POWDERPUFS-V

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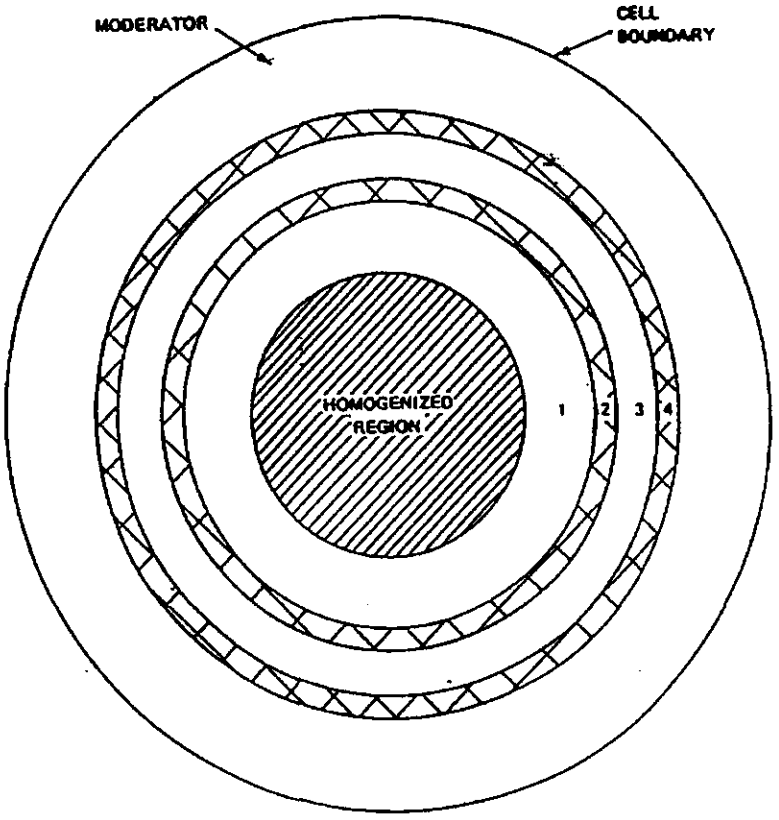
March, 2000

Powderpufs-V

- Cell code: calculates cross-sections for basic lattice cells
- Written specifically for CANDU lattices
  - D_20 moderator
  - U isotopic close to that of natural fuel
  - no appreciable Pu concentration
- Based on Westcott formulation
- Simple recipes and formulas which reproduce experimental results
- Incorporated within RFSP
- Works with simplified annular geometry of lattice cell



REGION:

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

Westcott Formulation

Neutron spectrum is well thermalized. Most neutrons are in thermal range.

Write spectrum as a Maxwellian distribution with a 1/*E* epithermal tail:

$$n(v) = N(1-f)\rho_m(v) + N\rho_e(\upsilon)$$

$\leq$

where:

N	=	total neutron density
f	=	fraction of total neutron density in epithermal spectrum (must be small a few per cent)
$\rho_m(v)$	=	Maxwellian spectrum
	=	$\frac{4}{\sqrt{\pi}} \frac{v^2}{v_T^3} e^{-(v/v_T)^2}$
v_T	=	velocity of neutron with energy kT_n
T_n	=	neutron temperature
$\rho_e(v)$	=	epithermal spectrum (tail)
		$v_T\sqrt{\mu}\frac{\Delta(v)}{v^2}$

Wescott Formulation (con't)

μ = 3.681 (Westcott convention)

$\Delta(v)$ = 0, for small energies ($E < kT$),

= 1, for large energies ($E > kT$)

Westcott Formalism (con't)

The Westcott formalism leads to the following form for the total reaction rate:

$$\text{Reaction Rate} = N v_0 \hat{\sigma}$$

where:

N	=	total neutron density
v_0	=	2200 m/s
$\hat{\sigma}$	=	microscopic Westcott cross-section, which can be written as: $\hat{\sigma} = \sigma_0 (g + rs)$

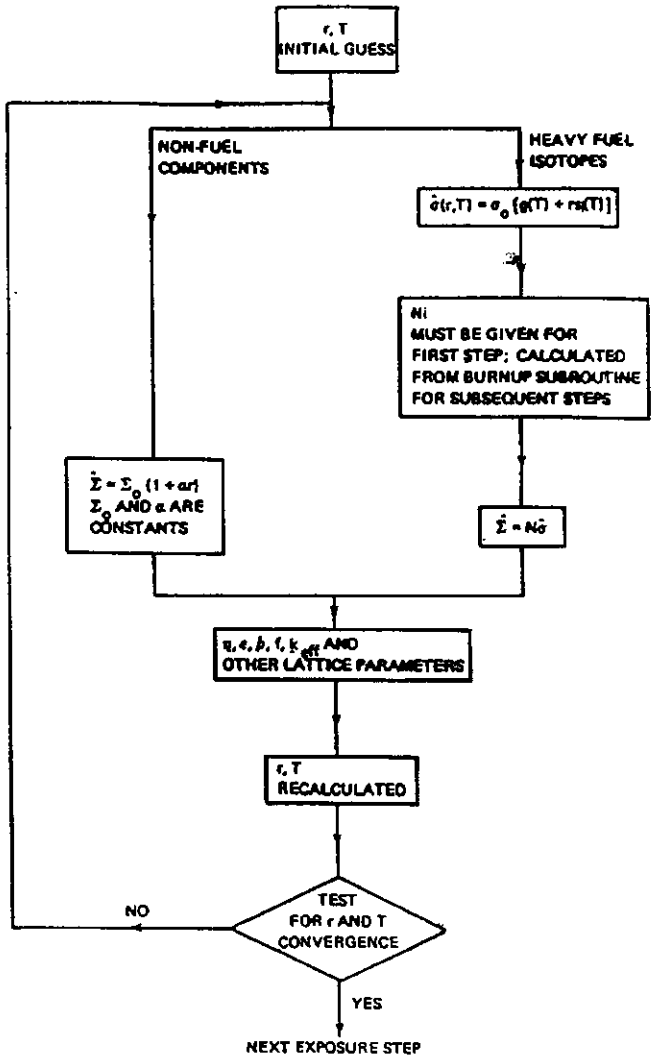
and,

σ_0	=	cross-section at 2200 m/s
r	=	epithermal index ("Westcott r") related to f
	=	$\frac{1}{4} f \sqrt{\pi\mu}$
g, s	=	microscopic quantities dependent on the nuclide (for a pure 1/v absorber, g = 1 and s = 0)

PPV Continued...

T_n and r

- All lattice properties are thus derived from the Westcott r and the neutron temperature (in fuel T_{nf}, annulus T_{na}, and moderator T_{nm} regions).
- T_n and r are calculated internally.
- This is an iterative calculation because r and T_n depend on the four-factor quantities, which are functions of r and T_n.


r, T
INITIAL GUESS
NON-FUEL
COMPONENTS
HEAVY FUEL
ISOTOPES
$\dot{\sigma}(r,T) = \sigma_0 [g(T) + rs(T)]$
$\dot{N}_i$
MUST BE GIVEN FOR
FIRST STEP; CALCULATED
FROM BURNUP SUBROUTINE
FOR SUBSEQUENT STEPS
$\dot{\Sigma} = \Sigma_0 (1 + \alpha r)$
Σ_0 AND α ARE
CONSTANTS
$\dot{\Sigma} = N\dot{\sigma}$
$\eta, \epsilon, p, f, k_{eff}$ AND
OTHER LATTICE PARAMETERS
r, T
RECALCULATED
TEST
FOR r AND T
CONVERGENCE
NO
YES
NEXT EXPOSURE STEP

PPV Continued...

Four-Factor Formula

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

k_∞ = lattice (infinite) multiplication constant

ε = fast-fission factor

p = resonance-escape probability

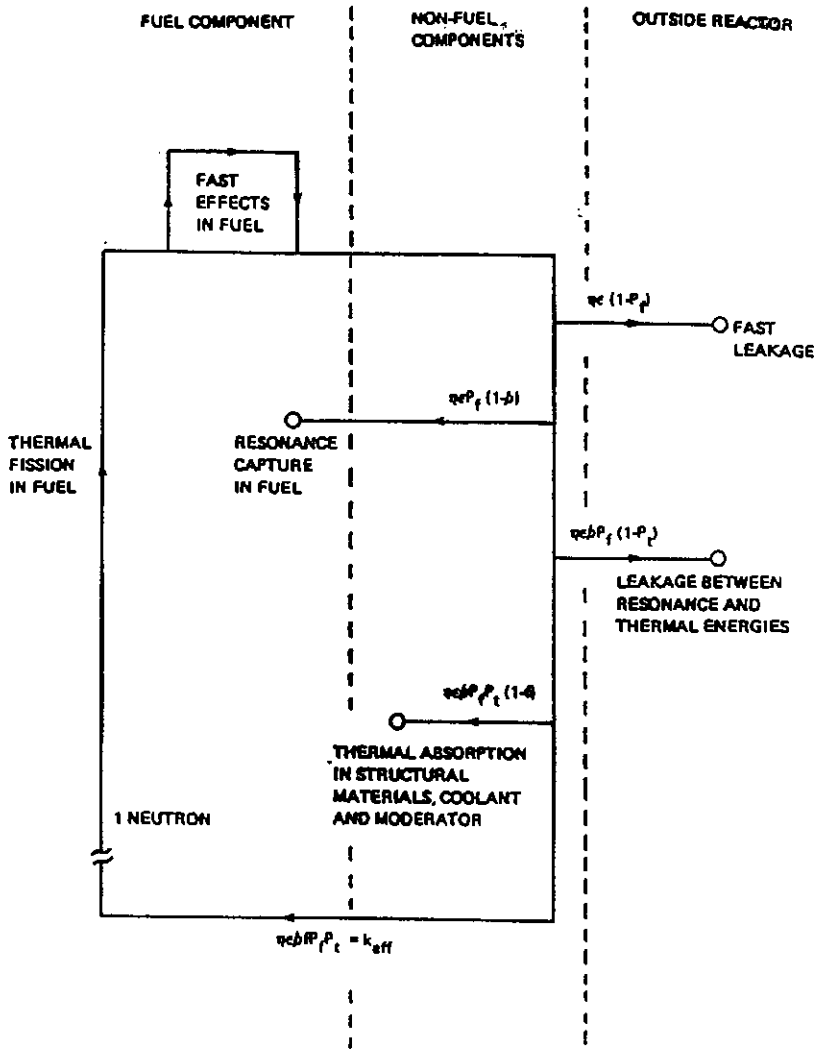
f = fuel utilization

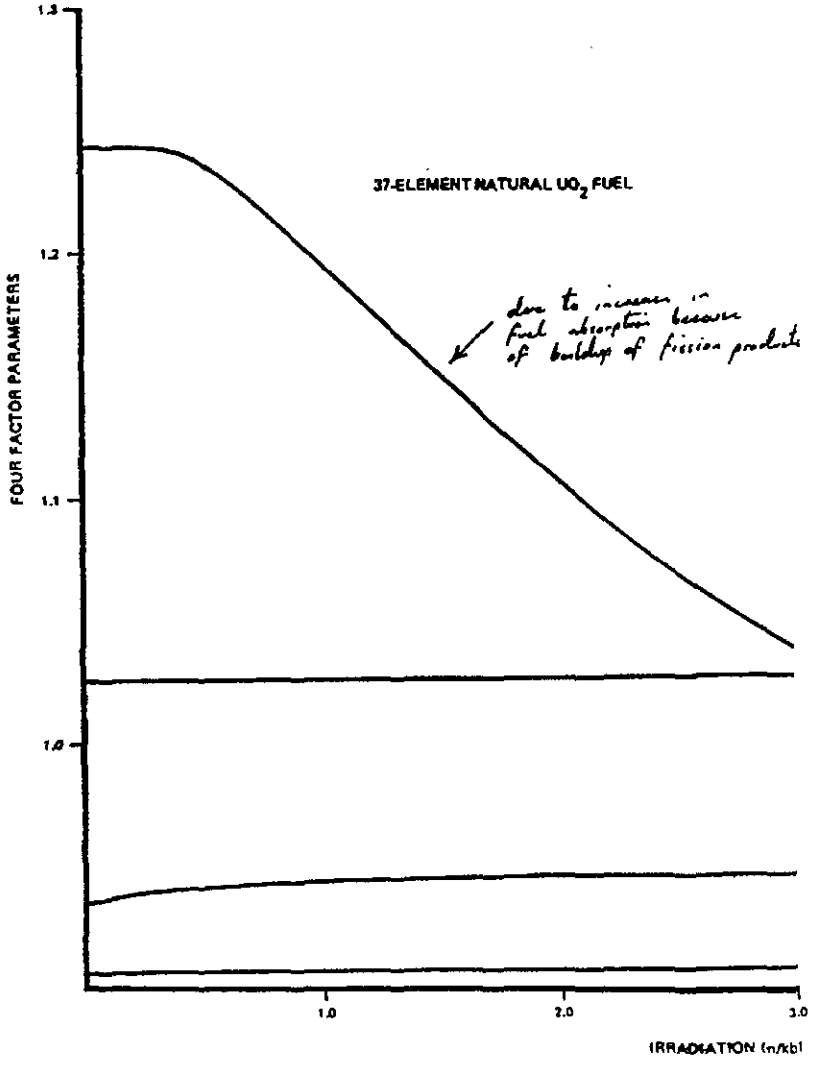
η = thermal reproduction factor (number of fast neutrons produced per thermal absorption in fuel)

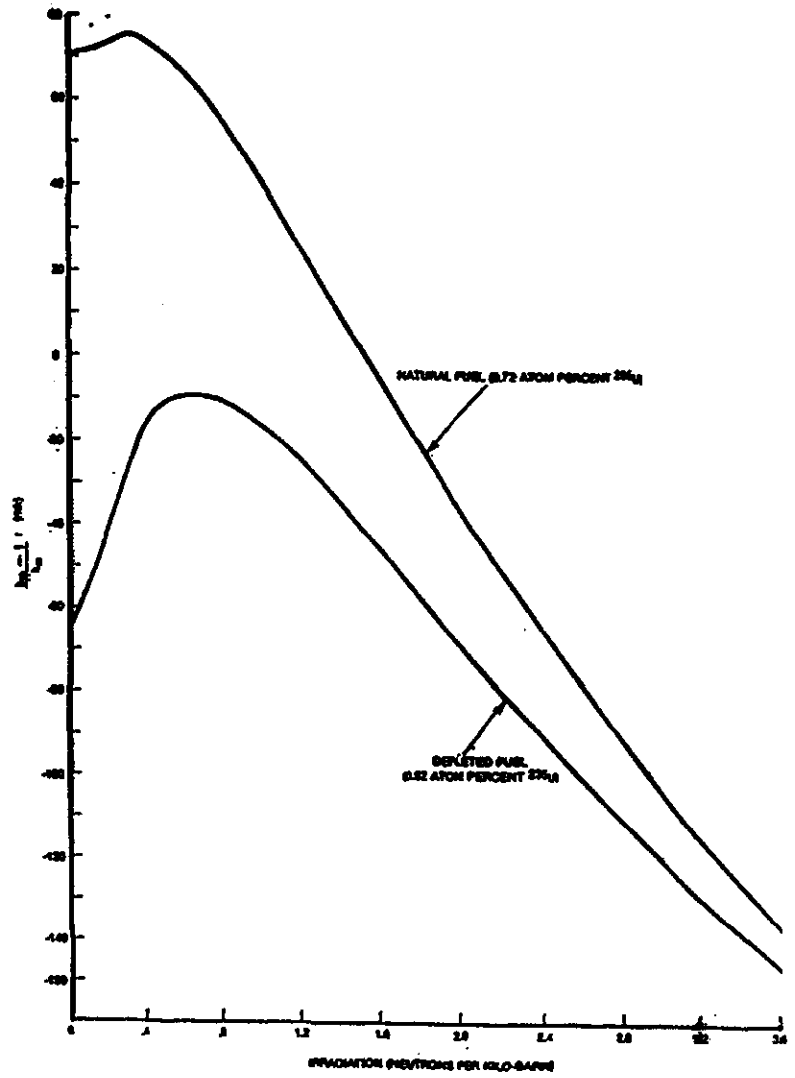
$k_{eff} = k_\infty P_f P_t$

P_f = fast non-leakage probability

P_t = thermal non-leakage probability


FUEL COMPONENT
NON-FUEL COMPONENTS
OUTSIDE REACTOR
FAST EFFECTS IN FUEL
FAST LEAKAGE
RESONANCE CAPTURE IN FUEL
THERMAL FISSION IN FUEL
LEAKAGE BETWEEN RESONANCE AND THERMAL ENERGIES
THERMAL ABSORPTION IN STRUCTURAL MATERIALS, COOLANT AND MODERATOR
1 NEUTRON


37-ELEMENT NATURAL UO_2 FUEL
FOUR FACTOR PARAMETERS
1.3
1.2
1.1
1.0
due to increase in fast absorption because of buildup of fission products
1.0
2.0
3.0
IRRADIATION (n/kb)


NATURAL FUEL (0.72 ATOM PERCENT ^{235}U)
DEPLETED FUEL
(0.52 ATOM PERCENT ^{235}U)

PPV Continued...

From the four factors, the 2-group cell cross-sections are computed.

This is done first at 0 irradiation (fresh fuel). The code then advances the irradiation value by a defined increment, solves the burnup equations to calculate the new isotopic concentrations, and then repeats the cell calculation.

The end result is a fuel table - table of cross-sections versus irradiation (for a given set of POWDERPUFS-V inputs).

Properties of any given bundle to which this input set applies are then obtained by interpolating in the fuel tables at the (known) bundle irradiation.

Powderpufs-V (Continued)

Powderpufs-V requires a set of 90 input values. This is the "R000" array.

The inputs can be grouped into a number of categories:

- Geometric specification of lattice cell
- Materials specification
- Atomic purities and isotopic compositions
- Physical properties such as densities and temperatures
- Saturating-fission-product control
- Initial guesses
- Run-control data
- Selection of major calculation options

TABLE 3.1
ITEMS IN POWDERPUFS-V INPUT

ITEM	DESCRIPTION
1	Wescott 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	Rubberband perimeter
12	Total fuel perimeter
13	Coolant thickness
14	Number of annuli
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
23	Outside radius of second annulus
24	Outside radius of third annulus
25	Outside radius of fourth annulus
26	Outside radius of fifth annulus
27	Coolant temperature
28	Total coolant volume
29	Flux ratio
30	Lattice pitch

TABLE 3.1 (CONTINUED)
ITEMS IN POWDERPUFS-V INPUT

ITEM	DESCRIPTION
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
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	DRUMS 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	ϕ / ϕ_{max}

TABLE 3.1 (CONTINUED)
ITEMS IN POWDERPUFS-V INPUT

ITEM	DESCRIPTION
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
75	Not used
76	Not used
77	Not used
78	Thermal Pu-239 production control
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_{ref} and r calculation control
86	Extrapolated length of reactor
87	Core radius
88	Reactor radius
89	Radial form factor
90	Total fission power

Geometric Quantities

Entries 11 - 14, 17 - 26, 28, 30, 46, 56, 72

- Lattice pitch
- Bundle length
- Radii of annuli (homogenized region, pressure tube, calandria tube, ...)
- Volumes of fuel, sheath, void
- Derived geometric quantities

Materials Specification and Purities

Entries 61 - 70

- **Initial isotopic composition of fuel - atom percent of the various U and Pu isotopes in fresh fuel**
- **POWDERPUFS-V can accommodate natural or depleted fuel, but is not designed for fuel too enriched in uranium or plutonium**

Entries 15, 52, 49

- **Moderator purity - very large effect on achievable burnup)**
- **Coolant purity - affects void reactivity**
- **Boron poison concentration in moderator - used to suppress excess reactivity in initial core or on return from an outage**

Densities and Physical Temperatures

Entries 3 - 5, 7, 27, 42, 60

- **Moderator temperature**
- **Moderator density (if set to zero, calculated internally from temperature)**
- **Coolant density - set to zero for calculation of void reactivity in "perturbation" option**
- **Coolant temperature**
- **Fuel temperature**
- **Heat rating (maximum thermal bundle power per unit length). This, together with entry 60 (ratio of average to maximum flux in core) determines the flux level (magnitude) at which the fuel is "burned"**

Saturating-Fission-Product Control

Entries 58, 79

- Entry 58 can be used to modify the xenon absorption cross-section built into the code - e.g., to turn the Xe-135 absorption off independently of other saturating fission products
- Entry 79 is the flag which turns all three groups of saturating fission products (Xe-135, Rh-105, the samarium group) on or off together
- Note: the calculation of all saturating fission products makes use of the fuel flux value, computed from entries 42 and 60

Initial Guesses

These are quantities which are recalculated internally by the program, but for which initial guess values are required.

Entries 1, 2, 8, 9, 37

- **Westcott r value (related to non-Maxwellian fraction of neutron spectrum)**
- **Neutron temperatures in fuel, annulus, and moderator**
- **Magnitude of flux in fuel**

Run Control

Entries 45, 53, 54

- Convergence criteria for iterative calculations

Entries 51, 55

- Initial and maximum irradiation values

Major Calculational Options

Entry 71

- Isotopic density indicator

This input is a flag which selects between the "instantaneous" (flag=2) and "reaction-rate-averaged" (flag=1) calculations of lattice properties.

The "instantaneous" option calculates the fuel table as a function of the instantaneous fuel irradiation in a given lattice cell. This fuel table is normally used in "snapshot" core models, where each fuel bundle has its own specific value of fuel irradiation at that instant. Snapshot core models are used when the reactor operating history is being tracked (e.g., with RFSP).

Major Calculational Options (con't)

The "reaction-rate-averaged" option is used in more simple-minded, "homogeneous", models, where average properties are assumed over large regions of the core. These properties are averaged over the irradiation range from zero to exit irradiation. They serve as a first approximation to the nuclear cross-sections in a core with continuous (or semi-continuous) and bi-directional refuelling. Separate properties can be used in different core regions (e.g., "inner core" and "outer core") with different average exit irradiations.

Major Calculational Options (con't)

Note that the time-average model in RFSP also requires properties averaged over irradiation. However, in the time-average model, the irradiation range and the bundle properties are bundle-specific. The *TIME-AVER module of RFSP therefore does its own averaging over irradiation (separately for each bundle), and consequently expects "instantaneous" fuel tables.

Major Calculational Options (con't)

Entry 73

- **Perturbation control**

This input is a flag which selects between a "burn" and a "perturbation" calculation.

The "burn" calculation is the normal one, where the fuel is being irradiated at the conditions specified, and the fuel table reflects the change in fuel isotopic as a result of this irradiation.

Major Calculational Options (con't)

- A "perturbation" is a "sudden" change in conditions in the lattice. Here, "sudden" means on a time scale which is insignificant with respect to irradiation changes, i.e., on the scale of seconds or minutes. (It can also apply to much longer time scales, e.g., days or weeks, if no irradiation is taking place, for example during a reactor shutdown).

Major Calculational Options (con't)

Examples of perturbations in the lattice are accidents (e.g., coolant voiding, LOCA), sudden changes in temperatures, purities, or moderator poison, etc..., or changes in saturating fission products as after a shutdown.

In a perturbation calculation, the fuel is not irradiated under the new conditions, but instead the fuel isotopics from the "burn" calculation are used to compute the new lattice properties. Therefore, a perturbation calculation cannot be done in isolation. It must always be preceded by a burn calculation which determines the fuel composition as a function of irradiation.

Major Calculational Options (con't)

Note: Reactivity coefficients are by definition the change in system reactivity due to a sudden unit change in a parameter (such as a temperature, density, etc...). Reactivity coefficients would then be calculated using POWDERPUFS-V properties in the perturbation option. The preferred way of evaluating reactivity coefficients is with full 3-d calculations in RFSP. If an approximate (point-model) value of the reactivity coefficient is desired, it can be obtained directly from the POWDERPUFS-V k-effective value, using the reaction-rate-averaged option (to capture the core-average effect).