The QCALC power profile model for calculating burnup dependent radial power distributions in light and heavy water reactor fuel pins

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ABSTRACT

For analysis of thermal and mechanical fuel rod behaviour, the fuel performance code CARO-E is used in KWU. In the current version of CARO-E radial power distributions are provided by the QCALC-module. QCALC predicts the radial power profiles in fuel pellets q(r) in dependence on the following design parameters: burnup (b), enrichment (e), pellet radius (R), gadolinium content (g), coolant void (v). The module uses interpolating curves and spline functions in the (r,b)-plane and a linear interpolation procedure in the (e, R, g, v)-subspace.

The derived spline coefficients are based on zone power radial profiles calculated by the pin cell code CIRTHE. Application of the method to recalculation of measurements involving relative concentrations of U-, Gd- and Pu-isotopes in burnt fuel assemblies as well as radial distributions of Pu-isotopes in partially burnt fuel pellets provided results that agreed with the measured values very well.

CIRTHE calculations were performed for pin cells of H_2O-lattices and pin cells of Halden-type D_2O-lattices. For the most important fuel pin types (U, MOX, Gd) a net of supporting points in the 6-space of the a. m. parameters was considered.

Introduction

The knowledge of the radial power distribution within the fuel rod pellet is one of the basic assumptions in calculating safety relevant parameters by fuel performance codes. For determination of the radial power profile, the spatial distribution of neutron spectrum and fission nuclide number densities are required.

The power density q(r,b) at the radial pellet position r and the burnup point b is given by

$$q(r,b) = \int_0^{10MeV} \phi(r,E,b) \sum_{i=1}^{n} (N^i(r,b)\,\sigma^i{}_f(E)\,\kappa^i(E))\,dE$$

$$\begin{aligned}
\phi(r,E,b) &= \text{neutron spectrum} \\
N^i(r,b) &= \text{number density of fission nuclide } i \\
\sigma^i{}_f(E) &= \text{fission cross section of nuclide } i \\
\kappa^i(E) &= \text{fission power of nuclide } i
\end{aligned}$$

From this expression follows that the accuracy of q(r,b) depends strongly from the exactness of the space and energy dependent neutron spectrum. Therefore, the calculation of reliable radial power profiles needs sophisticated pin cell codes. One-dimensional pin cell codes are normally the basic codes of the nuclear reactor analysis based on collision probability methods and are used for calculating homogenized group constants. In general, these codes use a certain energy group structure and a radial subdivision of the pin cell area in several concentric ring zones with the assumption of constant group fluxes and constant material properties in each zone. The calculation of precise results with these codes requires fine-meshed group structures and fine-meshed radial subdivisions of the cell area.

It turned out that the most adapted code available in KWU to meet the a. m. requirements is given by the spectral code CIRTHE.

Pin cell calculation

Pin cell code

CIRTHE is a one-dimensional collision-probability method with burnup. Development of CIRTHE began in the early sixties, led by Siemens and with contributions from AECL, Canada /1/ and CNEA, Argentine. Although primarily written for heavy water fuel rod cluster calculations, it can just be so applied to light water moderated fuel rod lattices.

In CIRTHE a sophisticated calculation of the thermal spectrum is performed. The main characteristics of the thermal spectrum calculation are:

- Calculation of the scattering kernel by Cadilhac’s secondary model /2/.

- Calculation of thermal group cross sections in each zone by using of an analytic representation of the energy dependent cross sections in form of a superposition of the Breit-Wigner formula with a 1/v-part.

$$\sigma_{a,f} = \frac{1}{\sqrt{E}}\left(a + \sum_{i=1}^{N_R} \frac{c_i}{b_i + (E - e_i)^2} \right) \qquad N_R = \text{number of resonances}$$

The quantities b_i, c_i, e_i have in most cases no physical meaning, but are to be understood only as fit parameters.

The great advantage of this method results from the following facts:

- The number of energy groups is in principle variable. In the present program version a maximum of 200 thermal groups can be considered.

- Number and volume of the concentric fuel zones and moderator zones are also variable. The actual version allows a maximum of 14 fuel zones and 20 pin cell zones in total.

- The group cross sections in each zone of the pin cell are calculated with its own actual burnup-dependent spectrum.

- Burnable absorber (BA) pins and U-pins affected by the absorber burnout of adjacent BA-pins, are modelled in CIRTHE using the <u>P</u>in <u>C</u>ell Radius <u>A</u>daptation (PRA)-method /3/.

Code validation

The D_2O version of CIRTHE was checked many years ago by recalculation of measurements concerning lattice parameters for several lattice pitches, fuel rod numbers and temperatures. In all cases a good agreement was found between theory and measurement.

CIRTHE calculations on PWR fuel rods have been checked against experiments involving capture rates of heavy nuclides, fuel temperature coefficients at full power conditions, relative concentrations of U- and Pu-isotopes in burnt fuel assemblies as well as radial distributions of burnable absorbers and Pu-isotopes in partially burnt fuel pellets. A very satisfactory agreement between calculation and experiment was obtained in all cases.

<u>Validation against measured radial distributions of Pu-isotopes and Nd148</u>

In the frame of the ARIANE program, Secondary Ion Mass Spectrometry (SIMS) examination of three MOX fuel specimens with an initial Pu_{fis}-enrichment of 4.2 w/o, irradiated in Beznau nuclear power plant up to 48.5 MWd/kgU has been performed /4/. Isotope distributions have been obtained across two perpendicular pellet diameters. The results of the recalculation by CIRTHE are shown in case of the Pu-isotope Pu239, Pu240, Pu241 in Fig. 1-3, in case of the radial burnup distribution in Fig. 4.

The measured burnup profiles across the pellet were determined by use of the Nd148 distributions. Small tilts occur in the burnup distributions, similar to the Pu239-distributions, due to azimuthal asymmetries in the flux distribution during irradiation. Unreal peaks within the distributions are caused by the presence of cracks in the specimen.

As can be seen, the measured dualism of breeding and fission at the periphery of the pellet is perfectly reproduced by the CIRTHE calculation.

<u>Validation against measurements of the isotopic fraction of Gadolinium /5/</u>

The measurements of isotopic fractions were performed for Gd-poisoned fuel rods belonging to an assembly in the second row of the Biblis-B reactor at EOC4.

In Fig.5 the measured gadolinium isotope concentrations in dependence on the burnup are compared with CIRTHE calculations for the relevant isotopes Gd155 and Gd157. As long as significant amounts of the main absorber nuclides Gd155 and Gd157 exist, measurement and calculation agree in good approximation.

Parameter variation

CIRTHE calculations were performed for pin cells of H_2O-lattices (PWR) and pin cells of Halden-type D_2O-lattices (HBWR). For the most important fuel pin types (U, MOX, Gd) the following set of parameter knots was considered:

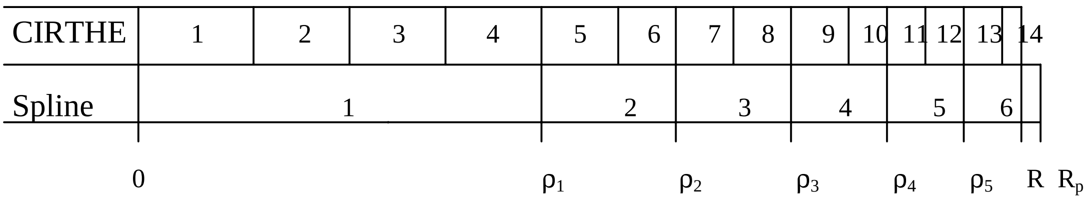
Burnup	(PWR)	b	=	0.0, 0.1, 0.2, . . . , 95, 100	MWd/kgU
	(HBWR)	b	=	0.0, 0.5, 1.0, . . . , 110, 120	MWd/kgU
Enrichment	(U, PWR)	e	=	0.71, 2.0, 3.5, 5.0	w/o U235
	(U, HBWR)	e	=	3.0, 6.0, 10, 13, 16, 20	w/o U235
	(MOX, PWR)	e	=	0.0, 2.0, 4.0, 6.0	w/o Pufis
	(MOX, HBWR)	e	=	3.0, 4.4, 5.8, 7.2, 8.6, 10.0	w/o Pufis
	(Gd, PWR)	e	=	0.71, 2.5. 4.0, 5.0	w/o U235
Pellet radius	(PWR)	R	=	0.41, 0.465, 0.54	cm
	(HBWR)	R	=	0.30, 0.40, 0.465, 0.50	cm
Gd_2O_3-amount	(PWR)	g	=	0.0, 3.0, 7.0, 10.0	w/o
Coolant void	(PWR, HBWR)	v	=	0.0, 40.0	%

QCALC module

Radial spline interpolation

CIRTHE yields the radial power profile in form of zone-averaged powers q^C_i for a limited number of fuel zones (outer radius r_i, i = 1, . . ,14). The transition of q^C_i to another zone subdivision, however, needs an analytical representation of q(r).

In order to obtain suited interpolation functions, the q^C_i values can be considered as supporting points. Oscillations of the interpolation functions can be avoided by using of spline interpolation with nodes at the spline zone borders ρ_j(j = 1, . . ,6). The allocation of the spline zones used in the interpolation procedure to the fuel zones used in CIRTHE is shown in the following figure.



Interpolating function within the j-th spline zone:

$$f_j(r) = a_{j1} + a_{j2} r^2 + a_{j3}/(R_p - r), \qquad j = 1,...,6$$

The 18 spline coefficients a_{jk} (j=1,6, k=1,3) can be deduced from the following equations:

8 identity conditions:

$$q^C_1 + q^C_2 = \frac{13}{R^2} \int_0^{r_2} f_1(r)\, r\, dr \qquad i = 1$$

$$q^C_{2i-1} + q^C_{2i} = \frac{13}{R^2} \int_{r_{2i-2}}^{r_{2i}} f_{i-1}(r)\, r\, dr \qquad i = 2,6$$

$$q^C_{13} = \frac{26}{3R^2} \int_{r_{12}}^{r_{13}} f_6(r)\, r\, dr \qquad i = 7$$

$$q^C_{14} = \frac{13}{3R^2} \int_{r_{13}}^{r_{14}} f_6(r)\, r\, dr \qquad i = 8$$

10 continuation conditions:

$$f_i(\rho_i) = f_{i+1}(\rho_i) \qquad i = 1{,}5$$

$$\left.\frac{\partial f_i(r)}{\partial r}\right|_{\rho_i} = \left.\frac{\partial f_{i+1}(r)}{\partial r}\right|_{\rho_i} \qquad i = 1{,}5$$

Separation of burnup

The quantities a_{jk} are functions of the parameters b, e, R, g, v and dependent on the pellet type. Since the burnup b has by far the greatest influence on the spline coefficients, the number of burnup supporting points is relatively high. In order to reduce the data flood of spline coefficients, the burnup dependence was separated in case of g=0, i.e. U-pellets (μ=1) and MOX-pellets (μ=2), by expanding a_{jk}^{μ} in even powers of b:

$$a_{jk}^{\mu}(b,s) = \sum_{\lambda=1}^{4} c_{\lambda jk}^{\mu}(s)\,\beta^{2(\lambda-1)} \qquad (e \geq 1.0)$$

$$a_{jk}^{\mu}(b,s) = \sum_{\lambda=1}^{2} \bar{c}_{\lambda jk}^{\mu}(s)\,\beta^{2(\lambda-1)} + \bar{c}_{3jk}^{\mu}(s) \Big/ \left[(1-\beta)\bar{c}_{4jk}^{\mu}(s) + x^{\mu}\right] \qquad (e < 1.0)$$

$$s = (e, R, g, v) \qquad \beta = b/100$$

Considering Gd-Pellets, the burnup expansion of spline coefficients leads to relatively inaccurate power profiles. Data reduction without significant loss of exactness was possible by reducing the number of burnup knots used in the CIRTHE calculation to the following 18 knots

0.0, 0.5, 1.0, 1.6, 2.2, 2.8, 3.4, 4.2, 5.0, 6.5, 8.0, 10., 15., 20., 30., 50., 70., 100.

and deriving the spline coefficients for the desired burnup point with aid of cubic spline interpolation.

Linear interpolation

Considering the remaining parameters e, R, g, v the used knot spacing allows the appliance of linear interpolation.

Let (e_0, R_0, g_0, v_0) be a certain point within the (e, R, g, v)-space with the following properties:

$$e_l < e_0 \le e_{l+1}$$
$$R_n < R_0 \le R_{n+1}$$
$$g_\nu < g_0 \le g_{\nu+1}$$
$$v_m < v_0 \le v_{m+1}$$

and let $V_{ijkk'}$ denote the following expression

$$V_{ijkk'} = |(e_{l+2-i} - e_0)(R_{n+2-j} - R_0)(g_{\nu+2-k} - g_0)(v_{m+2-k'} - v_0)|$$

than it follows for the radial power profile

$$q(r,b,e_0,R_0,g_0,v_0) = \sum_{k'=1}^{2}\left(\sum_{k=1}^{2}\left(\sum_{j=1}^{2}\left(\sum_{i=1}^{2}\left(q(r,b,e_{l-1+i},R_{n-1+j},g_{\nu-1+k},v_{m-1+k'})\,V_{ijkk'}\right)\right)\right)\right)$$

Interpolated power profiles

U-Pellet (PWR)

Fig. 6 and 7 show zone power radial profiles of PWR U-pellets in dependence on the burnup b for natural uranium and 4.0 w/o U-enrichment. In both cases, the powers q_i (i=1, . . ,20) of 20 volume-equal zones increase towards the pellet edge at each burnup point. The smallest power peaking occurs in fresh fuel pins. At the burnup b=0 the radial power profiles are determined by depression of the thermal flux within the fuel pellet. In this special case, the power peaking increases with an increase of the fuel-averaged thermal absorption cross section. Thus, the rim zone power of the natural uranium pellet starts with q_{20} = 1.037, in case of 4.0 w/o U-enrichment already with q_{20} = 1.060.

Screening effects in the thermal energy range and to a high degree at resonance energies lead to increasing fluxes toward the pellet edge and therefore to redistributions of all fuel nuclides, especially of the fission nuclides, during burnup evolution. Referring to power profiles in U-pins, the following effects are important:

1. Steep increase of the U238-resonance absorption and subsequent Pu239-buildup towards the pellet rim (i.e. strong increase of the power peaking at the pellet edge).

2. Amplified depletion of the initially uniform distributed isotope U235 and the breeded Pu-isotopes Pu239 and Pu241 in the outer fuel zones (i.e. reduction of the power peaking at the pellet edge).

The first effect is predominant at a low U235 content, like natural uranium. It is responsible for a steep growth of the radial power peaking from the very beginning, as shown in Fig. 6. With increasing U-enrichment the second effect becomes more and more important. This is indicated in Fig. 7, which shows the behaviour of $q_i(b)$ in case of 4.0 w/o U-enrichment.

MOX-pellet (PWR)

In similar fashion, Fig. 8 shows power profiles of a MOX-pellet with 4.0 w/o Pu_{fis}-content. Since the thermal absorption cross section of fresh MOX-fuel exceeds the corresponding value of fresh U-fuel with comparable enrichment approximately by factor 2.5, the initial power peaking surpasses the corresponding value of U-fuel considerably.

It is apparent that during the burnup evolution the above mentioned first effect (i.e. steep increase of the U238-resonance absorption and subsequent Pu239-buildup toward the pellet rim) is for MOX-fuel just so important than for U-pins. The second effect, however, is in case of MOX-fuel more complicated. The amplified depletion of Pu-isotopes in the outer fuel zones leads not only to a greater reduction of Pu239 but also to an amplified creation of the thermal fissionable isotope Pu241 through neutron capture in Pu240 during the first phase of burnup evolution. Therefore, the burnup related changes in the radial power profiles after transition to higher Pu-enrichments are less significant than in case of comparable enrichment changes in U-pins.

MOX-pellet (HBWR)

Differences of the radial power profile with burnup were found in heavy water moderated HBWR fuel rods against comparable light water moderated fuel pins. These differences are attributed to enormous spectral differences in the epithermal energy range.

The neutron energy spectrum at the Halden reactor is dominated by the thermal spectrum. Consequently, the enhanced Pu239-buildup at the pellet edge is subordinated compared to thermal effects. Especially in case of HBWR-MOX fuel pins, the radial power peaking up to approx. 30 MWd/kgU (see Fig. 9) is mainly affected by the enhanced Pu241-buildup at the pellet edge. Only at higher burnups the Pu239-buildup becomes more and more conspicuous.

Gd-pellet (PWR)

In case of Gd-pellets some additional affects are important to the radial power profiles:

- Strong peaking of the thermal flux toward the pellet edge; flat epithermal flux distribution.

- With increasing Gd-content the absorption and fission processes are more and more shifted to epithermal energies in consequence of spectral shift effects.

- Burnout of the strong absorbing isotopes Gd155 and Gd157 from the edge to the centre of the pellet.

In fresh Gd-pellets the rim zone power q_{20} increases with increasing Gd-content up to 3.0 w/o Gd_2O_3. One obtains values as follows:

q_{20} = 1.24 for e = 0.71w/o U235 and R = 0.41cm,
q_{20} = 1.40 for e = 5.00w/o U235 and R = 0.41cm,
q_{20} = 1.42 for e = 5.00w/o U235 and R = 0.54cm.

At higher Gd-concentrations the power peaking at the pellet edge is reduced again due to the a.m. spectral shift effects.

During the Gd-burnout phase up to approx. 10 MWd/kgU in case of usual initial Gd-loading, the radial power profiles are changed dramatically (see Fig. 10). At first, the power peaking at the pellet rim is strongly increased due to the amplified burnout of the Gd-isotopes in the outer fuel zones. With continual Gd-burnout, the radial power peaking reaches a maximum and decreases finally till an asymptotic distribution.

Concluding remarks

The implementation of the outlined interpolation scheme for radial power levels in the current version of CARO-E affects the results mainly in two ways.

In the frame of evaluation of temperature measurements made with instrumented HBWR-fuel assemblies, the burnup dependent power profiles play an important role. Accurately calculated power profiles of the test pins improve the worth of the measured data significantly, because the power levels influence calculated temperatures as well as calculated burnups.

The new radial PWR-power profiles deviate from those calculated with the previous model in some points considerably. Especially the increasing power peaking with increasing burnup at the pellet rim was drastically underestimated by the old model. With aid of the new profiles, measured fission gas release distributions can be predicted with excellent precision /6/.

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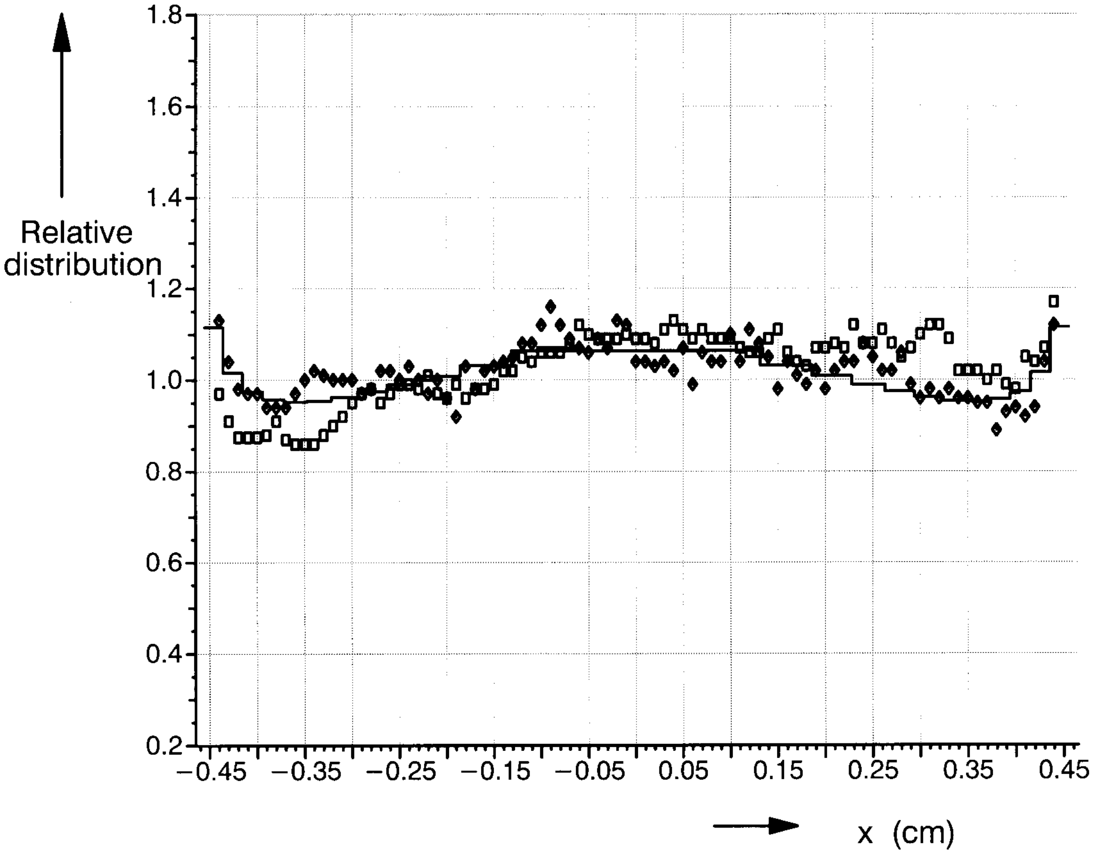
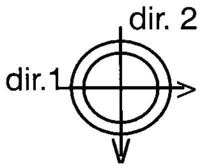
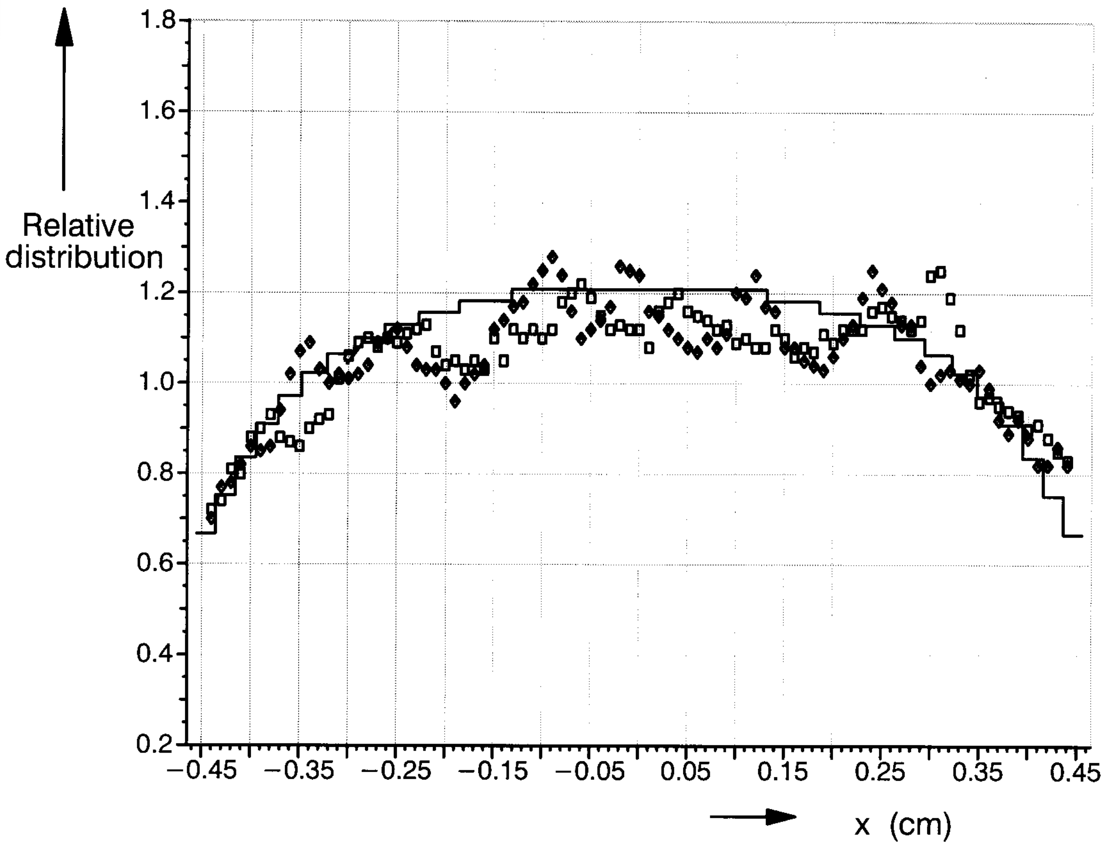


BEZNAU1, MOX, 4.2 w/o Pu_{fiss}, 48.5 MWd/kgU

Fig. 1 **Relative Pu239 isotopic distribution along the pellet diameter**

— CIRTHE
□ ARIANE measurement (direction 1)
◇ ARIANE measurement (direction 2)



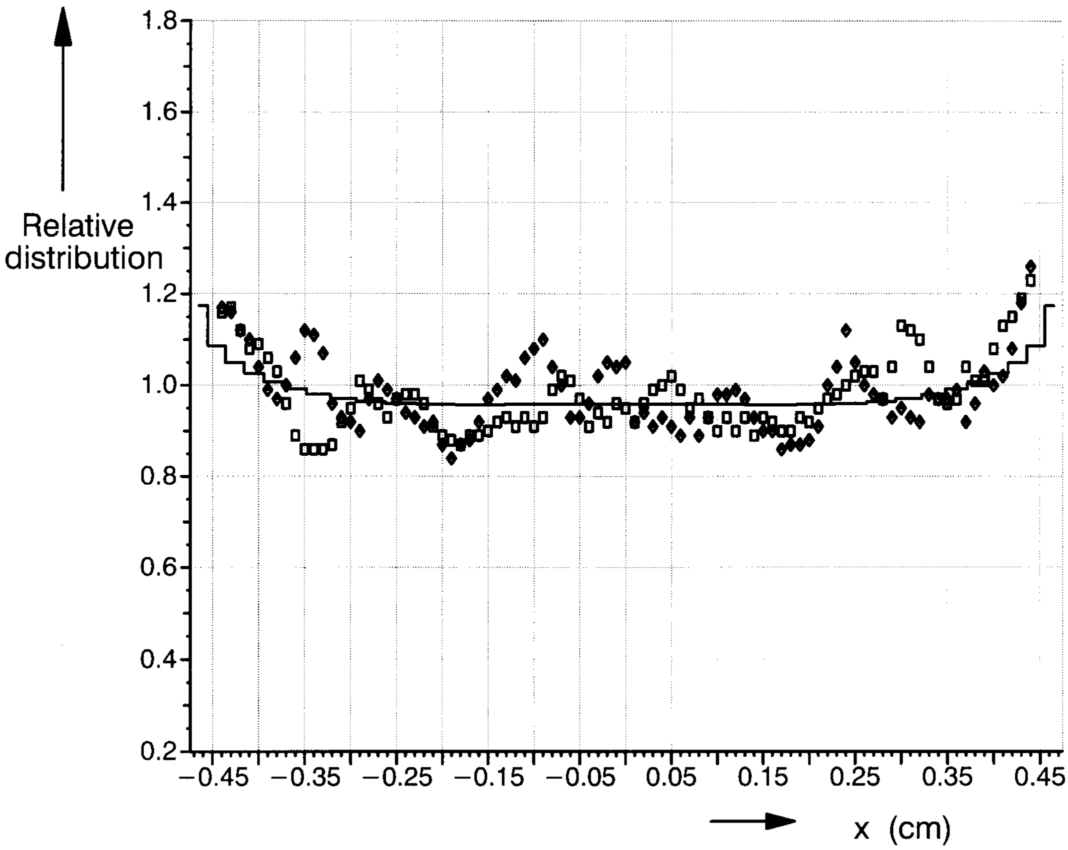


BEZNAU1, MOX, 4.2 w/o Pu_{fiss}, 48.5 MWd/kgU

Fig. 2 **Relative Pu240 isotopic distribution along the pellet diameter**

— CIRTHE
□ ARIANE measurement (direction 1)
◇ ARIANE measurement (direction 2)

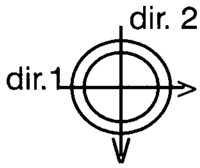
dir. 2
dir.1



BEZNAU1, MOX, 4.2 w/o Pu_{fiss}, 48.5 MWd/kgU

Fig. 3 **Relative Pu241 isotopic distribution along the pellet diameter**

— CIRTHE
□ ARIANE measurement (direction 1)
◆ ARIANE measurement (direction 2)



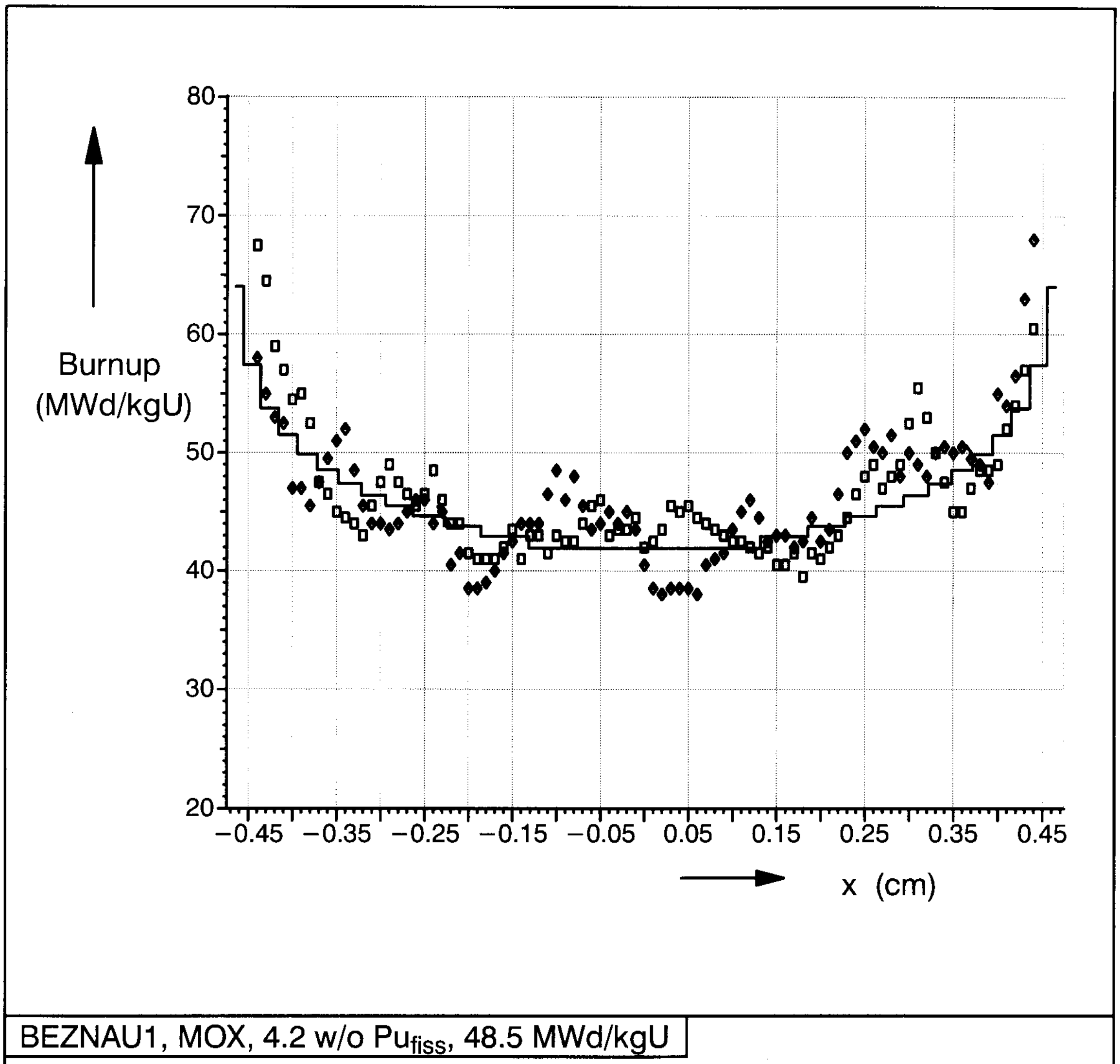
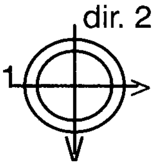
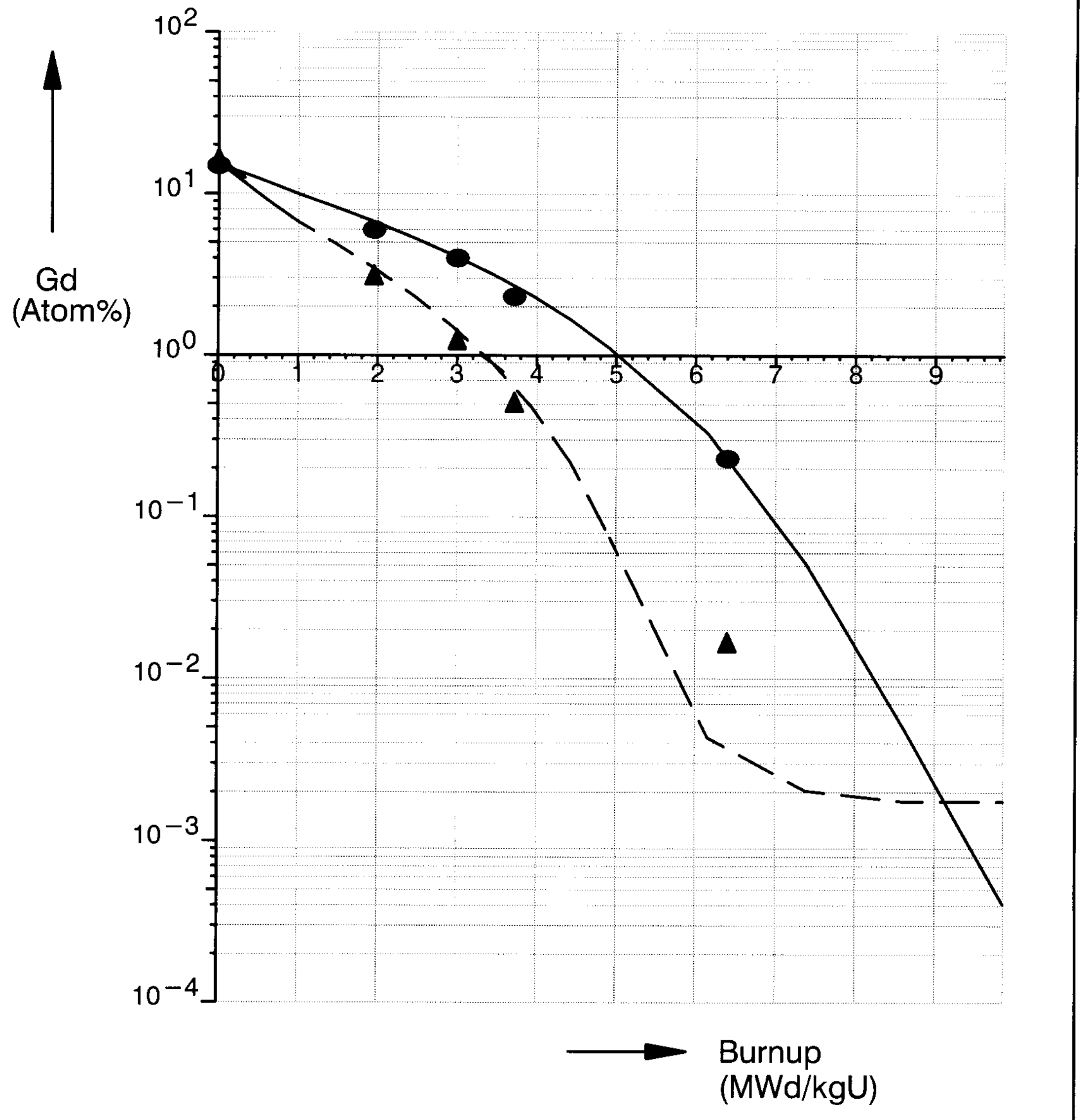


Fig. 4 Burnup distribution along the pellet diameter

— CIRTHE
□ ARIANE measurement (direction 1)
◇ ARIANE measurement (direction 2)

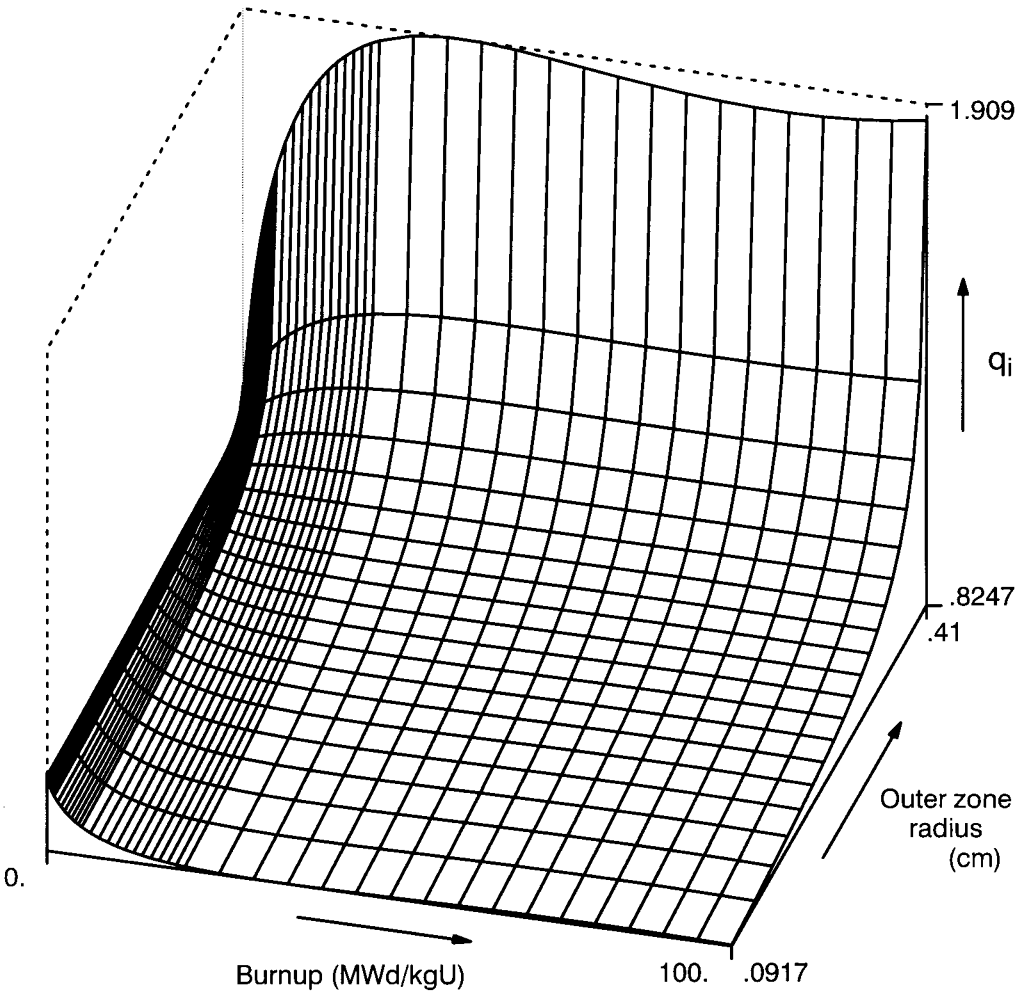




BIBLIS−B, 16x16−20 2.5w/o U235, 6.0w/o Gd_2O_3

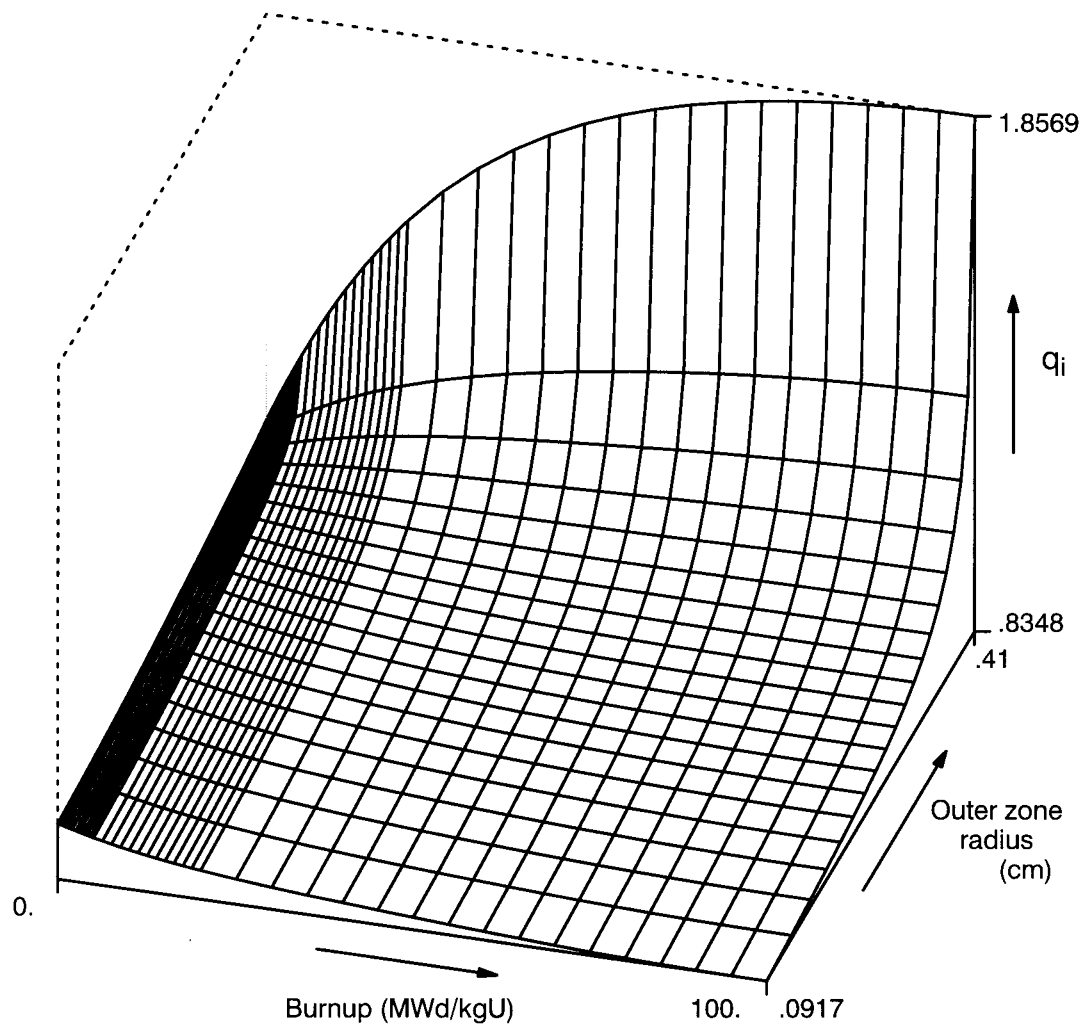
Fig. 5 Gd isotopic contribution vs. burnup

—	Gd155	CIRTHE
---	Gd157	
●	Gd155	Measurement
▲	Gd157	



U−pellet, PWR, R=0.41cm, 0.71w/o U235, 0 %Void

Fig. 6 Zone powers in dependence on burnup and radius



U−pellet, PWR, R=0.41cm, 4.00w/o U235, 0 %Void

Fig. 7 Zone powers in dependence on burnup and radius

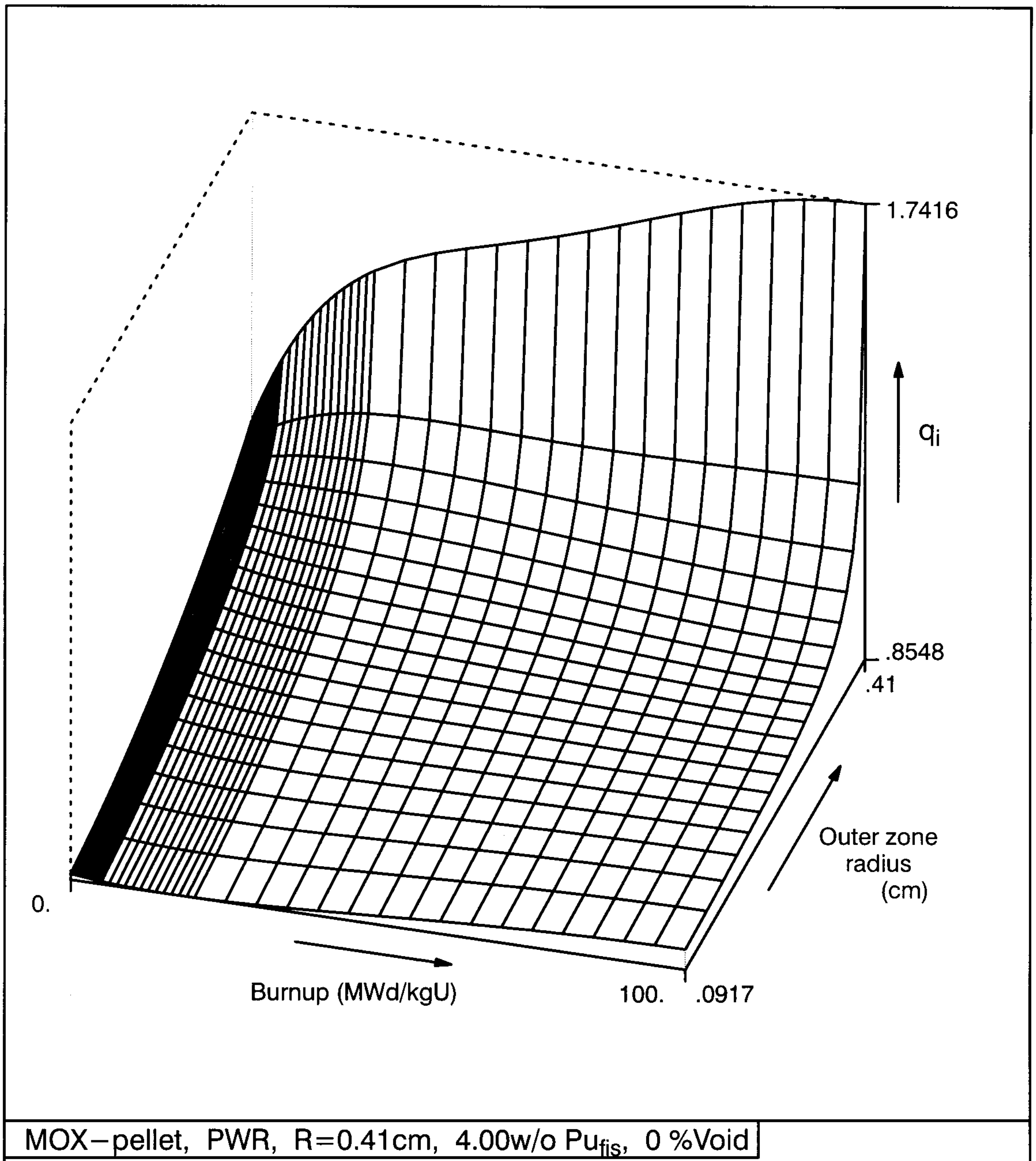
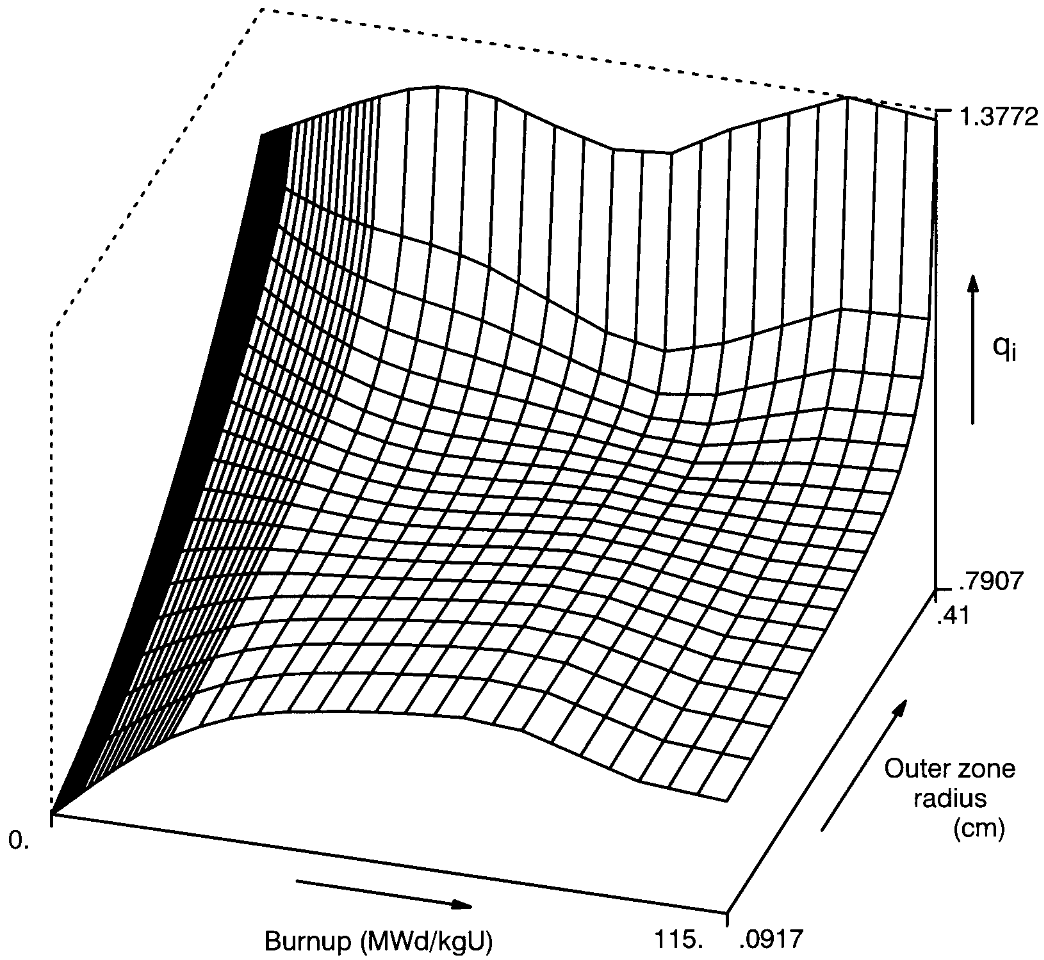
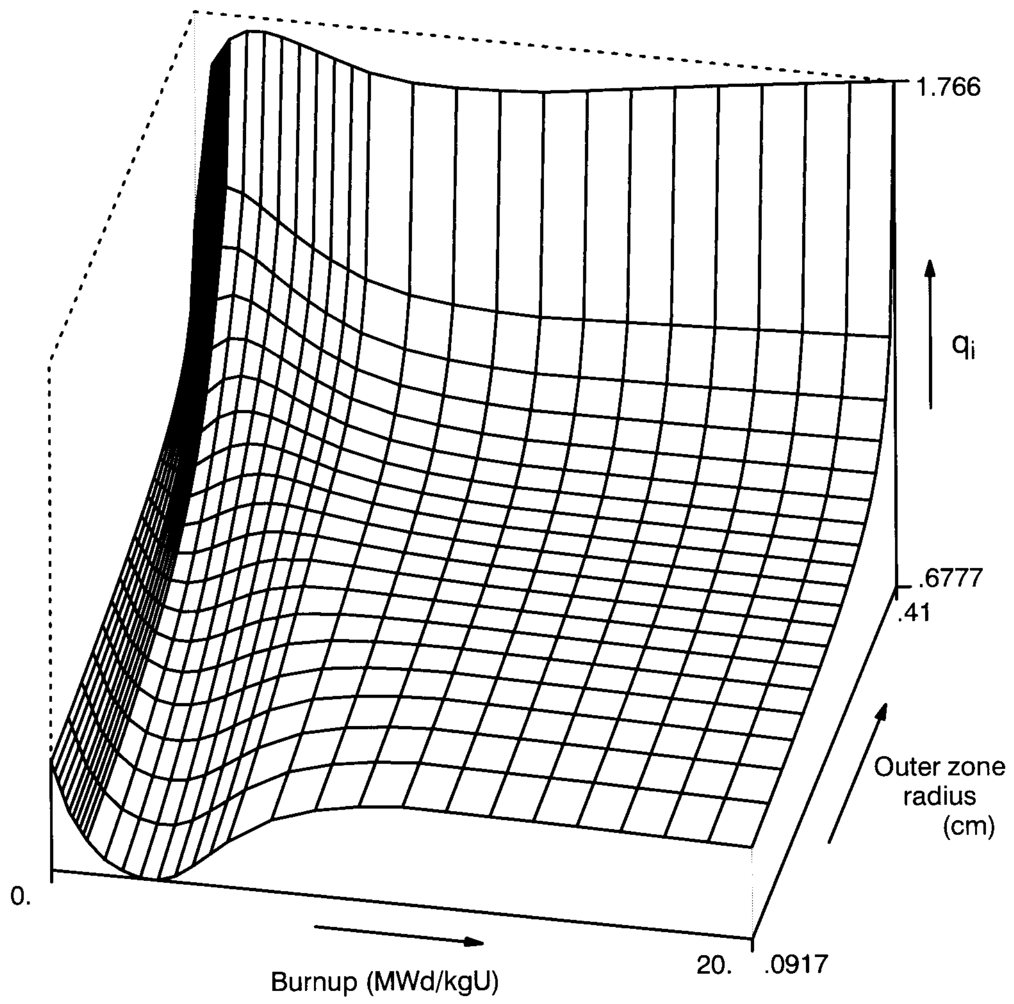


Fig. 8 **Zone powers in dependence on burnup and radius**



MOX−pellet, HBWR, R=0.41cm, 4.00w/o Pu_{fis}, 20 %Void

Fig. 9 Zone powers in dependence on burnup and radius



Gd–pellet, PWR, R=0.41cm, 2.00w/o U235, 8.00w/o Gd_2O_3, 0 %Void

Fig. 10 Zone powers in dependence on burnup and radius