



## ***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.



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## ***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  $r$ .



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## *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**

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

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

**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  $\mu kT$  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

$$\hat{\phi} = N v_0 \quad (4.4)$$

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  $\sigma_0$ , 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  $\text{UO}_2$ .**
- ♦ **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  $^{238}\text{U}$  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 % D<sub>2</sub>O, 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  $\omega$  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.



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## *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.



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## ***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.



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## ***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:**

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

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



## ***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::

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

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



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## ***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.