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H. Kumpf

Recriticality Calculations for Uraniumdioxide-Water Systems with MCNP

Herausgeber:
FORSCHUNGSZENTRUM ROSSENDORF
Postfach 51 01 19
D-01314 Dresden
Telefon (0351) 26 00
Telefax (0351) 2 69 04 61

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Recriticality Calculations for Uraniumdioxide-Water Systems with MCNP

H. Kumpf

Forschungszentrum Rossendorf e.V.

Abstract

With the aim of generating a certain feeling for the general dependencies of the multiplication factor k_∞ the first section provides some results for two classes of deformations of the original fuel pins. The main part examines UO_2-structures of increasing disorder, beginning with the hexagonal close package of fuel spheres and ending up with stochastic geometries. Among these structures the worst case, i.e. the one with the highest k_∞ but preserving mechanical stability is identified. The composition and geometric parameter of this case is used to calculate the critical thickness of a slab and critical radius of a sphere.

Contents

1 Introduction

Investigations of severe accidents in power rectors will hardly produce data on the geometry, composition and density distributions of fuel mixtures in such detail as demanded for criticality calculations. In view of this ill-conditionedness of the task one might consider the following objectives of a general contribution to the problem of recriticality in of a severe accident scenario:

- The generation of a certain feeling for the dependencies of the multiplication factor k_∞ on various parameters of fuel debris. This feeling is not too well developed even among specialists. In order to test one's ability one may try to guess the signs of changes in k_∞ due to deformations of the pins dealt with in the following section. This first section is devoted mainly to a didactic purpose.
- The search for the 'worst case', i.e. the composition and structure of arrangements with maximum multiplication. The fuel geometry with maximum k_∞ is a hexagonal close package of spheres with a certain radius, immersed in water. But this arrangement is mechanically unstable. Furthermore, the collapsed hexagonal close package with touching spheres is by no means optimal with respect to k. Thus mechanical stability is a necessary condition in the search for the worst case. The main part of the present paper deals with the determination of such a structure. In view of the complexity of the task rigorous mathematical demonstration is not expected to be successful. Instead one adheres to heuristic reasoning.
- Finally a worthwhile objective might be to develop and verify calculational tools for dealing with systems possibly emerging from severe accidents in order to have them ready on the shelf in the case of such an event. The present paper may be regarded as a small step in this direction, too.

The present parameter study pursues to some extent all of the enumerated aims. It makes use of the Monte Carlo Neutron Transport Program MCNP elaborated by LANL ([1]), together with continuous neutron data from the ENDF/B-VI library. The thermalization of neutrons is treated by means of the $S(\alpha, \beta)$ module implemented in the code.

2 Pin Deformations

The description of possible pin deformations is limited by the pool of cell boundaries available in MCNP. These are: 1) Planes, 2) Surfaces of second order such as cylinders, spheres, cones, ellipsoides and hyperboloides, 3) One kind of surfaces of fourth order, that is to say toroids.

The Babcock and Wilcox UO_2 benchmark experiment ([2]) serves as a starting point in this section. It represents an infinite quadratic lattice with a pitch of 1.6256cm containing cylindrical UO_2 fuel elements with 2.49% enrichment in ^{235}U and 0.51cm radius. The system is moderated by H_2O with an addition of 220ppm ^{10}B. By void substitution in the center of a finite mock-up with the cited properties it has been demonstrated experimentally, that the corresponding infinite system exhibits $k_\infty = 1$. MCNP reproduces this value within the error limits.

In the following two subsections the pins will be subjected to two kinds of deformations. In all cases the volumes of moderator and UO_2 are conserved, and neither edges nor corners of the deformed surfaces are tolerated.

The surface gain x due to the deformation serves as one of the deformation parameters.

2.1 Toroidal Deformations

This kind of deformation changes the cylindrical pin to a body similar to a high voltage insulator (see cross-section through the axis in fig.1). The outer boundary consists of tori with equal smaller radii, which can still be handled by MCNP. The transitions from inner to outer tori are smooth ones. Thus there are two parameters of the deformation transformation: Surface gain x and torus small radius r. All the pins in the lattice are deformed in the same way, without shifts along the axis.

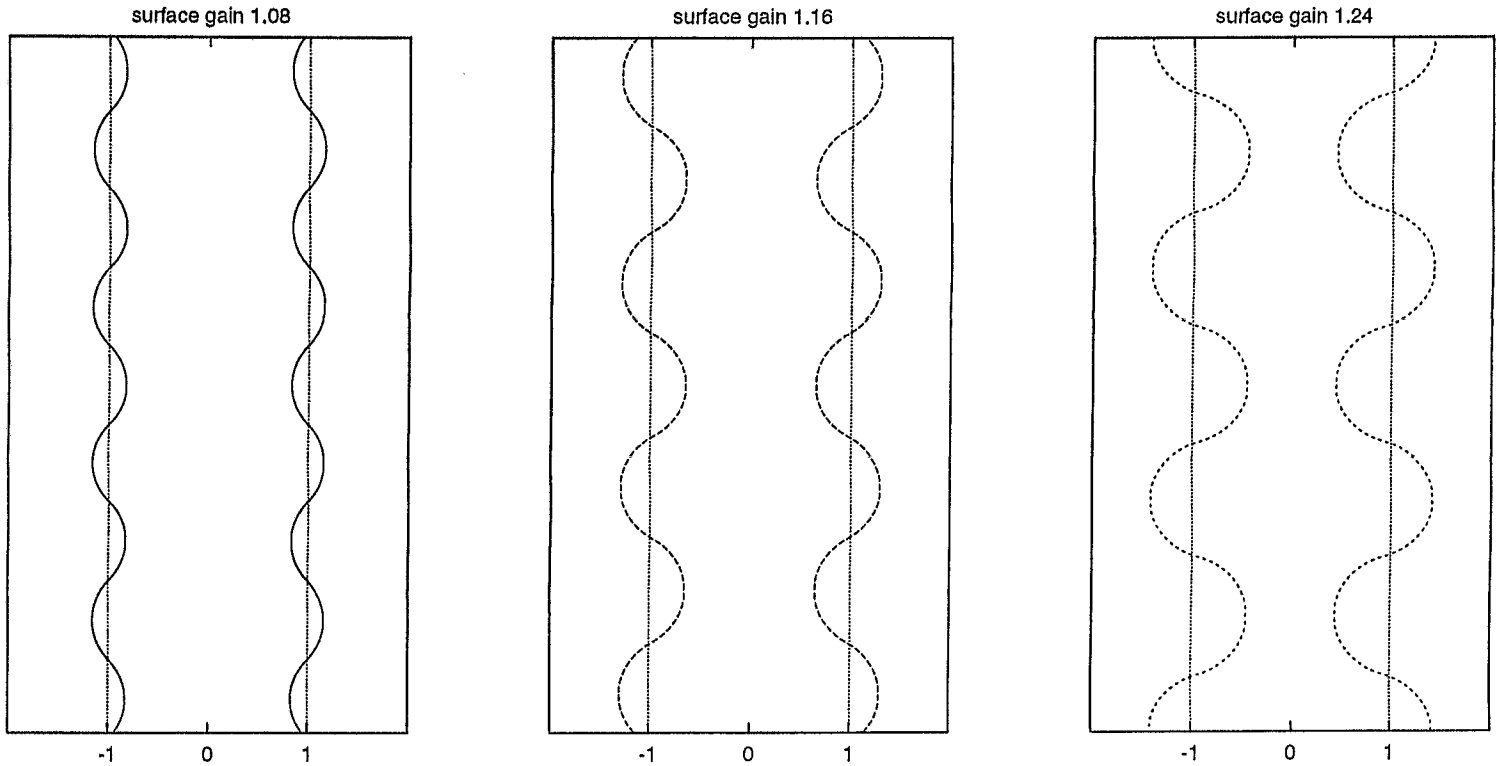

Figure 1: Longitudinal cross-section of toroidal pin distortion. Smaller toroidal radius= 0.7*pin radius. The pin in its original and deformed shape is shown. The side frame corresponds to the dimension of the cell.

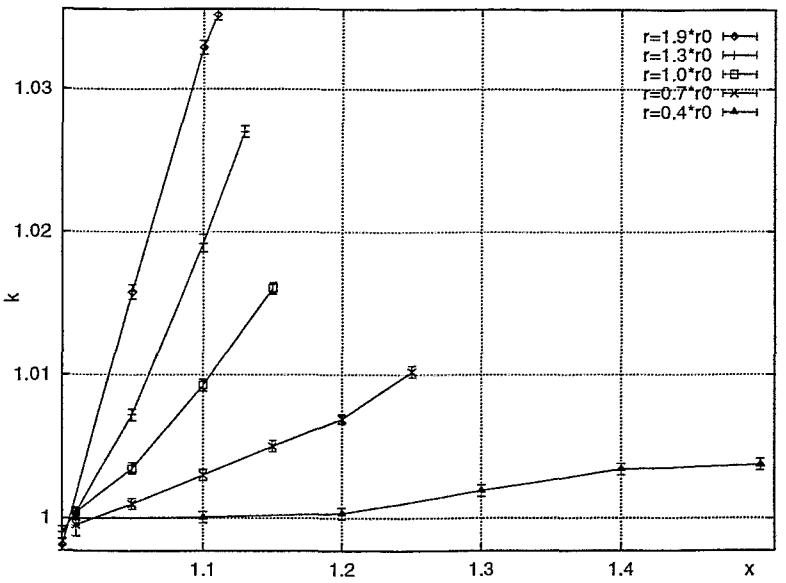

Figure 2: Results of k_∞ calculations (vertical axis). The horizontal axis represents x, the surface gain by toroidal deformation. The parameter of the family of curves is the smaller radius of tori r, i.e. the radius of curvature of the deformed surface of the pin. The pin radius r0 serves as a unit of length.

The results of k_∞ calculations after toroidal deformations are shown in fig.2 in dependence on the surface gain x with the radius of tori as a parameter of the family of curves. Generally, the curves terminate when neighbouring pins begin to touch.

The maximum reactivity increase amounts to about 3.5%.

One observes that a roughness with a small radius of curvature does not considerably change k_∞ even if it strongly increases the surface (lowest curve in fig.2).

2.2 Flute Deformations

This kind of deformations leads to bodies similar to channelled greek columns (see cross-section perpendicular to axis in fig.3). The boundary consists of cylinders with equal radii and smooth transitions. There are again two parameters of the transformation: Surface gain x and periodicity n (number of flutes around the circumference). The cylinders radii depend on n and x. They are falling monotonically with n or x rising. All the pins in the lattice are distorted in the same way, without rotations around the axis.

The results of k_∞ calculations after flute deformations are shown in fig.4 in dependence on the surface gain x with the periodicity n as a curves parameter. Generally the curves terminate when the hills of neighbouring pins begin to touch.

It's amazing, but reactivity change is negative with this kind of distortion!

There is no monotonic dependence on the periodicity, even and odd n behaving differently. This is an indication of the interaction of neighbouring pins. With even n the hills always meet the hills of their neighbours, while with odd n this is not true.

Again a small scale roughness (small $r \rightarrow$ big n) has a negligible influence on k_∞, even if the surface gain is considerable.

The above observations suggest the following *heuristic conclusions*:

Deformations approaching the geometry of the absolutely optimal case (hexagonal close package of spheres with a certain lattice constant and sphere radius, see below) lead to positive reactivity changes. Indeed, if the toroidal deformations are amplified more and more, they lead to a configuration similar to chains of spheres (see the rightmost part in fig.1).

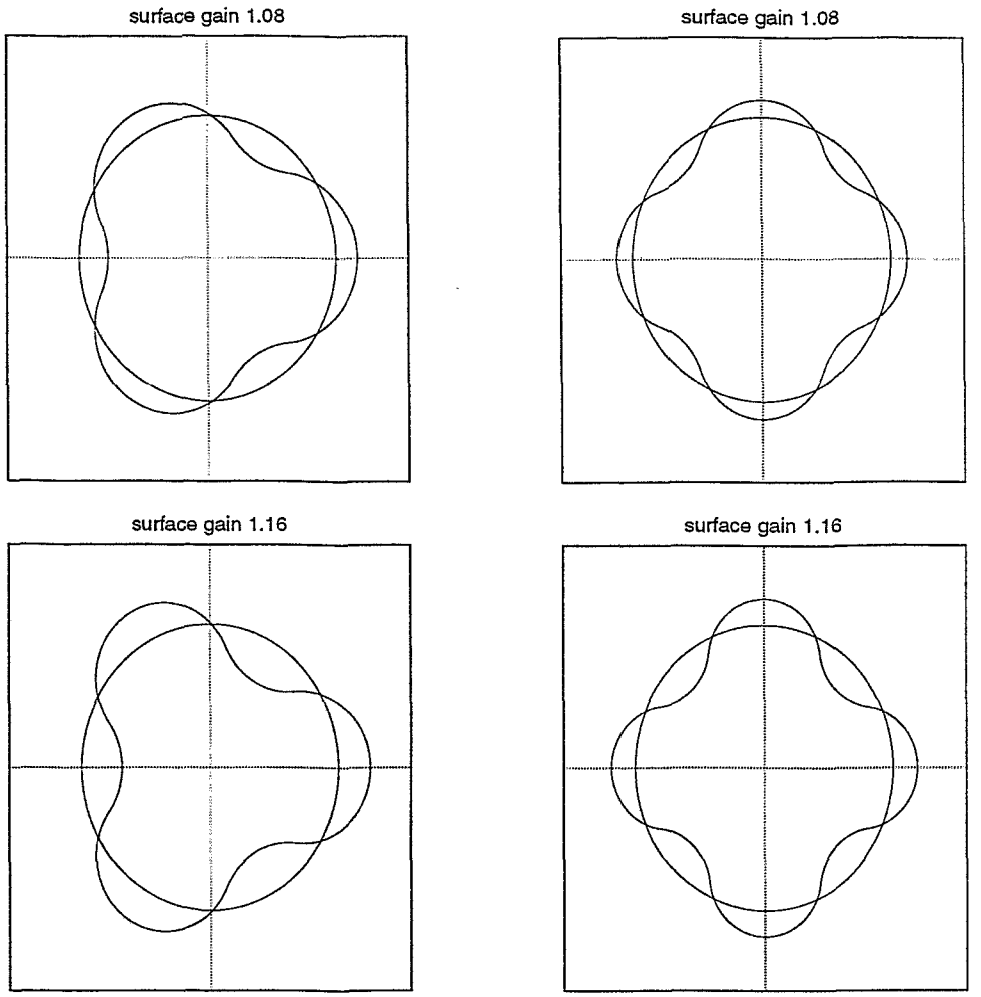

Figure 3: Flute shape pin distortions with 3 flutes (left) and 4 flutes (right).

Deformations leading further away from the optimal case induce negative reactivity changes. Indeed, if the flutes are deepened more and more, the resulting configuration is rather similar to a bundle of smaller cylinders an the place of the original pin.

An increase of the surface due to small scale roughness (characteristic radius $\ll$ sphere radius in the cited optimal case) has negligible consequences in k.

3 Fuel-Water Structures far away from the Normal State

In the following the condition of the same U/H_2O volume ratio as in the Babcock-Wilcox experiment will be dropped. The enrichment of 2.5% and the slight Boron content of 220ppm will be maintained.

3.1 Hexagonal Close Packing

According to the textbooks the fuel arrangement with the absolutely biggest k_∞ for a given enrichment is the hexagonal close packing of equal fuel spheres. Indeed, no complete demonstration of this statement is known to the author.

Fig.5 demonstrates the results for our case. The mechanically stable case of touching spheres is far from being optimal.

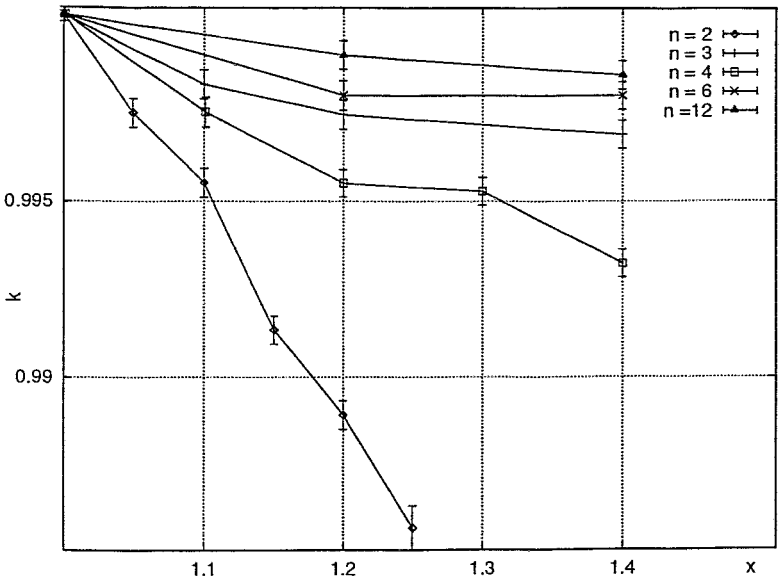

Figure 4: Results of k_∞ calculations (vertical axis). The horizontal axis represents x, the surface gain by flute deformation. The parameter of the family of curves is the periodicity, i.e. the number of flutes or hills around the circumference of the pin.

3.2 Heaps of Fuel Spheres

By means of a special code the MCNP input for a heap of touching fuel spheres without any lattice order, contained within a cubic box provided with reflecting walls, was generated. Due to limitations of the field dimensions in MCNP a total of less than 4000 spheres had to be used and the reflecting box had to be subdivided into smaller cubic cells. Of course, the box with reflecting walls does not exactly model an infinite heap. But by varying the dimensions of the box it could be shown, that the resulting error is negligible. The same comment applies to the other structures to be presented in the following.

The results are depicted in fig.6.

3.3 Stochastic Geometries of Overlapping Spheres

Fuel in Spheres, Moderator in Intermediate Space

By means of yet another special code the MCNP input for a structure of interpenetrating spheres, randomly distributed within a cubic box with reflecting walls, has been generated.

An important question concerns the threshold for the U/H_2O volume ratio, above which there may exist mechanically stable structures within the frame of the indicated model. Within the model of touching spheres, the only stable configuration exhibits a U/H_2O ratio of 0.83. If one wants to increase this ratio, the spheres were forced to interpenetrate. Therefore within the model of overlapping spheres we regard U/H_2O ratios below 0.83 as mechanically impossible. This postulate is strongly supported by regarding the corresponding pictures generated by the MCNP visualization code SABRINA.

The results for the geometry of overlapping fuel spheres are shown in fig.7.

Fuel in Intermediate Space, Moderator in Spheres

Oviously, the above geometry can be inversed by putting the fuel into the intermediate space and the moderator into the spheres. The corresponding results are contained in fig.8

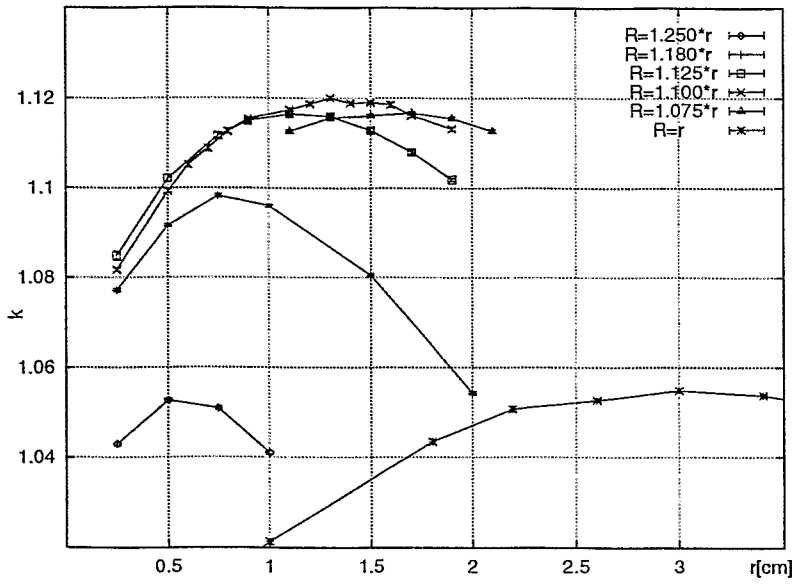

Figure 5: Results of k_∞ calculations (vertical axis) for a lattice of fuel spheres in hexagonal close package, surrounded by moderator. The horizontal axis represents the radius of spheres r. The parameter R characterizes the property of the lattice (sphere radius for the case of touching spheres). The lower right curve represents the case of touching spheres, the only configuration exhibiting mechanical stability. The curve showing the absolute maximum of k_∞ (R=1.1 0*r) corresponds to a volume ratio of $U/H_2O = 1.254$.

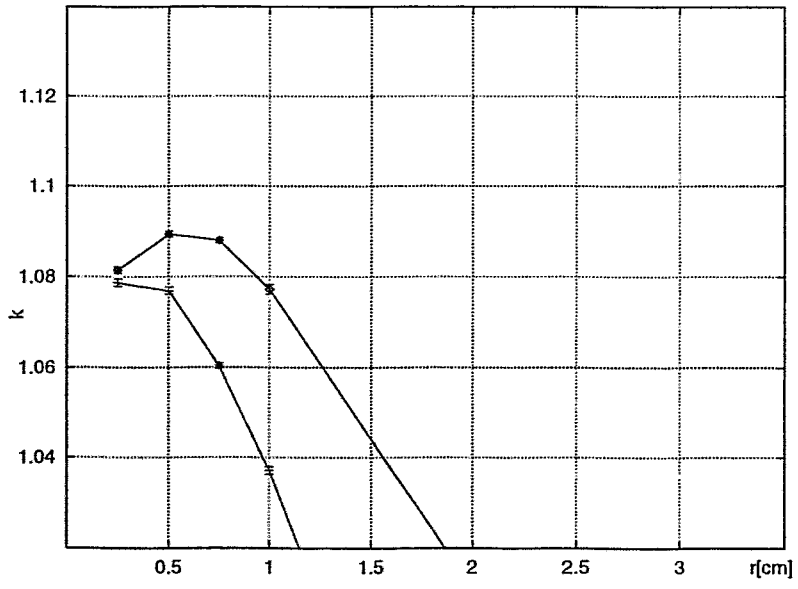

Figure 6: Results of k_{eff} calculations (vertical axis) for a heap of fuel spheres penetrated by moderator (upper curve) and the inverse case of closely touching moderator bubbles and fuel in between (lower curve). In both cases the horizontal axis represents the radius of spheres r. The volume ratio of $U/H_2O = 0.828$ in the direct case.

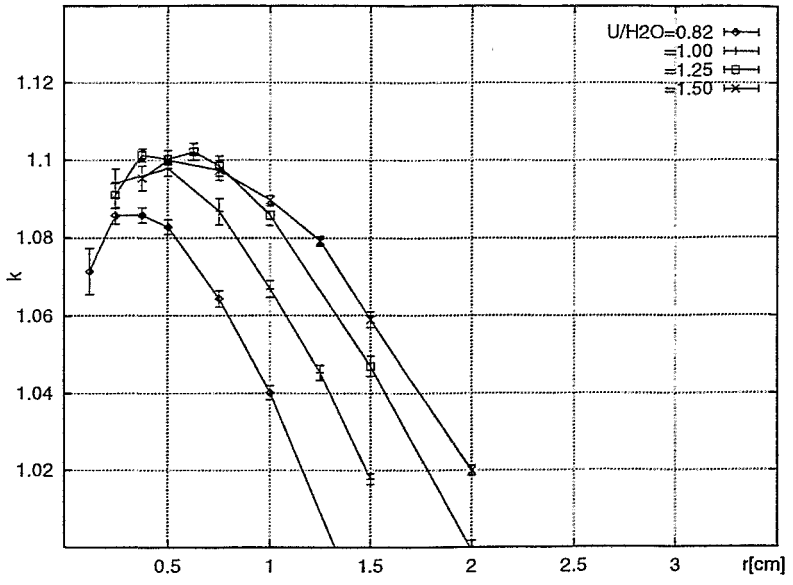

Figure 7: Results of k_{eff} calculations (vertical axis) for a structure of overlapping fuel spheres arranged stochastically in space, penetrated by moderator. The horizontal axis represents the radius of spheres r. Parameter of the family of curves is the volume ratio of U/H_2O.

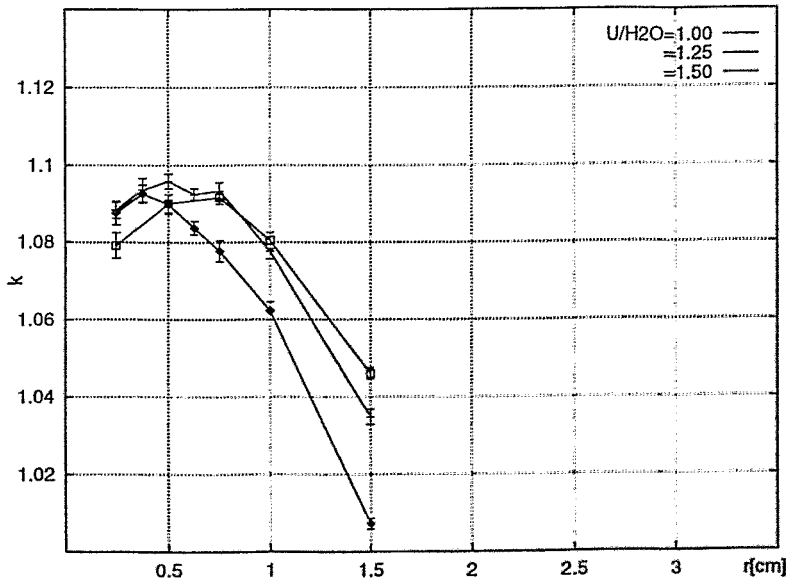

Figure 8: Results of k_{eff} calculations (vertical axis) for a structure of overlapping spherical moderator bubbles arranged stochastically in space with fuel filling the resulting gaps. The horizontal axis represents the radius of bubbles r. Parameter of the family of curves is the true volume ratio U/H_2O.

A Simple Chord Length Model

Up to now the results for stochastic direct and inverse geometries are not comparable, because in the first case the independent parameter is the radius of the fuel spheres, in the second case the radius of the moderator bubbles. Both parameters are of the dimension of a length, but they lack any general significance, being related to specific models.

A well proven approximation in reactor theory is the so called form independent approximation using the notion of the chord length. The definition of the uranium chord length S_U is:

$$S_U = \frac{4V_U}{O_U} \tag{1}$$

where V_U, O_U are volume and surface area of the fuel.

Thus the chord length depends exclusively on the fuel volume and the 'inner surface area'. For this reason it is a much more general parameter than e.g. the sphere radius.

We now try to derive expressions for the U chord length in the direct and inverse case of our model of overlapping spheres in stochastic geometry. To this end fuel volume and surface area are understood as functions of the number n of spheres placed inside the (large) total volume V_{tot}.

It is easy to see, that the volume V_U obeys the following differential equation:

$$\frac{dV_U}{dn} = \frac{4\pi r_U^3}{3}\frac{V_{tot} - V_U}{V_{tot}} \tag{2}$$

where r_U is our former radius of fuel balls. Using the following notations for dimensionless quantities:

$$x = \frac{V_U}{V_{tot}}$$
$$v_0 = \frac{4\pi r_U^3}{3V_{tot}}$$

we get:

$$\frac{dx}{dn} = v_0(1-x) \tag{3}$$

Using the initial condition $x = v_0$ at $n = 1$ the solution becomes:

$$x = 1 - (1 - v_0)e^{(1-n)v_0} \tag{4}$$

or if $n \gg 1$ due to $v_0 \ll 1$:

$$x = 1 - e^{-nv_0}, \tag{5}$$

a result to be expected.

Slightly more tricky is the derivation of a differential equation for the surface O_U, see fig.9, where the addition of one more sphere is depicted and where in this rather crude description the boundary U/H_2O is represented by a plane.

The wanted diff. equ. for the surface area O_U then becomes:

$$\frac{dO_U}{dn} = 4\pi r_U^2\frac{V_{tot} - V_U - r_U O_U}{V_{tot}} + \frac{O_U\int_{-r_U}^{r_U}\Delta O(z)dz}{V_{tot}} \tag{6}$$

The first term concerns the case, if the new sphere ($dn = 1$) as a whole fits into the space not occupied by fuel. The second term concerns the case, if the sphere crosses the fuel/moderator boundary. In this case the surface increase is $\Delta O(z)$ = cap - circle cut by sphere on boundary:

$$\Delta O(z) = 2\pi r_U(r_U - z) - \pi(r_U^2 - z^2) = \pi(r_U - z)^2 \tag{7}$$

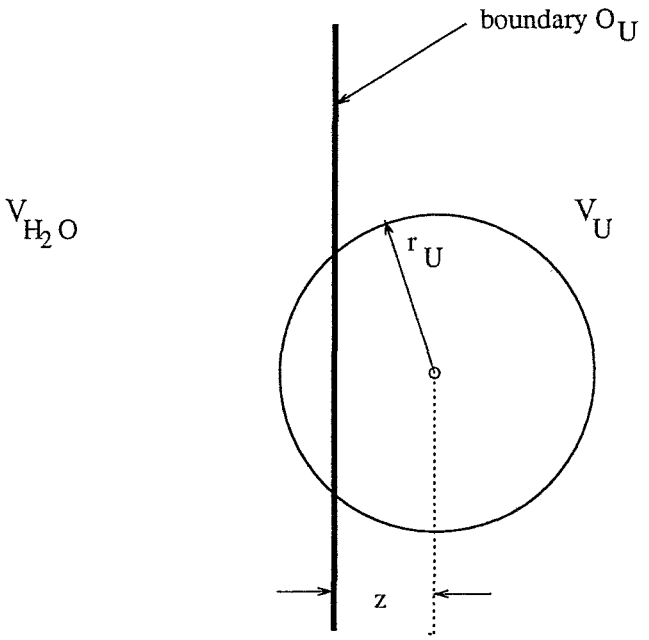

Figure 9: Derivation of a diff. equ. for the surface area O_U

With the notation $y = O_U/4\pi r_U^2$ after integrating we get:

$$\frac{dy}{dn} + v_0 y = 1 - x \tag{8}$$

With the initial condition $y(1) = 1$ due to $v_0 \ll 1$ the solution is:

$$y = ne^{-v_0 n} \tag{9}$$

The chord length expressed in the dimensionless quantities x, y und v_0 reads:

$$S_U = \frac{4V_U}{O_U} = \frac{4xV_{tot}}{y4\pi r_U^2} = \frac{4r_U x}{3yv_0} \tag{10}$$

Replacing n in equ.(9) by means of equ.(5) with x and substituting the obtained expression for y in equ.(10) the result is:

$$S_U = \frac{4r_U}{3} \frac{x}{(x-1)\ln(1-x)} \tag{11}$$

Similarly, in inverse geometry:

$$S_U^{inv} = -\frac{4r_{H2O}}{3\ln(x)} \tag{12}$$

Both these formulae for the chord lengths show the expected behaviour for $x \to 0$ and $x \to 1$. Thus for $x \to 0$ $S_U \to 4r_U/3$, the chord length for isolated spheres. Likewise for $x \to 1$ $S_U \to \infty$.

The fig.10 presents the results in direct and inverse geometries for overlapping spheres as well as for the heap of touching spheres in dependence on the fuel cord length S_U. Obviously, for identic fuel/moderator ratios the results roughly agree independent of the geometry. In view of the applied rather simple model of chord length, ideal coincidence may not be expected.

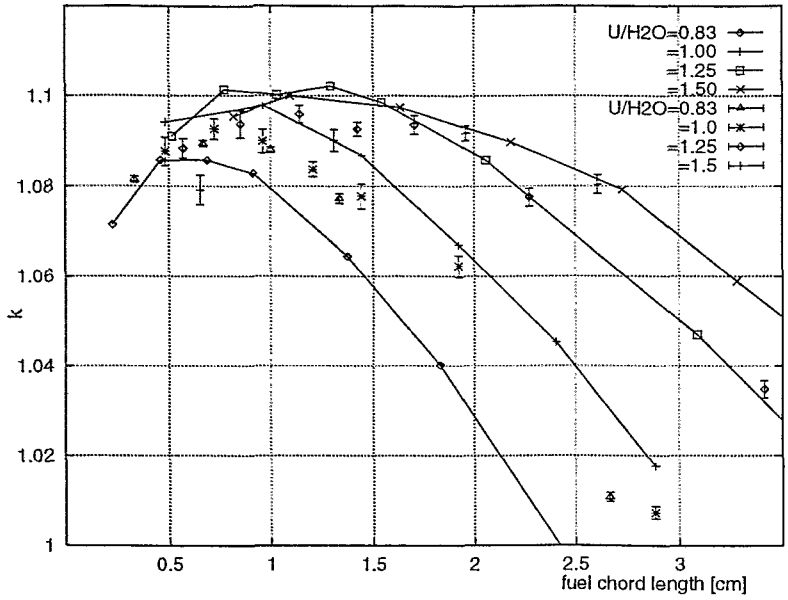

Figure 10: Results of k_∞ calculations (vertical axis) in dependence on the fuel chord length S_U. The continuous lines represent results for structures of overlapping fuel spheres. The points with triangles and errorbars refer to a heap of touching fuel spheres (U/H_2O=0.83). The other points with errorbars refer to the inverse geometry of overlapping moderator spheres (U/H_2O=1.0, 1.25 and 1.50).

The Worst Case for UO_2 - pure H_2O Mixtures

In the following we shall drop the boration of the moderator and will use pure H_2O instead. Furthermore, besides the enrichment of 2.5% values of 3.0 and 3.5% will be considered. The aim will be to determine the worst case. Fig.11 presents the results obtained with the model of overlapping fuel spheres. In contrast to the case of a slightly borated moderator, here the optimum is placed clearly outside the range of U/H_2O volume ratios securing mechanical stability (≥ 0.83 , see discussion above).

In the case of slightly borated moderator shown above (see fig.7 or 10), the maximum in k_∞ occurred at $U/H_2O = 1.25$, obviously within the region of mechanical stability. But with pure H_2O the theoretical maximum ist located at $U/H_2O = 0.45$, a value clearly causing mechanical instability. Therefore we take as the U/H_2O volume ratio in the worst case the value 0.83, realized for a heap of touching spheres. By observing cross-sections of arrangements of overlapping spheres generated as MCNP input using the SABRINA visualization program one can get a feeling, that stability is probably lost already above the threshold of 0.83. Furthermore the increase in k_∞ by reducing U/H_2O from the adopted 0.83 to the true optimal but unstable 0.45 is not too important (from 1.33 to 1.35).

Up to now we have used stochastic distributions in space but fixed radii of the spheres. Likewise we have done calculations with radii distributed around a mean $\bar{r}$ with a certain dispersion σ_r. In all cases results for k have been below those with r fixed at $\bar{r}$. This fact is easily understandable due to the convex shape of the dependence of k_∞ on r (existence of a maximum). In this respect too, the 'worst case' is really worst.

Thus we retain for further use as the worst case the model of overlapping spheres with sphere radius fixed at 0.87cm (or chord length = 4*(fuel volume)/(inner fuel surface)= 3.20cm). These structure parameters do not change if the enrichment is raised from 2.5 up to 3.5% ^{235}U. With the same results we could use the model of touching spheres with identical chord length and volume ratio.

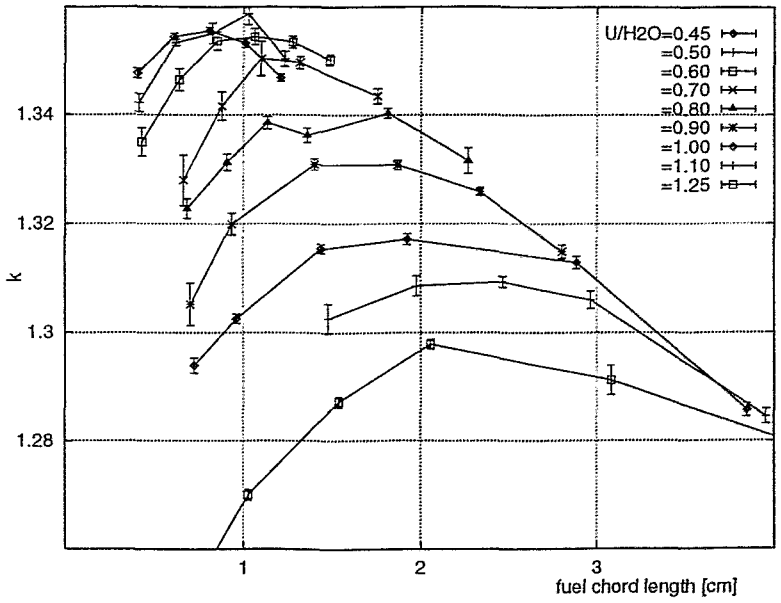

Figure 11: Results of k_∞ calculations (vertical axis) for 2.5% enrichment in ^{235}U in dependence on the fuel chord length S_U for UO_2 - pure H_2O mixtures in the model of overlapping fuel spheres. Parameter of the family of curves is the U/H_2O volume ratio.

4 Critical Slabs and Spheres in the Worst Case

A box with the worst structure defined above has been repeated in a threedimensional lattice. This lattice has been used to fill an infinite slab or a sphere and to calculate their k_{eff} by means of MCNP. Again the results are insensitive to small changes of the box dimensions. The results at three values of the enrichment in ^{235}U and in the presence or absence of an infinite water reflector are contained in the following table.

% ^{235}U			2.5	3.0	3.5
slab	d_{krit} $[cm]$	no reflector	29.8	27.8	26.5
		with reflector	19.9	17.6	16.5
	m_{krit} $[kg/m^2]$	no reflector	2480	2310	2210
		with reflector	1660	1460	1370
sphere	r_{krit} $[cm]$	no reflector	31.3	29.2	28.0
		with reflector	26.1	24.3	23.0
	m_{krit} $[kg]$	no reflector	1063	868	765
		with reflector	620	500	424

Table 1: Results of criticality calculations for an infinite slab and a sphere for the worst case (structure with fuel chord length 3.20 cm und fuel/moderator volume ratio 0.83). The masses refer to UO_2 with the given enrichment.

5 Conclusion

The present paper tries to create a certain intuitive feeling for the dependencies of the multiplication factor k_∞ of $UO_2 - H_2O$ mixtures.

Composition and structure of the corium in the 'worst case' have been proposed and made plausible.

The critical surface density of an infinite slab and the critical mass of a sphere of $UO_2 - H_2O$ mixtures *for the worst case with respect to their composition and structure* have been evaluated.

MCNP appears to be a proper tool for calculating any macroarrangement of a great number of small spheres modelling a stochastic structure.

References

[1] MCNP4A Monte Carlo N-Particle Transport Code System, contributed by Los Alamos National Laboratory, RSIC Code Package CCC-200, December 1993

[2] S. Sitaraman, MCNP: Light Water Reactor Critical Benchmarks, GE Nuclear Energy, NEDO-32028, March 1992