# **LECTURE 3: LATTICE PARAMETER CALCULATIONS**

# MODULE OBJECTIVES:

At the end of this module, you will be able to:

- 1. Describe the approximations used in a lattice parameter (POWDERPUFS) calculation.
- 2. Use the output of POWDERPUFS to explain the results of a physical core change.

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### INTRODUCTION

The preceding Lecture gave a brief summary of the scope of physics analysis that typically takes place in the process of designing a CANDU reactor. This Lecture deals with this process in detail and discusses some of the typical results we obtain from our analysis.

The two main objectives are:

- to provide an understanding of the methods we use
- to give a fairly detailed description of the physics characteristics of these reactors.

The organization of the next several Sections is based on the intent to follow a typical sequence of activities which take place in the process of performing the reactor physics analysis required to produce a CANDU reactor design.

CONCEPTUAL STAGE DESIGN ANALYSIS

- The basic building block of the CANDU pressure tube type reactor is the fuel channel.
- The design of the fuel, pressure tube and calandria tube and the separation of these assemblies from each other (the lattice pitch) determine the basic nuclear characteristics of the reactor core.
- Since there is a repeating array of these assemblies throughout the core, the basic nuclear characteristics can be determined by considering only one channel surrounded by the appropriate volume of heavy water moderator. This is



Figure 3-1: Arrangement of fue! channels & moderator.

commonly called a "unit cell". The nuclear characteristics of a unit cell are called lattice parameters.

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#### CALCULATION OF LATTICE PARAMETERS

- The boundary condition at the outer surface of the moderator associated with the unit cell is taken to be zero gradient of the neutron flux (no leakage of neutrons).
- The method which is applied in the unit cell calculation depends on the detail with which the reaction rates within the unit cell need to be known.
- For most purposes it is sufficient to know the reaction rates within the fuel bundle as a whole.
- Since the early days of the design of CANDU prototypes it was considered desirable to develop a fast and reasonably accurate cell code that could be used for survey and design purposes.
- The lattice parameter program POWDERPUFS is a fast and reasonably accurate cell code that is used for survey and design purposes.
- POWDERPUFS is the code most widely used to generate the lattice parameters needed for commercial core design and analysis.



Figure 3-2: Lattice Cell for 37element Fuel. FUEL ELEMENT D20 COOLANT PRESSURE TUBE AIR GAP CALANDRIA TUBE D20 MODERATOR

#### FUNCTIONAL DESCRIPTION OF LATTICE PARAMETER PROGRAMS

#### **Nuclear Reaction Rates**

- in the POWDERPUFS code the cell is assumed to be divided into three main regions:
  - $\Rightarrow$  1 a fuel region,
  - $\Rightarrow$  2 an annuli region (including the pressure tube and calandria tube and the gap between them)
  - $\Rightarrow$  3 a moderator region.
- Therefore the flux distribution in the cell is calculated using a simple one dimensional annular model.
- The moderator region is approximated by circular outer boundary rather than a square.
- The nuclear cross sections for the fuel are based on the Wescott convention, i.e. that the neutron spectrum has of a maxwellian & a 1/e part characterized by two parameters calculated in the program.
- The resonance integrals are based on a semi-empirical treatment and the resonance absorption is lumped into a single adjusted energy.
- Thermal absorption is calculated by a simple collision probability method.
- The calculations within this code are basically recipe type or semi-empirical type calculations.
- The ratio of moderator to fuel in a CANDU lattice is such that over 95% of neutrons in the moderator are thermalized i.e. have an energy distribution in equilibrium with the moderator atoms.
- The majority of neutrons absorbed are, therefore, thermal neutrons and the epi-thermal neutron absorption is conveniently grouped with thermal absorption using measured thermal-to-epi-thermal reaction rate ratios (an exception is resonance absorption <sup>238</sup>U).
- Neutron absorption in <sup>238</sup>U at the higher resonance energies is treated specifically and hence is not included in the Wescott cross sections. The total epi-thermal cross sections are measured in an experimental reactor and empirical expressions are derived based on data for various fuel geometries and fuel temperatures. While this method is quite simplified it does provide reliable results for lattices in the range of interest for natural uranium CANDU reactors.

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Power Distribution within a Fuel Bundle

- An important consideration in fuel design is the maximum heat flux produced in any one pin of the fuel bundle. This cannot be obtained from the POWDERPUFS code.
- Detailed power distribution data in the fuel cluster can be obtained from the LATREP lattice parameter program, or obtained directly from experimental data.
- The flux distribution is calculated in LATREP at several energy groups using collision probability methods.
- Resonance integrals of fertile materials are based on semi-empirical recipes but the resonance absorption is calculated in 32 groups.
- A single thermal group is assumed, using the Wescott convention for reaction rate calculations in nonfertile isotopes and in fissile isotopes.
- In the LATREP code the fuel pencils are smeared into annular rings so that the reaction rates can be calculated separately in each of these rings and from those results the power distribution across bundle can be determined.

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# MULTI-GROUP TRANSPORT CODES

• multi-group transport codes such as WIMS and HAMMER are used primarily to perform spot checks for the simpler and much faster codes.

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- A series of transport codes have also been developed at AECL.
  - ⇒ An R-Z code (PEAKAN) is used primarily for treating the bundle-end flux peaking
  - ⇒ An X-Y-Z code (SHETAN) is used to calculate reaction rates in absorbers of complex geometry.
  - $\Rightarrow$  GETRANS is a two dimensional version of SHETAN.
- There are also certain specific problems where even the so-called "hyperfine" distribution of flux within the fuel pin is important to determine. We have found an important difference in the variation of the hyperfine pin power distribution with *irradiation between the natural uranium fuel and* enriched fuel. We find that, because of the socailed "skin effect", resonance absorption occurs preferentially at the surface of the pin. The corresponding preferential plutonium production as the irradiation proceeds tend to cause a relatively larger proportion of power to be produced near the surface of the pin for irradiated natural fuel than for irradiated enriched fuel.
- The degree of sophistication of analytical methods used to perform unit cell calculations depends on the problem being dealt with. Our approach is to apply the multi-group codes only in those cases where their capabilities are demanded.





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## SPECIAL FEATURES FOR CANDU APPLICATIONS

- For conceptual design studies, the POWDERPUFS code is used to generate lattice parameters for various fuel geometries and pressure tube and calandria tube characteristics and also for various values of lattice pitch. Average cell parameters are produced for each case. These parameters are then put into a diffusion code to simulate a reactor core.
- The POWDERPUFS code has built within it the capability to perform a simple one dimensional analytical core calculation in which fuel can be assumed to be at different burnups in annular regions in the core and the heavy water reflector surrounding the fuel channels can be simulated. This is convenient for the very early conceptual stages of a design study as the fuel burnup achievable for various core sizes and various degrees of radial flattening in the core can be examined as well as the effect of changing reflector thickness all at very minimal cost.
- A feature which is important in respect to treating the bi-directional semi-continuous fuelling that occurs in a CANDU reactor at equilibrium burnup is the capability to average reaction rates over a burnup interval. The basic output of POWDERPUFS, as with most other cell codes, are the cell-average lattice parameters (in this case cross sections in two energy groups) as a function of the irradiation seen by the fuel.
- If we consider two adjacent channels in the CANDU reactor and assume ideally that they are being fuelled continuously in opposite directions, each channel would have fuel with irradiation ranging from zero to the discharge value from one end of the channel to the other. We find that if we calculate average reaction rates by integrating over this irradiation interval, the corresponding lattice properties are not very different than what would be obtained if the properties of two adjacent channels are averaged point by point along the channel.
- This feature provides a very convenient way to calculate lattice parameters for a reactor operating under equilibrium fuelling conditions for any given assumed discharged burnup. These average parameters can be calculated within the POWDERPUFS program.

## SPECIAL FEATURES FOR CANDU APPLICATIONS (continued)

- Another feature of the program which is very useful, is the capability to calculate the effect on these
  averaged properties of instantaneously changing the characteristics of the materials in the fuel channel
  e.g. changing fuel temperature, coolant temperature, coolant density, removing coolant completely etc.
  This feature is used to determine reactivity coefficients for the reactor during the conceptual stage, and
  in some cases the POWDERPUFS calculations are sufficiently accurate for the final design.
- In addition to giving the cell averaged cross sections used in two-group diffusion code simulation of the reactor core, the POWDERPUFS program also provides the classical "four factors" which determine the multiplication factor for the infinite lattice. The effective multiplication factor for a finite care having a given geometric buckling is also calculated as indicated in the following equations:

$$k_{\infty} = \eta \epsilon p f$$

$$k_{eff} = \frac{k_{\infty}}{(1 + L^2 B_g^2) (1 + L_g^2 B_g^2)}$$

- Note that the expression for effective multiplication factor includes terms which account for the leakage from a finite core for which the effective geometry buckling is  $B_{\alpha}^2$  an input quantity.
- This is valid, to the extent that this buckling can be estimated for a "real" system. The calculated k<sub>eff</sub> when based on reaction rate averaged cross-sections, gives a reasonable estimate of the multiplication factor of a reactor as a function of discharge burnup.
- This means that the POWDERPUFS code alone can be used to study sensitivity of discharged fuel burnup to changes in the fuel channel design characteristics and operating temperatures.

## SPECIAL FEATURES FOR CANDU APPLICATIONS (continued)

- The POWDERPUFS code alone can also be used to determine the impact of these changes on the reactivity coefficients which are important from the point-of-view of control and shutdown system implications. This is important in both the conceptual and detailed design stage as a large number of parameter variations can be studied at relatively small expense.
- The POWDERPUFS program has been incorporated into a comprehensive optimization program which ۲ considers all the other economic aspects of various design changes and arrives at a total unit energy cost for a given system.
- Some of the things which are "traded-off" in this optimization process are: .
  - $\Rightarrow$  the capital cost savings in minimizing the number of channels
  - the size of the calandria  $\Rightarrow$
  - $\Rightarrow$  increased fuelling cost associated with the need to flatten the power distribution to achieve the required energy output with a smaller reactor
- reducing the pitch of the fuel channels saves capital cost because of reducing the size of the calandria and the heavy water inventory but that would result in lower burnup and introduce design complications in respect to (many other variables are, of course, examined as well):
  - (a) the spacing of feeders from each channel and
  - (b) constraints imposed on the interstitial control and shutdown system devices.
- It is this kind of process which has led to the evolution of the CANDU PHW design from the smaller • channel and 19 element fuel bundles to the larger channel and 37-element fuel bundles in the current generation reactors.
- The basic fuel channel design including the fuel is generally arrived at by applying this optimization analysis using simple cell calculations to determine nuclear characteristics of the reactor with some one dimensional core simulations done to properly account for the effect of changing the radial power flattening and/or the reflector thickness on the reactor dimensions and fuel burnup.

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## **TYPICAL POWDERPUFS CALCULATIONS FOR CANDU-6**

# Four-Factor Data

- Figure 3-4 shows:
  - $\Rightarrow k_{\infty} \text{ the infinite multiplication factor versus} \\ neutron irradiation of the fuel$
  - $\Rightarrow \eta$  (neutrons produced per thermal neutrons absorbed)
  - $\Rightarrow$  f (thermal utilization)
  - $\Rightarrow \epsilon$  (fast fission factor) is essentially constant as a function of irradiation
  - ⇒ p (resonance escape probability) is essentially constant as a function of irradiation
- Note that the thermal utilization is also almost constant with irradiation, because:
  - ⇒ the absorption cross section of the fuel is dominated by the heavy elements which change very little, tending to increase only slightly with irradiation
  - ⇒ the buildup of plutonium isotopes due to capture in <sup>238</sup>U just about balances the burnout of the <sup>235</sup>U
  - ⇒ the η variation is very similar to the overall multiplication factor. The decrease with irradiation is primarily because of the buildup of fission products in the fuel.



Figure 3-4: Variation of Lattice parameters with Irradiation.

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**Fuel Temperature Reactivity Effects** 

- The fuel temperature reactivity coefficient is shown versus instantaneous irradiation \* in Figure 3-5.
- Note that it is significantly negative with fresh fuel and becomes less negative with irradiation.
- The value labeled "reaction rate averaged" is the value calculated using reaction rate averaged parameters for the irradiation which is typical of the average discharge from the reactor.
- The effect of heating up the fuel to the operating temperature is shown in Figure 3-6.



Figure 3-5: Fuel Temperature Reactivity Coefficient.



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Figure 3-7: Effect of instantaneously changing the coolant temperature on the reactivity of fuel as a function of irradiation.

Figure 3-8: Reactivity Change due to Change in Coolant Temperature, including Density Effect.

- Note in Figure 3-8 that although the coefficient (i.e. the slope of the curve) is positive at the operating temperature for both fresh and irradiated fuel, it is quite nonlinear for fresh fuel and in fact changes sign at low temperatures.
- There are two counter-balancing effects which take place as the temperature for the coolant is raised: the effect of making the coolant hotter than the moderator (which is typically kept at around 70°C) tends to harden the neutron spectrum in the fuel; on the other hand since the coolant density is decreasing, this spectrum hardening effect is less than it otherwise would be.

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Loss-of-Coolant Reactivity Effect

- Rupture of the primary heat transport system, although highly improbable, is one of the accidents which is postulated in design of the reactor safety systems.
- Since this accident leads to loss of coolant from some or all of the fuel channels the magnitude of this effect on reactivity is an important design parameter. Figure 3-9 shows the reactivity effect of simultaneously losing the coolant from all fuel channels for various fuel irradiations.
- Reactivity change due to losing the coolant is positive but not very large in magnitude and decreases with fuel irradiation.
  - ⇒ reducing coolant density results in an increase in the resonance escape probability due to lower resonance energy flux in the cluster;
  - ⇒ however, because the coolant is hot under normal steady state full power conditions, it tends to harden the spectrum of thermal neutrons coming from the moderator, which is a positive reactivity effect when plutonium is present in the fuel;





⇒ when the coolant is lost this hardening effect no longer exists which results in a decrease in reactivity, the magnitude of which is function of the concentration of plutonium isotopes in the fuel.

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#### Moderator Temperature Reactivity Effect

- The moderator temperature is not a parameter of much significance in the CANDU system because the moderator is essentially completely isolated from the fuel channel and the temperature of the moderator is relatively low and separately controlled.
- However it is of interest to know the reactivity effect associated with instantaneous changes in the moderator temperature to assess the impact on the reactor of changes that may occur due to upsets in the temperature control system of the moderator.
- The moderator temperature coefficient is plotted versus fuel irradiation in Figure 3-10.





**Reactivity Effect of Boron in the Moderator** 

- Adding "poison", in the form of dissolved natural boron or gadolinium to the moderator is the usual way of compensating for excess reactivity which exists when the reactor is initially loaded with all unirradiated fuel or during operation at equilibrium burnup when the reactor has been shut down for a significant period so that the <sup>135</sup>Xe in the fuel has decayed away.
- Therefore, the reactivity effect of changing the boron concentration in the moderator is a necessary design parameter.
- The effect of instantaneously changing the boron concentration for various fuel irradiations is plotted in Figure 3-11. In this case the calculations were done with reaction rate parameters for all cases. Note that the coefficient is not very dependent on the irradiation (the ordinate is an expanded scale).



Figure 3-11: Variation of Boron Coefficient with Irradiation.

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