Session 12
CANDU Physics Computational Scheme and Use of POWDERPUFS-V

by
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In this Session we will look at the general computational scheme for CANDU reactor-physics calculations. We will then initiate some specific lattice calculations with the code POWDERPUFS-V.

12. CANDU Reactor-Physics Computational Scheme

The computational scheme for CANDU neutronics consists of three stages. Computer programs have been developed to perform the calculations corresponding to each stage.

The three stages are:

- Lattice-Cell Calculation
- Reactivity-Device (Supercell) Calculation
- Finite-Core Calculation

12.1 Lattice Calculation

This first stage involves calculating the average nuclear properties ("homogenized-cell nuclear cross sections" for absorption, moderation, fission, etc.) for the basic lattice cell consisting of the fuel, coolant, pressure and calandria tubes, and moderator, but no reactivity device - see Figure 12.1 (not to scale).

Quantitatively, the lattice properties govern the neutron-multiplying behaviour of the reactor lattice. The lattice properties must reflect the configuration of the lattice. For example, if the coolant is assumed "voided" in a hypothetical loss of coolant, then the lattice properties must change accordingly.

The fuel burnup is the amount of fission energy a unit mass of fuel has generated since its first entry into the reactor. Burnup changes the fuel composition, as uranium is depleted and plutonium builds up. Therefore the lattice properties change with burnup (or irradiation), and must therefore be evaluated for each lattice cell in the reactor, as the fuel burnup varies with the position of the fuel in the reactor.

In addition, the lattice properties must also be calculated for spatial or temporal variations in cell conditions which result from normal changes inherent in reactor operation (e.g., changing poison concentration in the moderator) or from hypothesized accident scenarios (e.g., different coolant densities and fuel temperatures in loss-of-coolant accidents), etc.

D₂O
Primary
Coolant
Gas
Annulus
Fuel Elements
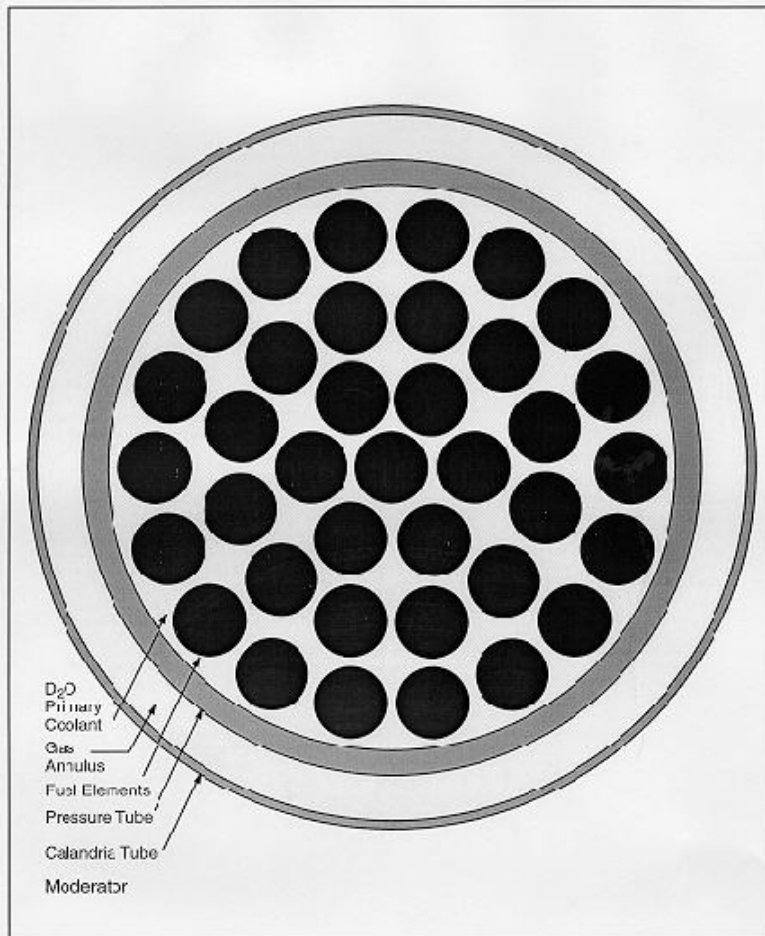Pressure Tube
Calandria Tube
Moderator

Figure 12.1
CANDU Basic-Lattice Cell (not to scale)

Because of the strong neutron-production and neutron-absorption properties of the nuclear fuel, diffusion theory cannot be used to calculate the average lattice properties. To calculate these properties from first principles, a computer code would have to be rooted in transport theory. WIMS-IST (IST meaning Industry Standard Tool) is such a computer code with a rigorous theoretical basis in neutron transport theory. It is being used increasingly to calculate lattice properties, especially in safety-analysis applications. Because it is a transport-theory code, WIMS-IST requires powerful computer resources and a relatively large amount of computer time for its calculations, especially if the number of lattice calculations to be performed is large.

However, the lattice code which was originally used for the design of most CANDUs is not a transport-theory code. It is POWDERPUFS-V. This is a semi-empirical code, which means that it uses simple "recipes", equations and approximations with parameters fitted to experimental results in natural-uranium, heavy-water-moderated lattices at Chalk River. Because of its design, POWDERPUFS-V demands very modest computer resources and its execution time is extremely short. POWDERPUFS-V has been used with a lot of success for over three decades at the operating CANDU stations. For this reason, it continues to be used to this day for normal-operation calculations at most of the stations, although there are plans at many of the sites to eventually replace it with WIMS-IST.

12.2   Reactivity-Device Calculation

This type of calculation determines the effect of a reactivity device on the nuclear properties in its vicinity. This effect is cast in the form of "incremental" cross sections which are to be added to the properties of basic cells in a modelled volume around the device, a "supercell" - see Figure 12.2.
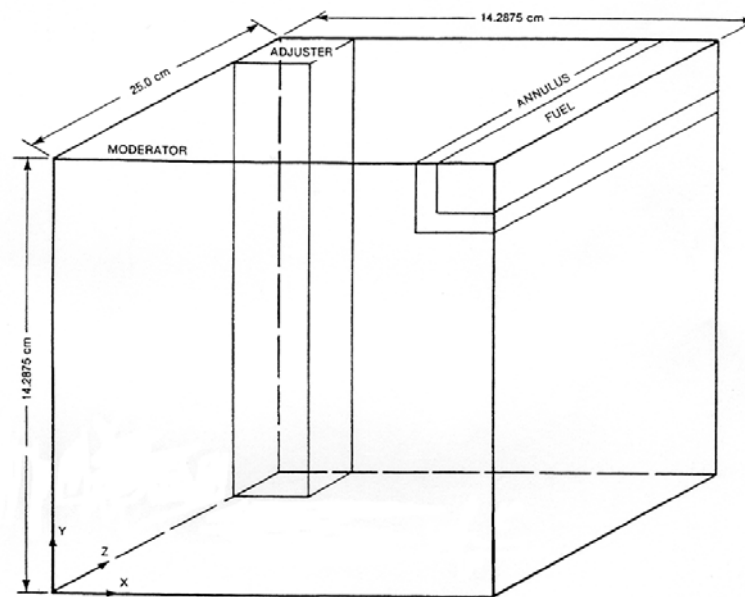

Figure 12.2 – Supercell for Calculation of Reactivity-Device Incremental Cross Sections

For instance, shutoff-rod incremental cross sections will dictate the local efficacy of the shutoff rods in absorbing neutrons and shutting down the fission chain reaction. The incremental cross sections of a device are obtained by calculating the differences in the supercell homogenized properties between the case when the device is inserted in the

supercell, and the case when it is withdrawn from it. These cross sections are then added to the lattice cross sections in the modelled volume around the device in the reactor core.

The supercell code associated with POWDERPUFS-V was MULTICELL. This has now essentially been superseded by the 3-d fundamental transport code DRAGON-IST, developed at École Polytechnique de Montréal.

12.3   Finite-Core Calculation

In this final stage, the entire reactor is modelled, incorporating both the basic-lattice cross sections and the incremental cross sections of reactivity devices in their appropriate locations. This model is used to calculate the 3-dimensional flux and power distribution in the core.

The finite-core computer code RFSP-IST is specifically designed for CANDU reactors. It was developed by merging AECL's RFSP (Reactor Fuelling Simulation Program) code with Ontario Power Generation's sister code, OHRFSP. RFSP-IST is a very large code (> 1500 subroutines), with many applications and many calculational options. In particular, it can be applied in both steady-state (time-independent) and kinetics (time-dependent) problems, the 3-d flux and power distributions being calculated in two energy groups (1 = fast, 2 = thermal) by solving the corresponding diffusion equation.

Other finite-core computer programs have also been used. One is SMOKIN, a code based on modal analysis and which has been used mainly at Ontario Power Generation and Bruce Power.

12.4   POWDERPUFS-V

POWDERPUFS-V was developed at the Chalk River Laboratories in the 1960s and early 1970s. It is a semi-empirical code, using the results of measurements in research reactors such as ZED-2, and it evolved from lattice recipes of Duret and Marriott. The work of many others also contributed to the development of the code over the years.

POWDERPUFS-V treats complex processes, such as resonance absorption, by simple approximations, thus reducing the computation time considerably. An abbreviated version of the Physics Manual for POWDERPUFS-V is available as an external report, AECL-11357, "Description of the Lattice Code POWDERPUFS-V", 1999, by B. Rouben (based on an early AECL internal report by E.S.Y. Tin and P.C. Loken).

In this Section we will discuss the inputs to POWDERPUFS-V and initiate some calculations.

12.4.1 POWDERPUFS-V Capabilities

POWDERPUFS-V has the following capabilities:

a) It solves the burnup ("depletion") equations to calculate the change in fuel isotopic composition as a function of fuel irradiation.
b) At each value of fuel irradiation or burnup in the range considered, it does the following:

It calculates the four-factor parameters (ε, p, η, f):

$$\varepsilon = \text{Fast-Fission Factor}$$
$$p = \text{Resonance-Escape Probability}$$
$$\eta = \text{Thermal Reproduction Factor}$$
$$f = \text{Fuel Utilization Factor}$$

From these it computes the infinite-lattice multiplication constant k_∞:

$$k_\infty = \varepsilon p \eta f$$

It also derives the finite-core multiplication constant k_{eff}:

$$k_{eff} = k_\infty / \text{Leakage}$$

It also calculates two-group cross sections (also known as lattice parameters) and diffusion coefficients for use in finite-reactor codes.
c) It has a "reaction-rate-average" feature, which provides lattice cross sections which many be considered core-average properties for "equilibrium-fuelling" conditions. With these cross sections, "point-model" calculations of reactor parameters and burnup can be made as a function of exit fuel irradiation.
d) It also has a "perturbation" feature, which can be used to calculate the reactivity effect (reactivity coefficients) of instantaneous changes in lattice parameters, e.g., fuel, coolant and moderator temperatures, coolant and moderator densities, etc. In a perturbed case, the isotopic fuel composition used is that generated by the preceding reference (or "burn") case; thus, the calculated reactivity effects are those arising from the changes in the cross sections associated with the perturbation only. This calculation is essential in predicting various reactivity coefficients and other important quantities such as the reactivity change on loss of coolant. Moreover, the variation of reactivity coefficients with fuel irradiation can also be calculated.

12.4.2 Lattice Representation

Figure 12.3 shows the model of the lattice cell used in the POWDERPUFS-V calculation. The fuel elements (fuel and sheath) and most of the coolant have been homogenized into one region. In the program, the homogenized-region radius is the radius of a circle having an area equal to the cross sectional area enclosed by a rubber band touching the sheath of each outermost element and wrapped around the bundle at its midplane. There is an annulus of coolant between the homogenized region and the pressure tube.

Not shown in Figure 12.3 are the bundle end regions, which contain end caps and end plates but no fuel. In POWDERPUFS-V, the total quantity of fuel and cladding material per bundle has been homogenized over the length of the bundle. The lattice cell is thus divided into three separate regions, viz. the homogenized fuel region, the annulus region, and the moderator region.

REGION:
1   COOLANT ANNULUS
2   PRESSURE TUBE
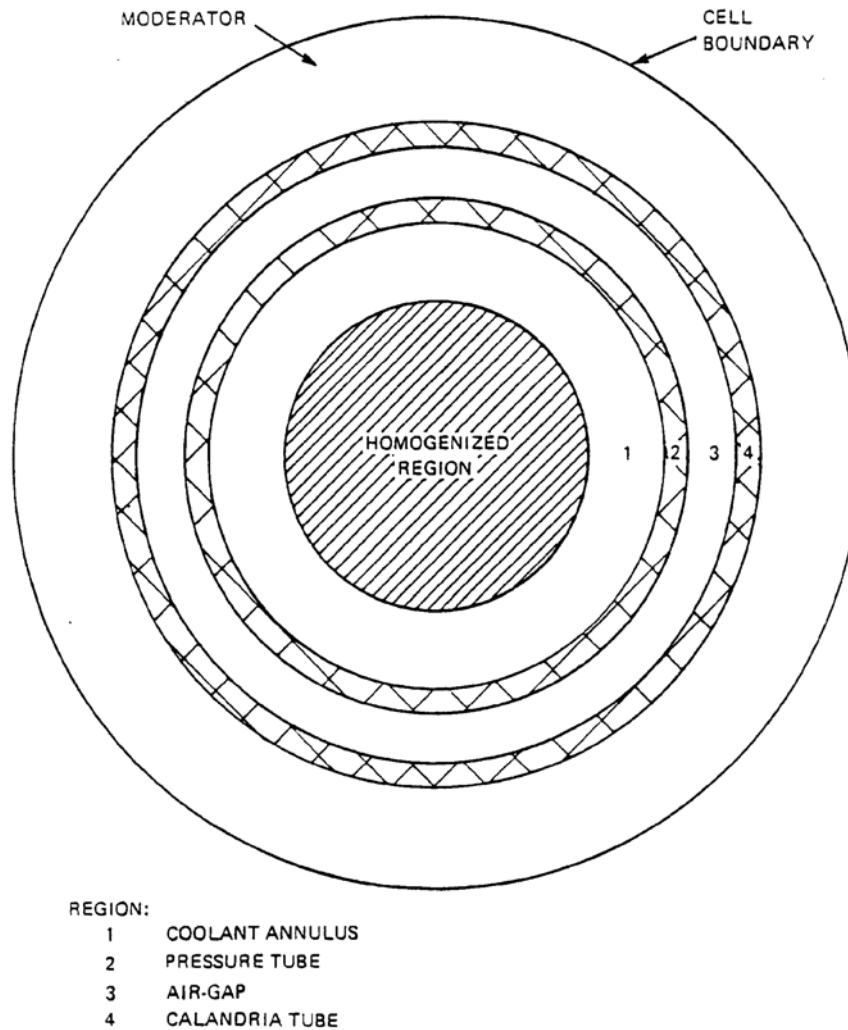3   AIR-GAP
4   CALANDRIA TUBE

Figure 12.3 – Lattice-Cell representation in POWDERPUFS-V

12.4.3 Inputs and Quantities for Study

The following section lists the various POWDERPUFS-V inputs and their meaning.

We do not have time to study all the inputs to POWDERPUFS-V. We shall focus on a few, which are very significant either from the point of view of their effect on achievable burnup or from the point of view of reactivity coefficients:
- Moderator purity
- Coolant purity
- Fuel temperature
- Moderator poison
- Coolant density

- Moderator temperature
- Pressure-tube thickness
- Calandria-tube thickness
- Lattice pitch
- Xe-135 concentration
- Saturated fission products

The important outputs we will be considering are:
- Irradiation
- Burnup
- k_∞
- k_{eff}
- Lattice cross sections

The important options we will be exercising are:
- Instantaneous or reaction-rate-average properties
- "Burn" or perturbation calculations

To calculate the basic-lattice properties at a given point in the reactor model, POWDERPUFS-V needs a number of numerical inputs which must be provided by the user. Table 12.1 lists these inputs. Figure 12.4 shows a sample POWDERPUFS-V input for a reference ("burn") instantaneous calculation. Figure 12.5 is the echo of this input as it appears in the POWDERPUFS-V output – this is easier to read because the inputs are labelled.

The input format is as follows:
1) A title line
2) A library identification (196902), which never changes
3) 90 input values (see next sections) arranged in 18 lines with 5 values each, in format (5E15.8, 5X)
4) 3 blank lines if the calculation is a "burn" case only; when it is desired to do also a perturbation case, the package of perturbation inputs replaces the second blank line.

The present discussion will not cover every single input, but it is appropriate to:
- review some of the most important quantities, especially those which are most likely to vary from one program execution to another
- point out their significance, and
- describe the manner in which the values input should be defined.

12.5.1 Categories of Input Items

The 90 items shown in Table 12.1 may be grouped into a number of categories. A possible categorization is as follows:

- **Geometrical quantities** - these define the geometry and dimensions of the basic lattice cell
- **Materials specification** - defining the materials in the cell
- **Atomic composition of fuel** - quantities which define or control the fuel nuclide densities
- **Atomic purities and other quantities affecting composition** - purities of moderator and coolant, moderator poison concentration, control variables relating to saturating fission products in the fuel
- **Initial guesses** - starting values for quantities which are internally recalculated by the code
- **Densities and temperatures**
- **Run control** - inputs which define the type of calculation desired.

These input categories will be discussed in turn in the following subsections, where item numbers always refer to Table 12.1.

12.5.2 Geometrical Quantities

In this category belong inputs which define the geometry of the basic cell (such as items 11-14, 56, and 72, as well as radii, areas/volumes, and derived dimensions (such as items 17-26, 28, 30, and 46).

These inputs are the most straightforward and the simplest to define. The numbers can essentially either be obtained from blueprints of the basic lattice cell, or be calculated therefrom using formulas given in Reference 2. Only a few of these quantities will be discussed here.

12.5.2.1   Pressure-Tube Radii

Items 22 and 23 are usually the inner and outer radii of the pressure tube respectively. The difference between these two numbers represents the pressure-tube thickness. Since the thickness has both a nominal value and a tolerance, one should use for the outer radius *a* realistic value which takes into account the variability of the thickness (e.g., the average "real" thickness). As for the inner radius, it of course determines the volume of coolant within the pressure tube.

Pressure-tube dimensions change with age, however, due to radial creep. For the corresponding lattice, the inner radius should be obtained for the crept condition. This can be calculated from a correlation (derived from experience at real plants) of creep with the number of years of operation and the average capacity factor. The outer radius can then be adjusted so that the mass of the tube per unit length is conserved. Accounting for the proper amount of creep is especially important in LOCA simulations, as the coolant volume increases with the amount of creep. If it is desired to model different degrees of creep in different parts of the core, then a number of lattice calculations have to be performed with different values for the radii.

12.5.2.2   Fuel and Sheath Volumes

Item 18 is the fuel volume per unit length along the axial dimension of the lattice cell. The physical quantity important to conserve in the model is the mass of fuel in the bundle. Thus item 18 (the fuel volume) must be connected with the fuel density (item 6) and the bundle length (item 46) to the known fuel mass in the bundle by the relation:

Fuel volume * bundle length * fuel density = Mass of fuel per bundle

The bundle length is 49.53 cm, and the value normally used for the density of UO_2 fuel is 10.67 g/cm^3. The mass of uranium per bundle is typically in the range 18 - 19.5 kg. The mass of actual fuel (UO_2) can of course be determined from the uranium mass. If, for example, a value of 19.1 kg(U) corresponds to 21.668 kg(UO_2). This is the value used to calculate the fuel volume (40.996 cm^2) shown in Figures 12.4 and 12.5.

Similarly, item 19 is the sheath volume per unit length. Because the cell model in POWDERPUFS-V is axially uniform, the bundle end plates, spacer pads and bearing pads must be lumped in within the "sheath" volume. Thus item 19 must be connected with the assumed zircaloy density (6.55 g/cm^3) to the total mass of zircaloy in the cell:

Sheath volume * bundle length * 6.55 g/cm^3 = Mass of zircaloy per bundle

A zircaloy mass of 2.292 kg per bundle results in the sheath volume of 7.065 cm^2 shown in Figures 12.4 and 12.5.

12.5.3 Materials Specification

Items 61-70 define the initial atomic composition of the fuel. The relative atomic densities of the various uranium and plutonium isotopes at zero irradiation must be provided. These quantities may be given in any relative units - not necessarily on an absolute scale. For natural uranium, the relative atomic densities are 0.7204 U-235, 99.2796 U-238.

The inputs for a cell containing depleted uranium would of course be different from those for a cell containing natural uranium. They would be different again for fuel with an initial plutonium content, or for fuel enriched in U-235. However, note that POWDERPUFS-V was developed for CANDU lattices, i.e., for D_2O moderator and for fuel which does not differ substantially from natural uranium.

12.5.4 Atomic Purifies and Other Quantities Affecting Composition

Items 15 and 52 are fairly straightforward. They define the atomic D_2O percentage in the moderator and coolant respectively. The D_2O percentage in the moderator has a very large effect on reactivity - the value input should therefore be the actual operating purity.

Item 49 is the moderator poison concentration, given in terms of ppm of natural boron. Note that the POWDERPUFS-V library cannot treat gadolinium; therefore if it is desired to simulate the presence of gadolinium in the moderator, one should represent it by an equivalent amount of boron. The correspondence for the naturally occurring mixtures of isotopes is approximately 1 ppm Gd = 3.4 ppm B.

Note that the presence of poison in the moderator increases the void reactivity (reactivity gain on loss of coolant). Thus, it is important in LOCA simulations to define the boron concentration for the desired scenario. For instance, if a LOCA is simulated for a reactor coming out of a long shutdown, one should account for the presence of poison which compensates for the absence of Xe-135 and other saturated fission products (SFP) in the fuel (these having decayed away during the shutdown). The requisite poison concentration should thus be determined beforehand.

Items 58 and 79 control the calculation of Xe-135 and the other SFP. Item 58 is the Xe-135 microscopic absorption cross section. An input value of exactly 0.0 for this quantity signifies that Xe-135 will be assumed **present** in a concentration in equilibrium with the flux level (as determined by POWDERPUFS-V). If it is desired to model the absence of Xe-135, one should input a very small, but non-zero, value for item 58; a value such as 10^{-10} or 10^{-15} is appropriate. A calculation without Xe-135 would, for example, apply to the simulation of conditions after a long shutdown.

Item 79 controls the calculation of **all SFP, including Xe-135**. A value of 0.0 signifies the SFP will be calculated at all irradiations, while a negative value means they will be assumed absent at all irradiations (whereas a positive value will result in the SFP being neglected only at strictly zero irradiation - i.e. fresh fuel). It should be remembered that "turning off" the SFP by means of input quantity 78 also turns off Xe-135, whereas quantity 58 controls xenon independently of the other SFP.

12.5.5 Initial Guesses

A number of values in the POWDERPUFS-V input serve as initial guesses. The corresponding quantities are recalculated internally by the code as the calculation proceeds.

The main quantities in this category are those which characterize the neutron spectrum inherent in the Westcott parametrization used in POWDERPUFS-V: these are the spectral parameter r (item 1) and the neutron temperatures in the fuel, annuli, and moderator (items 2, 8 and 9). Note that when item 1 is set identically to 0.0 the r value is calculated internally by the program (this should be the normal selection by the user, and item 54 defines the convergence criterion on r), otherwise the non-zero value is used without change. For items 2, 8, and 9, the input values are used without change if item 85 is set to a value greater than 1, and are treated as initial guesses if item 85 is set to a value less than 1. In this latter case, the neutron temperatures are internally recalculated until numerical consistency in the spectrum is achieved (note that item 45, typically set at 0.001, serves as the neutron temperature convergence criterion).

Another initial guess is item 37, the initial flux estimate for the average Westcott flux in the fuel. This average flux is used in the program to compute the level of the saturated fission products, such as Xe-135, as well as the concentration of plutonium in a "burn" calculation.

The flux is recalculated internally by the program, and is made consistent with the "effective" power level, as obtained by the product of two other inputs, item 42 and item 60. Item 42 is the fuel heat rating, or bundle thermal power per unit length. The bundle power normally used to compute item 42 is the maximum time-average bundle power, i.e. the maximum bundle power excluding refuelling ripple. If this latter value is taken, for example, as 800 kW, the fuel heat rating is 16.15 kW/cm, as shown in Figures 12.4 and 12.5. Item 60 is the ratio of flux-squared-weighted average flux to maximum flux in the core. This is best derived from a 3-dimensional flux distribution obtained from a full-core calculation. For a typical nominal flux distribution in a CANDU 6, the value of item 60 is in the range 0.75-0.80. The value shown in Figures 12.4 and 12.5, 0.764, was obtained from a previously-calculated nominal flux shape.

12.5.6 Densities and Temperatures

12.5.6.1   Moderator

The moderator density and temperature are represented by items 3 and 4 respectively. When item 3 is set to zero, the moderator density is internally calculated by the program for the temperature specified in item 4.

Normally a single, "average" value of moderator temperature is used to calculate lattice properties at all points in core. A value of 68 °C is in current use for the CANDU 6, as an educated guess of the "average" moderator temperature under normal operating conditions. However, if information is available on the spatial distribution of moderator temperature in the core, different values could conceivably be used in different core regions.

12.5.6.2   Coolant

The coolant density and temperature are items 5 and 27 respectively. Again, single "average" values of temperature and density are most often used for all points in core. However, the coolant density in particular can vary substantially from one point in the core to another, especially when there is boiling at the outlet ends of channels. The effect of this spatial variation can be obtained by using different values of density.

For LOCA simulations, the coolant density is of course the single most important quantity since it is the positive reactivity gain on loss of coolant which causes the power pulse. The variation of the coolant density with time must be captured to realistically simulate the positive-reactivity insertion.

12.5.6.3   Fuel Temperature

The fuel temperature is item 7. This quantity is closely related to power: the higher the power of a bundle, the higher the fuel temperature in that bundle. Through its relationship with bundle power, the fuel temperature is also connected to the absolute flux level, the concentration of saturated fission products. and the amount of plutonium at a given irradiation. As explained in an earlier section, the reactivity decreases with increasing fuel temperature.

At full power, the bundle-average fuel temperature can vary spatially in the core in the range of about 300 °C to about 900 °C. Yet most reactor calculations have traditionally used a single effective value of fuel temperature. A value of approximately 690°C is in current use for the CANDU 6.

12.5.7 Run Control

Several of the inputs to POWDERPUFS-V are flags which control the type of calculation desired.

12.5.7.1   Irradiation

First, note that the lattice properties are calculated and displayed as a function of irradiation. Item 51 is the irradiation interval (in n/kb) at which the lattice properties are tabulated; a typical interval is 0.1 or 0.05 n/kb. Item 55 is the maximum irradiation desired; a value of 3.0 n/kb is often used. The starting value of irradiation for the tabulation of the lattice properties is normally 0 n/kb. However, in a perturbation run (see discussion in Section 12.5.7.3) the user has the option of specifying the initial irradiation explicitly via item 44.

12.5.7.2   Instantaneous Versus Reaction-Rate Averaged Properties

Item 71 is the isotopic density indicator. This flag controls whether the calculation is for "instantaneous" or "reaction -rate- averaged" lattice properties.

In the "instantaneous" option (item 71 = 2.0), the irradiation against which the lattice properties are tabulated is the actual irradiation of the fuel. These results are appropriate to very detailed models (such as those used in fuel management) where the irradiation value unique to each bundle is considered.

In the "reaction-rate-averaged" option (item 71 = 1.0), the irradiation has the meaning of exit irradiation - i.e. the irradiation at which the fuel is expected to exit from the reactor. The lattice properties are then computed for a fuel mixture in which all irradiations, from 0 to the exit irradiation, are present. The properties are then tabulated against the exit irradiation. These results are appropriate to simplified "axially homogeneous" models, in which the basic-lattice properties are assumed uniform along the length of a channel. The "reaction-rate-averaged" properties for an exit irradiation ω_{exit} are normally close to,

but not identical to, the instantaneous properties at an irradiation $\omega_{inst} = 0.5 * \omega_{exit}$ since this ω_{exit} can be expected to be close to the "average" irradiation in the channel.

12.5.7.3   "Burn" Versus Perturbation Runs

Item 74 is the perturbation control, which distinguishes between "burn" (item 73 = 0.0) and "perturbation" (item 73 = 1.0) runs of the program.

In a "burn", or reference, run, the lattice properties are calculated by advancing the irradiation from 0 to the maximum value (item 55) in specified increments (item 51), all the while computing the fuel isotopic composition at each irradiation, consistent with all input data. That is, the fuel is "burned" through the irradiation range required.

A "perturbation" calculation cannot be performed on its own. It must follow a reference "burn" calculation. The perturbation input replaces the second blank line which follows the input for the burn calculation.

The format of the perturbation input is as follows (each field is 15 columns, column 1 must not be blank):
1) One card as follows:
    73.   1.
2) One card for each parameter perturbed, which gives the number of the parameter perturbed, and the perturbation value, for example, perturbing the moderator temperature to 78 degrees:
    4.   78.

That is, along with setting item 73 to 1.0, the user modifies one or more of the other physical inputs (say coolant density, fuel temperature, etc...) to new values which are interpreted to be perturbed values which the physical properties attain suddenly.

Figure 12.6 shows the input file for the reference case defined in Figure 12.4, followed by a perturbation calculation with the moderator temperature changed to 78 ^{o}C.

In a perturbation calculation, the isotopic composition of the fuel is not recalculated, but is taken to be identical to that of the fuel in the burn calculation at the same irradiation. Thus, the perturbation calculation gives the lattice properties for a fuel which is burned at certain assumed conditions, but which then suddenly experiences changes to those conditions at each irradiation tabulated.

The perturbation calculation thus applies to all "off-normal" or accident situations where one or more core parameters may change. The most typical example is the case of a LOCA, where at a certain irradiation a sudden loss of coolant occurs, with consequent changes to the coolant density, the coolant temperature, and the fuel temperature. As these changes may vary significantly from one location in core to another, many different sets of lattice properties may be required for an appropriate modelling of the LOCA.

TABLE 12.1
LIST OF ITEMS IN POWDERPUFS-V INPUT

ITEM	DESCRIPTION
1	Westcott spectral parameter r
2	Fuel neutron temperature
3	Moderator density
4	Moderator temperature
5	Coolant density
6	Fuel density
7	Fuel temperature
8	Annuli neutron temperature
9	Moderator neutron temperature
10	Sheath absorption factor
11	Rubber-band perimeter
15	Moderator purity
16	Sheath material code
17	Void volume
18	Fuel volume
19	Sheath volume
20	Coolant volume in homogenized zone
21	Radius of homogenized zone
22	Outside radius of first annulus
30	Lattice pitch
31	Coolant material code
32	Material code of first annulus
33	Material code of second annulus
34	Material code of third annulus
35	Material code of fourth annulus
36	Material code of fifth annulus
37	Initial flux estimate
38	U238 resonance capture fraction
39	Fast neutron yield cross section
40	Fast neutron non-escape probability
41	Fuel material code
42	Fuel heat rating
43	Power-to-coolant fraction
44	Initial exposure for a perturbed run

ITEM	DESCRIPTION
45	Neutron temperature convergence criterion
46	Bundle length
47	Pu-240 self shielding factor
48	Not used
49	Moderator poison concentration
50	Nuclei per mass of fuel
51	Exposure increment
52	D_2O coolant purity
53	DEEMS convergence criterion
54	Westcott spectral parameter convergence criterion
55	Maximum exposure
56	Lattice arrangement indicator
57	Geometrical buckling
58	Xenon macroscopic absorption cross section
59	Pu-240 convergence criterion
60	Ratio of flux-squared average to max
61	Initial Th-232 concentration
62	Initial U-233 concentration
63	Initial U-234 concentration
64	Initial U-235 concentration
65	Initial U-236 concentration
66	Initial U-238 concentration
67	Initial Pu-239 concentration
68	Initial Pu-241 concentration
69	Initial Pu-241 concentration
70	Initial Pu-242 concentration
71	Isotopic density indicator
72	Number of rods in fuel bundle
73	Perturbation control
74	Not used
79	Saturating-fission-product control
80	Printout control
81	Radial buckling of central region
82	EXTERMINATOR calculation control
83	PERIGEE calculation control
84	Burnup control
85	T~ and r calculation control

ITEM	DESCRIPTION
86	Extrapolated length of reactor
87	Core radius
88	Reactor radius
89	Radial form factor
90	Total fission power

Figure 12.4
Sample PPV Input File – Reference Case

1.0 Sample Fuel File - Reference Case
196902
 0.00000000E+00 0.22500000E+03 0.10856100E+01 0.68000000E+02 0.81812000E+00
 0.10593230E+02 0.68700000E+03 0.15200000E+03 0.78000000E+02 0.00000000E+00
 0.30950001E+02 0.14123000E+03 0.41890001E+00 0.40000000E+01 0.99750003E+02
 0.40000000E+02 0.78600001E+00 0.41591000E+02 0.68280001E+01 0.27892000E+02
 0.49540000E+01 0.51689000E+01 0.56032000E+01 0.64478002E+01 0.65875001E+01
 0.00000000E+00 0.28750000E+03 0.34734001E+02 0.10590000E+01 0.28575001E+02
 0.00000000E+00 0.20000000E+02 0.70000000E+02 0.00000000E+00 0.50000000E+02
 0.00000000E+00 0.90000000E+14 0.00000000E+00 0.24000000E-01 0.00000000E+00
 0.00000000E+00 0.16150000E+02 0.95612001E+00 0.00000000E+00 0.10000000E-02
 0.49529999E+02 0.00000000E+00 0.00000000E+00 0.24000000E-01 0.22300000E+22
 0.10000000E+00 0.99222000E+02 0.99999998E-02 0.10000000E-02 0.30000000E+01
 0.00000000E+00 0.76179997E-04 0.00000000E+00 0.10000000E-02 0.76400000E+00
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.72039998E+00 0.00000000E+00
 0.99279602E+02 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00
 0.20000000E+01 0.37000000E+02 0.00000000E+00 0.00000000E+00-0.10000000E+02
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.30000000E+01
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.20000000E+01 0.00000000E+00
 0.00000000E+00 0.31426999E+03 0.37973001E+03 0.82300001E+00 0.21560000E+04

Figure 12.5 – Echo of Sample Input in POWDERPUFS-V Output File

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11        POWDERPUFS-5 RUN ***Sampl- 1. ***      e Fuel File - Reference Case                                    DATE

 2 196902 THIS IS A CONTROLLED PGM,MODIFICATION MUST BE RECORDED IN PGM PACKAGE

 3        SPECTRAL PARAM. R        FUEL NEUT. TEMP.        MODERATOR DENSITY        MODERATOR TEMP.        COOLANT DENSITY
           .00000000E+00           .22500000E+03          .10856100E+01           .68000000E+02          .81812000E+00
 4         FUEL DENSITY            FUEL TEMP.             ANNULI NEUT. TEMP.       MOD. NEUT. TEMP.       SHEATHABS.XN.FACT.
           .10593230E+02           .68700000E+03          .15200000E+03           .78000000E+02          .00000000E+00
 5        RUBR BAND PERIM SO       FUEL PERIM. SA         COOLANT THICKNS D        NUMBER OF ANNULI       MOD. D2O ATOM PERC
           .30950000E+02           .14123000E+03          .41890000E+00           .40000000E+01          .99750000E+02
 6        SHEATH MATL. CODE        VOID  VOLUME           FUEL VOLUME             SHEATH  VOLUME         COOLANT VOL. IN RO
           .40000000E+02           .78600000E+00          .41591000E+02           .68280000E+01          .27892000E+02
 7        HOMGNIZD RADIUS RO       RADII  R1              R2                      R3                     R4
           .49540000E+01           .51689000E+01          .56032000E+01           .64478000E+01          .65875000E+01
 8         R5                      COOLANT TEMP.          TOT. COOLANT VOL.        FLUX RATIO C/F         LATTICE SPACING
           .00000000E+00           .28750000E+03          .34734000E+02           .10590000E+01          .28575000E+02
 9        COOLANT MATL CODE        MATL. INDIC. M1        MATL. INDIC. M2          MATL. INDIC. M3        MATL. INDIC. M4
           .00000000E+00           .20000000E+02          .70000000E+02           .00000000E+00          .50000000E+02
10         MATL. INDIC. M5         INITIAL FLUX GUESS      R                       SB                     PSUBF
           .00000000E+00           .90000000E+14          .00000000E+00           .24000000E-01          .00000000E+00
11        FUEL MATL. CODE          FUEL HEAT RATING       POWER TO COOLANT        FIRST STEP EXP         NEUT.TEMP.CONV.CRIT.
           .00000000E+00           .16150000E+02          .95612000E+00           .00000000E+00          .10000000E-02
12         BUNDLE LENGTH           PU-240 S-S. FACT.                               MOD. POISON.PPM        FUEL  RAV/MOW
           .49530000E+02           .00000000E+00          .00000000E+00           .24000000E-01          .22300000E+22
13         EXPOSURE STEP           COOLNT D2O ATM PER      DEEMS CONV. CRIT.        W-R CONV. CRIT.        MAXIMUM EXPOSURE
           .10000000E+00           .99222000E+02          .10000000E-01           .10000000E-02          .30000000E+01
14        SQU. OR HEX. IND.        GEOMETRIC BUCKLING     XENON MAC ABS XSN        PU240 CONV. CRIT.      EFF/MAX FLUX RATIO
           .00000000E+00           .76180000E-04          .00000000E+00           .10000000E-02          .76400000E+00
15         N02(0)                  N23(0)                 N24(0)                  N25(0)                 N26(0)
           .00000000E+00           .00000000E+00          .00000000E+00           .72040000E+00          .00000000E+00
16         N28(0)                  N49(0)                 N40(0)                  N41(0)                 N42(0)
           .99279600E+02           .00000000E+00          .00000000E+00           .00000000E+00          .00000000E+00
```

Figure 12.6
Sample PPV Input File – Reference Case Followed by Perturbation

1.0 Sample Fuel File - Reference Case
196902
 0.00000000E+00 0.22500000E+03 0.10856100E+01 0.68000000E+02 0.81812000E+00
 0.10593230E+02 0.68700000E+03 0.15200000E+03 0.78000000E+02 0.00000000E+00
 0.30950001E+02 0.14123000E+03 0.41890001E+00 0.40000000E+01 0.99750003E+02
 0.40000000E+02 0.78600001E+00 0.41591000E+02 0.68280001E+01 0.27892000E+02
 0.49540000E+01 0.51689000E+01 0.56032000E+01 0.64478002E+01 0.65875001E+01
 0.00000000E+00 0.28750000E+03 0.34734001E+02 0.10590000E+01 0.28575001E+02
 0.00000000E+00 0.20000000E+02 0.70000000E+02 0.00000000E+00 0.50000000E+02
 0.00000000E+00 0.90000000E+14 0.00000000E+00 0.24000000E-01 0.00000000E+00
 0.00000000E+00 0.16150000E+02 0.95612001E+00 0.00000000E+00 0.10000000E-02
 0.49529999E+02 0.00000000E+00 0.00000000E+00 0.24000000E-01 0.22300000E+22
 0.10000000E+00 0.99222000E+02 0.99999998E-02 0.10000000E-02 0.30000000E+01
 0.00000000E+00 0.76179997E-04 0.00000000E+00 0.10000000E-02 0.76400000E+00
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.72039998E+00 0.00000000E+00
 0.99279602E+02 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00
 0.20000000E+01 0.37000000E+02 0.00000000E+00 0.00000000E+00-0.10000000E+02
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.30000000E+01
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.20000000E+01 0.00000000E+00
 0.00000000E+00 0.31426999E+03 0.37973001E+03 0.82300001E+00 0.21560000E+04

73.   1.
4.   78.