4. Computational Scheme for CANDU Neutronics

- The computational scheme for CANDU neutronics consists of three stages:
- Cell calculation: to determine lattice properties for basic lattice cells
- "Supercell" calculation: to determine the "incremental" cross sections to be added to the basic-cell properties to account for the effect of reactivity devices
- Finite-core calculation: to solve the neutron-diffusion problem in the reactor core, to calculate the 3-dimensional flux and power distribution.

4. Computational Scheme for CANDU Neutronics

- **Computer programs have been developed to perform the calculations corresponding to each stage in the above process.**
- **These are now briefly discussed in the following sections.**

4.1 Cell Calculation and the POWDERPUFS-V Lattice Code

- **The cell calculation treats the "bare" CANDU basic lattice cell.**
- **"B are" here means the basic lattice cell without reactivity devices superimposed (refer to Fig. 1.2).**

4.1 Cell Calculation and the POWDERPUFS-V Lattice Code

- **The cell (or lattice) code which has traditionally been used for CANDU design and analysis is POWDERPUFS-V.**
- **This is an empirical-recipe code, based on the results of measurements made on heavy-water-moderated lattices in research reactors ZEEP and ZED-2 at Chalk River Laboratories.**
- **Although based on empiricism rather than a strong theoretical foundation, POWDERPUFS-V has been applied very successfully to CANDU design and analysis.**

4.1 Cell Calculation and the POWDERPUFS-V Lattice Code

- **POWDERPUFS-V uses the four-factor formula to calculate the infinite-lattice multiplication constant**

$$k_{inf} = \varepsilon p \eta f,$$

- **and to calculate homogenized-cell nuclear cross sections.**
- **It also utilizes the Westcott formulation for nuclide cross sections, a parametrization in terms of the neutron temperature and a spectral parameter r.**

4.1 Cell Calculation and the POWDERPUFS-V Lattice Code

- **The Westcott parametrization is applicable to highly thermalized neutron spectra,**
- **such as those in the CANDU lattice cell,**
- **where over 95% of neutrons in the fuel have a Maxwellian energy distribution.**

4.1 Cell Calculation and the POWDERPUFS-V Lattice Code

- **The nuclear cross sections are evaluated using the Westcott formula and other simple recipes,**
- **using parameter values obtained empirically from experiment.**
- **POWDERPUFS-V is applicable to CANDU reactors fuelled with natural uranium,**
- **where the amount of plutonium in the fuel is limited by the natural-uranium burnup.**

4.1 Cell Calculation and the POWDERPUFS-V Lattice Code

- **The Westcott convention for calculating the effective cross sections of fuel nuclides is based on assuming**
- **that the neutron spectrum can be written as the sum of a Maxwellian function and an epithermal function tending to 1/E:**

$$n(v) = N(1-f)\rho_m(v) + Nf\rho_e(v) \qquad (4.1)$$

where $\rho_m(v)$ and $\rho_e(v)$ are the Maxwellian and epithermal normalized density distribution functions, respectively, and

4.1 Cell Calculation and the POWDERPUFS-V Lattice Code

N = total neutron density

f = fraction of the total neutron density in the epithermal spectrum

$$\rho_m(v) = \frac{4}{\sqrt{\pi}} \frac{v^2}{v_T^3} e^{-(v/v_T)^2} \qquad (4.2)$$

$$\rho_e(v) = v_T \sqrt{\mu} \frac{\Delta(v)}{v^2} \qquad (4.3)$$

and v_T = velocity of a neutron of energy kT

4.1 Cell Calculation and the POWDERPUFS-V Lattice Code

- **$\Delta(v)$ is an empirical function describing the way the epithermal spectrum (with its 1/E "tail") joins the Maxwellian spectrum.**
- **It satisfies $\Delta(v) \rightarrow 0$ for $E < \mu kT$**
- **and $\Delta(v) \rightarrow 1$ for $E > \mu kT$,**
- **where μkT represents the lower limit of the 1/E spectrum and, by choice of convention, $\mu = 3.681$.**

4.1 Cell Calculation and the POWDERPUFS-V Lattice Code

- The Westcott flux $\hat{\phi}$ is defined as

$$\hat{\phi} = Nv_0 \qquad (4.4)$$

where $v_0 = 2200$ m/s

(i.e., as if the entire neutron distribution had a speed of 2200 m/s)

4.1 Cell Calculation and the POWDERPUFS-V Lattice Code

- and the effective (Westcott) cross section $\hat{\sigma}$
- of a given nuclide is defined so that its product with the Westcott flux gives the total reaction rate:

  Total reaction rate in nuclide

$$= \hat{\sigma}\hat{\phi} = \hat{\sigma} N \, \mathbf{v_0} \qquad (4.5)$$

- (By total reaction rate is meant the reaction rate in the entire spectrum, which includes the Maxwellian and the 1/E parts.)

4.1 Cell Calculation and the POWDERPUFS-V Lattice Code

- It can be shown that $\hat{\sigma}$ can be written in terms of 0, the 2200-m/s cross section, as follows:

$$\hat{\sigma} = \sigma_0(g + rs) \qquad (4.6)$$

- where g is the ratio of the reaction rate of the nuclide in a pure Maxwellian spectrum to the reaction rate of a 1/v absorber of the same 2200 m/s cross section
- (i.e., g is a measure of the 'non-1/v' character of the absorber in a Maxwellian spectrum), and
- r is a measure of the epithermal part (i.e., the 'hardness' of the spectrum).

4.1 Cell Calculation and the POWDERPUFS-V Lattice Code

- **r has a small value in the CANDU lattice:**
- **typically, r ~ 0.05 for a CANDU lattice fuelled with natural UO_2.**
- **This is what makes the Westcott formulation a good approximation in CANDU reactors.**

4.1 Cell Calculation and the POWDERPUFS-V Lattice Code

- **The g and s values for the various nuclides are obtained from experiment**
- **They are functions of the neutron temperature T_n, so that Eq. (4.6) is evaluated in fact as**

$$\hat{\sigma}(r, Tn) = \sigma_0(g(Tn) + rs(Tn)) \qquad (4.7)$$

4.1 Cell Calculation and the POWDERPUFS-V Lattice Code

- **In POWDERPUFS-V, the factors g(Tn) and s(Tn) are expressed as power series in the neutron temperature.**
- **With this database of g and s values for various nuclides, POWDERPUFS-V can calculate reaction rates in the fuel very quickly, using Eq. (4.7).**
- **For other materials, constant inputs or simple recipes are used.**

4.1 Cell Calculation and the POWDERPUFS-V Lattice Code

- **The methodology requires the evaluation of the spectral parameter r and the neutron temperature T_n**
- **in an iterative fashion from the lattice parameters via empirical relationships.**

4.1 Cell Calculation and the POWDERPUFS-V Lattice Code

- **In addition to the empiricisms, there are some approximations:**
- **Fast fission is taken into account in ^{238}U only, and is "lumped" into the thermal-fission cross section;**
- **also, up-scattering is ignored.**

4.1 Cell Calculation and the POWDERPUFS-V Lattice Code

- **One great advantage of POWDERPUFS-V is that, due to its semi-empirical nature and the simplifying assumptions used, it is very fast-running:**

- **A complete calculation (including depletion to exit burnup values) for a given lattice type is performed in less than 1 second of CPU time.**

4.1 Cell Calculation and the POWDERPUFS-V Lattice Code

- **POWDERPUFS-V provides "homogenized-cell" two-energy-group lattice properties for input into finite-core models and calculations.**
- **In standard "fuel-burn" mode, the lattice properties are provided as functions of fuel irradiation (or burnup)**
- **for specified values of lattice conditions, such as geometry, fuel, coolant, and moderator temperatures, power level, coolant density, moderator-poison concentration, etc.**
- **These conditions are entered as input to the code.**

4.1 Cell Calculation and the POWDERPUFS-V Lattice Code

- **For instance, the geometrical input and fuel mass may correspond to those for the 37-element-natural fuel lattice,**
- **the (average) fuel temperature may be entered as 687^{o} C,**
- **the (average) coolant temperature 290^{o} C,**
- **the moderator temperature 70^{o} C,**
- **the moderator and coolant purities may be 99.9 and 99.75 weight % D_2O, and**
- **the moderator poison may be set to 0 ppm B**

4.1 Cell Calculation and the POWDERPUFS-V Lattice Code

- **In addition to providing nuclear properties at various values of instantaneous irradiation,**
- **POWDERPUFS-V can do a "reaction-rate-averaged" calculation,**
- **where it averages the properties over irradiation ω from 0 to a specified exit value:**

$$\Sigma_{r.r.av.} = \left(\frac{1}{\omega_{exit}}\right)\int_0^{\omega_{exit}} \Sigma(\omega)d\omega$$

- **This calculation is extremely useful as a fairly good point-reactor model.**

4.1 Cell Calculation and the POWDERPUFS-V Lattice Code

- **A "perturbation" mode is also provided in POWDERPUFS-V,**
- **where lattice properties are evaluated assuming "instantaneous" changes in lattice conditions**
- **occurring at various values of fuel irradiation.**

4.1 Cell Calculation and the POWDERPUFS-V Lattice Code

- **POWDERPUFS-V has been used as the lattice code for CANDU reactors for about 30 years,**
- **where it has performed very well.**
- **One advantage of POWDERPUFS-V is that it is incorporated as a module within the finite-core code RFSP, described in Section 4.3 below.**

4.1 Cell Calculation and the POWDERPUFS-V Lattice Code

- **While POWDERPUFS-V has traditionally been the lattice code for CANDU design and analysis,**
- **it will eventually be replaced by a code with a stronger theoretical foundation, a multigroup transport-theory code such as WIMS-AECL.**
- **Calculating lattice cross sections with WIMS-AECL is, however, more complex and**
- **much more computationally intensive than with POWDERPUFS-V.**

4.2 Supercell Calculation

- **The effects of reactivity devices on the nuclear properties of the lattice in their vicinity are determined by a supercell calculation,**
- **performed with the computer code MULTICELL.**

4.2 Supercell Calculation

- A typical supercell is shown in Fig. 4.1.
- It is essentially a small model volume of the core around a portion of the reactivity device,
- including a portion of the neighbouring fuel channel (normally oriented perpendicularly to the device).
- The dimensions of the supercell are typically 1 lattice pitch x 0.5 lattice pitch x 0.5 bundle length.
- This represents a unit volume over which the effect of the reactivity device is modelled, utilizing the assumption of mirror symmetry about the supercell boundaries.

4.2 Supercell Calculation

- **The calculation provides incremental cross sections, which are to be added to the basic lattice cross sections over "homogenized" supercell volumes along the length of the device.**
- **MULTICELL applies pre-calculated boundary conditions (current-to-flux ratios) on internal surfaces which represent the reactivity device and the fuel (modified to Cartesian geometry). These boundary conditions are calculated using integral transport theory (Kushneriuk's method).**

4.2 Supercell Calculation

- **Outside the reactivity-device and fuel regions, MULTICELL applies diffusion theory to calculate the 3-dimensional flux distribution in the moderator.**
- **Except for zone controllers, which have a spectral effect, 1-group instead of 2-group diffusion is used, and the thermal-neutron source distribution is assumed flat in the moderator,**
- **based on the contribution to the slowing-down density of the multiple line sources represented by the fuel channels.**

4.2 Supercell Calculation

- Once the flux distribution in the supercell has been calculated, MULTICELL derives the homogenized-supercell cross sections.
- Then, from two MULTICELL calculations performed for the supercell:
  - a reference calculation with the device absent, and
  - a calculation with the device present
- device incremental cross sections are obtained by subtraction

4.3 Finite-Core Calculation and the RFSP Code

- **Once basic-lattice properties and reactivity-device incremental cross sections are available,**
- **the finite-core calculation can proceed.**
- **The finite-core computer code RFSP (Reactor Fuelling Simulation Program) is specifically designed for CANDU reactors.**

4.3 Finite-Core Calculation and the RFSP Code

- **It can calculate the steady-state 3-dimensional flux and power distributions in the reactor using two different methods:**
- **by solving the time-independent finite-difference diffusion equation in two energy groups, and**
- **by the method of flux mapping (described in Section 3.3), if the readings of the in-core vanadium detectors are available.**

4.3 Finite-Core Calculation and the RFSP Code

- **The time-independent neutron-diffusion equation solved in RFSP for eigenvalue problems in two energy groups with lattice properties from POWDERPUFS-V is:**

$$-\vec{\nabla} \cdot D_1(\vec{r})\,\vec{\nabla}\phi_1(\vec{r}) + (\Sigma_{a1}(\vec{r}) + \Sigma_{1\to 2}(\vec{r}))\,\phi_1(\vec{r}) - \frac{\nu\Sigma_f(\vec{r})}{k_{eff}}\phi_2(\vec{r}) = 0$$

$$-\vec{\nabla} \cdot D_2(\vec{r})\,\vec{\nabla}\phi_2(\vec{r}) + \Sigma_{a2}(\vec{r})\,\phi_2(\vec{r}) - \Sigma_{1\to 2}(\vec{r})\,\phi_1(\vec{r}) = 0$$

4.3 Finite-Core Calculation and the RFSP Code

- In this equation there are no fast-fission or
- up-scattering terms, consistent with the POWDERPUFS-V methodology
- However, for use with WIMS-AECL lattice properties, RFSP has the capability to solve a true-two-energy-group diffusion equation::

$$-\vec{\nabla} \cdot D_1(\vec{r})\,\vec{\nabla}\phi_1(\vec{r}) + (\Sigma_{a1}(\vec{r}) + \Sigma_{1\to 2}(\vec{r}))\,\phi_1(\vec{r}) - \left(\Sigma_{2\to 1}(\vec{r}) + \frac{\nu\Sigma_{f2}(\vec{r})}{k_{eff}}\right)\phi_2(\vec{r}) = 0$$

$$-\vec{\nabla} \cdot D_2(\vec{r})\,\vec{\nabla}\phi_2(\vec{r}) + \left(\Sigma_{a2}(\vec{r}) + \Sigma_{2\to 1}(\vec{r})\right)\phi_2(\vec{r}) - \left(\Sigma_{1\to 2}(\vec{r}) + \frac{\nu\Sigma_{f1}(\vec{r})}{k_{eff}}\right)\phi_1(\vec{r}) = 0$$

4.3 Finite-Core Calculation and the RFSP Code

- **A typical reactor model used with RFSP is shown in Fig. 4.2 a and b (face and top views respectively).**

4.3 Finite-Core Calculation and the RFSP Code

- **Major applications of RFSP are in:**
- **core-design calculations and analyses, including fuel-management design calculations, and simulations of reactor power histories**
- **core-follow calculations at CANDU sites, to track the actual reactor operating history, with burnup steps and channel refuellings.**

4.3 Finite-Core Calculation and the RFSP Code

- **Additional capabilities of the program include, among others:**

- **the calculation of flux distributions for various reactor configurations**
- **the simulation of $^{135}Xe/^{135}I$ transients**
- **the capability for simulating (quasi-statically) bulk control and spatial control**
- **the calculation of harmonic flux shapes for use in flux mapping,**

(cont'd)

4.3 Finite-Core Calculation and the RFSP Code

- **the calculation of the reactivity increase expected on refuelling of individual fuel channels**
- **the capability for solving neutron-kinetics problems by the Improved Quasi-Static (IQS) method.**
- **RFSP can therefore be used to analyze fast transients, such as those following hypothetical large-loss-of-coolant accidents (LOCA), and can be used to simulate and verify the performance of the shutdown systems.**