy through conventional critical reactors is also not devoid of problems. Safety, proliferation and management of nuclear waste are major issues related to the presently operating critical reactors.

Various innovative reactor designs addressing these issues are under development. An innovative reactor concept which is increasingly getting worldwide interest is the Accelerator Driven System. The ADS has superior safety characteristics as compared with critical reactors and can work as a fissile material breeder, a waste transmuter and as an energy amplifier.

Indian interest in accelerator driven systems (ADSs) has an additional dimension (Degweker et al., 2007a), which is related to the planned utilization of our large thorium reserves for future nuclear energy generation. Studies done by several researchers (Rubia et al., 1995; Degweker, 2001, 2002; Bowman, 2000; Furukawa, 1997) around the world have shown the achievability of

self-sustaining thorium-uranium cycles in ADSs. Globally, thorium is 3–4 times more abundant (IAEA-TECDOC-1450, 2005) than uranium and India in particular, has much larger thorium reserves compared to that of uranium. Thorium however does not contain any fissile isotope. The fertile Th^{232} has to be converted into the fissile U^{233} by neutron irradiation. In an ADS, the accelerator delivers additional neutrons over and above those coming from fission. Therefore the thorium fuel cycle in ADSs can be expected to give higher breeding and hence appears to be an attractive alternative for long term energy production. Moreover, the Th cycle generates much lower quantities of long lived radiotoxicity waste (IAEA Safety Standards, 2005).

These attractive features of ADSs have given a fillip to research activities in several countries (Abderrahim et al., 2001; Kapoor, 2001; Mukaiyama et al., 2001; Gohar and Smith, 2010) aimed towards development of high power accelerators, spallation targets and sub-critical reactor physics concepts. On the reactor front, the R&D effort is mainly geared towards development of accurate simulation tools, generating new nuclear data and conducting experiments oriented towards understanding the physics of accelerator driven sub-critical reactors. A programme and roadmap for development of ADSs has also been drawn up in India. This includes development of a high energy high current proton accelerator, development of target technology and basic theoretical and experimental studies in ADS reactor physics and nuclear data.

Evolving a suitable method of reactivity monitoring in ADSs is one of the areas of experimental reactor physics research. Besides deterministic methods such as pulsed neutron and source jerk methods, noise based methods are also being evaluated for this purpose. A considerable amount of theoretical work (Pazsit and Yamane, 1998a,b; Pazsit et al., 2005; Degweker, 2000,2003) has been carried out for understanding reactor noise in ADSs and its application to measurement of

the degree of sub-criticality. Several zero power experiments (YALINA, MUSE) devoted to reactivity monitoring of ADS have been carried out around the world and a number of reactivity measurement methods such as the Feynman-alpha and the Rossi-alpha methods, and pulsed neutron source methods were investigated. In BARC many such physics experiments are planned (Rasheed et al., 2010) in the newly created BRAHMMA sub-critical facility, at the Purnima laboratory. These experiments will be helpful in validation of reactor physics analysis tools and ADS related theoretical concepts developed in BARC.

The thesis discusses the theoretical work and computer code development performed for the design and analysis of experiments planned for determination of sub-criticality at the Brahma facility mentioned above. Deciding suitable locations of detectors, so that the effects of higher harmonics are minimal, is one of the problems addressed in this context. Knowledge of the zeros of the alpha-eigenmodes is required for fixing suitable locations of the detectors. In the thesis, we describe methods developed for calculation of alpha eigenmodes of the neutron diffusion equation. The other development pertains to simulation of deterministic and noise experiments for sub-criticality measurement. For this purpose we have developed a space time kinetics code based on diffusion theory. Though this is a deterministic code it can be used not only for the analysis of pulse neutron experiments but also for simulation of noise experiments. The diffusion theory code can also be used for simulating transient in power reactors (critical or ADS) as it also incorporate various feedback effects. Since a more accurate description is provided by the Monte Carlo method, we have also developed a transport theory based analogue Monte Carlo code (Singh and Degweker, 2014) specially developed for simulating the noise experiments planned at BARC. A description of this development is also contained in the thesis.

1.1. Spent fuel and its management

Handling and storing nuclear waste is one of the major obstacles in nuclear energy development. As per IAEA there are primarily three major classes of nuclear waste (IAEA technical report 2009; Ripani, 2013) which require attention for safe storage and disposal. The first category is Low level waste (LLW) having enough radioactivity content (annual dose rate to members of public < 0.01 mSv) to require action for the protection of people, but not so much that it requires shielding during handling, storage or transportation. The second category is Intermediate level waste (ILW) which because of its radioactivity content, (particularly of long lived radionuclides less than 4000 Bq/g of alpha-emitters) requires a greater degree of containment and isolation and requires disposal at greater depths. In the third category, we have the High level waste (HLW) containing large amounts of short and long-lived radio nuclides requiring both cooling and shielding which poses a great challenge with regard to storage and disposal.

Most of the HLW originates from the spent fuel of nuclear power plants. As per an estimate (Salvatores and Palmiotti, 2011) LWR spent fuel with a burnup of 33 GWd/t after a cooling of 10 years, consists of about 95.5% uranium, 0.2% short-lived fission products (Cs^{137}, Sr^{90}), 0.2% long-lived fission products (I^{129}, Tc^{99}, Zr^{93}, Cs^{135}), 0.8% plutonium, and 0.2% minor actinides (neptunium, americium, and curium). The half lives of these radio nuclides vary in the range between minutes and millions of years. For the first few hundred years, the spent fuel radiotoxicity (measure of hazard) is dominated by fission products. In the long run radiotoxicity of spent fuel arises from long lived plutonium, neptunium, americium and curium and also from some long-lived fission products such as iodine and technetium isotopes.

1.1.1. Nuclear waste management options

Finding a solution to the problem of nuclear waste management has been one of the thrust areas in nuclear energy research in last few decades. Several spent fuel management options have been suggested, varying from the direct disposal concept to proposals for reprocessing and recycling a various spent fuel components. The three major back-end fuel cycle options currently under consideration by various countries are: a once through fuel cycle option with direct disposal of spent fuel as HLW; reprocessing fuel cycle (RFC) with mixed oxide (MOX) recycle of U and Pu in light water or fast breeder reactors and disposal of minor actinides and fission products; an advanced fuel cycle, an extension of RFC in which the minor actinides and long lived fission products are partitioned and transmuted (P&T) to reduce the long-term radio toxicity. These options have different advantages and disadvantages and pose different challenges that vary in complexity to the management of nuclear wastes.

Partitioning and transmutation

To deal with the problem of disposal of nuclear wastes, plans have been made to permanently store them in solid state in deep geological formations. However, there is concern that geologic formation might change over millions of years and as a consequence it might turn out to be a potential risk to human society. Another long-term risk with repository burial is the possible leaching of the stored waste by underground water and its entry into the biosphere. As an alternative, a basically different strategy called partitioning and transmutation is also being explored.

Transmutation in fast reactors

Effective transmutation of long-lived actinides can be better achieved in fast reactors as compared to thermal reactors because the fast neutrons have a higher ratio of fission to capture probability as compared to thermal neutrons. Several feasibility studies (Wakabayashi, et al. 1997; Wakabayashi and Higano, 1998) have been performed in the recent past to investigate suitability of a fast reactor core for TRU and FP transmutation. But the general conclusion from these studies show that since safe reactor operation of fast reactors is crucially dependent on the delayed neutron fraction and negative fuel temperature (Doppler) reactivity coefficient which are rather low for minor actinides, critical fast reactors can be loaded with limited amount of minor actinides and they are not suitable for rapid transmutation of minor actinides.

ADSs for waste transmutation and breeding

Accelerator Driven Systems (Rubia et al., 1995; Stefan, 2003; Bowman et al., 1992) have been suggested to accomplish several tasks including transmuting minor actinides and fission products produced as a result of nuclear energy generation. ADSs can also breed fissile materials for subsequent use in critical or sub-critical systems. Many countries have proposed ADS concepts for power production utilizing thorium-based fuel to take advantage of some of its benefits, including greater natural abundance, proliferation resistance and significantly lower production of transuranic elements. For these reasons, many countries are carrying out theoretical and experimental studies to develop, demonstrate and exploit accelerator-driven systems technology for nuclear waste transmutation and power generation.

1.2. ADS historical background

The roots of the ADS concept can be found in the research works done on accelerator based fissile material breeding in early 1950s by Glenn Seaborg, E.O Lawrence and W.B Lewis, V.I. Goldanski, R.G. Vassylkov (Van Atta, 1977; Bartholomew, 1965; Vassylkov et al., 1978). Later there were studies on the Fertile-to-Fissile Conversion Program (Russel et al., 1988) with collaborative efforts of various laboratories. The idea of using spallation process directly to breed fissile material or transmutation of actinides and long lived fission products did not last long due to technological difficulties and high costs. In late 1980s and early 1990s, C. Bowman (Bowman et al., 1992) and H. Takahashi both independently came out with the idea of ADS promising to use high-energy proton beam from an accelerator to produce spallation neutrons which in turn would drive a sub-critical blanket. While Bowman conceived a thermal system for transmutation and energy production, Takahashi,s PHOENIX (Van Tuyle et al., 1991) project was based on a fast spectrum sub-critical blanket for incineration of actinides. The interest in ADSs got a major boost with the research work done by a group led by Carlo Rubbia (Rubia et al., 1995) who conceived the idea of the Fast Energy Amplifier, which is a Th-U fuelled sub critical reactor using lead as coolant, driven by external neutrons coming from spallation in Pb induced by a high energy (1 GeV) proton accelerator having a current of about 10 mA.

1.3. Basic principles of ADS

The basic idea of ADS (Rubia et al., 1995; Kadi and Revol, 2001) is to couple a subcritical core with neutrons coming from a spallation neutron source produced by impinging high energy proton from an accelerator (Linac or Cyclotron) on a heavy metal target. Spallation is a well-known nuclear reaction in which energetic particles (e.g. protons) interact with the target nucleus

producing high energy secondary particles (neutrons, protons, mesons, gammas). These particles, besides depositing a large amount of energy and generating spallation products in the target, release a large number of neutrons in the sub critical medium when they leave the target. The main safety advantages of ADSs are increased margin to prompt criticality and reduced dependence on delayed neutrons and reactivity feedbacks. These attractive features of ADSs offer a great promise for effective management of nuclear waste and safe nuclear power generation.

1.3.1. Spallation neutron sources

Typical industrial-scale ADS designs, having thermal power ratings in the range of 500 MW_{th} to 1500 MW_{th} are considered. To have adequate criticality safety margins typical K_{eff} values are generally chosen in the range 0.95-0.98. For the ADSs, the level of sub-criticality (Erikssona & Cahalan, 2002) being suggested is at least an order of magnitude larger (typically ~10$ subcritical or K_{eff}<0.98) because reactivity feedbacks will not be as effective a means in source-driven systems as they are in critical systems. Moreover stronger reactivity effects, from what is experienced in critical reactors, are necessary to have an effect on the source-driven system. In thermal ADSs, because of fission product reactivity load, a lower value of K_{eff} is chosen.

A rough estimate of neutron source strength which can drive an 800 MW_{th} (K_{eff}=0.95) reactor shows that the required source strength will be about $3x10^{18}$ neutron/sec. Such a strong source is not possible through any radioactive-decay type source. Achieving such a strong neutron source is however possible using the spallation reaction. At 1 GeV each proton will on the average expel 25 neutrons. Thus, the required proton intensity would roughly amount to $1.2x10^{17}$ protons/sec, which equals a beam current of roughly 20 mA or 20 MW of beam power. Though a

beam power of 20 MW is not available today, recent advances in accelerator technology promise the availability of such beam power in future.

1.4. Theoretical research in the area of ADSs

1.4.1 Computer codes and nuclear data

Reactor physics theories, nuclear data and computational methods developed for critical reactors need to be modified or adapted for applicability for ADS. The analysis of ADSs requires computer codes, capable of handling the transport of high energy hadrons (protons, neutrons, pions etc) in addition to those required for treating low energy (<10 MeV) neutronics. In the high energy physics area, the commonly used codes are LAHET, FLUKA and CASCADE (Prael and Madland, 2000; Ferrari and Sala, 1996; Kumawat and Barashenkov., 2005). These codes calculate the neutron yield per proton, the neutron energy spectrum, the heat deposition in the target and the creation of the spallation products. Criticality, neutron transport and multiplication, fuel depletion and generation of fission products are generally dealt with core and burn-up simulation codes based on deterministic and stochastic low energy transport codes based on nuclear data from ENDF files. Monte Carlo depletion codes such as MCNPX with CINDER'90 depletion capability, MCB, Monteburns (Cetnar et al., 1999; Poston et al., 1999) and other codes have been developed for analyzing the neutronics of ADSs and core follow-ups. In BARC also, development of continuous energy Monte Carlo code McBurn has been carried out (Ghosh and Degweker, 2004) for analysis of ADS. The greater use of Monte Carlo codes for statics and burnup calculations reflects both the increasing computing power available and the need to predict K_{eff} (or K_s) accurately throughout the burnup cycle as both the power that can be produced as well as the safety margin available are dependent upon these predictions. Multi-

group diffusion theory kinetics codes (Singh K.P. et al., 2011) have been recently developed keeping in view its application for steady state and transient analysis of ADSs. The SIMMER-III/IV (Maschek et al., 2000; Yamano et al., 2003) codes are under development for analyzing transients and accidents in critical waste incinerating reactors and in ADSs.

Augmentation of existing nuclear data files to include minor actinides and isotopes related to Th cycle is required as these nuclides have been studied less compared to the nuclides in U cycle. For target nuclides the nuclear data at higher neutron energies extending up to hundreds of MeV is required for ADS applications as opposed to critical reactors. Various laboratories and institutes are working towards developing (Takanori et al., 2011; Koning et al., 2007) a new nuclear data for ADSs. High-resolution nuclear data are being generated using neutron time-of-flight techniques in advanced facilities such as the 150 MeV electron LINAC (800 MHz, 10-400 m flight paths, 10 meV to 20 MeV neutron energy region) at Geel, Belgium, the 800 MeV proton LINAC at Los Alamos National Laboratory (20 Hz, spallation, <500 keV neutrons, 20 m path length). In CERN (CERN n TOF) new measurements of cross-sections using the neutron time-of-flight facility for applications to ADSs have provided an impetus towards generating new nuclear data.

1.4.2. Weighting Function and Reactivity Definitions

In conventional reactors the information about reactivity is derived from their effective multiplication constant which is also the largest eigenvalue of neutron transport/diffusion equation. However, the fundamental eigenvalue and eigenstate may not be suitable parameters to describe source-driven subcritical multiplying systems, since the stationary neutron distribution is strongly dominated by presence of the source and it can be very different from the

fundamental critical eigenstate. Here it is worth mentioning that though the parameter K_{eff} retains its significance as a measure of the margin of subcriticality, neutron multiplication may be a useful parameter, which can be used to characterise the properties of the entire system i.e. material, geometry and source. The corresponding multiplication factor Ks defined below has been introduced in this connection.

Weighting function is very important for defining reactivity and other parameters which are used in point kinetics equation and its proper value may improve the accuracy of point-kinetics computations. If the reactor is almost critical during the transient, the optimal weighting function is very close to the steady-state adjoint flux (Ott and Neuhold, 1985). In addition to the standard weighting function, the "unity" and the ''adjoint alpha mode'' have also been considered as weighting functions in the literature (Gandini, 1997; Gandini and Salvatores, 2002; Sandra Dulla et al., 2006; Kobayashi, 2005; Makai, 2008) for ADS studies and depending on the weighting function new definitions (Gandini, 1997; Gandini and Salvatores, 2002; Sandra Dulla et al., 2006) of reactor parameters have been introduced.

1.4.3. Source importance factor

In ADS, the external neutron source get amplified by a factor M called source multiplication factor. In the evaluation of M, the source importance factor plays very important role. The source importance factor (φ^*) is defined as the ratio of the average importance of a source neutron to the average importance of fission neutron.

For a subcritical system with an external source at steady state, the neutron multiplication M and the subcritical multiplication factor K_s are defined in the present study as follows:

$$M = \frac{F+S}{S}$$

$$F \equiv \int_{VOL} \int_0^\infty \nu\Sigma_f(r,E)\phi_s(r,E)dEd^3r$$

$$S \equiv \int_{VOL} \int_0^\infty s(r,E)dEd^3r$$

where $\phi_s(r,E)$ is the neutron flux in the subcritical system at position r(x, y, z) and energy E, $s(r,E)$ is the external neutron source, F and S are the total number of produced fission and source neutrons, respectively, per unit time, VOL is the whole system volume, ν is the average number of fission neutrons per fission reaction, and $\Sigma_f(r,E)$ is the fission cross-section.

In terms of the K_s the fission power can be written simply as $\frac{SK_s}{[\upsilon(1-K_s)]}$. On the other hand, in terms of the K_{eff}, the expression for power includes the source importance factor and is given by $\frac{S\varphi^* K_{eff}}{[\upsilon(1-K_{eff})]}$. Equating the two expressions for power, it is seen that the source importance factor can be related to the K_{eff} and K_s as follows:

$$\varphi^* = \frac{(1-1/K_{eff})}{(1-1/K_s)}$$

1.4.4. Noise theory in ADS

The behaviour of neutrons in a nuclear reactor can be represented as a stochastic process. Observation of the fluctuations and their correlation of the neutrons in a system are used to measure kinetics parameters of a reactor. Based on this principle, noise techniques have been

suggested (Behringer and Wydler, 1999; Carta and D'Angelo, 1999; Munoz Cobo et al., 2001) for monitoring the sub-criticality of ADS. Since noise methods do not require any perturbation of the system, they might be more suitable in situations where perturbations (Degweker and Rana, 2007) are not desirable. Early theoretical studies on various noise techniques for ADS (Pazsit and Yamane, 1998a,b; Behringer and Wydler, 1999) assumed the neutron producing source events in an ADS to form a Stationary Poisson Point Process with each such event (spallation) producing neutrons with a large multiplicity distribution. A new theoretical approach considering periodic pulsing and non-Poisson character of the source was proposed by (Degweker, 2000, 2003). The theory has, since then, been considerably expanded (Degweker and Rana, 2007; Rana and Degweker, 2009, 2011).

1.4.5. Studies on waste transmutation

There have been theoretical studies devoted towards advanced solutions related to waste transmutation based the use of accelerator-driven reactor systems to burn the Minor Actinides (MAs) Np, Am, and Cm and Long Lived Fission Products (LLFP). Most of these studies have been towards assessing the potential of such system, on the basis of a physics analysis of the main phenomena involved. Rubbia et al. (1995) showed that an accelerator could directly drive a sub-critical power reactor and that the neutron spectrum from a lead moderator would sweep the capture resonances of transuranic isotopes and consume long-lived wastes. Bowman et al, and Venneri et al., (Bowman et al., 1992; Venneri et al., 1993) have carried out studies on Accelerator-Driven Transmutation of Waste (ATW) at Los Alamos. The system is based on transmutation of both fission products and higher actinides using a thermal neutron flux of about 10^{16} n/cm^2/sec.

Studies on long lived fission product transmutation in ADSs have also been carried out by several other researchers (Nishihara et al., 2001, 2008; Tachi et al., 2009; Yokoyama et al., 2009). Theoretical studies (Song et al., 2004; Yang et al., 2004) of simultaneous transmutation of minor actinides and long lived fission product in ADS were carried out in a 1 GWth hybrid power extraction reactor (HYPER) and in Argonne National Laboratory on Accelerator Transmutation of Waste System (ATW) of 840 MWt power. The studies have shown that ADSs can burn significant amounts of all minor actinides and long lived fission products in readily controlled manner contrary to fast critical reactors.

Researchers under various thorium utilization programmes are investigating whether ADS can speed up the deployment of the ^{233}U-Th fuel cycle by breeding ^{233}U, which does not exist in nature. In India, ADSs can play key role in its 3-stage programme to develop a sustainable Th-U fuel cycle. In the recent years, various types of accelerator-driven transmutation technologies have been studied (Abanades and Perez- Navarro, 2007; Adam et al., 2007; Mukaiyama et al., 2001; Seltborg and Wallenius, 2006) to produce energy and transmute radioactive wastes.

1.5. Experimental Studies

Several experiments (Andriamonje et al., 1995; Soule et al., 2004; Carl-Magnus Persson et al., 2005; Kitamura et al., 2006) for selecting a suitable method for sub-criticality monitoring of ADS have been conducted around the world and several more are planned. Other parameters pertaining to operation of a future ADS have also been studied/planned in FEAT and TRADE experiments (Andriamonje et al., 1995; Imel et al., 2004). Recently the Guinevere experimental facility in Belgium has become operational (Billebaud et al., 2009). Experiments aimed towards

measurement and monitoring of sub-criticality and evolution of procedures for operation of an ADS are planned in this facility.

Generally the methods of reactivity determination are based on point kinetics model with some spatial correction applied to the evaluated value for inferring the sub-criticality. In the reactor noise methods the natural fluctuations in detector counts have potential information about sub-criticality. Similar experiments for demonstrating pulsed neutron and noise methods for sub-criticality measurement are planned in the upcoming Purnima facility at the Bhabha Atomic Research Centre (BARC), India. A brief description of these methods is summarized is below.

1.5.1. Pulsed Neutron Source (PNS) experiments

In sub-critical system, it is possible to determine the reactivity of the core by analysing the decay in detector response after a neutron pulse insertion. The methods used for analyzing a PNS experiment are slope fit method (Keepin, 1965) and area ratio method (Sjostrand, 1956). MUSE experiments (Soule et al., 2004) show that space and energy effects may introduce some bias in the results and detailed computer simulations should be used to take into account the spatial and energy effects. The PNS experiments in YALINA (Carl-Magnus Persson et al, 2005) were found in good agreement with those obtained by Monte Carlo calculations. The experiments showed that the slope fit method gives better results compared to area ratio method. However, in deep sub-criticalities, it may be difficult to find the correct slope.

1.5.2. Source Jerk method

Source jerk method (Keepin, 1965) is a dynamic method based on the utilisation of a time dependent external source for reactivity determination. In such technique, the external source is suddenly removed from the initial steady state condition, where there is the equilibrium of both

the delayed neutron precursors and the prompt neutron concentrations. Assuming a subcritical core at constant power driven by an external source, a neutron flux level somewhere in the core will be n_0. Suddenly, the external neutron source is removed very quickly. Then, the neutron flux changes rapidly to a asymptotic level n_1. The reactivity in dollars is given by

$$\rho(\$) = \frac{(n_0 - n_1)}{n_1}$$

The efficiency of source jerk experimental techniques for assessing a subcritical level was tested in RACE experiments (Jammes, Christian C. et al., 2006) by causing transient through the neutron generator shutdown (SJ-Gen) and standard source jerk technique (SJ-Cf) using the Cf-252 source. Among the methods used for reactivity determination, source jerk method provided less satisfactory results.

1.5.3. Noise experiments

Noise methods using Rossi alpha, Feynman alpha and CPSD (Soule et al., 2004) have been studied in MUSE experiments. The Rossi alpha and Feynman alpha methods were found suitable for low sub-criticalities. CPSD measurements demonstrated the inference of alpha through the break frequency. Rossi alpha measurements have been carried out at the Kyoto University Critical Assembly (KUCA) by using a D–T pulsed neutron source (Kitamura et al., 2006). Since the authors used a solution technique that is based on the Laplace transform, the formula derived by them contains infinite series expansion structure of the oscillating term. Therefore, it was difficult to fit the formula to the experimental data and only the correlated term was used to extract the value of alpha.

CHAPTER 2

Review of Computational Methods in Physics of Critical & Sub- critical Systems

The reactor physics of ADSs is quite different from that of critical reactors. This is due to the presence of the spallation source, which results in a different spatial and energy distribution. whereas in critical reactors the fundamental eigenmode prevails, in ADSs (Carta and D'Angelo, 1999; Rineiski et al., 2005; Degweker, et al., 2007) other modes also arise due to the fact that the spallation neutrons have different energy and spatial distributions different than that of fission source. Moreover, ADS cores are characterised by a very low fraction of delayed neutrons and by a low Doppler reactivity coefficient. In consequence these cores have very different dynamic response to any reactivity/source perturbation. The degree of sub criticality is one of the principal reactor parameters of ADSs because this not only assures criticality safety; it has a bearing on the energy gain and decides the accelerator power necessary for producing the design power of the ADS. Therefore, for proper design of ADSs, it is very important to accurately predict the sub-critical reactivity throughout the core life.

For these reasons, the methodologies and computer codes developed for critical reactors may be inadequate in their present form, and hence it is required to develop of new simulation tools. Development of on-line reactivity monitoring techniques and their qualification by sound computational and experimental methods will also be necessary.

Various techniques are used for determining the reactivity of subcritical systems as discussed in chapter-1 are based on measurement of fundamental alpha of the system. The reactivity predicted by these methods has a strong dependence on detector location due to presence of higher modes. Misawa et al. (1990) have shown that in a subcriticality measurement with the Feynman-aalpha method, it is important to quantify the effects of higher order alpha-modes. Higher alpha-modes are important in developing modal neutron kinetics where these modes form the expansion bases for neutron flux due to any perturbation.

Considering the importance of alpha modes, there has been considerable work done in the past (Dhal et al., 1983; Modak and Gupta, 2003; Sahni, D.C. et al., 1992; Paranjape, S.D. et al., 1993) to evaluate the same. The alpha modes evaluated by these researches are either limited to simpler one dimensional one energy group cases or limited to only few dominant prompt alpha modes. In our research work we have developed schemes which can efficiently evaluate higher prompt eigenvalues/eigenmodes and also evaluate higher delayed time eigenvalues/eigenmodes. The evaluation methodologies of higher prompt and delayed alpha-modes are discussed in detail in chapters 3&4.

Simulation of the deterministic and noise experiments for sub-criticality measurements and to analyse any reactivity initiated transient full three dimensional space time kinetics code is required. Though there are several such codes popularly in use for space time kinetics applications for critical reactors, the motivation behind the development of 3-dimensional space time kinetics code is to analyze the dynamical behavior of ADSs. The deterministic code developed can not only be used for the analysis of pulse neutron experiments but also for simulation of noise experiments. In chapter 5 we have brought out the theoretical bases for 3-D

space time code and results of benchmark problems to validate the code. We have also developed thermal model which can be useful for analyzing feedback effects.

As discussed in chapter-1, noise based techniques are more suitable method for assessment of sub-criticality. As part of the planning noise based experiments, a prior knowledge of the kinds of results that might be expected with different detector locations, counting and analyzing setups will be useful. Simulation of such experiments can accurately be done by Monte Carlo method. Simulations with standard existing code packages are not appropriate because of several non-analogue features built into such codes. For this reason we developed our own Monte Carlo code specifically intended to simulate noise based experiments and the detailed description is given in chapter-6.

In present chapter we present an overview of the computational reactor physics methods used for critical and sub-critical reactor analysis. We also introduce the time eigenvalue problem of the neutron diffusion equation which helps in the design and planning of experiments for sub-criticality determination.

2.1. Methods in computational reactor physics

Calculation of the reactivity, neutron flux, reaction rates and fission power distribution are of pivotal importance in the design of critical and sub-critical reactors. Several codes based on deterministic as well as stochastic approaches viz., transport theory, diffusion theory and Monte Carlo methods are in use. Diffusion theory is an approximation to transport theory, and the Monte Carlo method is a statistical approach based on random sampling. Each of these methods has its strengths and weaknesses in the areas of application mentioned above.

Reactor Physics calculations begin with the processing of nuclear data files in what is called the Evaluated Nuclear Data File (ENDF) format to produce multi-group or continuous energy data files for use in transport theory or Monte Carlo codes. Often readily available multi-group or continuous energy data files such as the Wims cross section data library or the ACE format libraries for use in continuous energy Monte Carlo calculation may be a starting point. Though the Monte Carlo calculations for the full reactor core can be carried out in one step and give good estimates of quantities such as the K_{eff}, detailed power distribution in the core and its variation with burn-up and during transients can be determined quickly only by deterministic methods. These are, even today, carried out in a series of steps which are described in the next section, since it is not possible at the present time to perform three dimensional whole core calculations using multi-group transport theory without homogenization. However it may be mentioned that in recent years, due to phenomenal increase in computing power, there have been suggestions/attempts to solve the multi group transport equation in a single step without homogenization (Hernandez et al., 2013).

2.2. Neutron transport equation

The neutron distribution inside a reactor core is well described by the linear Boltzmann transport equation. It is basically a statement of neutron balance in small volume element of phase space $d^3\mathbf{r}$. In its integro differential form it can be written as (Bell and Glasstone, 1970)

$$\frac{1}{v}\frac{\partial\phi(\underline{r},E,\underline{\Omega},t)}{\partial t}+\underline{\Omega}.\nabla\phi(\underline{r},E,\underline{\Omega},t)+\Sigma_t(\underline{r},E)\phi(\underline{r},E,\underline{\Omega},t)=S_{ext}(\underline{r},E,\underline{\Omega},t)+$$
$$\int_{4\pi}d\underline{\Omega}'\int_0^\infty dE'\Sigma_s(\underline{r},E'\rightarrow E,\underline{\Omega}'\rightarrow\underline{\Omega})\phi(\underline{r},E',\underline{\Omega}',t)+\frac{\chi(E)}{4\pi}\int_0^\infty dE'\nu(E')\Sigma_f(\underline{r},E')\phi(\underline{r},E',t) \qquad (2.1)$$

The Eq.(2.1) is a complicated equation not only because it is an integro-differential equation in seven variables but also because of cross sections being extremely complex functions of energy and position for any realistic reactor problem. For this reason the problem is solved in a series of steps and approximations like multi group formalism, lattice – pin cell calculation and assembly homogenisation and finally diffusion theory approximation.

2.2.1. Multi-group formalism

In multigroup formalism neutron transport equation is made computationally suitable by dividing complete neutron energy range into G number of discrete intervals. Indexing of these intervals is chosen so that group g contains neutrons with energies $E^g < E < E^{g-1}$. The structure of multigroup discretisation can be written as

$$\left\{0 = E^G < E^{G-1} < ---------- < E^g < E^{g-1} < ---- < E^1 < E^0 \to \infty\right\}$$

Neutron balance within group *g* can be obtained by integrating Eq.(2.1) over the group energy range and can be expressed as under

$$\frac{1}{v^g}\frac{\partial \phi^g(\underline{r},\underline{\Omega},t)}{\partial t} + \underline{\Omega}.\nabla\phi^g(\underline{r},\underline{\Omega},t) + \Sigma_t^g(\underline{r},E)\phi^g(\underline{r},\underline{\Omega},t) = S_{ext}^g(\underline{r},\underline{\Omega},t) +$$
$$+\sum_{g'=1}^{G}\int_{4\pi} d\underline{\Omega}'\Sigma_s^{g'\to g}(\underline{r},\underline{\Omega}'\to\underline{\Omega})\phi^{g'}(\underline{r},\underline{\Omega}',t) + \frac{\chi^g}{4\pi}\sum_{g'=1}^{G}\nu\Sigma_f^{g'}\phi^{g'}(\underline{r},t) \qquad (2.2)$$

Various terms in Eq.(2.2) are defined as below:

$$\phi^g(\underline{r},\underline{\Omega},t) = \int_{E^g}^{E^{g-1}} \phi(\underline{r},\underline{\Omega},E,t)dE$$

and assuming separation of energy and angle variables ie; $\phi(\underline{r},E,\underline{\Omega},t) = \phi(\underline{r},E,t)\,f(\underline{r},\underline{\Omega})$, group constants used in Eq.(2.2) are defined as under

$$\Sigma_t^g = \frac{\int_{E^g}^{E^{g-1}} \Sigma_t(r,E)\phi(\underline{r},E,t)dE}{\int_{E^g}^{E^{g-1}} \phi(\underline{r},E,t)dE}, \frac{1}{v^g} = \frac{\int_{E^g}^{E^{g-1}} \frac{1}{v}\phi(\underline{r},E,t)dE}{\int_{E^g}^{E^{g-1}} \phi(\underline{r},E,t)dE}, \chi^g = \int_{E^g}^{E^{g-1}} \chi(E)dE$$

$$\Sigma_s^{g'\to g}(\underline{r},\underline{\Omega}' \to \underline{\Omega}) = \frac{\int_{E^g}^{E^{g-1}} dE \int_{E^{g'}}^{E^{g'-1}} \Sigma_s(r,E' \to E,\underline{\Omega}' \to \underline{\Omega})\phi(\underline{r},E',t)dE'}{\int_{E^{g'}}^{E^{g'-1}} \phi(\underline{r},E',t)dE'}, \nu\Sigma_f^{g'} = \frac{\int_{E^{g'}}^{E^{g'-1}} \nu\Sigma_f(r,E')\phi(r,E',t)dE'}{\int_{E^{g'}}^{E^{g'-1}} \phi(\underline{r},E',t)dE'}$$

2.2.2. Lattice level calculations

Various numerical methods have been devised for obtaining the quantities of interest to the reactor systems by solving the multigroup neutron transport/diffusion equation. The calculations are done by discretizing each of the variables involved. The discretization of energy gives rise to the group structure as mentioned in the previous section, the discretisation of the spatial variables results in what is commonly referred to as the spatial mesh and the discrete neutron directions are defined by asymmetric quadrature set. Moreover differential scattering cross sections are expressed in terms of the orthogonal Legendre polynomials. There is variety of numerical methods like discrete ordinates (DSN), spherical harmonics (PN), method of characteristics and collision probability method (Bell and Glasstone, 1970) popularly used in transport calculations.

Transport calculations are done at the lattice level and diffusion theory codes are used for full core calculations. Transport theory based lattice codes WIMSD and CLUB (Askew, J.R. et al., 1966; Krishnani, P.D., 1992) are used to calculate neutron flux distribution and an infinite medium multiplication factor. Evaluated multi- group nuclear data ENDF/B-6 and geometrical as well as material descriptions of unit cell all together form the input data for the code to solve

transport equation. The flux and volume weighted homogenised macroscopic cross-sections of the lattice cell obtained are used for full core calculations.

2.3. Core calculations using diffusion theory

One generally uses neutron diffusion equation for reactor core calculations. The neutron diffusion equation does not account for the angular dependence of the flux. Neutron flux in space is assumed to be slowly varying and source is assumed to be isotropic. The diffusion theory model of neutron transport has played a crucial role in reactor theory since it is simple and sufficiently realistic to study many important design problems. Though the approximations used to derive neutron diffusion equation may not be valid in conditions of heterogeneity, anisotropy and strong absorption, some of these problems are taken care at lattice level transport calculation. The multi group diffusion equation is obtained using Fick's law of neutron diffusion as given below.

$$J = -D\nabla\phi$$

Here D is the diffusion coefficient, such that $D = \frac{1}{3(\Sigma_t - <\mu>\Sigma_s)} = \frac{1}{\Sigma_{tr}}$

The validity of Fick's law is dependent on the conditions given below:

1. Region is ~3 mean free paths away from either a neutron source or a surface of a medium boundary
2. Medium is weekly absorbing and strong scattering
3. Scattering is weekly anisotropic
4. The neutron flux is a slowly varying function of position

Using Fick's law, multigroup neutron diffusion equation can be written as under

$$\frac{1}{v^g}\frac{\partial}{\partial t}\phi^g(r,t) - \nabla.\, D^g \nabla\phi^g(r,t) + \Sigma_t^g(r)\phi^g(r,t) = \sum_{g'=1}^{G}\left[\Sigma_s^{g'\to g}(r)\phi^{g'}(r,t)\right] + \chi^g \sum_{g'=1}^{G}\left[\nu\Sigma_f^{g'}(r)\phi^{g'}(r,t)\right] + S_{ext}^g(r,t)$$

Defining group removal cross-section as $\Sigma_r^g = \Sigma_a^g + \sum_{g'\neq g}^{G}\Sigma_s^{g\to g'} = \Sigma_t^g - \Sigma_s^{g\to g}$

We get the following equation

$$\frac{1}{v^g}\frac{\partial}{\partial t}\phi^g(r,t) = \nabla.\, D^g \nabla\phi^g(r,t) - \Sigma_r^g(r)\phi^g(r,t) + \sum_{g'\neq g}^{G}\left[\Sigma_s^{g'\to g}(r)\phi^{g'}(r,t)\right] + \chi^g \sum_{g'=1}^{G}\left[\nu\Sigma_f^{g'}(r)\phi^{g'}(r,t)\right] + S_{ext}^g(r,t) \quad (2.3)$$

2.3.1. Solution of multi-group neutron diffusion equation

Neutron density in a reactor will be independent of time in either a critical reactor or a sub-critical reactor driven by external neutron source. Time independent neutron diffusion equation with external source can be written by equating the time derivative of flux to be zero as under:

$$-\nabla.\, D^g \nabla\phi^g + \Sigma_r^g\phi^g = \sum_{g'\neq g}^{G}\left[\Sigma_s^{g'\to g}\phi^{g'}\right] + \chi^g \sum_{g'=1}^{G}\left[\nu\Sigma_f^{g'}\phi^{g'}\right] + S_{ext}^g \quad (2.4)$$

From here onwards for convenience we have dropped explicitly displaying the space variable.

Numerical solution method

Over the years several schemes for solution of multigroup neutron diffusion equation have been developed and computer code packages made based on these methods. Notable among these methods are the nodal method (Lawrence, R.D., 1986), the finite difference method (Duderstadt and Hamilton, 1976; Lewins and Ngcobo, 1996) and the finite element method (Kang and Hansen, 1973). In the present work we have chosen a standard finite-difference approach. In the finite difference method, the second spatial derivative term is descretised in number of meshes each having uniform properties within it. The result of the finite difference discretisation is that

the partial differential equations are converted to a set of algebraic equations and for very fine mesh structure the method converges to the exact solution.

Two forms of finite difference theory equations (i) 'Corner mesh' equations and (ii) 'centre mesh equations' (Cacuci, D.G., 2010) are in use. We have used the centre mesh approximation for descretisation of diffusion equation in our research work. A derivation of the set of algebraic equations obtained using the scheme is given in Appendix 2A. The time dependent and steady state multigroup diffusion equation take the form of Matrix equations as given below:

$$\frac{1}{V}\frac{\partial \phi}{\partial t} = \chi F\phi - A\phi + S_{ext} \tag{2.5}$$

$$A\phi = \chi F\phi + S_{ext} \tag{2.6}$$

M is the matrix containing diffusion, removal and scattering terms and F is the matrix containing fission terms. The element of ϕ are arranged in such a way that all fluxes for group 1 precede those for group 2 and so on. A, M, F , χ are NGxNG matrices and ϕ and S_{ext} is NGx1 column vector.

λ - Eigenvalue problem

The Eq.(2.6) admits stationary solutions for a critical reactor (S_{ext}=0) which implies exact balance between production and removal. However, we can restore this balance for any system by dividing the fission source by a suitable quantity λ . In that case Eq.(2.6) is rewritten as

$$A\phi = \frac{1}{\lambda}\chi F\phi \tag{2.7}$$

The set of solutions of Eq.(2.7) are called the λ-modes and the corresponding values of λ are called the λ-eigenvalues. The highest eigenvalue is the K_{eff} of the system and the corresponding eigenfunction ϕ gives the flux distribution in a critical reactor.

Iterative solution procedure

The eigenvalue Eq.(2.7) is solved by power iteration (Duderstadt and Hamilton, 1976) method. There are two iterative processes involved in the evaluation of eigenvalue and eigenflux. One is called as the outer iteration or source iteration to evaluate the source distribution/eigenvalue with the obtained neutron flux until source distribution/eigenvalue converges. The other is called as the inner iteration for obtaining the flux distribution under the fixed source distribution. Starting with an initial 'guess' flux vector and a given eigenvalue we first obtain the 'fission source' by evaluating the RHS of Eq.(2.7). The resulting source problem

$$A\phi = S^{(0)}$$

is solved to obtain the new flux vector. This then used to obtain a new value of λ. Using these two a new fission source is obtained and the next iteration begins. It is easily seen that the above procedure is equivalent to repeatedly multiplying upon a guess vector with the matrix $A^{-1}F$ and normalizing. This is the standard algorithm to obtain eigenvalue of $A^{-1}F$. The solution of $A\phi = S^{(n)}$ is obtained by an iterative procedure. This is known as inner iteration. These set of linear equations are solved by various methods like Jacobi, Gauss-Seidel, conjugate gradients, Krylov subspace method. We have chosen the popular Gauss Seidel method for solution of system of neutron flux equations. The various iterative equations involved are given below:

$$A\phi^{(n+1)} = \frac{1}{\lambda^{(n)}} S^{(n)} \tag{2.8}$$

$$S^{(n)} = F\phi^{(n)} \tag{2.9}$$

$$K^{(n+1)} = \frac{\int d^3 r S^{(n+1)}}{\frac{1}{K^{(n)}} \int d^3 r S^{(n)}} \tag{2.10}$$

Solution of inhomogeneous diffusion equation in the presence of external source is important for evaluation of flux/power distribution in sub-critical reactor and this can be achieved by suitably modifying the iterative procedures used of eigenvalue evaluation. It is to be noted that contrary to eigenvalue problem wherein the ratio of fission source and lambda is maintained constant, in source problem only fission source is updated in outer iterations.

2.4. Time eigenvalue of neutron diffusion equation

Solution of the eigenvalue problem discussed in previous section is required for studying the criticality behaviour and for obtaining the stationary power distribution in nuclear reactors. Supercriticality, criticality or sub-criticality of a reactor is determined by the value of the largest value of λ often called fundamental lambda-eigenvalue which is identified with the effective multiplication factor K_{eff}. Besides the lambda-eigenvalue problem, there is another eigenvalue problem commonly referred to as the prompt time-eigenvalue or alpha-eigenvalue problem (Bell and Glasstone, 1970). In this problem, the eigenvalue appears in the form of a (positive or negative) 1/v absorber.

2.4.1. Prompt alpha eigenvalue

To define prompt α-eigenvalue problem, the space-energy and time dependent neutron flux is assumed to be exponentially varying in time as given below:

$$\phi^g(r,t) = \phi^g(r)\exp(\alpha t) \tag{2.11}$$

If the Eq.(2.11) is substituted in the multi-group time dependent diffusion equation Eq.(2.5), we obtain on separating the time variable from the space and energy variables,

$$F\phi - A\phi = \frac{\alpha}{v}\phi \tag{2.12}$$

The values of α for which non trivial solutions exist are called the α-eigenvalues and the corresponding solutions are the α-modes.

2.4.2. Prompt and delayed alpha eigenvalue

The time-dependent multi group neutron diffusion equation describing the flux distribution in various energy groups in a reactor in the presence of 6 groups of delayed neutrons is

$$\frac{1}{v^g}\frac{\partial \phi^g}{\partial t} = D^g \nabla^2 \phi^g - \Sigma_r^g \phi^g + \sum_{g' \neq g}^{G} \left(\Sigma_s^{g' \to g} \phi^{g'} \right) + (1-\beta)\chi_p^g \sum_{g'=1}^{G} \nu \Sigma_f^{g'} \phi^{g'} + \sum_{i=1}^{i=6} \chi_{di} \lambda_i C_i \tag{2.13}$$

$$\frac{\partial C_i}{\partial t} = \beta_i \sum_{g'=1}^{G} \nu \Sigma_f^{g'} \phi^{g'} - \lambda_i C_i \tag{2.14}$$

Eq.(2.13) and Eq.(2.14) can be written more compactly using the removal and fission operators as follows

$$\frac{1}{V}\frac{\partial \phi}{\partial t} = (1-\beta)\chi_p F\phi - A\phi + \sum_i \lambda_i \chi_{d_i} C_i \tag{2.15}$$

$$\frac{\partial C_i}{\partial t} = \beta_i F\phi - \lambda_i \chi_{d_i} C_i \tag{2.16}$$

To define the prompt and delayed α-eigenvalue problem, the space-energy and time dependent neutron flux is assumed to be exponentially varying in time as given below

$$\phi^g(r,t) = \phi^g(r)\exp(\alpha t) \tag{2.17}$$

$$C_i = C_{i0} e^{\alpha t} \tag{2.18}$$

If the Eq.(2.17) and Eq.(2.18) are substituted in multi-group time dependent diffusion equation and Eqs.(2.15) and (2.16), we obtain on separating the time variable from the space and energy variables,

$$(1-\beta)\chi_p F\phi + \sum_i \frac{\beta_i \lambda_i \chi_{di} F\phi}{(\lambda_i + \alpha)} - A\phi = \frac{\alpha}{V}\phi \qquad (2.19)$$

The values of α for which we obtain non trivial solution for flux and precursor concentration are called the α -eigenvalues and the corresponding solutions are called the α -modes.

2.5. Solution of space time kinetics equation

Time dependent spatial power distribution is required for the transient and safety analysis of reactors and this is normally obtained by solving the coupled time dependent multigroup neutron diffusion equation and equations for the precursor concentration as expressed by Eqs.(2.15) and (2.16). The numerical solution of these equations is obtained using various methods which have been discussed in detail in a book entitled "Nuclear reactor Physics" by W.M Stacey (Stacey, 2001). The solution methods (Sutton and Aviles, 1996) that are broadly categorised as: direct methods, space-time factorisation methods. In direct methods, neutron diffusion equations are converted to a set of first-order differential equations in each volume element and that can be solved by the finite difference method over small time interval for all volume elements and energy groups. During each of the time steps certain parameters are kept constant enabling the time dependent diffusion equation to be transformed into steady state equation. Indirect methods involve a factorization of the flux into space and time parts.

If we combine Eqs(2.15) & (2.16) and writing the group fluxes and precursor densities at every mesh point as a column vector ψ and writing the terms of the multigroup neutron and delayed

neutron precursor balance equations at each spatial point as a matrix H, the space time neutron kinetics equations can be written as a coupled set of ordinary differential equations

$$H\psi = \dot{\psi} \tag{2.20}$$

Forward-Difference Method

The simplest approximate solution to Eq.(2.20) is obtained by a simple forward difference algorithm,

$$\psi(p+1) = \psi(p) + \Delta \mathrm{t}\ \mathrm{H(p)}\psi(p)$$

where, $\psi(p+1), \psi(p)$ denote the values of column vector ψ at time t_{p+1} and t_p and $\Delta \mathrm{t} = \mathrm{t}_{p+1} - t_p$.

This algorithm suffers from a problem of numerical stability. Stable solution requires very small time steps. Numerical stability of the solution depends on fundamental and higher eigenvalues of operator H. It has been proved that for ensuring stability of the solution, $\left| (1-\omega_n \Delta t) \right|$ should be less than unity where ω_n $(n \geq 2)$ are higher eigenvalues of the operator H. Numerical studies have shown (Stacey W. M., 2001) that Δt necessary for convergence should be less than the reciprocal of $(\mathrm{v}^{\mathrm{g}}\Sigma_{\mathrm{a}}^{\mathrm{g}})$ which forces very small time steps (~10^{-7} sec) because of large neutron velocities in fast group.

Backward-Difference Method

The numerical stability problem associated with the preceding method can be all but eliminated by the backward-difference algorithm**:**

$$\psi(p+1) = [I - \Delta \mathrm{t}\ \mathrm{H(p+1)}]^{-1}\psi(p)$$

The method is unconditionally stable. The difficulty with the backward-difference method arises from the necessity of inverting a matrix at each time step. Thus, although much larger time steps

can be taken with the implicit method than with the explicit method, the computation time needed for the matrix inversions may more than offset this advantage. The size time step used in the backward-difference method is usually limited by the effect of truncation error accuracy of the solution rather than by numerical stability.

Alternating direction implicit method

For multidimensional problems, the matrix inversion associated with the implicit methods poses a formidable and time-consuming task. To reduce the time required for this matrix inversion, another technique is the alternating direction implicit (ADI) method**.** The basis of the ADI method is to make the algorithm implicit for one space dimension at a time and to alternate the space dimension for which the algorithm is implicit. Weight et al. (1971) have introduced an approximate solution of the multigroup neutron diffusion kinetics equations with delayed neutrons in two-dimensional geometry by matrix splitting methods based on an ADI scheme. However, this conventional ADI method is unstable for heterogeneous problems unless extremely small time steps are used. Recently, the suitability of the ADI method for parallel computation has been demonstrated by Chen et al. (1992). This method becomes extremely attractive for parallel computer applications. Since, it is based on the solution of a system of independent block-tridiagonal matrix equations that can be solved in parallel by improving the stability of the ADI method.

Improved Quasistatic method

The most popular of the indirect method is improved quasi-static method (IQS). In this method the time and space dependent neutron flux is expressed as the product of a shape function,

$\psi(r,E,t)$ which is slowly varying in time and a purely time dependent amplitude function, $T(t)$. In this method, we have to follow a normalization condition as given below.

$$\int \frac{\psi(r,E,t)\psi^*(r,E,t)}{V(E)} d^3r dE = \text{constant}$$

$\psi^*(r,E,t)$ is the adjoint flux that must be found via solution of the steady state adjoint diffusion equation during each time increment. After putting the time and space part of neutron flux in time dependent neutron diffusion and precursor concentration equations, the transient problem is expressed as an amplitude equation and a delayed precursor equation as given below.

$$\frac{dT(t)}{dt} = \left(\frac{\rho(t) - \bar{\beta}(t)}{\Lambda(t)} \right) T(t) + \sum_i \lambda_i C_i$$

$$\frac{dC_i(t)}{dt} = \left(\frac{\beta_i(t)}{\Lambda(t)} \right) C_i(t) + \lambda_l C_l(t)$$

The shape equation resembles the steady state diffusion equation. The kinetic parameters (Stacey, 2001) are defined in terms of direct and adjoint fluxes.

2.6. Monte Carlo methods

As seen in previous sections, deterministic transport or diffusion calculations require various approximations at different stages. The Monte Carlo method not only can handle the complex reactor geometry exactly and treat the neutron energy as a continuous variable. These codes are capable to mimic exact physical phenomena in the reactor. As a consequence Monte Carlo based simulation methods are more accurate. Hence Monte Carlo methods are much more appropriate for the analysis of ADSs because the tolerance in predicting quantities such as ks, k_{eff} throughout the burnup cycle is much lower. Here it is also important to mention that for noise based

reactivity assessment method, the analog Monte Carlo methods with point-wise cross-sections can provide lot of information that are seldom available with deterministic codes.

There is, an extensive literature devoted to Monte Carlo which provides a sound theoretical basis (Hammersley and Handscomb, 1967; Lux and Koblinger, 1991). Neutron transport calculations by Monte Carlo Methods (Forrest and William, 1984) are performed by following a large number of individual particle histories from birth to death with the help of number of probability distribution functions and scoring the results to form average quantities. The sampling process is carried out by generating pseudorandom numbers uniformly distributed on the unit interval. By applying a suitable transformation these are then transformed to obtain sample value of the desired variable over the range of interest and distributed according to the relevant probability distribution. A Monte Carlo calculation for a neutron transport problem consists of selecting a small number of source neutrons and observing their paths through a system. Neutrons are assumed to travel in straight lines between collisions. Distance between collisions is calculated from the mean free path. In analog Monte Carlo, the when a collision occurs, the decision concerning absorption is made probabilistically; if outcome is indeed absorption, the particle history is terminated, and if not, the particle history is continued. Any scoring during the random-walk consists of adding one to an appropriate tally bin.

In non-analog Monte Carlo, the PDF's derived from physical laws are altered, i.e. particle behaviour is biased to improve the chances of an eventual particle score in some place of interest. To avoid biasing the results, a particle weight is defined and this weight is altered in such a way as to conserve probability. It is the weight which is tallied for a particular event rather than one. Thus, in analog Monte Carlo, all particles which undergo a particular event

contribute a score of one to the tally of interest; in non-analog Monte Carlo, particle scores for particular events consist of the particle weight which may have been adjusted many times during the random-walk. The advantage of non-analog Monte Carlo is that more particles (with reduced weights) can be directed toward a phase space region of interest, increasing the number of particles contributing to a particular tally.

Considering the importance of reactivity monitoring in ADSs as discussed in chapter 1, there is increasing trend in the use of Monte Carlo methods in the recent years to simulate the experiments aimed at reactivity determination of sub-critical system. Ficaro and Wehe (1994), Valentine and Mihalczo, (1996) have successfully used analog Monte Carlo technique for reactor noise simulations. We also have developed an analog Monte Carlo Simulator to simulate pulse neutron and reactor noise experiments. Here it is worth mentioning that the reactor noise simulations by analog Monte Carlo technique in general take a long computation time. Recently Szieberth and Kloosterman (2004, 2010 a,b) have developed a theory and methods to apply the non-analog Monte Carlo simulations to neutron noise measurements by modifying conventional variance reduction techniques to make the non-analog Monte Carlo method possible for reactor noise simulations.

CHAPTER 3

Iterative Schemes for Obtaining Dominant Alpha-modes of Neutron Diffusion Equation

In chapter-2 we have described time eigenvalue of multigroup neutron diffusion equation and its importance in modal neutron kinetics, identification of suitable detector locations for noise based and pulse decay experiments conducted for reactivity determination. In this chapter we present some numerical schemes for the evaluation of alpha modes of diffusion equation. In section 3.1, the existing methods for the solution of alpha eigenvalue problems are briefly reviewed. In section 3.2, two newly developed methods are described. In section 3.3, numerical results obtained using these schemes are presented. In section 3.4, the relation between fundamental λ-eigenvalue, α-eigenvalue and prompt neutron generation time is discussed. We show that the relation is universal provided the generation time is defined appropriately.

3.1. Review of existing methods to find λ and α modes

The methods that have been developed can be classified into two classes: 1) Methods which exploit the fact that extreme (largest or smallest) eigenvalues are needed, and 2) other methods which are unrelated to this fact. The two classes are described separately in sections 3.1.1 and 3.1.2.

3.1.1. Methods for extreme eigenvalues

In case of λ-eigenvalue problem, usually one is interested in computing the largest λ-value called k_{eff}, next few dominant λ-values and corresponding eigenvectors. In α-eigenvalue problem as defined in chapter-2 by Eq.(2.12) (assuming that α's are real, which is generally true for dominant modes in diffusion theory), in general, α can be positive or negative. Algebraically the largest eigenvalue corresponds to the fundamental mode. It is positive, zero and negative for super-critical, critical and sub-critical reactor. If the reactor is sub-critical, all α-values are negative. In that case, the dominant α-values of interest are those with smallest magnitudes, corresponding to the slowest decay in time. It is possible to rewrite the λ and α eigenvalue problems given by Eqs.(2.7) and (2.12) as:

$$A^{-1}F\phi = \lambda\phi \tag{3.1}$$

$$[A-F]^{-1}V^{-1}\phi = -(\frac{1}{\alpha})\phi \tag{3.2}$$

For any physically realizable set of multigroup parameters, it is proved (Wachspress, E.L., 1966) that there is a unique real, positive eigenvalue of operator $A^{-1}F$ [Eq.(3.1)] which is greater in magnitude than any other eigenvalue. Though in general higher lambda eigenvalues can be complex, however we are often interested in only few dominant lambda eigenvalues and eigenfunction of physically realizable reactors which are generally positive.

So far as alpha eigenvalues are concerned, we have assumed that all alpha's are real, which is generally true for dominant modes in diffusion theory. In general fundamental alpha can be positive or negative depending upon sub-crititicality or supercriticality of a reactor. For a subcritical reactor fundamental alpha is negative, so all other higher time eigenvalues are

expected to be negative. Since the eigenvalues of $[A-F]^{-1}V^{-1}$ are $(-1/\alpha)$, hence we expect all eigen values of $[A-F]^{-1}V^{-1}$ [Eq.(3.2)] to be positive. The largest eigenvalue and eigenvector of these operators can be found by the Power Iteration method.

The Power Iteration method

It is well-known that the largest eigenvalue of any matrix P (with positive eigenvalues) can be found by **P**ower **I**teration (**PI**) method. In this method, one starts with a guess vector x. It is multiplied by P and normalized, repeatedly. The resulting vector gradually approaches the eigenvector of P corresponding to largest eigenvalue.

Use of PI for λ eigenvalue problem

In order to implement PI for Eq.(3.1), one needs a capability to multiply any flux vector x by the matrix operator $A^{-1}F$. This can be done (Duderstadt and Hamilton, 1976) as follows. First y = Fx is computed, which is fission source vector. Then, for finding $A^{-1}y$, one solves the following external source problem Eq.(3.3) using several methods such as Gauss Siedel, Krylog sub-space and LU decomposition method. However we have used Gauss Siedel method for solving the following equation:

$$Az = y \tag{3.3}$$

Here y is the source vector and the computed solution z is the flux vector. z is the required quantity $A^{-1}Fx$. Hence PI can be implemented to find the fundamental λ-mode. In fact, the PI method is the most common routine method used to find fundamental λ-mode solution of Eq.(3.1).

Use of PI for α eigenvalue problem

In order to implement the PI for Eq.(3.2), one should be able to compute $[A-F]^{-1}V^{-1}x$ for any guess flux vector x. For this, first, $y = V^{-1}x$ is computed. Then, $[A-F]^{-1}y$ is computed by solving an external source problem in multiplying medium defined by

$$(A-F)z = y \tag{3.4}$$

by using neutron diffusion code. Here y is the source vector and the computed solution z is the flux vector. z is the required quantity $[A-F]^{-1}V^{-1}x$. Hence, PI method can be implemented to find the most dominant mode. However, fundamental mode of Eq.(3.2) corresponds to largest ($-1/\alpha$) only for sub-critical reactors (Lathouwers, 2003). Thus, the method would be applicable only for sub-critical reactor. However, as will be seen later in section 3.2.2, this restriction can be removed and PI method can be used even for super-critical reactor.

Evaluation of next dominant λ and α modes

The above procedure to implement matrix vector product (by external source calculations) has to be supplemented with additional techniques to obtain a set of dominant modes of the matrix rather than just the fundamental mode. This has been done in three different ways in the literature as described below:

i) **Elimination method**: After finding fundamental mode by PI's, the contribution of fundamental mode is removed from guess vector. The continuation of PI's then leads to next dominant mode having second largest eigenvalue. The procedure is continued to find next dominant modes. This method has poor convergence for closely spaced

eigenvalues. Roy et al. (Roy et al., 1990) have used this scheme to find dominant λ-modes of a PHWR model in diffusion theory.

ii) **Sub-Space Iteration method (SSI):** One starts with a set of 'p' independent guess vectors rather than just one guess vector. The number p is slightly bigger than the number of required modes. By using the capability of finding product of matrix with these vectors, one first determines the sub-space spanned by dominant p eigenvectors. The p dominant eigenvectors can be easily obtained later by solving a small sized $(p \times p)$ matrix eigenvalue problem. This scheme has been used by Doring et al., Verdu et al., Modak et al. and Modak and Jain (Doring et al., 1993; Verdu et al., 1994; Modak et al., 1994; Modak and Jain, 1996) to find dominant λ-modes of neutron diffusion equation. The SSI method has much better convergence properties than elimination method.

iii) **Arnoldi Method:** This is a Krylov sub-space method. It also requires a capability to compute product of matrix (whose eigenvalues are to be found) with any given vector. Verdu et al. (Verdu et al., 1999) have used Arnoldi method to find dominant λ-modes of diffusion equation while Warsa et al. (Warsa. et al., 2004) have used it to find dominant λ-modes of 3-D transport equation. Lathouwers (Lathouwers, 2003) has found dominant α-modes of multi-group transport equation in which the matrix vector multiplication was found by solving external source problem in multiplying media. This method, however, does not seem to have been applied to the simpler case of α-modes of diffusion equation.

3.1.2. Other methods

The method based on Orthomin(1) algorithm belongs to this class. It was introduced by Suetomi and Sekimoto (Suetomi and Sekimoto, 1991) as an efficient alternative to power iteration method to find fundamental λ-mode. It is based on minimization of the norm of residual error vector by a gradient method. Modak and Gupta (Modak and Gupta, 2006, 2007) have shown that it can be used to find higher λ-modes as well as α-modes of diffusion equation by simply changing the initial guess vector.

Being based on completely different principles, Orthomin(1) method has some advantages and disadvantages relative to the methods in section 3.1.1. In Orthomin(1), the fact that extreme eigenvalues are needed is irrelevant. The evaluation of a selected higher mode does not require prior evaluation of any lower mode. Different eigensolutions can be computed completely independently by trying different guess vectors. Closely spaced eigenvalues do not have any direct effect on convergence. The disadvantage is that it is difficult to ensure that no eigenvalue is missed. Secondly, the robustness of algorithm needs to be studied for a range of cases. The α-modes obtained by Modak and Gupta (Modak and Gupta, 2007) by Orthomin(1) have been used to validate the proposed methods.

3.2. Proposed schemes for α - modes

The two proposed schemes are discussed in sections 3.2.1 and 3.2.2. The first scheme, called "1/v absorber method", is based on prior evaluation of λ-modes. The second scheme finds α-modes directly using the sub-space iteration method.

3.2.1. The 1/v absorber method

In this method, we solve the α eigenvalue problem by solving a sequence of lambda eigenvalue problems. For a particular eigenvalue α_i, Eq.(2.12) given in chapter-2 can be written as:

$$(A + \alpha_i / V)\phi = F\phi \tag{3.5}$$

However, this equation is identical to the λ-eigenvalue problem [Eq.(2.7) in chapter-2] if λ_i is replaced by 1.0 and A is replaced by $(A + \alpha_i / V)$. This shows that α_i is a number such that additional absorption by an amount α_i / V makes some eigenvalue λ_i equal to unity. This is true for all eigenvalues λ_i. Based on this, following procedure can be used to find α modes.

The j^{th} α -eigenvalue α_j is found as follows. First of all, j dominant λ-modes (λ_1, λ_2, … λ_j) for a given reactor model are found out by any one of the three methods listed in section 3.1. In the present work, the SSI method as described by Modak and Jain (Modak and Jain., 1996) was used. Then, certain guess value of α_j is chosen which can bring λ_j closer to unity and removal cross-sections of all materials in all groups are changed by α_i / V. The j number of λ-modes are again calculated by SSI. If λ_j is not unity, guess value of α_j is appropriately modified and the procedure is repeated till λ_j is close to 1.0 within certain error criterion. The corresponding α_j is desired eigenvalue and the flux distribution is the α-eigenvector.

All the above procedure is repeated for desired values of j = 1, 2, 3,…..,J. With this, J alpha modes are obtained. The starting guess for α_j can be inferred from the approximate formula $\alpha_j = (\lambda_j - 1)/ l$ with a reasonable value of lifetime *l*. This method is laborious since several λ-mode calculations are needed. It may not work for extremely large sub-criticalities because the

absorption cross section can become negative and hence inner iterations in SSI may not converge. Moreover this method is based on the assumptions that there is one to one correspondence between the α and λ-modes. This assumption might not be valid in all situations.

3.2.2. The modified power iteration method

3.2.2.1. Scheme for sub-critical reactor

Let us assume that the reactor being modeled is subcritical so that all alpha eigenvalues are negative. The dominant values are those with smallest magnitude (or slowest decay). The α eigenvalue equation is considered in the form of Eq.(3.2) in section 3.1.1. Thus, it is an eigenvalue problem for the matrix $M=[A-F]^{-1}V^{-1}$. The eigenvalues of M are $(-1/\alpha)$ which are all positive and largest values of $(-1/\alpha)$ form the dominant modes to be computed. In general, any of the three methods in section 3.1.1 can be used to find eigenvectors of M. Here, the SSI method is used since it is very efficient. This requires a capability to evaluate of product of M with any given flux guess vector x of size NG. As mentioned in section 3.1.1, this can be achieved by solving an external source problem in multiplying medium given by Eq.(3.4). M is a square matrix of order ($NG \times NG$), where N is number of mesh points and G is number of energy groups. In practical 3-D problems of multigroup diffusion equation, NG is very large. It is difficult to explicitly form the matrix M by inversion. Moreover, M will be a full matrix and its storage is difficult. On the other hand, while solving a source problem to find Mx, the sparsity of A and F is exploited. Thus effect of M on a vector is found without explicitly forming M.

3.2.2.2. Extension for Super-critical reactor

As mentioned earlier, the above scheme cannot be used straightaway for supercritical reactors for two reasons. Firstly, at least one of the dominant alpha eigenvalues will be positive while many

others will be large negative. The positive value need not be larger in magnitude than all the negative eigenvalues. Hence, the dominant modes required do not have largest/smallest magnitude. Therefore, neither power iteration nor any of the three methods mentioned in section 3.1.1 can be used to find the dominant modes. Secondly, the external source problem in multiplying medium given by Eq.(3.4) has no solution if the medium is super-critical.

This problem of super criticality is avoided by subtracting $(\beta/v)\phi$ from both sides of the α eigenvalue Eq.(2.12) where β is a suitable real constant.

This gives:

$$[-(A+\frac{\beta}{V})\phi + F\phi] = \frac{(\alpha-\beta)}{V}\phi \tag{3.6}$$

By choosing a suitable value of β one can assure the sub-criticality of reactor. Thus, $(\alpha-\beta)$ is negative for all modes. Then the procedure in section 3.3.1 can be used. Solution of eigenvalue Eq.(3.6) then gives $(\alpha-\beta)$ as eigen values. From this α eigen values can be calculated by addingβ.

3.2.3. Iteration steps

The full iteration scheme to obtain dominant alpha eigenvalues and eigenvectors is as follows:

(a) Let‘s’ be the number of α-modes to be found out. We choose p number of linearly independent vectors $x_m^1, x_m^2, x_m^3, ...x_m^p$ each containing NG elements. Here p is chosen such that it is more than‘s’. Here s and p both are much smaller than NG. The sub-script m is iteration index. For initial guess, the value of m is one. Let X_m denote an $NG \times p$ matrix formed by $x_m^1, x_m^2, x_m^3, ...x_m^p$ as columns.

(b) Let M stands for the term $\{ [A - F]^{-1} \}$ in Eq.(3.2). M and V^{-1} are $(NG \times NG)$ matrices. The matrix $(MV^{-1}X_m)$ is found out without explicitly knowing (MV^{-1}). The scheme runs as follows. The first column of (MV^{-1}) is estimated as detailed below:

Compute the $(NG \times 1)$ vector $V^{-1}x_m^1$. Now an external source of magnitude $V^{-1}x_m^1$ is assumed to be present in different meshes and energy groups. A source calculation is done using standard diffusion code and the steady state fluxes in all meshes and G energy groups are obtained. Steady state fluxes in all meshes and energy groups form the first column of $(MV^{-1}X_m)$. Similarly other column vectors matrix $(MV^{-1}X_m)$ are estimated. Thus after 'p' external source calculations, full matrix $(MV^{-1}X_m)$ is known. It is $NG \times p$ matrix

(c) The matrix $A_m = (MV^{-1}X_m)^T (MV^{-1}X_m)$ is calculated. A_m a small $(p \times p)$ matrix. Complete eigenvalue problem $A_m Q_m = Q_m \Delta_m$ is solved. Q_m is square matrix of order p formed by normalized eigen vectors of A_m. Here Δ_m is a diagonal matrix containing eigenvalues of A_m as diagonal elements.

(d) The matrix $T_m = Q_m (\Delta_m)^{-1/2}$ is evaluated.

(e) The matrix $X_{m+1} = (MV^{-1}X_m)$. T_m is estimated. The columns of this matrix form a set of 'p' orthonormal vectors denoted by $x_{m+1}^1, x_{m+1}^2, x_{m+1}^3, ...x_{m+1}^p$

(f) Steps (b-e) form one sub-space iteration.

(g) Step (f) is repeated till eigenvalues Δ_m and Δ_{m+1} are sufficiently close. At this stage, suppose $(n-1)^{th}$ iterations are over. After $(n-1)^{th}$ iteration X_n is known at the end of

step(e). From this, $(MV^{-1}X_n)$ is found out. The non-symmetric matrix B of order pXp, given by B= $X_n^T(MV^{-1}X_n)$ is found out. The full eigenvalue problem for matrix B is numerically solved.

$$BU = U\Lambda \tag{3.7}$$

U is a $(p \times p)$ square matrix containing the eigenvectors of B as columns, while the diagonal matrix Λ contains the eigenvalues of B, which are also the required eigenvalues of matrix (MV^{-1}). The eigen values of (MV^{-1}) will be in the form of $(-\frac{1}{\alpha_i})$ from which α_i can be found out.

(h) The matrix C = $(MV^{-1}X_n)$ U is evaluated. Its columns are the required eigen vectors of matrix (MV^{-1}).

(i) The required dominant eigenvectors of (MV^{-1}) are now already known. The elements of these column vectors represent the fluxes in all meshes and energy groups.

In the above scheme, the required number of dominant eigenvectors is obtained without any explicit evaluation of adjoint modes. In contrast, in the elimination method the adjoint modes are also required to find higher modes. Moreover, in sub-space iteration, all the required modes are calculated simultaneously. It is much more economical than the 1/v absorber method.

3.3. Numerical results

3.3.1. Problem description

In this section we present numerical results obtained by the two schemes described above. The α-eigenvalues and eigenfunctions of a 3-D realistic PHWR model given by Judd and Rouben (Judd and Rouben, 1981) are evaluated. This test case consists of two radial fuel zones in the XY plane surrounded by reflector (Figure-3.1). In the axial Z direction, the reactor extends up to 600 cm and has uniform material properties. There is no reflector in axial Z direction. The two-group cross-sections for two fuel zones and reflector given by Judd and Rouben (Judd and Rouben, 1981) are listed in Table-3.1. The spatial discretisation is done by using a total of 3240 meshes in XYZ geometry. Only one type of mesh structure (18x18x10) has been considered. The neutron velocities in fast and thermal groups are 10^7 cm/sec and $3x10^5$ cm/sec respectively. The two group fission spectrum is $\chi_1 = 1.0$ *and* $\chi_2 = 0.0$.

3.3.2. Results

3.3.2.1. Standard benchmark (near-critical case)

A total of nine dominant α-eigenvalues were calculated for the model (section 3.3.1) by both the proposed methods. The first 9 λ-modes had also to be calculated while implementing the 1/v absorber method. All the computed λ and α-eigenvalues are given in the Table-3.2. In the 1/v absorber method, which is a parameter search method, we have obtained eigenvalues only up to 4 significant digits. All the 9 λ-values computed in these studies agree with those given by Modak and Jain (Modak and Jain, 1996). The α-values computed by the two proposed methods also agree well with each other and with those given by Modak and Gupta (Modak and Gupta,

2007). The shapes of thermal flux in first, third and ninth α-modes in mid XY plane of the PHWR model have been plotted and are shown in Figures 3.2, 3.3 and 3.4.

It may be mentioned that the shapes α-modes are similar to those of corresponding λ-modes. The initial guess flux vectors for starting the iteration process (step a of section 3.2.3) were taken to be roughly similar to that of corresponding λ-modes. It is found that even randomly generated vectors numbers can be used as initial guess vectors. However, the convergence in that case is slower.

3.3.2.2 Highly sub-critical case

A case study for estimation of α-eigenvalues for a highly sub-critical reactor was also done. The PHWR test case was modified to make it highly sub-critical by reducing the value of fission spectrum χ_1 from 1.0 to 0.7. The χ_2 was kept 0.0 as before. Though it is right to correct ν rather correcting χ to recreate criticality but because the value of χ in two groups is 1.0 and 0.0 and value of $\nu\Sigma_f$ in second group is 0.0, the effect of altering χ is same as altering ν. We have evaluated three dominant α _ modes as well as λ-modes for this highly sub-critical reactor by SSI method. It is seen that even in this case of high sub-criticality, the shape of fundamental λ-mode is similar to that for the test reactor model with K_{eff} = 1.00355. On the other hand, the shape of α-mode for sub-critical reactor (Figure-3.5) is significantly different from shape in the test-case. Flux in α -mode of a highly sub-critical reactor is higher in reflector region than in the inner fuel region. This observation agrees with the earlier work by Modak and Gupta (Modak and Gupta, 2007). The peculiar flux shape is expected on physical grounds because while neutrons are rapidly lost by absorption in highly sub-critical core, they survive for a long time in the heavy water reflector. Moreover subtraction of (α / v) from removal cross-section in the reflector region

may make the effective removal cross-section very small or even negative and consequently enhancing the flux in the reflector region.

In all the calculations reported here, the point wise relative flux convergence criterion as well as the eigenvalue convergence criterion was 10^{-7}.

The modified power iteration based on sub-space iteration has very good convergence properties. If there are 'p' given vectors, the convergence of ith mode depends on (α_{p+1}/α_i). The problem due to closely spaced eigenvalues in the elimination/subtraction method is drastically reduced. Of course, Arnoldi method has also been shown to be highly efficient scheme for which free software is available. However, all 'p' calculations are completely independent and can be carried out in parallel. Thus SSI is very suitable for Coarse Grain paralleization and can give good speed-up.

3.4. Relation between fundamental k and α and definition of prompt neutron generation time Λ

A relation between the K_{eff} of a system, denoted by K and the fundamental eigenvalue α is often used to estimate K from the measured values of α by either pulsed neutron or noise based experiments. The relation is:

$$\alpha = \frac{(k-1)/k}{\Lambda} \tag{3.8}$$

The validity of this relation has been questioned for among others, highly subcritical systems (Perdu et. al., 2003). This is no doubt due to a simplistic calculation of the neutron lifetime i.e. without proper weighting, which is also true of the normal MCNP calculation of the neutron lifetime. For their analysis of pulsed neutron experiments at Yalina (Persson et al., 2005)

compute both k and α using MCNP and use Eq. (3.8) to define the neutron generation time. Even with proper adjoint weighting the relation Eq.(3.8) might not hold if the k and α modes are very different. However, we show that by use of a suitable weighting function in different contexts, we can define a generation time such that Eq.(3.8) is valid even if shapes of k and α-modes are vastly different.

Assume that the flux is in the fundamental alpha mode. If we take the scalar product of Eq.(2.12) in chapter-2 (section 2.3) with any arbitrary vector χ we get the following relation

$$\alpha = \frac{\left[1 - \frac{(\chi, A\phi)}{(\chi, F\phi)}\right]}{\left[(\chi, \frac{1}{V}\phi)/(\chi, F\phi)\right]} \tag{3.9}$$

If weight function χ is chosen such that

$$A^{+}\chi = \frac{1}{K}F^{+}\chi \tag{3.10}$$

i.e. as the adjoint eigenfunction of the fundamental lambda-mode, relation Eq.(3.8) follows with the following definition of the generation time (note that $K = \frac{(\chi, F\phi)}{(\chi, A\phi)}$)

$$\Lambda = (\chi, \frac{1}{V}\phi)/(\chi, F\phi) \tag{3.11}$$

then K in the Eq.(3.8) is same as K_{eff} of the system. Hence if we choose weight function χ to be the fundamental adjoint λ-mode and ϕ to be fundamental α-mode, the value of prompt neutron generation time Λ can be calculated with the help of Eq.(3.11) and the validity of the relation between α and K Eq.(3.8) can be established. Alternatively, if the flux is in the

fundamental lambda mode and we choose the adjoint alpha eigenfunction as the weighting function, by using similar argument, we can establish the validity of Eq.(3.8)

We have estimated prompt neutron generation times for standard PHWR test case and also for the highly sub-critical reactor system using Eq.(3.11) and checked the validity of Eq.(3.8). These results are given in Table-3.3. Λ obtained from Eq.(3.8) and Eq.(3.11) agrees exactly for near-critical case as well as for sub-critical case.

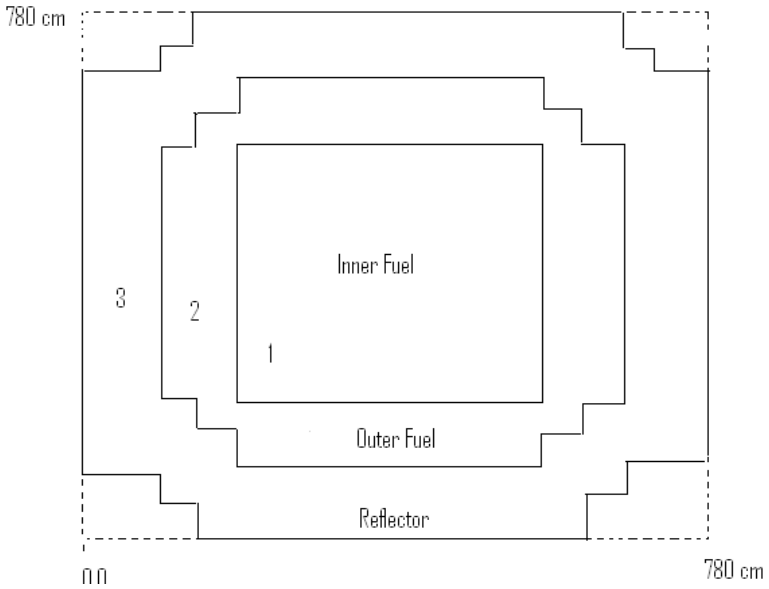


Figure-3.1: XY representation of PHWR test reactor

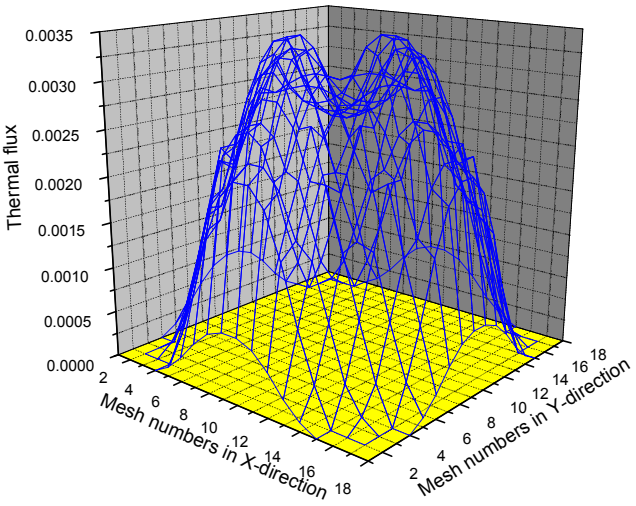


Figure-3.2: Shape of first alpha-mode in mid XY-plane

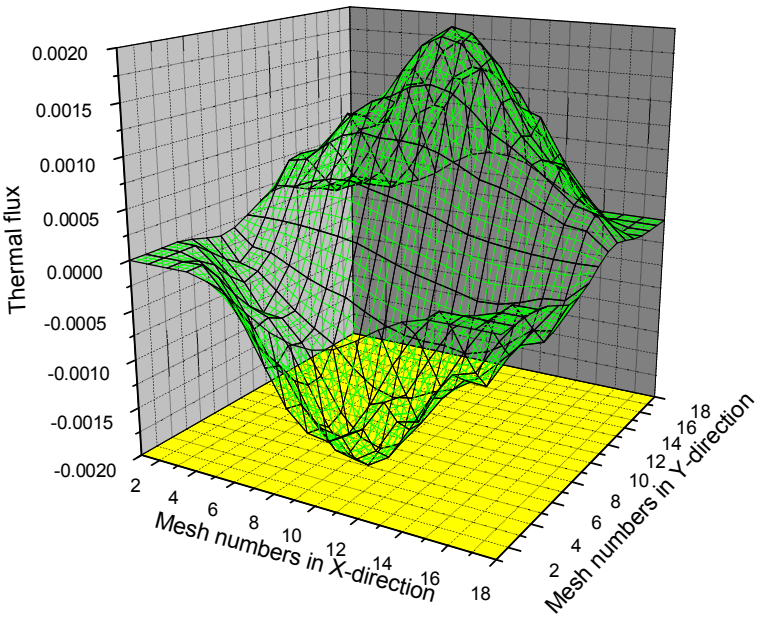


Figure-3.3: Shape of third alpha-mode in mid XY-plane

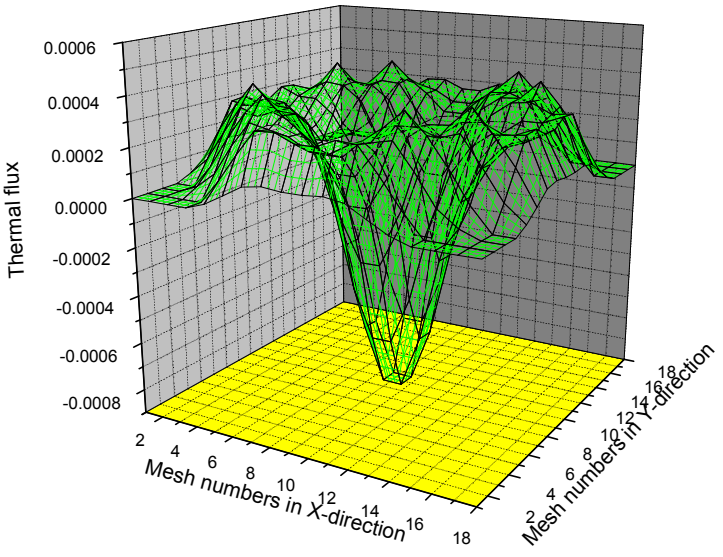


Figure-3.4: Shape of ninth alpha-mode in mid XY-plane

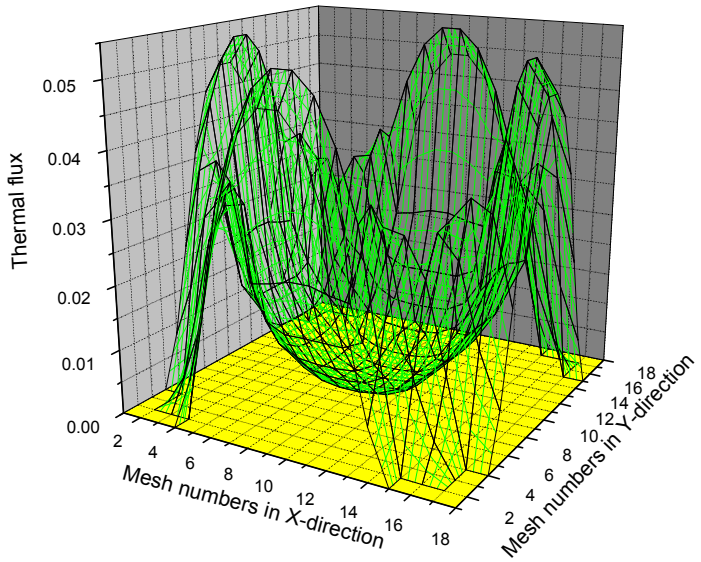


Figure-3.5: Shape of fundamental alpha-mode for highly sub-critical reactor

Table-3.1: Two group nuclear data in different regions of PHWR test reactor

Cross-section Type	Region-1 (inner fuel)	Region-2 (outer fuel)	Region-3 (reflector)
D1	1.2640E-00	1.2640E-00	1.3100E-00
D2	9.3280E-01	9.3280E-01	8.6950E-01
$\nu\Sigma_1^f$	0.0000E-00	0.0000E-00	0.0000E-00
$\nu\Sigma_2^f$	4.5620E-03	4.7230E-03	0.0000E-00
Σ_1^r	8.1540E-03	8.1540E-03	1.0180E-02
Σ_1^r	4.1000E-03	4.0140E-03	2.1170E-04
$\Sigma_{1\to2}$	7.3680E-03	7.3680E-03	1.0180E-02

Table-3.2: Comparison of alpha-eigenvalues obtained from different methods

Mode No.	λ	α^{*} (sec^{-1}) power iteration	α^{**} (sec^{-1}) 1/v absorber	α^{***} (sec^{-1}) Modak & Gupta
1	1.003555	4.06193	4.06	4.06182
2	0.990110	-11.11236	-11.11	-11.11245
3	0.990110	-11.11239	-11.11	-11.11245
4	0.973204	-31.24028	-31.24	-31.24051
5	0.966964	-36.70895	-36.71	---
6	0.964895	-38.89598	-38.90	---
7	0.960096	-45.78450	-45.80	-45.78395
8	0.960095	-45.78456	-45.80	---
9	0.938221	-71.42670	-71.40	---

Table-3.3: Prompt neutron generation time by two different methods

Case	Prompt neutron generation time (sec)	
	Λ_c	Λ_d
PHWR test reactor k=1.003555	0.000872086	0.000872099
Highly sub-critical reactor k=0.702488	0.002003580	0.002003590

CHAPTER 4

Iterative Schemes for Obtaining Dominant Prompt and Delayed Alpha-modes of the Neutron Diffusion Equation

The eigenvalue problems discussed in chapter 3 assume that all neutrons are prompt. For a complete description of a pulsed neutron experiment, however, the delayed neutrons should be taken into account in defining the eigenvalue problem. An expansion in these modes is more appropriate for describing transients in which delayed neutron effects are to be included. There have been a few studies for obtaining (Hoogenboom, 2002) alpha modes with the inclusion of delayed neutrons. However these evaluations have been limited to only fundamental modes. In this chapter we have the proposed method to evaluate higher prompt and delayed-alpha modes.

Substituting an exponential time dependence of the flux (as in the case of the alpha modes) results in the "delayed-alpha" eigenvalue problem, (also referred to as natural modes). Corresponding to each alpha mode there is one prompt mode and six delayed modes. In this chapter describe the numerical methods for the evaluation of alpha modes of diffusion equation including delayed neutrons. In section 4.1, we describe the method to evaluate fundamental alpha mode with delayed neutrons. In section 4.2, we discuss the method to evaluate higher alpha mode with delayed neutrons. In section 4.3, validation of the proposed method to evaluate higher alpha mode have been discussed. Numerical schemes for demonstration of the method are discussed in section 4.4.

4.1. Method to evaluate fundamental α with delayed neutrons

Eq.(2.19) given in chapter 2 can be rearranged to form an eigenvalue problem as under

$$\left[(1-\beta)\chi_p + \sum_i \frac{\beta_i \lambda_i \chi_{di}}{(\lambda_i + \alpha)}\right] F\phi - (A + \frac{\alpha}{V})\phi = 0 \tag{4.1}$$

In Eq.(4.1), the factor $\left[(1-\beta)\chi_p + \sum_i \frac{\beta_i \lambda_i \chi_{di}}{(\lambda_i + \alpha)}\right]$ can be interpreted as effective fission spectrum which is not normalized to unity. Eq.(4.1) can be written as a modified lambda-eigenvalue problem (with λ =1.0):

$$A'\phi = \frac{1}{\lambda} F'\phi \tag{4.2}$$

Where, $(A + \frac{\alpha}{V})\phi = A'\phi$ and $\left[(1-\beta)\chi_p + \sum_i \frac{\beta_i \lambda_i \chi_{di}}{(\lambda_i + \alpha)}\right] F\phi = F'\phi$

By assuming some initial guess value of α, we can solve Eq.(4.2) by the usual power iteration method to obtain the fundamental λ-eigenvalue of the Eq.(4.2). The value of α is repeatedly adjusted till the fundamental λ-eigenvalue of the Eq.(4.2) becomes unity.

The initial guess of alpha can be found by solving in-hour Eq.(4.3) given below.

$$\rho = \alpha\Lambda + \sum_{i=1}^{N} \frac{\beta_i \lambda_i}{(\alpha + \lambda_i)} \tag{4.3}$$

The reactivity ρ in this equation can be obtained from the solution of unmodified form of the λ-eigenvalue problem given by Eq.(4.2). By unmodified form, we mean Eq.(4.2) in which α =0.0 and χ_{di} is equal to χ_p.

Eq.(4.3) can be solved by polynomial solver and the roots of the polynomial give us the initial guess value of α. These values of α can be classified into two categories. Those of the order of decay constants of delayed neutron groups correspond to delayed modes. There is one value of α which is much larger in magnitude than the decay constants. It corresponds to the prompt α-mode.

The scheme for finding α is implemented as follows:

1. We make an initial guess of the value of α using Eq.(4.3).
2. We solve Eq.(4.2) using a standard criticality code to find the highest eigenvalue λ and the corresponding eigenvector.
3. If the eigenvalue is 1.0, then the guess value of α is the desired eigenvalue and the iteration is stopped.
4. If eigenvalue is not 1.0 then depending upon the value of λ, we reduce or increase the value of α and find another estimate for the highest value of λ using the criticality code. The search procedure to find α can be facilitated by the Regula Falsa algorithm.
5. We repeat the step 3 until we get λ equal to 1.0 to within 1.0E-05.

The steps 1-5 above are repeated for each α-value which is solution of Eq.(4.3). This gives us prompt as well as delayed α-modes corresponding to the fundamental spatial mode.

4.2. Method to evaluate higher α modes

A numerical method for calculating the higher α -modes has been developed. It makes use of the well-known subtraction method or elimination method to find higher modes of the λ-eigenvalue problem. This is explained in the Appendix 4A.

1. We first choose an initial guess value for alpha. The initial guess values for the prompt and delayed modes are taken from the solution of the in-hour equation, ρ is calculated using the K_{th} eigenvalue of the unmodified lambda eigenvalue problem. The generation time is assumed to be the same as for the fundamental mode. This does not cause any difficulty as we are only obtaining an initial guess value of alpha.

2. Using the guess value of α, obtain ϕ_K and ϕ_K^* and the eigenvalue λ_K corresponding to the modified eigenvalue problem Eqs.(4.1) and (4.2) by a elimination method (explained in Appendix 4A). If the value of λ_K equals 1.0 stop the calculation, otherwise make new guess on alpha and again find λ_K. The value of alpha for which the corresponding λ_K is 1.0 to within a specified accuracy, gives the final estimate of alpha and the corresponding ϕ_K and ϕ_K^* are the desired alpha-modes.

3. Step 2 is repeated for each guess value of α that was found in step 1. This gives one prompt mode and as many delayed modes as is the number of delayed groups.

4.3. Validation of the proposed method

To test the validity of the methodology for obtaining prompt and delayed-modes, described above, a simple 1-D problem with two energy groups and one group of delayed neutron is

solved using the proposed method as well as by a direct diagonalization of the matrix obtained after finite differencing of the diffusion equation for the problem. The number of matrix elements is small for the problem described above and this makes it possible to evaluate eigenvalue and eigenvectors directly.

The set of Eqs.(2.15) and (2.16) given [chapter-2] with two energy groups and one delayed neutron group can be written as a matrix eigenvalue equation as follows:

$$H\psi = \alpha\psi \tag{4.4}$$

where H is 3Nx3N matrix including fission, diffusion, removal, scattering and delayed neutron terms and ψ is 3Nx1 column vector representing two group fluxes and precursor concentration in all N meshes.

$$\psi = \begin{pmatrix} \varphi^1 \\ \varphi^2 \\ C \end{pmatrix} \tag{4.5}$$

and

$$\begin{pmatrix} v_1((1-\beta)\nu\Sigma_{f1} - A_1) & v_1(1-\beta)\nu\Sigma_{f1} & v_1\lambda I \\ v_2\Sigma_{1\to 2} & -v_2A_2 & 0 \\ \beta\nu\Sigma_{f1} & \beta\nu\Sigma_{f2} & -\lambda I \end{pmatrix} \tag{4.6}$$

Here $\Sigma_{1\to 2}$, $\nu\Sigma_{f1}$, $\nu\Sigma_{f2}$, I are NxN diagonal matrices corresponding to the 1st or 2nd group containing the respective cross section pertaining to a particular mesh, A_1, A_2 are the NxN matrices containing diffusion and removal terms.

The one dimensional slab reactor chosen for the purpose of testing is 450 cm thick and is represented by 18 meshes. In transverse directions leakages are assumed to be zero. With two energy groups and one group of delayed neutrons H is a 54x54 matrix. The two group cross-section data and delayed neutron data are summarized in Table-4.1. Since the matrix is small in size, the eigenvalue Eq.(4.4) is easily solved by a standard computer program. Orthogonal similarity transformations are used to reduce the matrix H in Hessenberg matrix and QR algorithm is used to compute the eigenvalues and eigenvectors of matrix H.

In Table-4.2 we compare the alpha eigenvalues for four prompt and four delayed modes by the direct diagonalization method and the proposed iterative method described in the previous section. The close agreement between the results by the two methods clearly shows the effectiveness of the proposed method.

4.4. Numerical studies for demonstration of the method

4.4.1. Problem description

In this section we describe the problem undertaken for demonstrating the method for computing the fundamental and higher alpha-modes with delayed neutrons. The pressurized heavy water reactor (PHWR) model problem described by Judd and Rouben (Judd and Rouben, 1981) is used for this purpose. The model problem consists of two radial fuel zones surrounded by a reflector (Figure-4.1). In the axial Z-direction, the reactor extends up to 600 cm and uniform material properties. There is no reflector in axial Z-direction. Three cases are studied for the purpose of the demonstration. The first is a study involving two energy groups and one delayed neutron group and is based exactly on the original problem description given by Judd and Rouben. The second study is in three energy groups and six delayed neutron groups and brings out the effect

of the difference in the spectra of prompt and delayed neutrons. Finally we have studied this three energy group case for a sub-critical reactor. The reactor is made sub-critical by increasing the burn-up of the fuel zones.

4.4.2. Evaluation of Alpha modes

4.4.2.1. Alpha modes in two energy groups

The two-group cross-sections for two fuel zones and reflector given by Judd and Rouben are listed in Table-4.3. The spatial discretisation is done by using a total of 3240 meshes in XYZ geometry. Only one type of mesh structure (18x18x10) has been considered. The neutron velocities in fast and thermal groups, the prompt and delayed neutron used for this calculation, fission neutron spectra and one group delayed neutron fraction and precursor decay constant are shown in Table-4.4. In the two group calculation, the fission neutron spectrum for delayed neutrons is assumed to be same as that for prompt neutrons. Figure-4.2 gives general shapes of modes in radial and axial directions.

A total of eight dominant α-eigenvalues, corresponding to the first four prompt and the first four delayed modes were calculated. All the computed prompt and delayed α-eigenvalues, are given in Table-4.8. The entries in brackets are the initial guess values used (corresponding to the roots of in-hour equation). The entries without braces are the converged values obtained by the parameter search method. The thermal components of the prompt and delayed α-modes in the central x-y plane of the reactor are shown in Figures-4.3-4.6. It can be seen that the difference between the prompt and the delayed modes is greater for the higher modes and this difference is most visible in the reflector region.

4.4.2.2. Alpha modes in three energy groups

To examine the effect of the softer spectrum of delayed neutrons (which cannot be seen in two energy groups) we have calculated three group diffusion theory parameters. The burn-ups in the two zones were adjusted such that the k_{eff} of the core in the three group calculation is close to that of the two group value. Two cases have been analysed. In first case we have considered one group of delayed neutrons and in the second case 6 groups of delayed neutrons have been considered. The three group cross-section for the two fuel zones and the reflector are given in Table-4.5. Delayed neutron data used are displayed in Table-4.6. The three group neutron kinetics data, the prompt and delayed neutrons spectrum used for this calculation are presented in Table-4.7.

For the case of one group of delayed neutrons, a total of eight dominant α-eigenvalues, corresponding to four prompt and four delayed modes were calculated. These are presented in Table-4.9. For the case of six groups of delayed neutrons, a total of 28 dominant α-eigenvalues corresponding to four prompt and 24 delayed modes were calculated. The 28 prompt and delayed α-eigenvalues are presented in Table-4.10. Two dimensional plots of thermal components of the prompt and delayed α-modes are displayed in Figures-4.7-4.10. From the figures it can be seen that the prompt and delayed modes are quite different. It can also be seen that the difference between prompt and delayed modes is more pronounced in the higher prompt and delayed modes.

4.4.2.3. Alpha-modes in three energy groups for a sub-critical reactor: Results

The third case study is for estimation of α-eigenvalues for a sub-critical reactor. The PHWR test case was modified to make it sub-critical by increasing the value of burn up in two zones. Three group cross-sections for two fuel zones and reflector given in Table-4.11. All other kinetic

parameters and delayed neutron data were kept same as given in Tables-4.6 and 4.7. We have obtained four prompt α-modes and 24 delayed modes for the sub-critical reactor as in the previous sub-section. The eigenvalues are presented in Table-4.12. Figures 4.11-4.14 show the two dimensional plots for the prompt and delayed modes. The difference in the nature of prompt and delayed modes is more pronounced for fundamental as well as for higher modes of sub-critical reactors. The fundamental prompt and delayed modes differ in the central as well as in the reflector regions of the core the case of a sub-critical reactor.

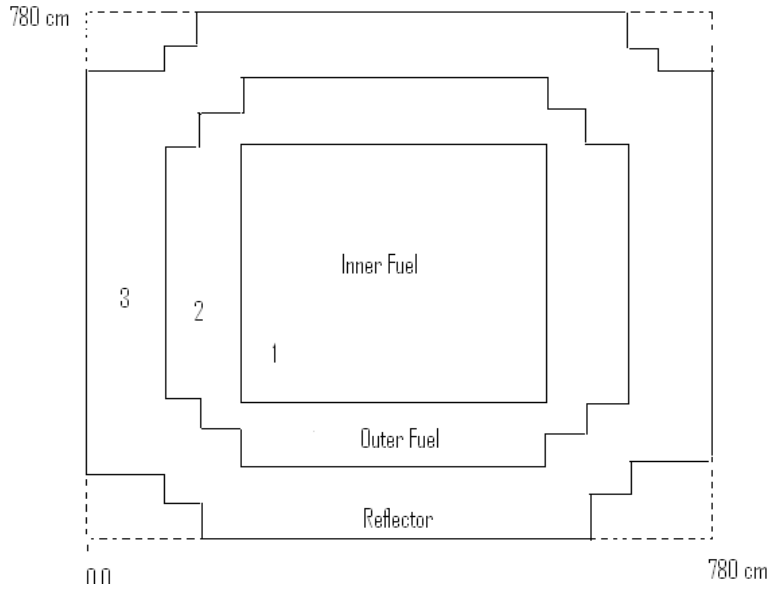


Figure-4.1: XY representation of PHWR test reactor

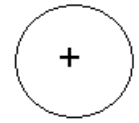
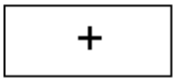
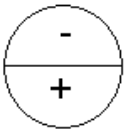
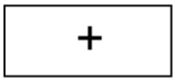
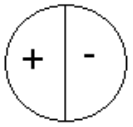
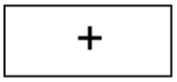
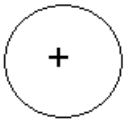
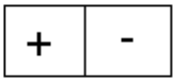
Mode No.	Schematic diagram		K-Eigenvalue
	Radial Plane(XY)	Axial direction(Z)	
1			1.0035548
2			0.9901118
3			0.9901118
4			0.9732067

Figure-4.2: Shape of various modes in radial and axial directions

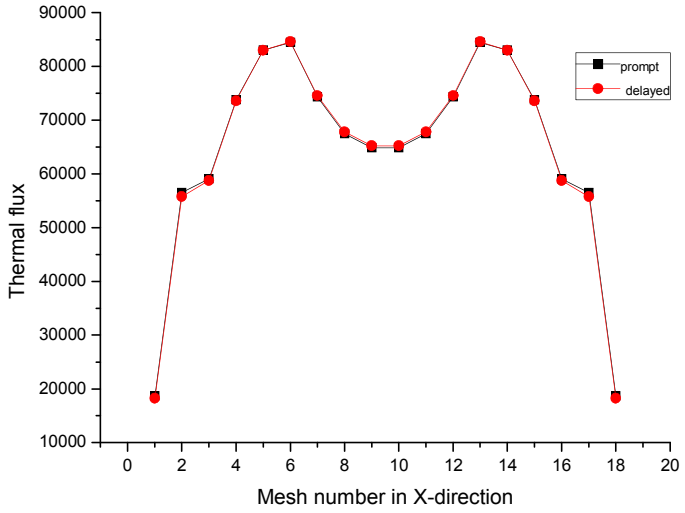


Figure-4.3: Fundamental prompt and delayed mode (2 group PHWR model, one group of delayed neutron) in X-direction

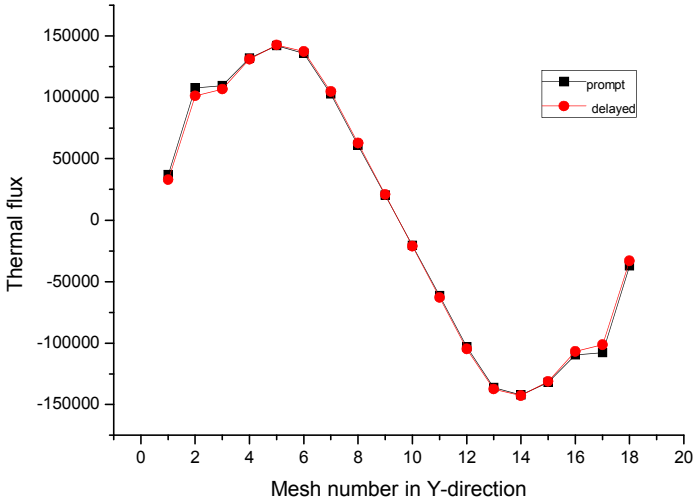


Figure-4.4: Second prompt and delayed mode (2 group PHWR model, one group of delayed neutron) in Y-direction

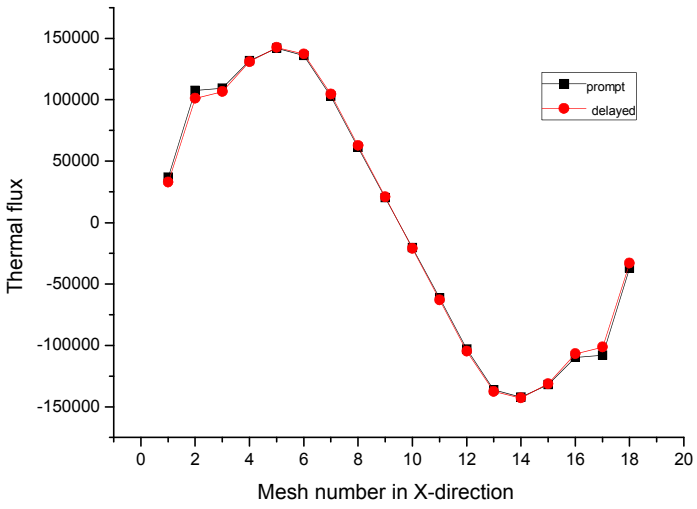


Figure-4.5: Third prompt and delayed mode (2 group PHWR model, one group of delayed neutron) in X-direction

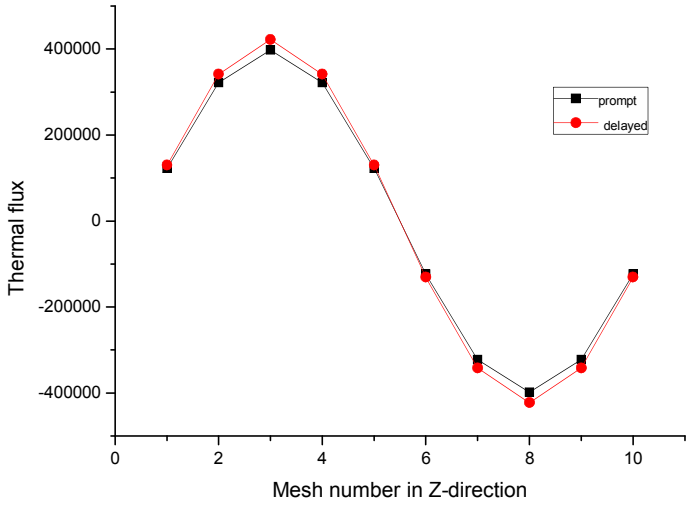


Figure-4.6: Fourth prompt and delayed mode (2 group PHWR model, one group of delayed neutron) in Z-direction

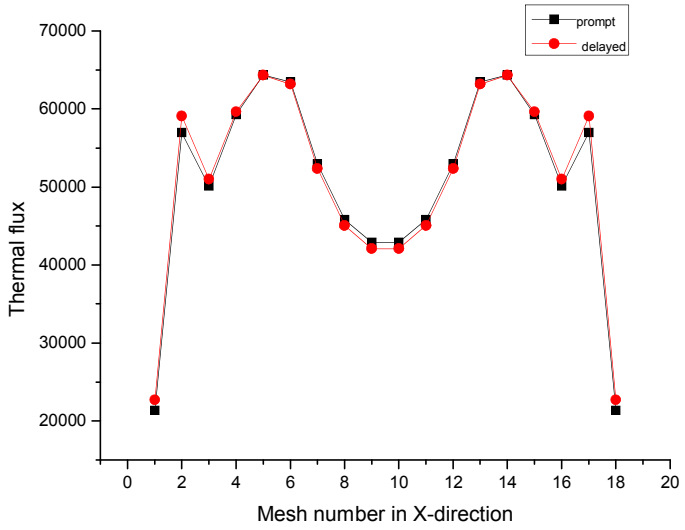


Figure-4.7: Fundamental prompt and delayed mode (3 group PHWR model, one group of delayed neutron) in X-direction

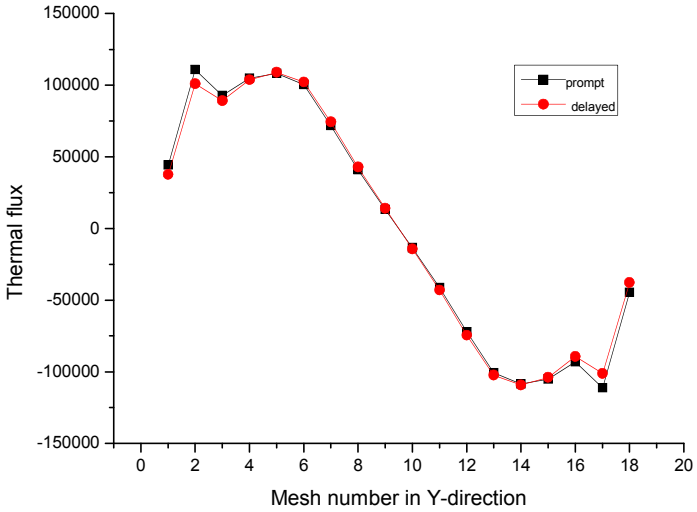


Figure-4.8: Second prompt and delayed mode (3 group PHWR model, one group of delayed neutron) in Y-direction

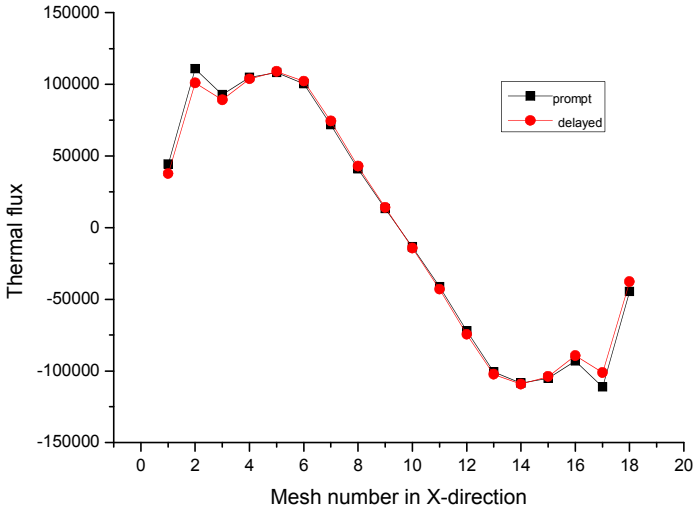


Figure-4.9: Third prompt and delayed mode (3 group PHWR model, one group of delayed neutron) in X-direction

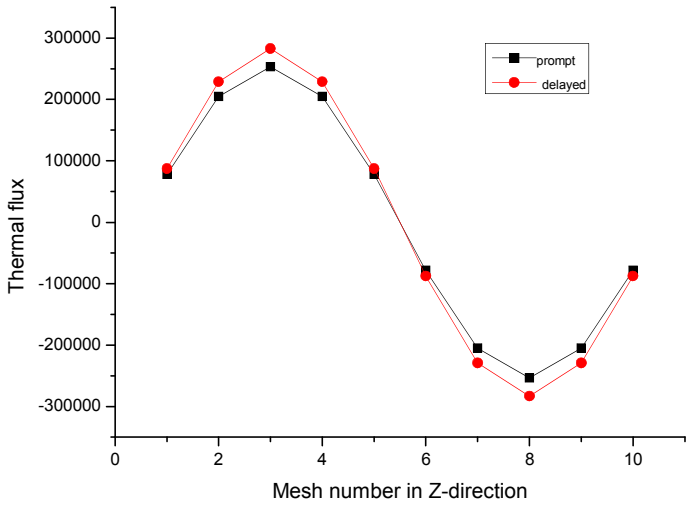


Figure-4.10: Fourth prompt and delayed mode (3 group PHWR model, one group of delayed neutron) in Z-direction

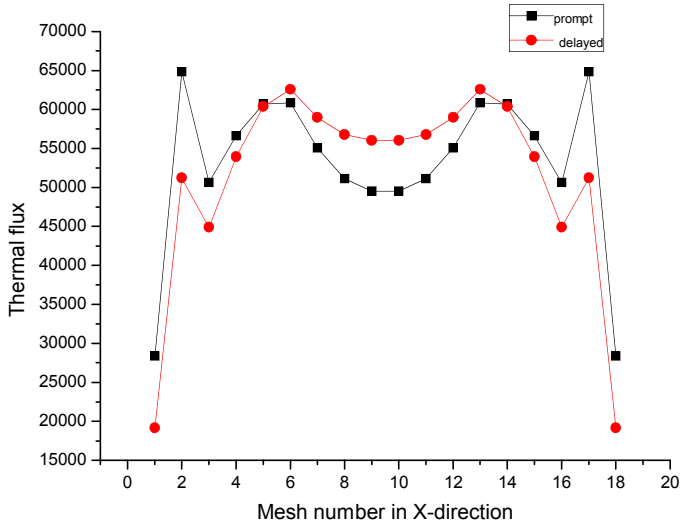


Figure-4.11: Fundamental prompt and corresponding first delayed modes (3group PHWR model, 6 group of delayed neutron) in X-direction: a case of sub-critical reactor

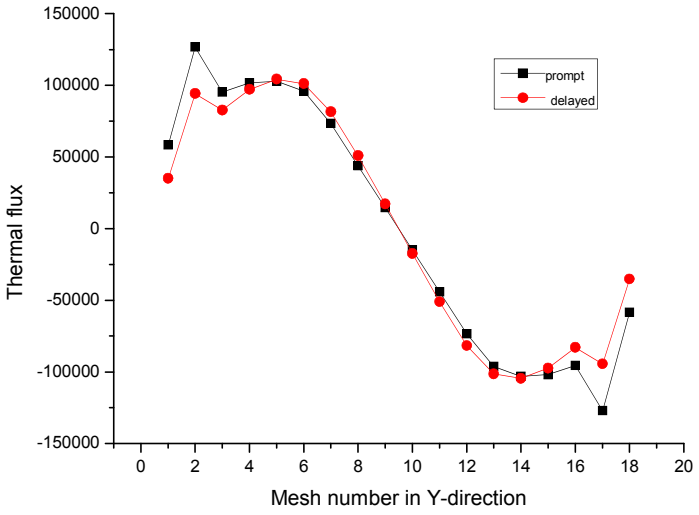


Figure-4.12: Second prompt mode and corresponding first delayed mode (3group PHWR model, 6 group of delayed neutron) in Y-direction: a case of sub-critical reactor

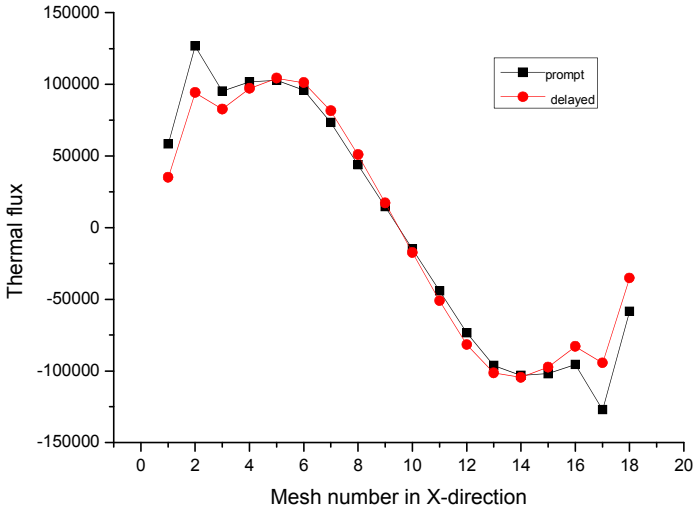


Figure-4.13: Third prompt mode and corresponding first delayed mode (3group PHWR model, 6 group of delayed neutron) in X-direction: a case of sub-critical reactor

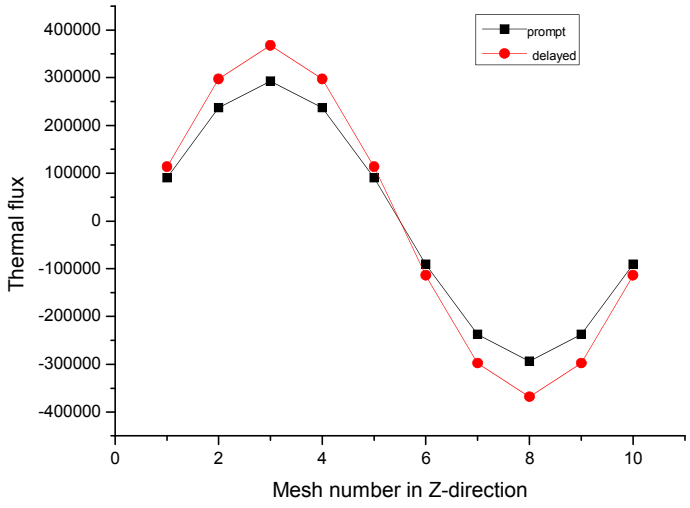


Figure-4.14: Fourth prompt mode and corresponding first delayed mode (3group PHWR model, 6 group of delayed neutron) in Z-direction: a case of sub-critical reactor

Table-4.1: Two group nuclear and delayed neutron data used for validation

Cross-section type	Values
D_1	1.2640E-00
D_2	9.3280E-01
$\nu\Sigma_f^1$	0.0000E-00
$\nu\Sigma_f^2$	4.5620E-03
Σ_r^1	8.1540E-03
Σ_r^2	4.1000E-03
$\Sigma^{1\to2}$	7.3680E-03
$\beta = 0.0065$	$\lambda = 0.084\ s^{-1}$

Table-4.2: Comparison of prompt and delayed modes for validation

S.No	λ -eigenvalue	Prompt alpha		Delayed alpha	
		Matrix method	Iterative method	Matrix method	Iterative method
1	0.98698	-23.834	-23.84	-0.0562	-0.0561
2	0.93516	-89.789	-89.77	-0.0768	-0.0770
3	0.85898	-195.31	-195.3	-0.0808	-0.0807
4	0.76976	-334.57	-334.6	-0.0822	-0.0824

Table-4.3: Two group nuclear data for PHWR model

Cross-section Type	Region-1 (inner fuel)	Region-2 (outer fuel)	Region-3 (reflector)
D_1	1.2640E-00	1.2640E-00	1.3100E-00
D_2	9.3280E-01	9.3280E-01	8.6950E-01
$\nu\Sigma_f^1$	0.0000E-00	0.0000E-00	0.0000E-00
$\nu\Sigma_f^2$	4.5620E-03	4.7230E-03	0.0000E-00
Σ_r^1	8.1540E-03	8.1540E-03	1.0180E-02
Σ_r^2	4.1000E-03	4.0140E-03	2.1170E-04
$\Sigma^{1\to2}$	7.3680E-03	7.3680E-03	1.0180E-02

Table-4.4: **Two group kinetics data**

Group Number	Group velocities(cm/sec)	Prompt spectrum	Delayed spectrum
1	$1.0x10^7$	1.0	1.0
2	$3x10^5$	0.0	0.0
Delayed neutron fraction (β) = 0.0065, Decay constant (λ) = 0.084 sec-1			

Table-4.5: Three group nuclear data for PHWR model (Near critical case)

Region-1			
Data	Neutron energy Group		
	g=1	g=2	g=3
D^g	2.413000E+00	1.2419000E+00	8.879800E-01
Σ_r^g	6.554500E-02	1.1445000E-02	4.976200E-03
$\nu\Sigma_f^g$	4.626100E-03	2.5413000E-04	5.565100E-03
Σ_{1g}	7.259560E-02	6.3543000E-02	0.0000000E+00
Σ_{2g}	0.0000000E+00	2.5696100E-01	9.530700E-03
Σ_{3g}	0.0000000E+00	8.2040000E-05	3.704080E-01
Region-2			
Data	Neutron energy Group		
	g=1	g=2	g=3
D_g	2.413700E+00	1.2426000E+00	8.8839000E-01
Σ_g^r	6.554500E-02	1.1445000E-02	4.8859000E-03
$\nu\Sigma_{fg}$	4.6280000E-03	2.8054000E-04	5.6811000E-03
Σ_{1g}	7.2550600E-02	6.3546000E-02	0.0000000E+00
Σ_{2g}	0.0000000E+00	2.5682300E-01	9.6041000E-03
Σ_{3g}	0.0000000E+00	0.8192900E-04	0.3703834E+00
Region-3			
Data	Neutron energy Group		
	g=1	g=2	g=3
D_g	2.517800E+00	1.2538000E+00	8.3990000E-01
Σ_g^r	8.185600E-02	1.2126000E-02	1.1557000E-04
$\nu\Sigma_{fg}$	0.000000E+00	0.000000E+00	0.000000E+00
Σ_{1g}	0.000000E+00	8.2083000E-02	0.0000000E+00
Σ_{2g}	0.0000000E+00	0.0000000E+00	0.000000E+00
Σ_{3g}	0.0000000E+00	4.4884000E-05	0.000000E+00

Table-4.6: **6 group delayed neutron data**

Group	1	2	3	4	5	6
B	0.000215	0.00142	0.00127	0.00257	0.00075	0.00027
λ (sec-1)	0.0124	0.0305	0.111	0.301	1.1	3.0

Table-4.7: 3 group kinetics data

Group Number	Group Velocities	Prompt spectrum	Delayed spectrum
1	1.95E+09	0.74522	0.0
2	9.15E+06	0.25478	1.0
3	3.18E+05	0.0	0.0

Table-4.8: PHWR model in 2 groups (one group of delayed neutron)

S.No	k-Mode	Alpha-mode without del neutron	Eigenvalue alpha-mode with one group of delayed neutron	
			prompt	Delayed
1	1.003555	4.061	-3.565 (-3.583)	0.0955 (0.0956)
2	0.9901115	-11.1126	-18.752 (-18.335)	-0.0508 (-0.05079)
3	0.9901113	-11.1126	-18.335 (-18.335)	-0.0508 (-0.05079)
4	0.9732065	-31.24	-38.56 (-37.9935)	-0.06793 (-0.067927)

Values in the bracket is the guess value

Table-4.9: PHWR model in 3 energy groups (one group of delayed neutrons) (Near critical case)

S.No	k-Mode	Alpha-mode without del neutron	Eigenvalue alpha-mode with one group of delayed neutron	
			Prompt	Delayed
1	1.001275	1.885	-7.841 (-7.892)	0.0171 (0.02019)
2	0.9918013	-11.837	-21.02 (-21.83)	-0.048 (-0.04694)
3	0.9918013	-11.837	-21.02 (-21.83)	-0.048 (-0.04694)
4	0.976771	-35.165	-44.49 (-44.033)	-0.06645 (-0.06594)

Values in the bracket is the guess value

Table-4.10: prompt and delayed alpha eigenvalues (for the PHWR model) in 3 energy groups (6 groups of delayed neutrons, near critical case)

Mode	Prompt	Delayed					
1	-8.2901	0.0211	-0.013534	-0.05851	-0.18028	-0.9557	-2.8111
2	-21.16	-0.01205	-0.026102	-0.09804	-0.24933	-1.04595	-2.9417
3	Do	do	do	do	do	do	do
4	-44.55	-0.012287	-0.02881	-0.1057	-0.2758	-1.07355	-2.97292

Table-4.11: Three group nuclear data for PHWR model (sub critical case)

Region-1			
Data	Neutron energy Group		
	g=1	g=2	g=3
D_g	2.41280E+00	1.24170E+00	8.87900E-01
Σ_g^r	6.55430E-02	1.14480E-02	4.99470E-03
$\nu\Sigma_{fg}$	1.90313E-03	1.01794E-04	2.26815E-03
Σ_{1g}	7.26091E-02	6.35420E-02	0.00000E+00
Σ_{2g}	0.00000E+00	2.57001E-01	9.51170E-03
Σ_{3g}	0.00000E+00	8.21140E-05	3.704230E-01
Region-2			
Data	Neutron energy Group		
	g=1	g=2	g=3
D_g	2.41320E+00	1.24210E+00	8.883900E-01
Σ_g^r	6.55460E-02	1.14410E-02	4.953900E-03
$\nu\Sigma_{fg}$	4.62720E-03	2.61910E-04	5.681100E-03
Σ_{1g}	7.25506E-02	6.35460E-02	0.0000000E+00
Σ_{2g}	0.0000000E+00	2.56823E-01	9.6041000E-03
Σ_{3g}	0.0000000E+00	0.8211400E-04	0.3704230E+00
Region-3			
Data	Neutron energy Group		
	g=1	g=2	g=3
D_g	2.517800E+00	1.2538000E+00	8.3990000E-01
Σ_g^r	8.185600E-02	1.2126000E-02	1.1557000E-04
$\nu\Sigma_{fg}$	0.000000E+00	0.000000E+00	0.000000E+00
Σ_{1g}	0.000000E+00	8.2083000E-02	0.0000000E+00
Σ_{2g}	0.0000000E+00	0.0000000E+00	0.0000000E+00
Σ_{3g}	0.0000000E+00	4.4884000E-05	0.0000000E+00

Table-4.12: Prompt and delayed alpha eigenvalues (for the PHWR model) in 3 energy groups [6 groups of delayed neutrons, sub-critical case]

Mode	Prompt	delayed					
1	-43.225	-0.01228	-0.02877	-0.01055	-0.2753	-1.07303	-2.9723
2	-56.96	-0.01232	-0.02933	-0.09804	-0.1073	-1.08307	-2.9804
3	do	do	Do	do	do	do	do
4	-79.09	-0.01223	-0.02965	-0.10828	-.2871	-1.08540	-2.9848

CHAPTER 5

Development of a 3-D Space Time Kinetics Code with Feedback

Prediction of reactor behavior during transient is one of important requirements for design and licensing of a nuclear reactor. Most popular of the available methods is point kinetic method which can analyze successfully many of the reactor transients. The codes MRIF, SECMOD (Ballaraman and Trasi, 1981; Secker, Jr., 1969) are based on the assumption that spatial flux shape does not change with time. For small reactors, this model may not lead to large errors in estimates of peak power densities. But in large reactors as well as in ADSs where space time effect is very important in determining fission power/temperature distribution in the reactor, the method does not provide accurate analysis. The motivation behind the development of 3-dimensional space time kinetics code is to analyze the dynamical behavior of large ADSs. Apart from power ADS analysis, it helps in simulating pulse neutron and noise experiments as shown in next chapter.

There is variety of numerical methods for solving space time kinetics equation. We have already provided a brief review of some of the methods popularly in use in chapter 2. With the advent of fast computation capability direct methods for solution of the space time kinetics equations are perhaps the most straightforward of the procedures for solving the time-dependent few group diffusion equation. We have developed a 3- dimensional reactor space time reactor kinetics code KINFIN (Singh K.P. et al., 2014) based on direct integration method. The validation of the method has been carried out by comparison of the results with existing 3-Dimensional PHWR

and LWR benchmarks. We have also developed thermal model which can be useful for analyzing feedback effects.

5.1. Theoretical model

In direct integration method, problem space is partitioned into a finite number of elemental volumes as described in Chapter 2 (section 2.2.2). Based on this spatial partitioning, one may then obtain spatially-discretized forms of coupled diffusion and precursor equations. Transient finite difference methods are simply the extension of the well known procedures for solving the static diffusion equation as described in Appendix 2A of Chapter 2. Using same discretization technique, the space time multigroup diffusion equation with delayed neutrons can be written as under

$$V^{-1}\frac{d\phi}{dt} = (1-\beta)\chi_p F\phi - M\phi + \sum_{i=1}^{N_d}\lambda_i\chi_{di}C_i \tag{5.1}$$

$$\frac{dC_i}{dt} = \beta_i F\phi - \lambda_i C_i \qquad (i = 1, ----N_d) \tag{5.2}$$

where $\phi = \phi(t)$ and $C_i = C_i(t)$

Combining Eqs.(5.1) and (5.2) we get

$$V^{-1}\frac{d\psi}{dt} = H\psi \tag{5.3}$$

where ψ is (G+Nd) element column vector and H is ((G+Nd)x(G+Nd)) operator matrix. We use a simple first order implicit scheme for evaluating the time derivative. Implicit time-differencing of Eq.(5. 3) leads to

$$\frac{\psi^{l+1} - \psi^{l}}{\Delta t} = H\psi^{l+1} \Rightarrow \psi^{l+1} = (I - V\Delta tH)^{-1}\psi^{l}$$

The implicit solutions are unconditionally stable and therefore permit the use of relatively large values of time step. However the solution of equation requires a very expensive matrix inversion

at each time step. So as in case of steady state calculation here also we apply iterative method for obtaining solution. The equations are modified to the iterative forms as given below:

$$V^{-1}\frac{(\phi^{l+1}-\phi^{l})}{\Delta t}=(1-\beta)\chi_p F\phi^{l+1}-M\phi^{l+1}+\sum_{i=1}^{N_d}\lambda_i\chi_{di}C_i^{l+1}$$

$$\frac{(C_i^{l+1}-C_i^{l})}{\Delta t}=-\lambda_i C_i^{l+1}+\beta_i\sum_{g'}^{G}\nu\Sigma_f^{g'}\phi_{g'}^{l+1}$$

$$C_i^{l+1}=\frac{C_i^{l}+\Delta t\beta_i F\phi^{l+1}}{1+\lambda_i\Delta t}$$

$$V^{-1}\frac{(\phi^{l+1}-\phi^{l})}{\Delta t}=(1-\beta)\chi_p F\phi^{l+1}+\sum_{i=1}^{N_d}\left(\frac{\chi_{di}\Delta t\lambda_i\beta_i F\phi^{l+1}}{1+\lambda_i\Delta t}\right)-M\phi^{l+1}+\sum_{i=1}^{N_d}\frac{\lambda_i\chi_{di}C_i^{l}}{1+\lambda_i\Delta t}$$

$$(M+\frac{I}{v\Delta t})\phi^{l+1}-(1-\beta)\chi_p F\phi^{l+1}-\sum_{i=1}^{N_d}\left(\frac{\chi_{di}\Delta t\lambda_i\beta_i F\phi^{l+1}}{1+\lambda_i\Delta t}\right)=\frac{I}{v\Delta t}\phi^{l}+\sum_{i=1}^{N_d}\frac{\lambda_i\chi_{di}C_i^{l}}{1+\lambda_i\Delta t}$$

$$\left[(M+\frac{I}{v\Delta t})-(1-\beta)\chi_p F-\sum_{i=1}^{N_d}\left(\frac{\chi_{di}\Delta t\lambda_i\beta_i}{1+\lambda_i\Delta t}\right)F\right]\phi^{l+1}=\frac{I}{v\Delta t}\phi^{l}+\sum_{i=1}^{N_d}\frac{\lambda_i\chi_{di}C_i^{l}}{1+\lambda_i\Delta t} \qquad (5.4)$$

Eq.(5.4) is similar to solving a source problem ($M'\phi-F'\phi=S$)

where, $M'=(M+\frac{I}{v\Delta t})$, $F'=(1-\beta)\chi_p F+\sum_{i=1}^{N_d}\left(\frac{\chi_{di}\Delta t\lambda_i\beta_i}{1+\lambda_i\Delta t}\right)F$, $S=\frac{I}{v\Delta t}\phi^{l}+\sum_{i=1}^{N_d}\frac{\lambda_i\chi_{di}C_i^{l}}{1+\lambda_i\Delta t}$

Initial starting source is given as under:

$C_i^0=\beta_i F\phi^0$, $S^0=\frac{I}{v\Delta t}\phi^0+\sum_{i=1}^{N_d}\frac{\lambda_i\chi_i^d C_i^0}{1+\lambda_i\Delta t}$, Here ϕ^0 critical steady state flux distribution

5.2. Description of computer code KINFIN

Computer code 'KINFIN' is finite difference based reactor kinetics code written in FORTRAN-77. The code is based on mathematical model as described in section 5.1. 'KINFIN' can simulate transient and steady state scenarios in reactors of rectangular pitch. The code can be used for

analyzing transients in PHWRs, LWR and sub-critical reactors. It can take variable meshes in X-Y-Z direction and also can simulate prompt and delayed neutrons in any group. One, two and three dimensional core models can be easily represented by using appropriate boundary conditions. Few group nuclear data generally computed by transport theory code WIMS, reactor core dimensional description mostly in the form of mesh width in X-Y-Z direction are major input data of the software. The time dependent insertion of reactivity devices in the core is modeled by changing the nuclear data of affected meshes where these reactivity devices pass through.

5. 3. Application to three dimensional reactor problems without feedback

5.3.1. The Three-dimensional PHWR Kinetic Problem (Judd and Rouben, 1981)

The description of the problem

This benchmark problem models a super delayed-critical transient for a very small reactivity insertion rate. The asymmetric insertion of reactivity devices is taken as protection system to arrest the transient. The reactivity initiated accident has been modeled by linear decrease in the thermal absorption cross-section. The absorber rods begin to move in horizontal (-Y) direction at 0.6 sec. The transient is studied for a total time of 2.5 sec. Maximum ~6.5 mk positive reactivity is added in the reactor. The geometrical and material descriptions of the initial and perturbed core of the benchmark are depicted in Figures 5.1-5.5. The relevant nuclear data for the problem is given in Tables-5.1&5.2.

The positive reactivity insertion due to the LOCA is simulated by decreasing the thermal absorption cross-section in regions 5, 6, 10, 11, 17, 18, 22 and 23 in the following way:

$$\frac{\partial \Sigma_2}{\partial t} = \begin{Bmatrix} -1.0\text{E}-04 \quad (\text{cm.s})^{-1} \quad \text{for } t \le 0.4\text{sec} \\ -8.88889\text{E}-06 \quad (\text{cm.s})^{-1} \text{for } t > 0.4\text{sec} \end{Bmatrix}$$

The negative reactivity due to asymmetric insertion of shutdown devices is simulated by adding $\Delta\Sigma_2 = 6.15\text{E}-04 \quad \text{cm}^{-1}$ to the thermal absorption cross-section in regions 2, 4, 7, 9, 12, 14, 16, 18, 19 and 21-24. The absorber insertion starts at 0.6 sec with a constant velocity of 520 cm sec^{-1} in the Y-direction. The moving absorber boundary is parallel to the X-Z plane. The change in cross-section is additive whenever perturbation overlap. The combined result of the positive reactivity due to the LOCA and the negative reactivity due to the asymmetric insertion of shutdown devices makes the transient a super delayed-critical transient.

Results and discussions

The three dimensional code KINFIN was used to model the PHWR problem described in Section-5.3.1. Different node sizes were used in the code, 60 cm inside the core and 30 cm near the reflector. The reactor core and reflector region (780*780*800 cm) were represented by a total 3240 meshes. Though the code has an option for estimating the suitable time step depending upon power variation, the uniform time step of 1 milli second has been chosen for all flux/power calculation during transient. Average power of reactor and thermal flux shapes during transient were compared with results given by code CERKIN (Judd and Rouben, 1981). The static multiplication factors (Table-5.3) estimated by both methods are in close agreement. The thermal and fast fluxes at various time points were estimated by KINFIN. The values were in close agreement with the values as estimated by CERKIN code. Figure-5.6 shows the variation of average power density as a function of time for this transient obtained by KINFIN and CERKIN.

5.3.2 The LMW problem

The description of the problem

This problem (Langenbuch, et al., 1977) is related with an operational transient in a LWR for a very small reactivity insertion rate in square geometry. This problem has been solved taking prompt neutrons in two energy groups and 6 delayed neutron precursors groups. The core configuration and the control rods positions are shown in Figures-5.7 & 5.8. The core is composed of two kinds of fuel regions surrounded by water reflector. The relevant nuclear data for the problem is given in Tables-5.4. The control rods of the rod group 1 are inserted from the upper water reflector to the axial mid-plane of the core, and the control rods of the rod group 2 are set in the upper axial reflector in the initial state. Transient is initiated by withdrawing the control rods of the rod group 1 at the constant speed of 3 cm/sec until they are fully withdrawn. At 7.5 sec into the transient, the control rods of the group 2 start to move in at the same speed and continue to move in for 40 sec.

Results and discussions

The quarter core was represented in code KINFIN. The core dimension in X-Y directions are 220 cm whereas in Z-direction it extends up to 200 cm. The uniform mesh size of 10 cm has been chosen to represent the quarter core in KINFIN. A total of 1210 meshes are used to represent the quarter core.

The reference solution was calculated by the CUBBOX code with a time step of 0.125 sec. The time variation of the average power as well as the power densities at some places of the reactor was compared. The time variation of average power density in the core has been plotted in

Figure-5.9. Table-5.5 gives the comparison of the average power as predicted by KINFIN and for CUBBOX.

5.4. Inclusion of feedback effects

Analyses of nuclear reactor safety have increasingly required coupling of full three dimensional neutron kinetics core model with system transient thermal hydraulics code. The objective of thermal- hydraulic model is to obtain fuel pellet, clad and coolant temperature distribution under steady state and transient conditions. The results will be used for calculating reactivity feedback due to voiding and Doppler effect. The thermal hydraulic feedback mechanism is primarily provided through cross sections to the space time neutron kinetics code that are temperature and density dependent. Through the space time kinetics code the power distribution in the reactor is estimated and the estimated power distribution is the input to thermal hydraulic module. The temperature effects are described by considering distinct temperatures corresponding respectively to the coolant fuel and clad. This enables reactivity feedback to include all the major contributions, namely, moderator temperature/density effects and fuel temperature effects and thus permits a more realistic description of various transients in critical or sub critical ADS reactors.

We have chosen a simple thermal hydraulic model as the aim is to obtain various reactivity feedbacks to the space time kinetics code rather than a detailed thermal hydraulic analysis of the reactor. To demonstrate these effects, a typical tank type research reactor with pin/cluster type fuel elements rectangular cooled and moderated with heavy/light water was selected as a reference reactor. For other coolant such as Lead-Bismuth used in ADS, various correlations evaluating heat transfer coefficients have been included in the code. The theoretical thermal

hydraulic model and temperature evaluation methodology are discussed in the following sections.

5.4.1 Theoretical modeling

The reactor core is modeled by parallel cooling channels which can describe one or more fuel elements. The parallel channels are coupled hydraulically by the condition of equal pressure drop over all core channels. The assumptions in the modeling are as below

(i) The core fuel element and coolant channels are essentially intact

(ii) No heat transport between sub-channels

(iii) Pressure change induced by boiling in one sub-assembly does not affect other sub-assemblies

For the fuel heat transfer model, since heat conduction is of relatively small importance in the axial and circumferential direction for the class of problems under consideration, a radial one-dimensional heat-flow model has been adopted, with the channel divided into axial segments, temperature calculations being performed for each of the segments in succession following the direction of coolant flow. The radial gaps between typical fuel elements envisaged would be filled with either gas or liquid metal. Following figure represents a typical fuel element and coolant clad corresponding to one sub-assembly.

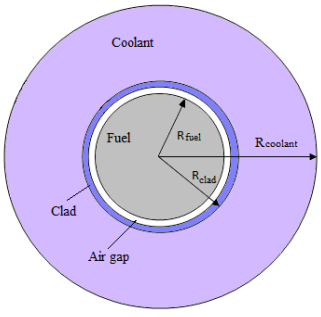


Figure: Cylindrical Fuel-Clad-Coolant system

The time-dependent radial temperature profile is obtained by solving the conduction equation (Todreas and Kazimi, 2011, Nikolay, 2009) in cylindrical geometry.

The Fourier conduction equation for cylindrical fuel is

$$\rho \mathrm{Cp} \frac{\partial T}{\partial t} - \frac{1}{r} \frac{\partial T}{\partial r} \left(\lambda r \frac{\partial T}{\partial r} \right) = \dot{q}''' \tag{5.5}$$

where, ρ is density, Cp is specific heat and λ is the thermal conductivity. To solve this equation by finite difference the fuel region is divided in N radial zones. Thermo dynamical properties averaged over temperature and space of each zone is taken into account for finite difference equation. Volume average temperatures i.e T_1, T_2, T_N and corresponding average radius i.e. $\overline{r}_1$, .., $\overline{r}_i$,…, $\overline{r}_N$ are determined for each zone. For i^{th} annular zone the average radius is defined as $\overline{r}_i^2 = \frac{(r_i^2 + r_{i+1}^2)}{2}$. Similarly effective conductivity λ_{ij} between i^{th} and j^{th} zones are estimated.

Integrating (5.5) from $r = 0$ to $r = r_1$

$$\rho \mathrm{Cp} \frac{\partial T}{\partial t} = \dot{q}_1''' + \lambda \frac{2}{r_1} \frac{\partial T}{\partial r} \tag{5.6}$$

The L.H.S is the time dependent heat energy. The first term of R.H.S is the heat generation rate per unit volume in zone 1 and the second term is the heat loss rate to outer zone per unit volume. To develop finite difference equation we replace $\lambda \frac{\partial T}{\partial r}$ by volume averaged $\overline{\lambda}_{12} \frac{T_2 - T_1}{\overline{r}_2 - \overline{r}_1}$ in (5.6). where, T_1 & T_2 are volume averaged temperatures of zones 1 & 2. Similarly, $\overline{r}_1$ & $\overline{r}_2$ are average radii of zones 1 & 2. λ_{ij} is the effective conductivity between i^{th} and j^{th} zones. For central zone of the fuel i.e. for *i=1*, the finite difference equation is given by

$$\rho_1 \mathrm{Cp}_1 \left(\frac{T_1^{k+1} - T_1^k}{t^{k+1} - t^k} \right) = \dot{q}_1''' - \bar{\lambda}_{12} \frac{2}{r_1} \left(\frac{T^k{}_1 - T^k{}_2}{\bar{r}_2 - \bar{r}_1} \right) \tag{5.7}$$

For annular zones, integrating (5.5) from $r = r_i$ to $r = r_{i+1}$ .The indices k stands for kth time step.

of the fuel i.e. for zones *i*=2, 3, .. , N-1, the finite difference equation has the form

$$\rho_i \mathrm{Cp}_i \left(\frac{T_i^{k+1} - T_i^k}{t^{k+1} - t^k} \right) = \dot{q}_i''' + \bar{\lambda}_{i-1,i} \frac{2r_{i-1}}{\left(r_i^2 - r_{i-1}^2 \right)} \left(\frac{T^k{}_{i-1} - T^k{}_i}{\bar{r}_i - \bar{r}_{i-1}} \right) - \bar{\lambda}_{i,i+1} \frac{2r_i}{\left(r_i^2 - r_{i-1}^2 \right)} \left(\frac{T^k{}_i - T^k{}_{i+1}}{\bar{r}_{i+1} - \bar{r}_i} \right) \tag{5.8}$$

For outer zone of the fuel i.e. for *i*= N, the finite difference equation has the form

$$\rho_i \mathrm{Cp}_i \left(\frac{T_i^{k+1} - T_i^k}{t^{k+1} - t^k} \right) = \dot{q}_i''' + \bar{\lambda}_{i-1,i} \frac{2r_{i-1}}{\left(r_i^2 - r_{i-1}^2 \right)} \left(\frac{T^k{}_{i-1} - T^k{}_i}{\bar{r}_i - \bar{r}_{i-1}} \right) - \frac{2}{\left(r_i^2 - r_{i-1}^2 \right)} \left(\frac{T^k{}_i - T^k{}_{clad}}{R_{th,FC}} \right) \tag{5.9}$$

where, $R_{th,FC}$ is the effective thermal resistance between fuel-clad interface

$$R_{th,FC} = \frac{1}{\lambda_{fuel}} \ln \left(\frac{R_{fuel}}{\bar{r}_N} \right) + \frac{1}{\lambda_{air}} \ln \left(\frac{R_{fuel} + \delta_{gap}}{R_{fuel}} \right) + \frac{1}{\lambda_{clad}} \ln \left(\frac{R_{fuel} + \delta_{gap} + \delta_{clad}/2}{R_{fuel} + \delta_{gap}} \right) \tag{5.10}$$

For clad to coolant heat transfer, the finite difference equation has the form

$$\rho_i \mathrm{Cp}_i \left(\frac{T_i^{k+1} - T_i^k}{t^{k+1} - t^k} \right) = \dot{q}_i''' + \frac{2}{\left(R_{clad}^2 - R_{fuel}^2 \right)} \left(\frac{T^k{}_i - T^k{}_{clad}}{R_{th,FC}} \right) - \frac{2}{\left(R_{clad}^2 - R_{fuel}^2 \right)} \left(\frac{T^k{}_{clad} - T^k{}_{coolant}}{R_{th,C}} \right) \tag{5.11}$$

where, $R_{th,C}$ is the effective thermal resistance between clad-coolant interface.

$$R_{th,C} = \frac{1}{\lambda_{clad}} \ln \left(\frac{R_{clad}}{R_{clad} - \delta_{clad}/2} \right) + \frac{1}{R_{clad} H_{eff}} \tag{5.12}$$

H_{eff} is the heat transfer coefficient for clad-coolant interface

5.4.2 Heat transfer coefficient

5.4.2.1 Single phase flow of the coolant

Heat transfer coefficient for single phase flow of coolant in the heated channel is expressed as

$$H_{eff} = \frac{N_u \lambda}{D_e} \tag{5.13}$$

where, N_u is Nusselt number, λ is thermal conductivity and D_e is the effective hydraulic diameter of the flow channel. Nusselt number is calculated using Dittus - Boelter correlation (Dittus and Boelter, 1930)

$$N_u = 0.023 R_e^{0.8} P_r^{0.4} \tag{5.14}$$

$$\text{where, Reynolds Number, } R_e = \frac{\rho V D_e}{\mu}$$

$$\text{Prandtl Number, } P_r = \frac{C_p \mu}{\lambda}$$

$$\text{And, } D_e = \frac{4 \times \text{Flow area}}{\text{Wetted perimeter}}$$

5.4.2.2 Two phase flow of the coolant

In case of two phase-flow of the coolant, the heat transfer coefficient has two component viz. convective part and nucleate boiling part (Chen, 1963). Therefore the total heat transfer coefficient is written as sum of two component i.e.

$$H_{2\phi} = h_c + h_{NB} \tag{5.15}$$

The convective part is a modified Dittus-Boelter correlation given by

$$h_c = 0.023 \left(\frac{G(1-x) D_e}{\mu_f} \right)^{0.8} P_{rf}^{0.4} \frac{\lambda_f}{D_e} F \tag{5.16}$$

where, $F = 1 \quad for \quad \frac{1}{X_{tt}} < 0.1$

$$F = 2.35 \left(0.213 + \frac{1}{X_{tt}} \right)^{0.736} \quad for \quad \frac{1}{X_{tt}} > 0.1$$

and, $$\frac{1}{X_{tt}} = \left(\frac{x}{1-x} \right)^{0.9} \left(\frac{\rho_f}{\rho_g} \right)^{0.5} \left(\frac{\mu_g}{\mu_f} \right)^{0.1}$$

The steam flow quality *x* is defined as $x = \frac{h_m - h_f}{h_{fg}}$

The heat transfer coefficient due to nucleate boiling is based on the Forster-Zuber (Forster and Zuber, 1955) equation with a suppression factor S

$$h_{NB} = 0.00122 \times S \left(\frac{\left(\lambda^{0.79} Cp^{0.45} \rho^{0.49} \right)_f}{\sigma^{0.5} \mu_f^{0.29} h_{fg}^{0.24} \rho_g^{0.24}} \right) \Delta T_{sat}^{0.24} \Delta P^{0.75} \tag{5.17}$$

where,

$$S = \frac{1}{1 + 2.53 \times 10^{-6} R_l^{1.17}}$$

$$R_l = R_e F^{1.25}$$

$$\Delta T_{sat} = T_{wall} - T_{sat}$$

and

$$\Delta P = P\left(T_{wall}\right) - P\left(T_{sat}\right)$$

5.4.3 Pressure difference along vertical fuel channels

Consider the coolant in a fuel channel as a mixture of liquid and vapor flowing upward. Assuming G_m and ρ_m as the mean mass flux rate and mean density of the homogenized liquid-vapor mixture. The momentum equation for a vertical constant area flow channel has the form

$$\frac{\partial G_m}{\partial t} + \frac{\partial}{\partial z}\left(\frac{Gm^2}{\rho_m^+}\right) = -\frac{\partial p}{\partial z} - \frac{fG_m|G_m|}{2D_e\rho_m} - \rho_m g.\cos\theta \tag{5.18}$$

where, ***f*** *is* friction factor and ***g*** is the acceleration due to gravity. D_e is the thermal hydraulics diameter of the flow channel.

5.4.3.1 Single phase pressure drop

In single phase liquid flow the physical property change along the heated channel can be assumed to be negligible. For constant flow area the mass flux (G_m) is constant and for $\rho_m^+ = \rho_l \approx$ constant, the pressure drop due to acceleration is negligible.

$$p_{in} - p_{out} = \frac{fG_m|G_m|}{2D_e\rho_l}\left(Z_{out} - Z_{in}\right) + \Delta p_{form} + \rho_l g\left(Z_{out} - Z_{in}\right) \tag{5.19}$$

5.4.3.2 Two phase flow of the coolant

The pressure drop across a channel in which boiling takes place at z=Z_B can be written as

$$p_{in} - p_{out} = \left(\frac{G_m^{\,2}}{\rho_m^+}\right)_{out} - \left(\frac{G_m^{\,2}}{\rho_m^+}\right)_{in} + \int_{Z_{in}}^{Z_B} \rho_l g dz + \int_{Z_B}^{Z_{out}} \rho_m g dz + \frac{f_{lo} G_m |G_m|}{2 D_e \rho_l}\left(Z_B - Z_{in}\right) + \frac{\overline{\phi_{lo}^2} f_{lo} G_m |G_m|}{2 D_e \rho_l}\left(Z_{out} - Z_B\right) + \sum_i \left(\phi_{lo}^2 K \frac{G_m |G_m|}{2\rho_l}\right)_i \tag{5.20}$$

This equation can be written as

$$\Delta p = \Delta p_{acc} + \Delta p_{gravity} + \Delta p_{fric} + \Delta p_{form}$$

where,

$$\Delta p_{acc} = \left(\frac{G_m^{\,2}}{\rho_m^+}\right)_{out} - \left(\frac{G_m^{\,2}}{\rho_m^+}\right)_{in}$$

$$\Delta p_{gravity} = \int_{Z_{in}}^{Z_B} \rho_l g dz + \int_{Z_B}^{Z_{out}} \rho_m g dz$$

$$\Delta p_{fric} = \frac{f_{lo} G_m |G_m|}{2 D_e \rho_l}\left(Z_B - Z_{in}\right) + \frac{\overline{\phi_{lo}^2} f_{lo} G_m |G_m|}{2 D_e \rho_l}$$

$$\Delta p_{form} = \sum_i \left(\phi_{lo}^2 K \frac{G_m |G_m|}{2\rho_l}\right)_i$$

The frictional pressure loss term Δp_{fric} is the pressure loss due friction from channel wall surface. f_{lo} is the friction factor for liquid only case while ϕ_{lo}^2 is the homogeneous friction pressure drop coefficient when the effect of viscosity is neglected. The term Δp_{form} is the pressure drop because of spacers and the factor K depend s upon the geometry/type of the spacers. The factor K has to be determined experimentally for the channel. The Friction Factor (f) depends upon flow velocity . Higher the flow rate higher will be the frictional pressure loss. For laminar flow i.e. Re< 2100, the friction factor is evaluated by

$$f = \frac{64}{\mathrm{Re}}$$

For turbulent flow in a smooth tube i.e. 2100< Re < 30000, the friction factor may be given by the Blasius relation

$$f = 0.316\,\mathrm{Re}^{-0.25}$$

for a smooth tube where 30000 < Re < 1000000, the friction factor is given by the McAdams relation

$$f = 0.184\,\mathrm{Re}^{-0.2}$$

5.4.4 Thermo physical properties of materials

The present purpose of this report is only concerned within thermo dynamical region where fuel and clad do not undergo any phase changes. Keeping this in mind the thermo-physical properties data were taken only for the solid alpha phase of fuel and cladding materials. The MATPRO-recommended expression (IAEA-TECDOC-949, 1997) was used to calculate specific heat and thermal conductivity of metallic Uranium and Uranium dioxide (Table-5.6). Thermo physical property for cladding materials i.e. Al, Zr-2 and SS are summarized in (Table- 5.7). Correlations for saturation properties of Light and Heavy water (Crabtree and Siman-Tov, 1993) were used to evaluate thermo physical properties. Tables-5.8 & 5.9 lists the correlations for Light water and Heavy water respectively. Table-5.10 lists the correlations for thermo physical properties of LBE.

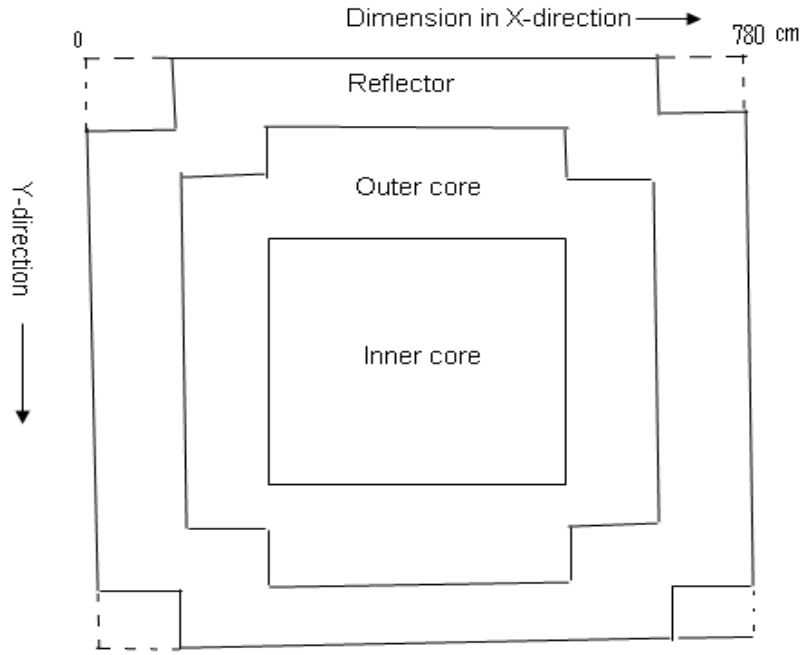


Figure-5.1: Vertical cross section and material assignment

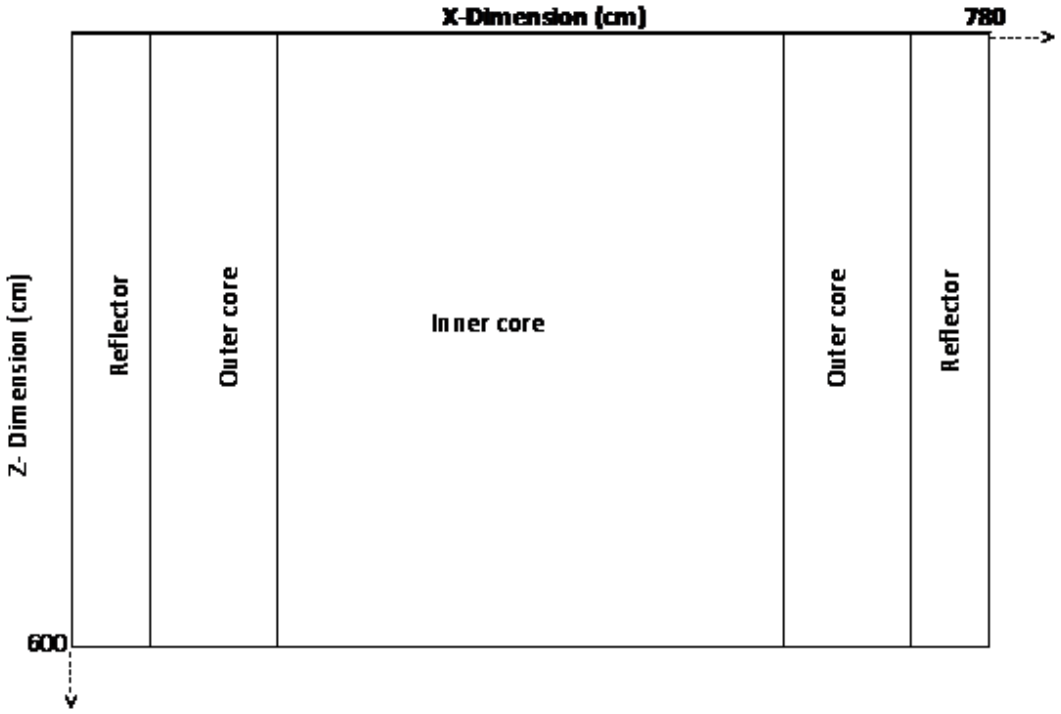


Figure-5.2: Horizontal cross section at Y=390 cm and material assignment

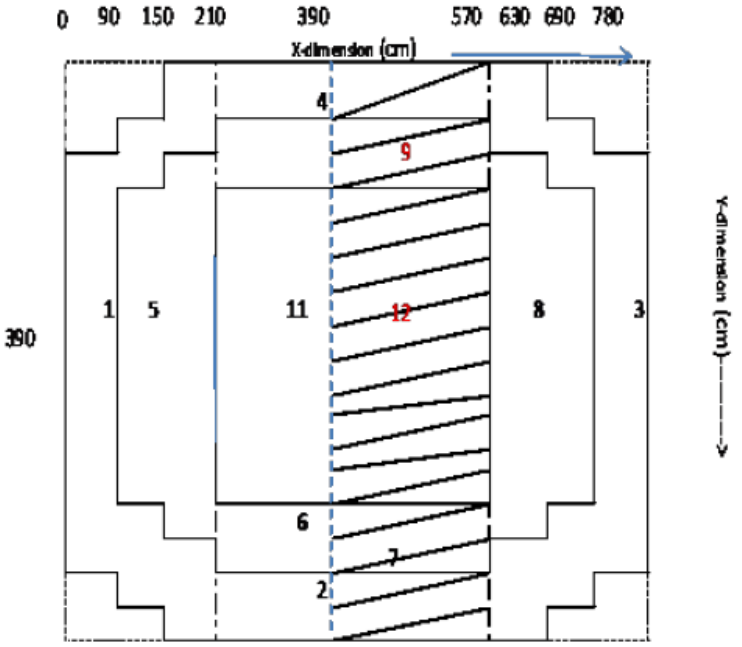


Figure-5.3: Vertical Cross section at Z=0; region affected by absorber (hached region)

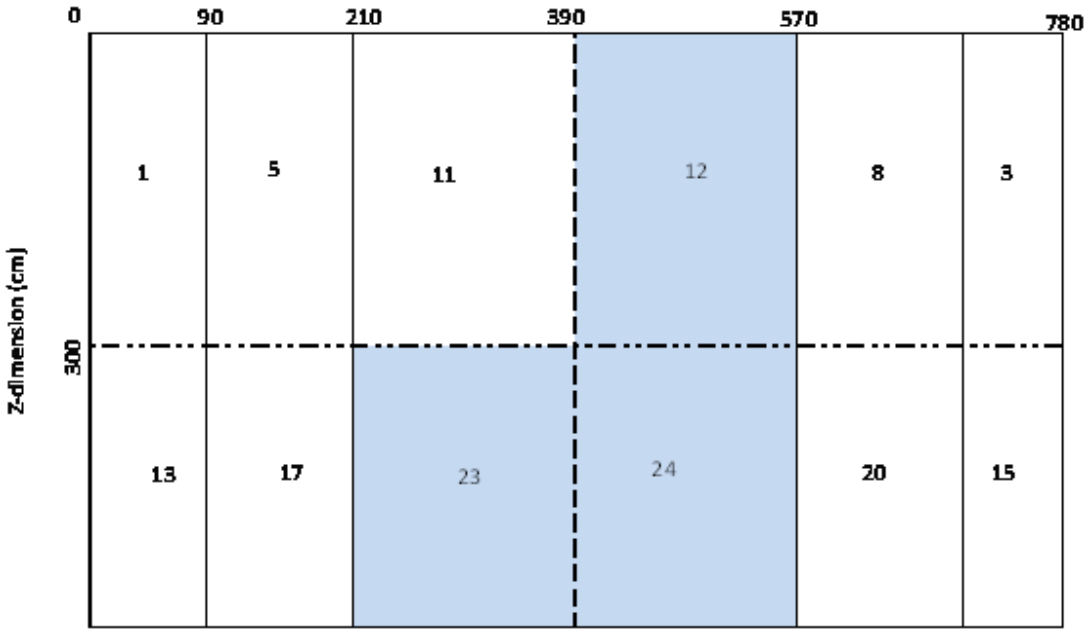


Figure-5.4: Horizontal cross section at Z=390; absorber path shown as shaded region

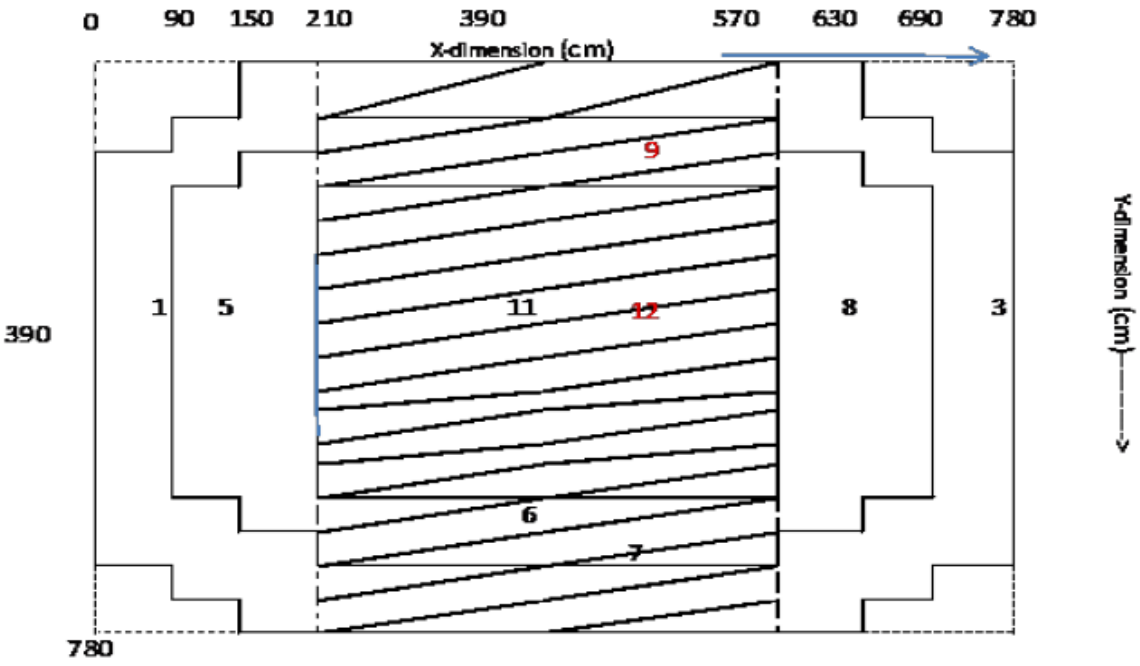


Figure-5.5: Vertical cross section at Z=600 cm; regions affected by absorber (hached)

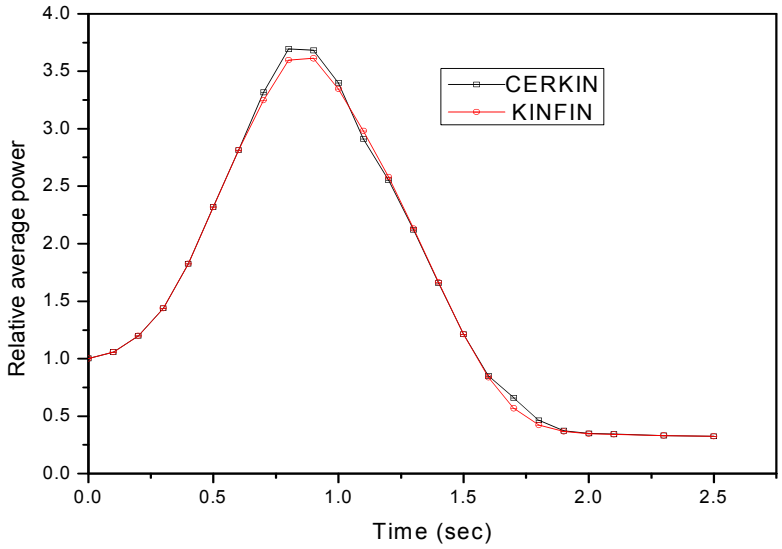


Figure-5.6: Average power density variation with time

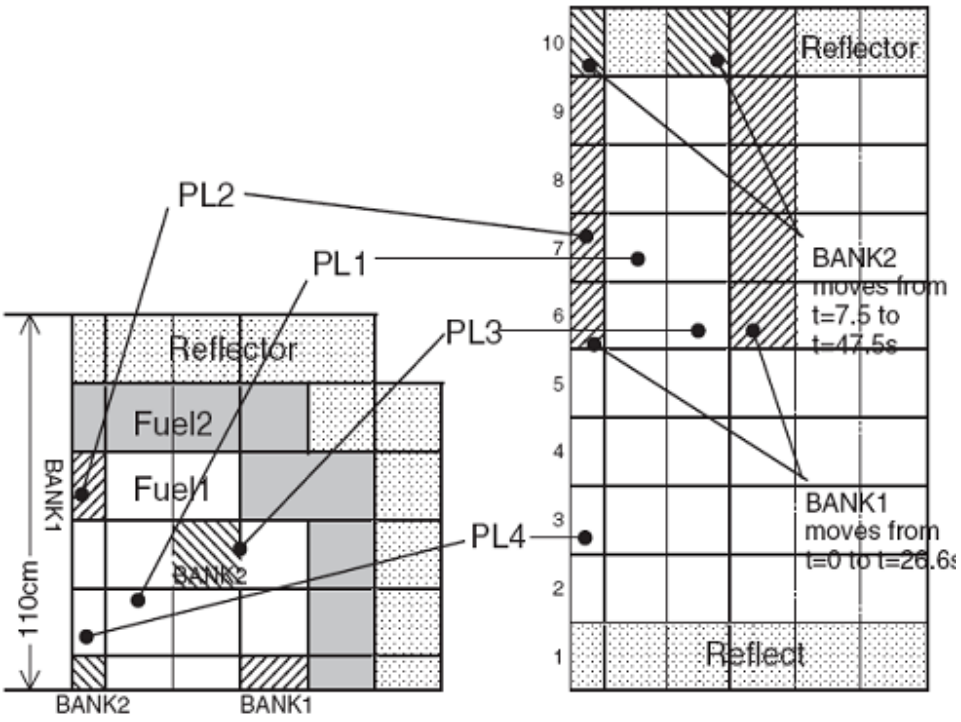


Figure-5.7: Cross sectional view and initial positions of absorber rods in LMW reactor

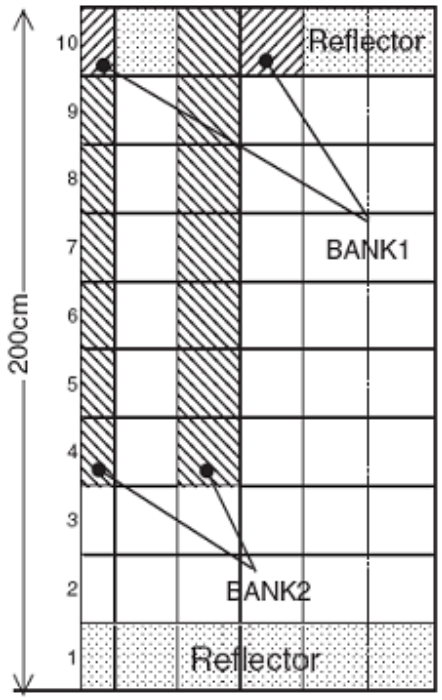


Figure-5.8: Final positions of absorber rods in LMW reactor

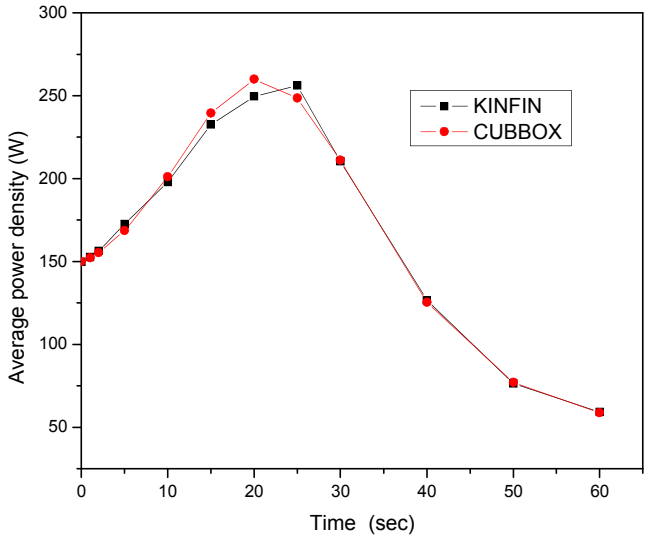


Figure-5.9: Variation of average power densities with time

Table-5.1: Two group nuclear data for PHWR model

Cross-section Type	Region-1 (inner fuel)	Region-2 (outer fuel)	Region-3 (reflector)
D1	1.2640E-00	1.2640E-00	1.3100E-00
D2	9.3280E-01	9.3280E-01	8.6950E-01
$\nu\Sigma_1^f$	0.0000E-00	0.0000E-00	0.0000E-00
$\nu\Sigma_2^f$	4.5620E-03	4.7230E-03	0.0000E-00
Σ_1^r	8.1540E-03	8.1540E-03	1.0180E-02
Σ_1^r	4.1000E-03	4.0140E-03	2.1170E-04
$\Sigma_{1\to2}$	7.3680E-03	7.3680E-03	1.0180E-02

Table-5.2: **Two group kinetics data**

Group Number	Group Velocities(cm/sec)	Prompt spectrum	Delayed spectrum
1	$1.0x10^7$	1.0	1.0
2	$3x10^5$	0.0	0.0

Delayed neutron data

Type	β_i	λ_i (sec^{-1})
1	4.170E-04	1.244E-02
2	1.457E-03	3.063E-02
3	1.339E-03	1.139E-01
4	3.339E-03	3.079E-01
5	8.970E-04	1.198E+00
6	3.200E-04	3.212E+00

Table-5.3: Steady state eigenvalues as estimated by KINFIN

Time (sec)	Keff
0.0	1.00355
0.4	1.00972
1.35	1.00508
2.10	0.99540
2.50	0.99625

Table-5.4: Two group nuclear data for 3-D LMW

Cross-section Type	Region-1 (inner fuel)	Region-2 (outer fuel)	Region-3 (reflector)
D1	1.423913E-00	1.2640E-00	1.3100E-00
D2	3.563060E-01	9.3280E-01	8.6950E-01
$\nu\Sigma_1^f$	0.0000E-00	0.0000E-00	0.0000E-00
$\nu\Sigma_2^f$	4.5620E-03	4.7230E-03	0.0000E-00
Σ_1^r	8.1540E-03	8.1540E-03	1.0180E-02
Σ_1^r	4.1000E-03	4.0140E-03	2.1170E-04
$\Sigma_{1\to2}$	7.3680E-03	7.3680E-03	1.0180E-02

Table-5.5: Variation of average power densities with time

Time	Average power density(W/cc)		Local power density (W/cc)							
			CUBBOX				KINFIN			
(sec)	KINFIN	CUBBOX	p11	p12	p13	p14	p11	p12	p13	p14
0	150.00	150	279.86	186.17	258.26	231.45	283.65	185.38	260.43	230.5
1	152.77	152.39	284.26	189.54	262.38	235.04	288.11	188.74	264.58	234.08
2	156.42	155.54	290.07	194.07	267.85	239.63	294	193.25	270.1	238.65
5	172.62	168.79	314.65	212.75	290.87	258.81	318.91	211.85	293.31	257.75
10	198.09	201.11	375.25	264.48	346.94	305.75	380.33	263.36	349.85	304.49
15	232.64	239.63	447.09	327.75	413.47	361.63	453.14	326.36	416.94	360.15
20	249.70	260.03	483.4	360.42	449.62	393.94	489.95	358.89	453.4	392.32
25	256.26	248.79	455.64	343.5	425.48	380.04	461.81	342.04	429.05	378.48
30	210.65	211.26	381.17	290.28	350.96	327.2	386.33	289.05	353.91	325.86
40	126.87	125.46	224.76	173.04	197.27	196.48	227.8	172.31	198.93	195.67
50	76.49	77.07	140.38	108.34	121.73	115.94	142.28	107.88	122.75	115.46
60	59.45	58.94	107.47	82.95	93.12	88.49	108.93	82.6	93.9	88.13

Table-5.6: Thermo physical property of fuel materials

Fuel Material	Density (kg/m^3)	Specific heat capacity, Cp ($J/kg/K$)	Thermal Conductivity, λ ($kW/m/K$)
Metallic Uranium [MATPRO]	*18900*	*for 300 K< T< 938 K* $Cp=104.82+5.3686\times10^{-3}T+10.1823\times10^{-5}T^2$ *for 938 K < T< 1049 K* $Cp = 176.41311$ *for 1049 K< T< 1405.6 K* $Cp = 156.80756$	$\lambda=20.457+1.2047\times10^{-2}T-5.7368\times10^{-6}T^2$
UO_2 [Finnemann, 1991]	*10240*	$Cp=162.3+0.3038T+2.391\times10^{-4}T^2+6.404\times10^{-8}T^3$	$\lambda = 1.05+\frac{2150}{T-73.15}$

Table-5.7: Thermo physical property of fuel materials

Cladding Material	Density (kg/m^3)	Specific heat capacity, Cp ($J/kg/K$)	Thermal Conductivity, λ ($kW/m/K$)
Aluminum	2700	*0.91*	*2.176*
Zircoloy-2	6504	Cp=252.54+ 0. 11474T	$\lambda = 7.51+2.09\times10^{-2}T-1.45\times10^{-5}T^2+7.67\times10^{-9}T^3$
SS-304	7900	For 300 < T < 1558 K, $Cp = 326 + 0.298\ T - 9.56\times10^{-5}\ T^2$ For T > 1558 K, Cp = 558.228	For 300 < T < 1671 K λ = 7.58 + 0.0189 T *W/m/K* For 1671 < T < 1727 K λ = 610.9393 - 0.3421767 T For T > 1727 K λ = 20

Table-5.8: Summary of the correlations for saturation thermophysical properties of light water

Property, parameter	Correlation	constants
Saturation Temperature (ºC)	$T_{sat} = \frac{A + CX}{1 + BX + DX^2}$ $X = log(P)$	A = 179.9600321 B = -0.1063030 C = 24.2278298 D = 2.951e-04
Saturation pressure (MPa)	$P_w = \exp\left(\frac{A+CX+EX^2}{1.0+BX+DX^2+FX^2}\right)$ $X = T$	*A = -7.395489709* *B = 4.884152e-03* *C = 3.6337285e-02* *D = 4.308960e-06* *E = 2.651419e-05* *F = -4.14934e-09*
Liquid density (kg/m^3)	$\rho_l = A + BX + CX^2$ $X = 1.8T + 32$	*A = 1004.789042* *B = -0.046283* *C = -7.9738e-04*
Vapour density (kg/m^3)	$\rho_g = \frac{A+CX+EX^2+GX^3}{1+BX+DX^2+FX^3+HX^4}$ $X = T_{sat}$	*A = -4.375094e-04;* *B =-6.947700e-03* *C = 7.662589e-04* *D = 2.418897e-05* *E = -5.963920e-06* *F = -4.227966e-08* *G = 2.867976e-07* *H = 2.594175e-11*
Liquid Enthalpy (kJ/kg)	$H_l = \frac{A +CX+EX^2}{1+BX + DX^2}$ $X = T$	*A = 0.786889159* *B = -0.001874457* *C = 4.163042560* *D = -3.334e-07* *E = -0.007798602*
Latent heat of vaporization (kJ/kg)	$x = T$ $H_{fg} = \sqrt{A + BX + CX^2 + DX^3}$	*A = 6254828.560* *B = -11742.337953* *C = 6.336845* *D = -0.049241*
Specific heat (kJ/kg/K)	$Cp = \sqrt{\frac{A + CX}{1 + BX + DX2}})$ $X = T$	*A = 17.48908904* *B = -1.67507e-03* *C = -0.03189591* *D = -2.8748e-06*
Thermal conductivity (W/m/K)	$\lambda = A + BX + CX^2 + DX^3$ $X = T$	*A = 0.5677829144* *B = 1.8774171e-03* *C = -8.1790e-06* *D = 5.6629477e-09*
Liquid dynamic viscosity (kg/m/sec)	$\mu_f = \exp\left(\frac{A+CX}{1+BX+DX2}\right)$ $X = T$	*A = -6.325203964* *B = 8.705317e-03* *C = -0.088832314* *D = -9.657e-07*
Surface Tension (Nm/m)	$\sigma = AX^B(1.0 + CX)$ $X = \frac{(373.99-T)}{647.15}$	A = 235.8e-03 B = 1.256 C = -0.625

Table-5.9: Summary of the correlations for saturation thermophysical properties of heavy water

Property, parameter	Correlation	constants
Saturation Temperature (ºC)	$T_{sat} = \exp(A + BX + CX^2 + DX^3)$ $X = log(P)$	A = 5.194927982 B = 0.236771673 C = -2.615268E-03 D = 1.708386E-03
Saturation pressure (MPa)	$Pw = \exp(A + \frac{B}{X} + C.\log(X) + DX)$ $X = T+273.15$	A = 95.72002 B = -8439.470752 C = -13.496506 D = 0.01201
Liquid density (kg/m^3)	$\rho_l = (A + BX + CX^2)$ $X = 1.8T+32$	A = 1117.772605 C = -8.42E-04 B = -0.077855
Vapour density (kg/m^3)	$\rho_g = \exp\left(\frac{A + CX + EX^2}{1 + BX + DX^2}\right)$ $X = T$	A = -5.456208705 B = 2.386228E-03 C = 0.060526809 D = -1.15778E-05 E = -1.11360E-04
Liquid Enthalpy (kJ/kg)	$H_l = A + BX^2 + \frac{CX}{\log(X)}$ $X = Tsat$	A = -81.40815291 B = 0.00274496 C = 21.13005836
Latent heat of vaporization (kJ/kg)	$H_{fg} = \sqrt{A + BX + CX^2}$ $X = 371.49 - T$	A = 508093.6669 B = 17006.921765 C = -1 1.009078
Specific heat (kJ/kg/K)	$Cp = (A + BX + CX^2 + DX^3)$ $X = (1.8T + 491.67) \times 10^{-4}$	A = 2.237124 B = 122.217151 D = 13555.737878 C = -2303.384060
Thermal conductivity (kW/m/K)	$\lambda = (A+BX+CX^2+DX^3) \times 10^{-3}$ $X=(1.8T+ 491.67) \times 10^{-4}$	A = -0.4521496 B = 36.0743280 D = 924.0219962 C = -357.9973221
Liquid dynamic viscosity (kg/m/sec)	$\mu_l = (A + BX + \frac{C}{X} + \frac{D}{X^2})$ $X = 1.8T+32$	A = -1.111606e-04 B = 9.46E-08 C = 0.0873655375 D = 0.4111103409
Surface Tension (N/m)	$\sigma = AX^B(1.0 + CX)$ $X = \frac{(371.49 - Tsat)}{444.65}$	A = 2.44835759E-01 B = 1.269 C = -6.60709649E-01

Table-5.10: Summary of the recommended correlations for thermophysical properties of molten LBE (p ~ 0.1 MPa)

Property, parameter	Correlation	Temperature range (K)	Estimated error ±
Melting temperature (K)	$T_{melt} = 397.7$	n/a	0.6
Latent heat of melting (kJ/kg)	$Q_{melt} = 38.6$	n/a	0.2
Boiling temperature (K)	$T_{boil} = 1943$	n/a	10
Latent heat of boiling (kJ/kg)	$Q_{boil} = 854$	n/a	2.0
Saturated vapour pressure (Pa)	$P_s = 11.1 \times 10^9 \exp(-22552/T)$	508-1943	50%
Surface tension (N/m)	$\sigma = (437.1 - 0.066T) \times 10^{-3}$	423-1400	5.0%
Density (kg/m^3)	$\rho = 11096 - 1.3236T$	403-1300	0.8%
Sound velocity (m/s)	$u_{sound} = 1773 + 0.1049T - 2.873 \times 10^{-4}T^2$	403-1300	-
Bulk modulus (Pa)	$B_s = (35.18 - 1.541 \times 10^{-3}T - 9.191 \times 10^{-6}\ T^2) \times 10^9$	430-605	0.05%
Isobaric specific heat (J/kg/K)	$Cp = 159 - 2.72 \times 10^{-2}T + 7.12 \times 10^{-6}T^2$	430-605	7%
Dynamic viscosity (Pa.s)	$\eta = 4.94 \times 10^{-4} \cdot \exp(754.1/T)$	400-1100	5%
Electric resistivity (Ω m)	$r = (86.334 + 0.0511 \cdot T) \cdot 10^{-8}$	403-1100	6%
Thermal conductivity (W/m/K)	$\lambda = 3.61 + 1.517 \times 10^{-2}T - 1.741 \times 10^{-6} \cdot T^2$	403-1100	5%

CHAPTER 6

Transport Theory Based Analog Monte Carlo for Simulating Noise Experiments in Sub-critical Systems

Experiments (Rasheed et al., 2010) are planned at the Bhabha Atomic Research Centre (BARC) with the aim of demonstrating pulsed neutron and noise methods for measuring the sub-critical reactivity of ADS. A new theory of Reactor Noise in ADS taking account of the non-Poisson character of the source has been developed at BARC (Degweker, 2000, 2003; Degweker et al., 2007; Rana and Degweker, 2009). One of the aims of the experiments would be to verify the theory and interpret the results in terms of the theory. The system planned is a natural uranium sub-critical assembly moderated by water or high density polyethylene (HDPE) and driven by a D-D or D-T neutron generator. The maximum k_{eff} of the assemblies is expected to be about 0.9. Though noise based experiments with such low k_{eff} are difficult because of modal effects, these can be performed with suitable location of detectors where modal effects are minimal.

As part of the experimental planning, a prior simulation of the kinds of results that might be expected with different detector locations, counting and analyzing setups is necessary, particularly in view of the difficulty mentioned above. It would be necessary to know the magnitude of say the Feynman Y function for given values of system parameters such as k_{eff}, detection efficiency etc., and how it compares with the background random noise for a given counting time or the magnitude of the space dependent effects, delayed neutron effects, dead time effects that inevitably appear in the experiment. This allows us to assess the feasibility of

carrying out measurements of parameters such as sub-critical reactivity, the errors that will appear and hence the kind of accuracy that may be expected from such a measurement. All this is possible only if the simulation is completely analog. Simulations with standard code packages (Gupta, 1991; MCNP, 1987) are not appropriate because of several non-analogue features built into such codes.

Since analogue simulations are generally very time consuming, we developed a diffusion theory based noise simulator which could be implemented quickly and was much faster to run than a transport theory Monte Carlo code. Simulations using the diffusion theory code (Rana, et al., 2013) have provided us with valuable information about the feasibility of the proposed experiments and the kind of accuracy that can be expected from such measurements.

However, a more realistic description of the experiments will be provided by transport theory based analog Monte Carlo. In this chapter we discusses the development of such a code specifically intended for simulating the noise based experiments such as Rossi-alpha and Feynman-alpha. The simulator generates a detailed time history of counts in the detector so that any method of analysis can be carried out. The code is based on delta neutron tracking method (Woodcock et al., 1965; Coleman, 1968) (also called Woodcock or Coleman method) which results in fast and relatively simple handling of complex geometries. The code has been validated with some criticality and noise benchmark problems. We also present results of simulation of the proposed ADS noise experiments at the PURNIMA facility obtained using the code. We also present a comparison with computed values of the Feynman alpha and Rossi alpha functions using a space-time kinetics code.

In Section 6.1, we give a brief description of reactivity measurement by noise methods. We discuss the basic experimental procedures used in noise methods and the theoretical basis of these methods. In particular we obtain general expressions for the Rossi alpha and Feynman alpha distributions and describe the computation of these distributions using a space-time kinetics code. We also discuss a novel application of the space time kinetics code KINFIN described in chapter 5 for obtaining Rossi alpha & Feynman alpha distribution. In Section 6.2, we describe the Transport Monte Carlo code developed by us for simulation of noise experiments. In Section 6.3, we discuss validation of the code. The results obtained for Purnima sub-critical facility are presented in Section 6.4.

6.1. Reactivity determination by noise method

When a neutron is injected into a system from an extraneous source, it randomly undergoes a number of events such as fission, scattering, capture or detection. The time between nuclear events is also a random variable. In reactor physics, these neutron fluctuations caused by the above types of sources due to inherent nuclear effects are called zero power reactor noise. Zero power noise carries information about reactor parameters such as reactivity. Suggestions for using this inherent noise for measuring reactor kinetics parameters were made as early as the Manhattan project and noise based methods such as Feynman-alpha and Rossi-alpha, among others, were further developed during the 1950s and 1960s to determine the reactivity of a sub-critical system (Saito, 1979). They are both based on the measurement of the second moment of the statistics of the detector counts. The methods have attracted renewed attention recently for measurement of sub-criticality of accelerator driven reactors.

In the following sub-section, we present a brief description of various noise methods for measurement of sub-critical reactivity and in Section 6.1.1, we derive general expressions for the Rossi alpha and Feynman Y functions in terms of the stationary flux and the time dependent solution of the backward adjoint equation. Finally, in Section 6.1.2, we describe a method used by us for computing the Rossi alpha and Feynman Y functions using a space-time kinetics code.

6.1.1. Brief description of various methods

6.1.1.1. The Rossi alpha method

In the Rossi-alpha method (Williams, 1974) one seeks to measure the probability of obtaining a detector count in an infinitesimal time interval dt_2 around time t_2 given that a count has been recorded at an earlier time t_1. While, in general, this is a function of both the time variables t_1 and t_2, for a stationary system this is a function of the time difference $\tau = t_2 - t_1$. The probability is traditionally measured by the use of delayed coincidence counting circuits (Saito, 1979) but with modern fast electronics, it is possible to simply record the entire time history of counts in a detector and the required probability distribution can be obtained by an off-line analysis of the recorded data. The second count need not be recorded in the same detector and often the use of two detectors might be preferred; particularly in fast systems where the time separations are of the order of 1 micro second.

It is clear that the probability consists of two parts: the first on account of neutrons which are uncorrelated with the one observed at t_1 (the so called 'accidental' coincidences) and, the second due to neutrons which are correlated with the one observed at t_1. In the point model (valid for

small systems and systems not too far from critical), it is possible to derive the following expression for this probability distribution:

$$P(\tau) = A + B\exp(-\alpha\tau) \tag{6.1}$$

Where $\tau = t_2 - t_1$ The prompt neutron decay constant α is determined by fitting the measured distribution to the above function. The method works best in systems where the power is very low so that the contribution of the first term is not overwhelmingly large compared to that of the second term. At higher powers, the auto-correlation or cross-correlation function method described below is more suitable. As we will see in the next sub-section, the general space energy dependent theory gives a much more complicated formula which reduces to that given by Eq. (6.1) in the point model (uni-modal approximation).

6.1.1.2. The auto correlation function method

This method is similar in principle to the Rossi alpha method but both the recording and analysis of the data are different. Here we seek to measure the auto correlation function (ACF) of the number of neutrons in the system at a given time with that at a later time. The ACF has a form similar to that given in Eq. (6.1) and alpha is inferred by fitting the data to Eq. (6.1). In practice, one measures N_i, the number of counts in successive short time intervals of width Δt labeled by the index i (or the current in an ion chamber sampled at times $i\Delta t$), and forms the average:

$$\langle N(t)N(t+\tau)\rangle = \frac{1}{n}\sum_{i=1}^{n} N_i N_{i+j} \tag{6.2}$$

where $\tau = j\Delta t$ is the separation between the two intervals and Δt is the width of each interval. The prompt neutron decay constant is estimated by fitting the measured ACF to an expression of the form given in Eq.(6.2)

6.1.1.3. The variance to mean (Feynman Alpha) method

In the Feynman-alpha method, one merely records the number of neutron counts registered in a detector in a large number of short time intervals each of length T (of the order of the prompt decay time i.e. inverse of alpha). The mean (m) and the variance V of the number of counts are calculated and the ratio V/m is determined. This is repeated for intervals of different lengths by varying T. Thus, one obtains a table of the V/m or the relative variance for different values of T. In the point model, the ratio of the variance to the mean is given by the expression

$$V/m = 1 + Y_T \tag{6.3}$$

Here Feynman function Y is defined by following relation

$$Y_T = \frac{\varepsilon_f D}{(\beta-\rho)^2}\left(1-\frac{1-\exp(-\alpha T)}{\alpha T}\right)$$

where D is the Diven factor and ε_f the fission detection efficiency of the detector. The prompt neutron decay constant α is obtained by fitting the data to the theoretical expression given in Eq.(6.3).

6.1.2. Theoretical expressions for the Rossi alpha and Feynman alpha functions

In the section 6.1.1, we saw how the measured quantities are given by simple functions of time involving various reactor kinetics parameters and how the latter can be inferred by fitting the measurements to the Feynman alpha and Rossi alpha functions. These expressions are valid in the point model approximations, but the actual situation is quite complicated and can be well described by stochastic transport theory. We show this in the present section. The more important point we wish to make is that these functions can be actually computed using space-

time kinetics codes suitably modified for this purpose. This provides with another method for validation of the results of our Monte Carlo simulator.

6.1.2.1. The Rossi alpha distribution

Let $p(r,\Omega,E,t;n_1,n_2)$ be the probability of the number of detections in two intervals of length Δt_1 and Δt_2 around the times t_1 and t_2 ($t_2 > t_1$) due to a neutron injected at (r,Ω,E,t). The corresponding probability generating function (PGF) is then defined by the following equation.

$$G(r,\Omega,E,t;z_1,z_2) = \sum_{n_1,n_2} p(r,\Omega,E,t;n_1,n_2) z_1^{n_1} z_2^{n_2} \tag{6.4}$$

The PGF obeys the backward stochastic transport equation (Bell, G.I, 1965; Pal, 1958)

$$\begin{aligned} &-\frac{1}{v}\frac{\partial G}{\partial t} - \Omega.\nabla G + \Sigma G = \Sigma_c + z_1\Sigma_{d1} + z_2\Sigma_{d2} + \int \Sigma_s(\Omega,E\rightarrow\Omega',E')G(r,\Omega',E',t;z_1,z_2)d\Omega'dE' \\ &+\Sigma_f f\left[\int \frac{\chi(E')}{4\pi} G(r,\Omega',E',t;z_1,z_2)d\Omega'dE'\right] \end{aligned} \tag{6.5}$$

In equation (6.5), f is the PGF of the number of neutrons in a fission reaction. The PGF $G_S(z_1,z_2)$ with a steady source $S(r,\Omega,E)$ of the Poisson type is given by the Bartlett formula (Bartlett, 1955)

$$G_S(z_1,z_2) = \exp\left[-\int\{S(r,\Omega,E,t)G(r,\Omega,E,t;z_1,z_2)-1\}drd\Omega dEdt\right] \tag{6.6}$$

The Rossi alpha formula is obtained by differentiating Eq. (6.6) twice with respect to z_1 and z_2 and setting $z_1 = z_2 = 1$

$$\begin{aligned} &P(t_1,t_2)dt_1dt_2 = \int S(r,\Omega,E,t)G_{z_1z_2}(r,\Omega,E,t;z_1,z_2)drd\Omega dEdt \\ &+\left(\int S(r,\Omega,E,t)G_{z_2}(r,\Omega,E,t;z_1,z_2)drd\Omega dEdt\right)\left(\int S(r,\Omega,E,t)G_{z_1}(r,\Omega,E,t;z_1,z_2)drd\Omega dEdt\right) \end{aligned} \tag{6.7}$$

where the derivatives w.r.t. z_1 or z_2 are to be evaluated at $z_1 = z_2 = 1$. On differentiating Eq. (6.7) with respect to z_1 or z_2 and successively with respect to z_1 and z_2 and setting $z_1 = z_2 = 1$ we obtain Eqs. (6.8), (6.9) and (6.10) for these derivatives i.e. the first and second moments

$$L^{\dagger}G_{z_1} = \Sigma_{d1} \tag{6.8}$$

$$L^{\dagger}G_{z_2} = \Sigma_{d_2} \tag{6.9}$$

$$L^{\dagger}G_{z_1z_2} = \overline{\nu(\nu-1)}\Sigma_f\left(\int\frac{\chi(E')}{4\pi}G_{z_1}(r,\Omega',E',t;1,1)d\Omega'dE'\right)\left(\int\frac{\chi(E')}{4\pi}G_{z_2}(r,\Omega',E',t;1,1)d\Omega'dE'\right) \tag{6.10}$$

The equation for the flux due to the source can be written as follows using the ordinary stationary forward equation:

$$L\phi = S \tag{6.11}$$

In Eqs. (6.8) - (6.11) we have used the symbols L and $L^{\dagger}$ for the time dependent backward (adjoint) and forward transport operators defined below:

$$L^{\dagger}G_{z_1} = -\frac{1}{v}\frac{\partial G_{z_1}}{\partial t} + H^{\dagger}G_{z_1} = -\frac{1}{v}\frac{\partial G_{z_1}}{\partial t} - \Omega.\nabla G_{z_1} + \Sigma G_{z_1} - \int\Sigma_s(\Omega,E\rightarrow\Omega',E')G_{z_1}(r,\Omega',E',t;1,1)d\Omega'dE'$$
$$-\bar{\nu}\Sigma_f\int\frac{\chi(E')}{4\pi}G_{z_1}(r,\Omega',E',t;1,1)d\Omega'dE' \tag{6.12}$$

$$L\phi = \frac{1}{v}\frac{\partial\phi}{\partial t} + H\phi = \frac{1}{v}\frac{\partial\phi}{\partial t} + \Omega.\nabla\phi + \Sigma\phi - \int\Sigma_s(\Omega',E'\rightarrow\Omega,E)\phi(r,\Omega',E',t)d\Omega'dE'$$
$$-\chi(E)\int\frac{\bar{\nu}\Sigma_f}{4\pi}\phi(r,\Omega',E',t)d\Omega'dE' \tag{6.13}$$

where H and $H^{\dagger}$ are the corresponding time independent transport operators.

Using: i) the fact that the various terms on the RHS in Eq. (6.7) are scalar products between the source and the functions G_{z_1} etc. ii) Eqs. (6.8), (6.9) and (6.10) iii) the properties of mutually adjoint operators, we can rewrite Eq. (6.7) as follows

$$P(t_1,t_2)dt_1dt_2 = \left(\int \Sigma_{d1}\varphi(r,\Omega,E,t;z_1,z_2)drd\Omega dEdt\right)\left(\int \Sigma_{d2}\varphi(r,\Omega,E,t;z_1,z_2)drd\Omega dEdt\right)$$
$$+\int \varphi(r,\Omega,E,t)\overline{\nu(\nu-1)}\Sigma_f\left(\int\frac{\chi(E')}{4\pi}G_{z_1}(r,\Omega',E',t;1,1)d\Omega' dE'\right)\left(\int\frac{\chi(E')}{4\pi}G_{z_2}(r,\Omega',E',t;1,1)d\Omega' dE'\right)drd\Omega dEdt$$

(6.14)

where, we have omitted the time variable for the flux, as we are considering a stationary Poisson source. The first term in Eq. (6.14) is merely the product of the average number of counts in the two intervals and is the uncorrelated term whereas the second term is due to fission chain correlations. It is this term that allows the estimation of α from Rossi alpha [or Auto Correlation Function (ACF)] measurements. Thus, it is possible to express the Rossi alpha function (and in a similar manner the Feynman Y function) in terms of the forward and adjoint solutions. While the forward solution gives the stationary flux, the two adjoint solutions are the Green's functions corresponding to a delta function adjoint source (i.e. a detection at times t_1 and t_2). Eq. (6.10) can be obtained (Rana and Degweker, 2011) if we assume that the functions $G_{z_1}(r,\Omega,E,t;1,1)$ can be represented as a single alpha mode corresponding to the fundamental mode.

6.1.2.2. The Feynman alpha method

The PGF $G(r,\Omega,E,t;z)$ for one interval probability function $p(r,\Omega,E,t;n)$ giving the probability of obtaining n counts in an interval of length T due to a neutron injected at (r,Ω,E,t) is defined by Eq. (6.15).

$$G(r,\Omega,E,t;z) = \sum_{n_1,n_2} p(r,\Omega,E,t;n)z_1^{\,n} \qquad (6.15)$$

By using Eq. (6.15) and following a method similar to that in Section 6.1.2.1, we obtain the Eq. (6.16) for the second factorial moment M_2 of the number of counts in the interval T.

$$M_2 = \left(\int \Sigma_{d1} \varphi(r,\Omega,E,t) dr d\Omega dE dt \right)^2 + \int \varphi(r,\Omega,E,t) \overline{\nu(\nu-1)} \Sigma_f \left(\int \frac{\chi(E')}{4\pi} G_z(r,\Omega,E,t;1) d\Omega' dE' \right)^2 dr d\Omega dE dt \quad (6.16)$$

The function $G(r,\Omega,E,t;1)$ is the solution of the adjoint (backward) transport equation with a source equal to Σ_d, the detector cross section in the time interval $t \in [0,T]$ and zero otherwise. The first term is simply the square of the mean count rate M_1 and $\phi(r,\Omega,E,t)$ is the stationary flux distribution in the presence of the external source. The variance to mean can be computed using Eq.(6.17).

$$V/m = (M_2 + M_1 - M_1^2)/M_1 \quad (6.17)$$

6.1.3. Computation of stochastic descriptors using a space-time kinetics code

In Section 6.1.2, it was seen that it is possible to obtain the Rossi alpha and Feynman alpha functions from the stationary flux distribution in the presence of the external source and the solution of the time dependent adjoint equation in the presence of a source (detector cross section for the adjoint problem). For this purpose we have used the three dimensional space time kinetics code [KINFIN]. The spatial discretisation in KINFIN is done using the finite difference method in which the space can be divided into rectangular meshes. A centre mesh finite differencing method is used for the spatial derivatives. The time integration is carried out using the backward Euler scheme. The code has provision to take thermal hydraulic feedback effects into account. For sub-critical systems, kinetics problems in the presence of a source can be solved. The code also has the capability to compute the time independent adjoint function.

The code [KINFIN] was modified to obtain the solution of the time dependent adjoint equation in the presence of an external source (the detector cross section). With this modification, the code can calculate the backward functions $G_{z_1}(r,\Omega,E,t;1,1)$, $G_{z_2}(r,\Omega,E,t;1,1)$ or $G_z(r,\Omega,E,t;1)$ and the forward function $\phi(r,\Omega,E,t)$ which are required to evaluate the various integrals in Eqs. (6.14) and (6.16) for computing the Rossi alpha and the Feynman Y functions respectively. Results of our calculations of these functions using KINFIN are described in Section 6.3.2.

6.2. The transport Monte Carlo code

The analogue Monte Carlo method is most obvious choice for simulating a proposed noise experiment. In its most general form it does not impose restrictions on the geometry nor does it require discretisation of the space, energy angle and time variables. In this method, each particle is followed from its birth till death. By counting the number of detection reactions [say (n,α)] in the volume of the detector, we can simulate the counts in the detector and prepare a complete time history of detected neutron counts which can be further processed depending upon the requirement. At this stage, detector effects such as dead times etc can also be included. Thus the outcome of a Monte Carlo numerical simulation is similar to a real experiment. In analog Monte Carlo method, when a collision occurs, the decision concerning events is evaluated probabilistically; if the outcome is indeed absorption, its history is terminated.

General Monte Carlo codes (MCNP, 1987; Gupta, 1991) that are used for criticality safety evaluations are typically meant for evaluation of integral reactor parameter such as k_{eff} and also for evaluation of flux. Even those that have time dependent features are not directly suitable due to several non-analogue features built into them and therefore cannot be used in reactor noise

applications. Either these codes should be modified (Szieberth and Klujber, 2010 a&b; Yamamoto, 2011) or new code should be written to suit the new application. In this section, we describe such a code developed by us. To begin with, we have kept the modeling rather simple. Thus, we do not attempt the continuous energy treatment characteristic of MC codes. Instead, we rely on the multi-group method with cross sections taken from the WIMS library (Askew, et al., 1966). The treatment of scattering is limited to isotropic scattering. An additional simplification is achieved by using the delta algorithm for tracking the neutron paths. Figure-6.1 gives the algorithm of the code. Details of the procedure followed from birth to removal are described in Sections 6.2.1 through 6.2.6.

6.2.1. Random number generator used

In the computations based on Monte Carlo method, the generation of uniform pseudo-random numbers between 0 and 1 is of utmost importance. Since accuracy of the simulations based on Monte Carlo methods depends on random number, the randomness of the same will affect the results. In view of this, it is important that the random numbers should have high quality. The random number generator should pass all reasonable statistical tests of randomness and should be portable and fast. Random number generator should have higher cycle length and there should be minimal correlation between generated numbers.

Several algorithms for generating random numbers have been developed and are being used. A wide range of references and overviews (Marsaglia, 1985; Anderson, 1990; Park and Miller, 1988) about random number generators are available. Though there are congruential, Fibonacci and combination generators, we have used well-known and most widely used congruential generator proposed by Park and Miller (Park and Miller, 1988). The congruential generators are

simplest and fastest random number generators and the simulations based on analog Monte Carlo like ours, a fast generator of reasonable quality is desired. Minimal random number generator algorithm has withstood the test of time. Several empirical tests of the randomness of its output have been published in literature and its important theoretical properties have been analyzed. A linear congruential sequence is a series of numbers based on the recurrence relation formula:

$$Z_n = (aZ_{n-1} + c) \bmod m \tag{6.18}$$

where a, c and m are suitable integers called the multiplier, increment and modulus respectively. In the special case where c is taken as zero we have what is called as a multiplicative generator. Many acceptable combinations of modulus and multiplier have been proposed. In our program, we have implemented the Minimal Standard Generator suggested by Park and Miller. The resulting sequence from m = 2,147,483,647 and a = 16,807 is recommended as the bare minimum for random number generators (though Park and Miller now recommend a = 48,271 for better statistical properties). The period for the generator is ~2x10^9 which is quite reasonable for our application.

6.2.2. Sampling source variables

In a multi-group calculation three space variables $\vec{r} = (x, y, z)$, three direction cosines $\vec{\Omega} = (\Omega_x, \Omega_y, \Omega_z)$, the group index g and the time t are associated with each neutron as it is tracked. The calculation begins by sampling the above variables for an external source neutron. The source position must be sampled from the source distribution. However, in our problem the D-T source is very small in extent and is treated as a point source located at a fixed position.

The angular distribution is assumed to be isotropic, which is a very good approximation for D-T sources. The isotropic distribution is sampled by noting that the azimuthal angle φ is uniformly distributed between 0 and 2π i.e. as $d\varphi/2\pi$ and the distribution of the polar angle θ is as $\frac{1}{2}\sin\theta d\theta$. In terms of the variable Ω_z the distribution is simply uniform between -1 and +1. Thus we draw two random numbers ξ_1, ξ_2 and obtain the direction cosines as follows

$$\Omega_z = 2\xi_1 - 1 \tag{6.19a}$$

$$\Omega_x = \sqrt{1-\Omega_z{}^2}\cos 2\pi\xi_2 \tag{6.19b}$$

$$\Omega_y = \sqrt{1-\Omega_z{}^2}\sin 2\pi\xi_2 \tag{6.19c}$$

Another important technique for sampling the direction variables for an isotropic source is due to Von Numann (Von Numann, 1951). The method avoids the need to compute the sine and cosine functions of the azimuthal angle and can be implemented using the following equations.

$$\cos\varphi = \frac{\eta^2 - \rho^2}{\eta^2 + \rho^2} \tag{6.20a}$$

$$\sin\varphi = \frac{2\eta\rho}{\eta^2 + \rho^2} \tag{6.20b}$$

where η and ρ are two uniformly distributed random numbers in the intervals (-1, 1) and (0, 1) respectively,

For the D-T source, the group index is sampled simply as the highest neutron energy group. More generally the source is sampled from a discrete cumulative distribution function derived from the source spectrum.

Finally, the times of occurrence of each of the source events for the case of a Poisson source is sampled as follows

$$t_{n+1} = t_n - \frac{1}{S}\ln\xi \tag{6.21}$$

where t_n is the time of occurrence of the nth source event and S is the source strength. We choose $t_0 = 0$.

6.2.3. Sampling distance to the next collision

In an infinite homogeneous medium, the neutron path lengths are distributed according to the exponential distribution $\Sigma_t \exp(-\Sigma_t s)ds$. By forming the cumulative distribution and inverting the same, we obtain the following formula for transforming from ξ distributed uniformly in [0, 1] to the exponential distribution

$$s = -\frac{1}{\Sigma_t}\ln\xi \tag{6.22}$$

Once the distance is obtained, the position of the collision point is updated using the equation

$$\vec{r} = \vec{r_0} + s\vec{\Omega} \tag{6.23}$$

and the time is updated as follows

$$t = t_0 + s / v_g \tag{6.24}$$

where $\vec{r_0}$ is the current position, t_0 is the current time and v_g is the average neutron speed in group g.

6.2.3.1. The delta tracking algorithm

The expression Eq.(6.22) for the sampled distance to the next collision assumes an infinite homogeneous medium. A reactor is more likely to be made up of piece wise homogeneous

media. Such media are normally treated in one of the following two ways. The distance to the next collision is estimated according to the above formula using the cross section of the medium in which the particle is currently located. The distance to the surface from which the particle will exit the current medium is calculated by solving the equation of the line representing the neutron track and the bounding surfaces. In case this distance is greater than the estimated collision distance, the point of collision is accepted. In case it is less, then there are two possible ways. In one, the particle is transported to the point of intersection on the interface between the two media and a new collision distance (from this point into the adjoining medium) is estimated using the above equation with the cross section of the adjoining medium and the process is repeated till a collision point is accepted. Alternatively, a new collision distance (from the point of intersection) can be calculated as follows

$$s' = \frac{1}{\Sigma'_t}(s-u)\Sigma_t \tag{6.25}$$

where Σ'_t is the cross section in the adjoining medium and u is the distance to the exiting surface. Again the process is repeated till a collision point is accepted.

The estimation of path length in various regions of the geometry consisting of many homogeneous regions requires information about the distance to the nearest boundary surface, calculation of intercepts made by the line in the different regions that the neutron travels before collision. All this makes the algorithm quite complex to model. It can also be very time consuming.

All the complexities of conventional ray-tracing algorithm can be by passed by an alternate method known as delta tracking method (Woodcock et al., 1965; Coleman, 1968). To begin with,

the maximum total macroscopic cross-section of all materials in the geometry at the particle energy is found. If this is called as Σ_m, then the distance to the next collision (irrespective of the cross section of the medium in which the particle is located) is sampled using

$$s = -\frac{1}{\Sigma_m} \ln \xi \tag{6.26}$$

If Σ_t is the actual cross section at the point of collision, the point is accepted as a collision site with a probability Σ_t / Σ_m and rejected with a probability $1 - \Sigma_t / \Sigma_m$. The method requires the program to only determine the medium at any given point which is much simpler than ray tracing. The method does not calculate track lengths in any region and hence it is not possible to estimate the track length flux using this method. However this is no limitation for our problem where we are interested only in the number of collisions in the detector that give rise to counts in it.

6.2.3.2. The geometry model and options available

The code uses geometry modeler based on combinatorial geometry logic. Combinatorial geometry describes general three-dimensional (3-D) material configurations by considering unions, differences, and intersections of simple bodies such as spheres, boxes, cylinders, etc. This method allows space to be subdivided into unique zones of arbitrary shape. In the code the task of assigning three-dimensional material configuration of the problem is accomplished in three distinct steps. First the regular body shapes to be used - rectangular parallelepiped, cylinder, sphere, etc. - their dimensions, location and orientation are defined. For a rectangular parallelepiped whose six plane surfaces are perpendicular to the co-ordinate axes, we specify the minimum and maximum values of x, y and z coordinates of the planes perpendicular to the

corresponding axis. A sphere is defined by radius and co-ordinates of centre. For a right circular cylinder, we specify the radius, the centre and the projection of its height on x, y and z axes. After defining the necessary geometrical bodies, entire problem geometry is segmented into zones and materials are assigned to these zones.

6.2.4. Sampling reaction events at a collision and tallying

Upon collision it is next required to determine the fate of the neutron. This is simply decided by the probability of various reactions such as fission (Σ_f / Σ_t), capture (Σ_c / Σ_t) or scattering (Σ_s / Σ_t). In case of scattering, (treated as isotropic) in our program, the procedure described in Section 6.2.2 is used to sample the direction cosines. It is also required to decide the group to which the neutron will be scattered. The probability for scattering to group g' from group g is $\Sigma_{s,g\to g'} / \Sigma_t$.

In case of fission the number of neutrons is sampled from the discrete distribution $p(\nu)$ giving the probability of ν neutrons being produced in a fission which is available for various nuclides in the literature (Jerome et al., 2010). Each of the fission neutrons is assigned the position and the time of the collision. The energies of each of the fission neutrons are sampled from the discrete (group) fission spectrum. The directions of each of the fission neutrons are sampled from the isotropic distribution as in Section 6.2.2. In case of a capture, or incase the neutron escapes the reactor volume, the history is terminated. The collisions inside the detector volume that give rise to a detection reaction (eg. (n,p)) in a He-3 detector are recorded as detections and the particle history is terminated.

6.2.5. Estimation of the effective multiplication factor (k_{eff})

Though the computer code has been written specifically intended to noise simulation, we have also included an option to evaluate k_{eff} as this is an important system parameter and also to check the correctness of geometry and overall computational algorithms by comparing with available benchmarks. Evaluation of k_{eff} is done by finding the ratio of number of neutrons in successive generations. The total number source neutrons for successive generations are kept around the initial source neutrons. This is achieved by increasing or decreasing the probability of emission of source neutrons for next generation using the ratio of source neutrons in the current and previous generations. The initial few k_{eff} cycles are ignored in final estimation of average k_{eff} to ensure that the distribution of source neutrons has reached the fundamental mode.

6.2.6. Time history of counts and its processing

When a (user specified) large number of source particle (histories) has been executed we are left with the detection times. However these are not arranged in chronological order since there is always some overlap of chains. A chronological ordering of this data is carried out to obtain the time history of counts as would be obtained in an actual experiment. This is then processed to obtain the various descriptors such as Rossi alpha, Feynman alpha, etc. Dead time effects can also be incorporated as per the standard paralysable or non-paralysable dead times.

6.3. Validation of the code

Validation of noise simulation code has been done in a number of different ways. At one level, the code has been validated by computing the keff for a number of one-group criticality benchmark problems. At another level, noise parameters calculated by the code have been compared with the diffusion Monte Carlo code. Yet another validation has been provided by

comparing Feynman alpha and Rossi alpha functions obtained by the code with theoretical results obtained by the diffusion theory code KINFIN as discussed in Section 6.1.4.

6.3.1. Comparison of K_{eff} results by the Code with benchmarks

6.3.1.1. Analytical benchmarks

We have chosen a set of benchmark problems (Sood et al., 2003) with analytical solutions of the k_{eff} eigenvalue problem of the neutron transport equation. This compilation consists of 75 criticality problems for which very accurate k-effective values are available. A set of 7 problems (Problems 2, 4, 7, 8, 10, 46, 58) was selected. The chosen problems are for slab, cylindrical, and spherical geometries in one- and two-energy groups, one- and two-media. In all these problems, the neutron scattering is isotropic. Full geometrical description and cross section of the problems are given in a research paper by Sood et al. (Sood et al., 2003). Table-6.1 gives a comparison of results obtained by our code with the analytical results given in the report (Sood et al., 2003). We see that for all the problems studied by us, the agreement is within the standard deviation and provides a source of validation of the geometry and tracking subroutines of the code.

6.3.1.2. Keff of the World problem

Another problem we have analysed is the one energy group version of the "K_{eff}-of the- world" problem (Taro, Ueki & Forrest, B. Brown, 2002). The "K-effective of the World" problem was introduced by G. E.Whitesides in 1970. The basic idea behind the "K_{eff}-of the- world" problems is to caution Monte Carlo code users that, even with the use of sophisticated codes, correct results can be obtained only if attention is paid to source convergence in the Monte Carlo iterations and to running a sufficient number of neutron histories to adequately sample all significant regions of the problem.

The system consists of a 7×7×7 array of identical cubes with the side length of 6 cm and macroscopic cross sections of Σ_t = 0.31997 cm^{-1}, Σ_a = 0.09916 cm^{-1} and $\nu\Sigma_f$ = 0.22711 cm^{-1}, placed at a pitch of 24 cm. The surfaces of the neighboring cubes are faced parallel to each other. The space between the cubes has macroscopic cross sections of Σ_t=0.05 cm^{-1}, Σ_a=0.001cm^{-1} and $\nu\Sigma_f$ = 0 cm^{-1}. The space up to 9 cm away from the outermost surfaces of the cubes has the same non-fissile cross sections. k_{eff} of this system by our code is computed to be (0.87617±0.00015) which is quite close to the value (0.87609 ±0.00028) given in literature. Here the geometry is more complicated and the good agreement obtained by us gives further confidence in the integrity of the coding.

6.3.2. Comparison of noise descriptors by transport MC with diffusion MC and space-time kinetics

As a part of validation of the code, we have analysed a bare homogeneous reactor in the shape of a rectangular parallelepiped which is described by one group nuclear data with the source located at the centre. This problem has been solved by diffusion based Monte Carlo method (Rana, et al., 2013) to obtain to obtain reactor noise parameters by diffusion Monte Carlo code. We have compared our results with those obtained by Rana and Degweker (Rana and Degweker, 2013). The dimensions and other properties are listed in Table-6.2 and are chosen to roughly correspond to natural uranium fuelled and High Density Poly Ethylene (HDPE) moderated assembly likely to be used in the first phase of the experiments. For the bare assembly, the point of intersection of the zeros of the first set of symmetric modes is easily seen to be at the coordinates $(\pm 14, \pm 14, \pm 20)$.

Figure-6.2 shows a comparison between results of auto-covariance by diffusion and transport Monte Carlo with eight detectors centered at the coordinates. After exponential fitting the fundamental alpha was found to be 4252 ±61 sec-1 whereas the same as calculated by diffusion Monte Carlo (Rana and Degweker, 2013) was found to be 4342±104 sec-1. Figure-6.3 shows plot of the variance to mean ratio (with the counting interval length) obtained by transport Monte Carlo. The results by transport Monte Carlo are quite close to that obtained by diffusion Monte Carlo. It is probably due to large size and homogeneous nature of the problem. Figure-6.4 shows the plot of auto-correlation obtained by space time kinetics code in adjoint mode. After exponential fitting the fundamental alpha was found to be 4219 sec-1.

6.4. Results for proposed PURNIMA experiments

6.4.1. The PURNIMA core and selected detector locations

A facility for carrying out experiments on the physics of ADS and for testing the simulation methods under development is being set up at PURNIMA laboratory, BARC. A 14-MeV neutron generator has been in existence in this laboratory for several years for performing fusion blanket neutronics studies. It consists of an accelerator, which produces a 200 mA current of deuterons accelerated to energy of 300 KeV. These deuterons fall on a Ti target loaded with tritium. The 14-MeV neutrons are produced by the D-T fusion reaction resulting in a continuous source of about $3x10^9$ n/s. Efforts are on to increase its strength and to have pulsed mode of operation for pulsed neutron source-based experiments. A simple sub-critical assembly [Figure-6.5] of natural U and light water was chosen for the purpose of basic reactor physics experiments. It consists of U metal rods of 3.45 cm diameter clad in 1 mm thick Al placed horizontally in Al tubes arranged in a hexagonal lattice of pitch 5.6 cm. A central axial Al tube

houses the tritium target. The core length is 100 cm and a loading of 300 rods gives a k_{inf} that is about 0.87.

6.4.2. Results of simulations using the Code

The full-scale 3-D heterogeneous geometry of PURNIMA facility has been modeled using our code. The model includes a 3D description of reactor vessel, actual fuel rod, clad and the tube through which fuel will be guided in the core. It also describes the neutron source tube at the centre of the core. Three group neutron cross-section for fuel, clad, tube, moderator and air has been calculated by transport theory code WIMS. Though there is no binding in neutron energy group from code point view, we have chosen three group energy structures to account for fast (10 MeV-0.821 MeV), epithermal (0.821 MeV-0.625 eV) and thermal (0.625 eV- 0) neutrons. In this structure source neutrons having energy ~14 MeV are covered in first group. Figure-6.6 shows the plot of auto-covariance. Leaving the first data point, a single exponential fits the data well and gives a value of alpha 3338 sec-1 with a variance of ±164. The first data points may be contribution from higher symmetric modes which are not suppressed by placement of detectors.

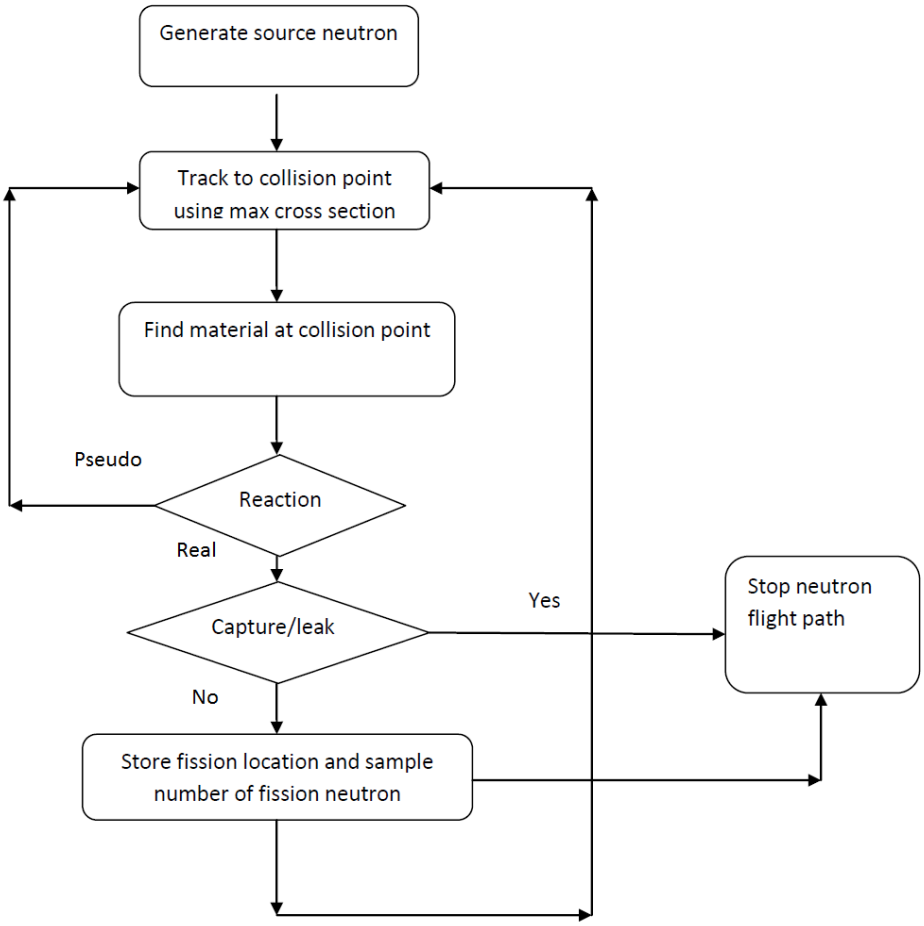


Figure-6.1: Flow chart of analog Monte Carlo code

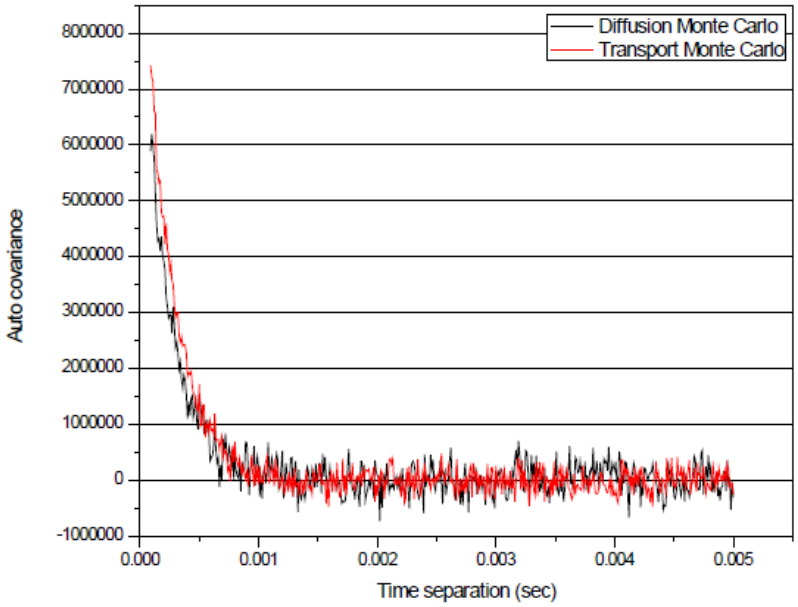


Figure-6.2: Comparison between results of auto-covariance by diffusion and transport Monte Carlo with eight detectors centered at the coordinates $(\pm 14, \pm 14, \pm 20)$ for a bare homogeneous reactor in the shape of a rectangular parallelepiped

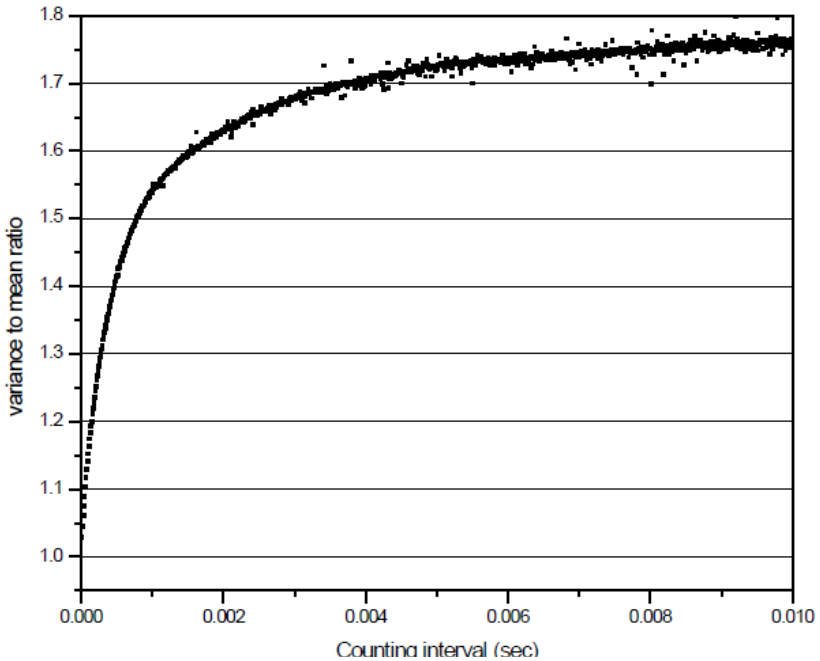


Figure-6.3: Plot of the V/m ratio (with the counting interval length) obtained by transport Monte Carlo with eight detectors centered at the coordinates $(\pm 14, \pm 14, \pm 20)$ for a bare homogeneous reactor in the shape of a rectangular parallelepiped.

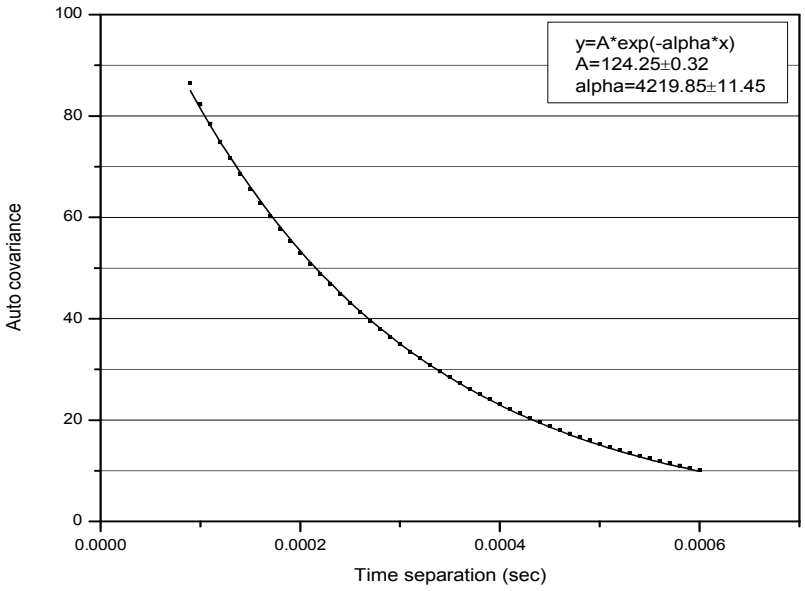


Figure-6.4: Plot of auto-correlation obtained by space time kinetics code in adjoint mode.

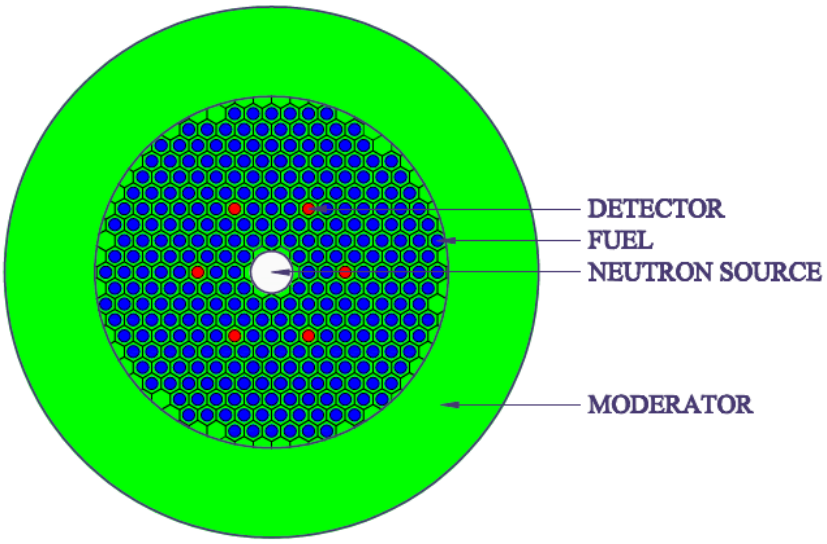


Figure-6.5: Core layout of the proposed natural U and light water sub-critical assembly for the experiments.

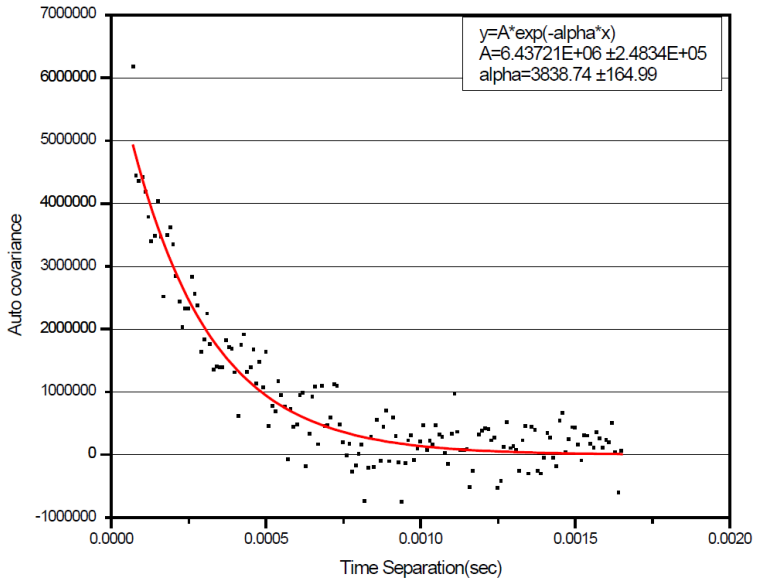


Figure-6.6: Plot of the auto covariance of the count rate with the time separation

Table-6.1: **Comparison of results obtained by Analog MC code with the analytical results**

Case	**Geometry**	**Neutron energy group**	**Exact Results**	**Our code**	
			Keff	**Keff**	**Std-dev**
Problem 2	One media Slab	One	1.00000	1.00012	0.00012
Problem 4	Two media slab	One	1.00000	0.99997	0.00016
Problem 7	One media cylinder	One	1.00000	0.99993	0.00013
Problem 8	One media sphere	One	1.00000	1.00002	0.00020
Problem 10	Two media cylinder	One	1.00000	0.99996	0.00016
Problem 46	One media sphere	Two	1.00000	1.00009	0.00022
Problem 58	Two media slab	Two	1.00000	1.00014	0.00031

Table-6.2: Geometrical and nuclear data of the experimental facility

Width and height (a,b)	84 cm
Length	120 cm
D	0.879 cm
$\nu\Sigma_f$	0.001 cm-1
Σ_c	0.00151
Σ_s	0.354

CHAPTER 7

Summary and Conclusions

Accelerator-driven systems (ADS) have been considered as a viable option to deal with the transuranic elements generated mainly from nuclear reactors. For development of such system several countries have initiated research activities in the area of development of high power accelerators, suitable targets and new reactor physics concepts. For desired power gain and assured criticality safety margin, ADSs would require constant reactivity monitoring. Compared with a critical reactor, the reactivity measurement and monitoring in ADS is a more challenging issue. Since these systems will never go critical, the reactivity calibration methods applicable for critical reactors will not be possible to use for ADSs. Therefore around the world additional reactivity measurement techniques are being validated and qualified. Generally these techniques are based on analysing the neutron flux/detector response for a short neutron pulse and fitting the fall of detector response to exponential curve and inferring the reactivity. Reactor noise techniques are also considered to be suitable for determining reactivity. Theoretical analysis supported by experiments has revealed that detectors placed at different locations may indicate different reactivity due to presence of higher harmonics. Alpha-modes are useful for the analysis of spatial effects in reactivity measurement experiments. The knowledge of zeros of the alpha-modes is important for identification of suitable detector locations.

In our research work we have developed two schemes which can efficiently solve prompt time eigenvalue problems. We call these as the 1/v absorber and the modified power iteration

schemes. The latter technique appears to have some advantages over the other methods. Alpha modes are not directly estimated in the 1/v absorber method. We have to first evaluate λ -modes and then we have to guess for α . This is a cumbersome process. The advantage of 1/v absorber method is that if a code for finding dominant λ-modes is available, it can be straightaway used to find α-modes without any further development work.

The modified power iteration based on sub-space iteration has very good convergence properties. If there are 'p' given vectors, the convergence of i^{th} mode depends on (α_{p+1}/α_i). Hence the problem due to closely spaced eigenvalues in the elimination method is drastically reduced. Of course, Arnoldi method has also been to be highly efficient scheme for which free software is available. However, we wish to point out one advantage of sub space iteration scheme. The main computational effort in SSI is to carry out 'p' number of external source calculations in a sub-critical medium. However, all 'p' calculations are completely independent and can be carried out in parallel. Thus one can implement a MASTER-SLAVE type of parallelization. Thus SSI is very suitable for Coarse Grain paralleization and can give good speed-up. On the other hand, in Arnoldi method the external source calculation have to be performed one by one and hence cannot be paralleized. It may be mentioned here that, the SSI method for λ -modes (Modak and Jain, 1996) was paralleized on a distributed memory processor ANUPAM of BARC, Mumbai and gave excellent speed-up.

In the context of the long computing associated with multiple source calculations during each iteration. So the above scheme cannot be used straightaway for supercritical reactors. This problem of super criticality is avoided by subtracting (β/v)Φ from both sides of the alpha eigen value equation. While it is enough to choose a magnitude such that the reactor is rendered

subcritical for the solution of the source problem, it might be profitable to use a larger value from the computational point of view, since the source iterations are expected to converge faster for a system that is far from criticality than one near criticality. Of course, this can also affect the dominance ratio and hence an optimum value of β can be found. The relation of this optimum value to the system properties as well as means to find such an optimum value is interesting problems for further study.

In the thesis we have also discussed the validity of relation between fundamental α and k. We have shown that by the use of an appropriate weighting function to define generation time, the validity can be extended to all situations. Numerical demonstration is provided by evaluating prompt neutron generation time for near-critical PHWR test case and also for a highly sub-critical reflected reactor. It is seen that the relation between α and k ie; $\alpha = \frac{(k-1)/k}{\Lambda}$ holds good irrespective of sub-criticality magnitude of the reactor.

For complete description of pulse neutron experiments, a method for obtaining α modes of the diffusion equation with delayed neutrons has also been developed. The method is based on the usual subtraction technique. Using this method, a model PHWR problem has been studied in two and three energy groups. In the case of the PHWR problem in two energy groups, the difference in prompt alpha modes and delayed alpha modes is not significant. This is due to the fact that in two energy groups, the fission spectra for prompt neutrons and delayed neutrons are identical. In three neutron energy groups the prompt and delayed neutron spectra are quite different and we observe a distinct difference between the prompt and the delayed modes. Moreover, the

difference between the two is more pronounced for the higher modes as compared to that for the fundamental modes.

The difference between prompt and delayed alpha modes is seen to be greatest in the reflector region. Since the alpha modes are equivalent to adding (subtracting) 1/v absorption, this is expected to have greatest effect in the reflector region since in this region absorption is minimum and therefore any addition has greater effect. Finally, in case the reactor is sub-critical the difference between prompt and delayed modes is found to be significant even for the fundamental modes. Since the prompt modes and delayed modes are approximately like the alpha modes and lambda modes respectively, and since these are known to be very different from one another for highly sub-critical systems, this may be the reason for the greater difference in the case of sub-critical systems.

Using the subtraction technique, we have been able to evaluate the fundamental and three higher (prompt and delayed) modes. Higher order delayed modes could not be obtained due to convergence related difficulties. An attempt was made to calculate higher prompt and delayed modes using the sub-space iteration methods but was not successful. Even for the sub-space method, the modes have to be computed one at a time, which defeats the very purpose of the sub-space iteration technique. Moreover the sub-space iteration method can be used for evaluation of delayed alpha modes only in sub-critical reactors. For a supercritical reactor, a 1/v absorption cross section is required to be added to make it sub-critical. Subsequently the coefficient of this 1/v absorber is subtracted from the computed alpha eigenvalue. Since the delayed alpha eigenvalues are small in magnitude in comparison to the added 1/v absorber, subtraction of the same from the computed delayed alpha eigenvalue results in loss of accuracy due to round off

errors. It would be interesting to develop a method for computing higher prompt and delayed modes which do not suffer from these difficulties.

In addition to alpha mode evaluation, we have also developed 3 dimensional space time kinetics code KINFIN to predict reactor behaviour during transient. The code is KINFIN based on direct integration method. The validation of the method has been carried out by comparison of the results with existing 3-Dimensional PHWR and LWR benchmarks. The code is proposed to be used in analyzing the neutron pulse experiments in PURNIMA facility. We have also developed thermal model which can be useful for analyzing feedback effects.

As a part of the planning of noise and pulse experiments in the Purnima sub-critical facility and also for validation of the theory of finding zeros of alpha modes for detector location, we have developed a time dependent transport theory based analog Monte Carlo code. The simulator is capable of treating the geometries commonly occurring in nuclear reactors. The delta tracking method (also called Woodcock and Coleman method) is used, which results in fast and relatively simple handling of complex geometries. The code has been validated by comparing with criticality benchmarks and with results of the previous simulator code based on diffusion theory as well as with Feynman alpha and Rossi alpha calculations based on solutions of the forward and adjoint equations.

We have also carried out simulation of a full 3-dimensional representation of one of the proposed designs of the Purnima sub-critical facility. The simulations show that proper location of detectors gives an almost single exponential (fundamental mode) response making alpha measurements by the noise methods possible even in deeply sub-critical systems. This is a confirmation of a result obtained using the diffusion theory based Monte Carlo simulator.

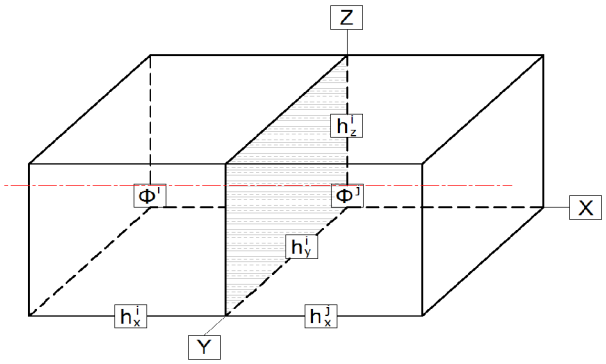
In the analogue Monte Carlo code for simulating various experiments, we have simplified our problem by treating the energy variable by the method of groups and by assuming isotropic scattering. Further work in this direction would be to develop a code capable of continuous energy treatment with anisotropic scattering.

APPENDIX 2A

Steady state multigroup neutron diffusion equation can be expressed by following equation

$$-\nabla.D_g\nabla\phi_g+\Sigma_g^r\phi_g=\sum_{g'\neq g}^{G}\left[\Sigma_{g'\to g}^{s}\phi_{g'}\right]+\chi_g\sum_{g'=1}^{G}\left[\nu\Sigma_{g'}^{f}\phi_{g'}\right]+S_g^{ext} \qquad (2A.1)$$

Eq.(2A.1) is integrated over rectangular mesh box i of volume V^i as shown in figure given below:



For a given cell we define the cell average flux of group g: $\phi_g^i \equiv \frac{1}{V^i}\int_{V^i}\phi_g dV$

Using Gauss divergence theorem first term of equation Eq.(A.1) can be simplified as under:

First Term of Eq.(2A.1)

$$-\frac{1}{V^i}\int_{v^i}\nabla.D_g\nabla\phi_g\,dV=-\frac{1}{V^i}\int_{S_i}D_g^i\hat{n}.\nabla\phi_g\,ds=-\sum_n D_g^i\left(\frac{d\phi}{dn}\right)_i A^{i(n)}$$

where, $A^{i(n)}$ = Area of surface in direction 'n' of i^{th} mesh

$\left(\frac{d\phi}{dn}\right)_i$ = Derivative of flux in the direction normal to surface 'n ' of i^{th} mesh

Here superscript ‘n’ denotes the neighbor of mesh i. ‘n ‘ can take value from (E, W, N. S, U, D) depicting directions (East, West, North, South, Up, Down). For example $D_g^{i(E)}$ is the diffusion coefficient in g^{th} group of the mesh which is in East direction of mesh i.

Let us consider the flux at common surface $A^{i(E)}$ is $\phi_g^{1/2}$ then with help of continuity equation one can write current from left and right hand side

$$J_{LHS}^{i(E)} = -D_g^i \frac{(\phi_g^{1/2} - \phi_g^i)}{\frac{h_x^i}{2}} A^{i(E)}$$

$$J_{RHS}^{i(E)} = -D_g^i \frac{(\phi_g^{i(E)} - \phi_g^{1/2})}{\frac{h_x^{i(E)}}{2}} A^{i(E)}$$

Now applying current continuity condition we get

$$\frac{1}{V^i}\int_{S_i} D_g \hat{n}.\nabla\phi_g ds = \sum_n D_g^{i(n)}(\phi_g^i - \phi_g^{i(n)})A^{i(n)}$$

$$\overline{D_g^{i(n)}} = \frac{2D_g^{i(n)}.D_g^i}{[D_g^{i(n)}.h_r^i + D_g^i.h_r^{i(n)}]}$$

Here, $h_r^i = h_x^i$ (mesh width in East direction)

$h_r^i = h_y^i$ (mesh width in North direction)

For boundary nodes the term $D_g \hat{n}.\nabla\phi_g$ are derived by putting boundary conditions on the boundary surfaces of the nodes In the boundary surfaces the leakages are evaluated by different formulations. In the boundary surfaces the leakages are evaluated as given below:

Let i^{th} mesh be a boundary mesh ie; the surface $A^{i(W)}$ be a boundary surface where flux is assumed to be zero. In this condition the leakage from this surface is expressed as under:

$$\text{Leakage} = -D_g^i \frac{(\phi_g^{1/2} - \phi_g^i)}{\frac{h_x^i}{2}} A^{i(W)}$$

Putting $\phi_g^{1/2}$ =0 in the equation, we have Leakage= $2D_g^i \frac{\phi_g^i}{h_x^i} A^{i(W)}$

Second term (Removal term)

$$-\frac{1}{V^i}\int_{V^i} \Sigma_g^r \phi_g dV = -\Sigma_g^{ri}\phi_g^i = -\Sigma_g^{ri}\phi_g^i$$

Third term (Scattering term)

$$\frac{1}{V^i}\int_{V^i} \sum_{g' \neq g}^{G} \left[\Sigma_{g' \to g}^{s} \phi_{g'}\right] dV = \sum_{g' \neq g}^{G} \left[\Sigma_{g' \to g}^{si} \phi_{g'}^i\right]$$

$$\frac{1}{V^i}\int_{V^i} (\chi_g \sum_{g'=1}^{G} \left[\nu\Sigma_{g'}^{f} \phi_{g'}\right] dV = \chi_g \sum_{g'=1}^{G} \left[\nu\Sigma_{g'}^{fi} \phi_{g'}^i\right]$$

For steady state case (critical reactors) the above formulations lead to a matrix equation as written below:

$$M\phi = \frac{1}{\lambda}\chi F\phi$$

M is the matrix containing diffusion, removal and scattering terms and F is the matrix containing fission terms. Here for convenience the element of ϕ are arranged in such a way that all fluxes for group 1 precede those for group 2 and so on. M, F, χ are NGxNG matrices and ϕ is NGx1 column vector. These are expressed as below:

$$\phi = \begin{pmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_G \end{pmatrix}, \quad M = \begin{pmatrix} [A_1] & [0] & \cdots & [0] \\ [-\Sigma_{1->2}^{s}] & [A_2] & \cdots & [0] \\ \vdots & \vdots & & \vdots \\ [-\Sigma_{1->G}^{s}] & [0] & \cdots & [A_G] \end{pmatrix}, \quad F = \begin{pmatrix} [\nu\Sigma_1^f] & [\nu\Sigma_2^f] & \cdots & [\nu\Sigma_G^f] \\ [0] & [0] & \cdots & [0] \\ \vdots & \vdots & & \vdots \\ [0] & [0] & \cdots & [0] \end{pmatrix}$$

$$\chi = \begin{pmatrix} [\chi_1] & [0] & \cdots & [0] \\ [\chi_2] & [0] & \cdots & [0] \\ \vdots & \vdots & & \vdots \\ [\chi_G] & [0] & \cdots & [0] \end{pmatrix}$$

Here $\Sigma_{g->g'}, \nu\Sigma_{f_g}, A_g$ are all diagonal matrices and A_g's matrices containing diffusion and removal terms.

Appendix 4A

The elimination method to find higher λ-modes

Let ϕ_n and ϕ_m^* be the eigenfunctions of the lambda eigenvalue equation Eq.(4.A.1) and the corresponding adjoint Eq.(4.A.2) written below:

$$A'\phi_n = \frac{1}{\lambda_n} F'\phi_n \qquad (4.A.1)$$

$$A'^t\phi_m^* = \frac{1}{\lambda_m^*} F'^t\phi_m^* \qquad (4.A.2)$$

Here ϕ_m^* is orthogonal to ϕ_n and the orthogonality relation between them is

$$(\frac{1}{\lambda_m^*} - \frac{1}{\lambda_n})\left\langle \phi_m^* F'\phi_n \right\rangle = 0 \quad \text{for } m \neq n \qquad (4.A.3)$$

The eigenvalues are real positive and they can be arranged as $\lambda_0 > \lambda_1 > \lambda_2 > \lambda_3$ … and so on. The fundamental eigenvalue λ_0 and corresponding flux can be found by the well-known power iteration method. This is done by starting with a guess flux ϕ and multiplying it repeatedly by

$A^{-1}F$ (and normalizing). The flux tends to ϕ_0. The higher modes are obtained by continuing with power iterations but periodically subtracting contribution of already determined modes.

Let $\phi_0, \phi_1, \phi_2, ...\phi_n$ be the direct modes and $\phi_0^*, \phi_1^*, \phi_2^*, ...\phi_m^*$ be the corresponding adjoint modes. If ϕ and ϕ^* are the starting (guess) flux and adjoint distributions respectively, then we can expand these in terms of the direct and adjoint modes as shown below

$$\phi = a_0\phi_0 + a_1\phi_1 + a_2\phi_2 + a_3\phi_3 + ... \qquad (4.A.4)$$

and

$$\phi^* = b_0\phi_0^* + b_1\phi_1^* + b_2\phi_2^* + b_3\phi_3^* + ... \qquad (4.A.5)$$

where a_k and b_k are the expansion coefficients. The expansion coefficients can be expressed as:

$$a_k = \frac{<\phi_k^* F'\phi>}{<\phi_k^* F'\phi_k>} \text{ and } b_k = \frac{<\phi^* F'\phi_k>}{<\phi_k^* F'\phi_k>} \qquad (4.A.6)$$

The procedure to find higher modes is as follows:

1) First find ϕ_0 and ϕ_0^* by power iterations.
2) Start with a fresh guess ϕ. Find coefficients a_1 and b_1. Find revised guess flux as $\phi - a_1 \phi_0$. This removes component along the fundamental mode. Continue power iterations for direct equation with periodical filtering of fundamental mode. The iterations converge to next mode ϕ_1.

3) Start with a fresh guess ϕ^*. Find revised guess flux as $\phi^* - b_1 \phi_0^*$. Continue power iterations for adjoint equation with periodical filtering. This generates next mode ϕ_1^*.

4) Compute coefficients a_2 and b_2.

5) Start with a fresh guess ϕ. Find revised guess flux as $\phi - a_1 \phi_0 - a_2 \phi_1$. This removes contribution of first two modes. Continue power iterations with periodic filtering of known modes. This generates ϕ_2.

6) In a manner analogous to step 5, ϕ_2^* can be found.

The procedure can be continued till required higher modes ϕ_K and ϕ_K^* are obtained. One has to subtract contributions of already known modes $\phi_0, \phi_1, \phi_2, \phi_3 ..... \phi_{K-1}$.

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