



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**
$$k_{\text{inf}} = \epsilon p \eta f,$$
- ◆ **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 $1/E$:

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

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

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

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

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**

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

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

$$= \hat{\sigma} \hat{\phi} = \hat{\sigma} N \mathbf{v}_0 \quad (4.5)$$

- ◆ (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 σ_0 , the 2200-m/s cross section, as follows:

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

- ◆ 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, $r \sim 0.05$ 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

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



4.1 Cell Calculation and the POWDERPUFS-V Lattice Code

- ◆ **In POWDERPUFS-V, the factors $g(T_n)$ and $s(T_n)$ 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° C,
- ◆ the (average) coolant temperature 290° C,
- ◆ the moderator temperature 70° C,
- ◆ the moderator and coolant purities may be 99.9 and 99.75 weight % D₂O, 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:**

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

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



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::

$$\begin{aligned} -\vec{\nabla} \cdot D_1(\vec{r}) \vec{\nabla} \phi_1(\vec{r}) + (\Sigma_{a1}(\vec{r}) + \Sigma_{1 \rightarrow 2}(\vec{r})) \phi_1(\vec{r}) - \left(\Sigma_{2 \rightarrow 1}(\vec{r}) + \frac{\nu \Sigma_{f2}(\vec{r})}{k_{eff}} \right) \phi_2(\vec{r}) &= \mathbf{0} \\ -\vec{\nabla} \cdot D_2(\vec{r}) \vec{\nabla} \phi_2(\vec{r}) + (\Sigma_{a2}(\vec{r}) + \Sigma_{2 \rightarrow 1}(\vec{r})) \phi_2(\vec{r}) - \left(\Sigma_{1 \rightarrow 2}(\vec{r}) + \frac{\nu \Sigma_{f1}(\vec{r})}{k_{eff}} \right) \phi_1(\vec{r}) &= \mathbf{0} \end{aligned}$$



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 $^{135}\text{Xe}/^{135}\text{I}$ 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.**