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# On the Capability of SMORES to Account for Self-Shielding in Search for Maximum $k_{eff}$

Yonathan Karni[1], Ehud Greenspan[1], Sedat Goluoglu[2] and Calvin Hopper[2]
[1]*University of California, Department of Nuclear Engineering, Berkeley, CA 94720, USA*
[2]*Oak Ridge National Laboratory, P.O. Box 2008, Oak Ridge, 37831, TN USA*

This study investigates the capability of SMORES – a new prototypic analysis sequence of SCALE-5, to identify the maximum $k_{eff}$ composition of 5% enriched uranium – water systems having fixed fuel mass. The effects of resonance self-shielding are accounted for. Simplified one-dimensional slab geometry systems are considered. It is found that SMORES is capable of identifying nearly optimal lumped composition of cores fueled with low enriched fuel the $k_{eff}$ of which can increase by increasing the resonance self shielding. The near optimal composition can be identified starting from either homogeneous or non-optimally lumped composition. The deviation of the converged lumped composition from the absolutely optimal depends on the amplitude of density change per iteration in addition to the initial composition. Large density changes per iteration may impair convergence and result in far from optimal lumped composition.

***KEYWORDS: SMORES, SCALE-5, Criticality safety, Maximum $k_{eff}$, Self-shielding, Low-enriched uranium***

## 1. Introduction

A new prototypic analysis sequence, SMORES (Scale Material Optimization and REplacement Sequence), was recently developed for incorporation into the SCALE-5 code package [1]. SMORES provides for a semi-automatic search for either the maximum $k_{eff}$ of a given amount of specified fissile material, or the minimum critical mass.

Most of the problems SMORES has been applied to so far [2-5] involved highly enriched fuel. Only one problem involved a thermal system that uses low enriched uranium [6]. Starting from homogeneous initial composition, SMORES automatically lumped the fuel in a fraction of the zones in the core, filling the other zones by moderator only [6]. The lumping increases $k_{eff}$ by virtue of self-shielding. The objective of the present work is to investigate the capability of SMORES to converge to the optimal lumped composition and its sensitivity to the initial composition and to the amplitude of material density variation per iteration.

The study is done for simplified one-dimensional systems made of 10.96 g/cm$^3$ $UO_2$ enriched to 5 weight % $^{235}U$ and water moderator and reflector. The illustrations are done for simplified slab geometry problems. The theoretical basis for the optimization and procedure used by SMORES are described in references 3 and 6.

There are three parts to this study. The first (Section 2.1) is a "brute-force" optimization in which the initial composition is a uniform homogeneous distribution of $UO_2$ in water. The second (Section 2.2) is a "lumped" optimization in which the initial composition is a lattice of fuel lumps of a fixed pitch. The third (Section 2.3) explores the effect of material density amplitude change per iteration on the number of iteration required for convergence and on the converged results while the fourth (Section 2.4) considers fuel lumps of variable location in the system.

## 2. Results

### 2.1 Homogeneous Initial Composition

We consider a slab core that is 19.95 cm thick and is surrounded by an effective infinite water reflector. The core is divided into 0.1 cm thick zones. The leftmost zone has a thickness of 0.05 cm. The boundary conditions are reflective on left and vacuum on right. The $UO_2$ mass is 13.152 g per square centimeter of slab surface area and is kept constant. The optimization searches for the maximum $k_{eff}$ the $UO_2$ can configure itself to have. The initial $UO_2$ concentration is homogeneous; it decreases linearly from the core center to zero in the outermost core zone.

Figure 1 shows the optimal composition SMORES arrived at as well as the corresponding Equal Volume Replacement Reactivity Worth (EVRRW) distribution (dotted red line; denoted as "rel.HRZ"). The EVRRW gives the reactivity effect of replacing a small volume of water at a given zone by the same volume of fuel; it is calculated by SMORES using first order perturbation theory. For an optimal system the EVRRW values should be the same in all fuel containing zones and smaller in non-fuel containing zones [3, 6].

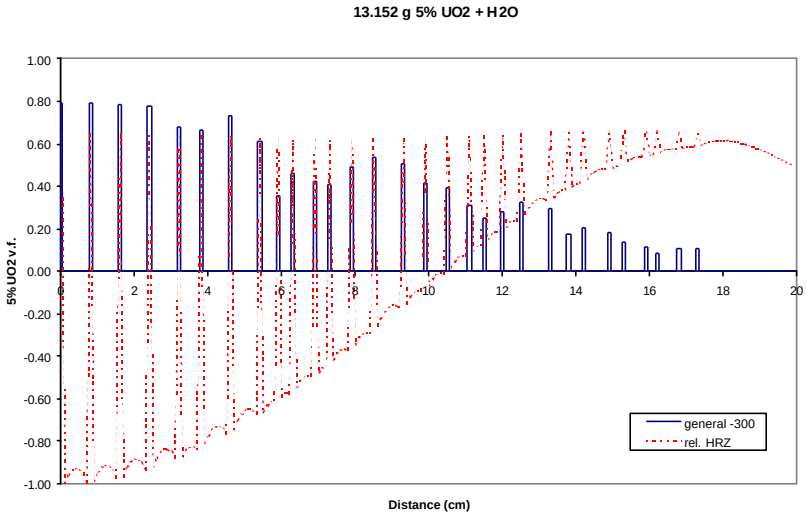


**Fig. 1** Optimal lumped composition of slab system fueled with 5% enriched $UO_2$ obtained starting from a homogeneous composition

It is seen that the spacing between the fuel lumps SMORES arrived at is not uniform but the EVRRW values in the fueled zones is pretty close to constant. $k_{eff}$ increased from 1.173 to 1.235. The next question considered is how close to the absolute optimal is the optimal system arrived at by SMORES. The answer to this question is sought by performing a sequence of optimizations starting from lumped initial composition of different lattice pitch; that is, with different number of water zones in between fuel zones. The maximum $UO_2$ concentration permitted in the zones that initially contain no fuel is set to zero, so the location of the fuel is fixed to the predefined zones. In Section 2.4 we perform optimization in which the location of the fuel lump is variable.

Similar results were obtained for spherical geometry systems.

## 2.2 Lumped Initial Composition with Fixed Fuel Zones

Figure 2 shows the optimal lumped composition and corresponding EVRRW distribution arrived at when starting with a uniform lumped composition having 5 water gaps in between fuel containing zones. Figure 3 gives the maximum value of $k_{eff}$ arrived at and the number of iterations required for reaching the optimal composition; it is significantly smaller than the number of iterations required for convergence when starting from homogeneous composition.

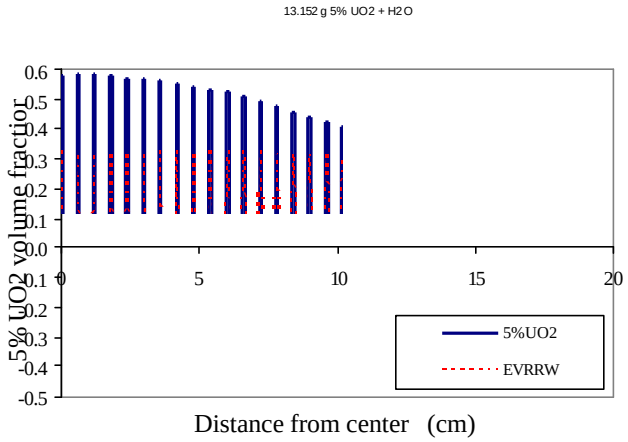


**Fig. 2** Optimal lumped composition of slab system fueled with 5% enriched $UO_2$ obtained starting from a uniform lumped composition with 5 water gaps between fueled zones

Figure 3 shows that the maximum value of $k_{eff}$ of the initially lumped problems vary significantly as a function of the number of water gaps initially chosen between the fuel lumps. The largest $k_{eff}$ is obtained for a uniform lattice having six-zone water gaps. This maximum $k_{eff}$ value SMORES arrived at (the horizontal pink line in Figure 3) by "brute force" optimization, i.e., starting from a homogeneous composition, is only slightly smaller.

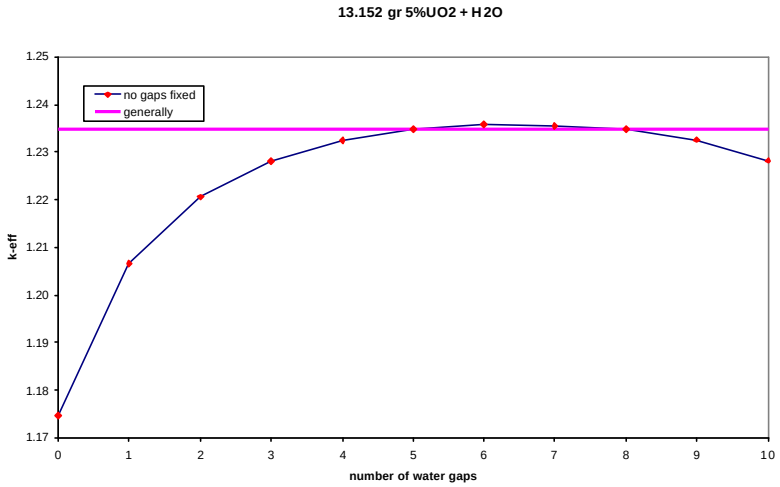


**Fig. 3** Maximum $k_{eff}$ SMORES converged to starting with different initial composition of the 5% enriched uranium dioxide fueled water moderated slab problems. Straight line corresponds to $k_{eff}$ of the optimal system of Figure 1.

Figure 4 shows the effect of the initial composition on the $k_{eff}$ evolution with number of iterations. The "0 gap" case corresponds to the initially homogeneous composition addressed in Section 2.1. It is observed that starting with a lumped initial composition of uniform amplitude results in much faster convergence than when starting with a homogeneous composition. However, if the initially lumped composition has significantly larger or smaller water gap in between the fuel lumps the $k_{eff}$ value SMORES converges to is lower than the maximum.

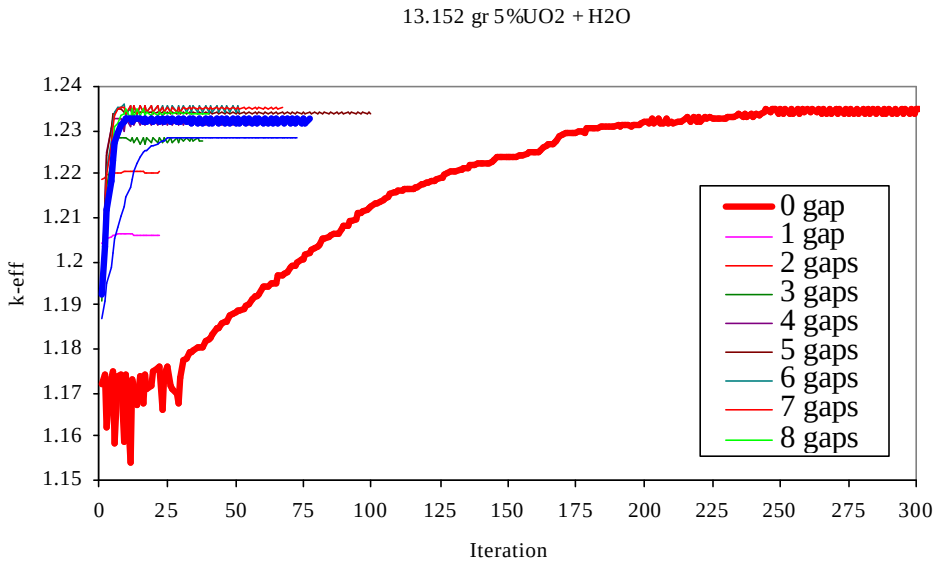


**Fig. 4** Maximum $k_{eff}$ SMORES converged to starting with different initial composition and 0.1 cm zones. "0 gap" corresponds to the initial homogeneous composition leading to the optimal composition of Figure 1.

Figure 5 compares the $k_{eff}$ evolution when starting with different initial composition when the zone width is 0.25 cm. The phenomena observed are consistent with those of Figure 4. It

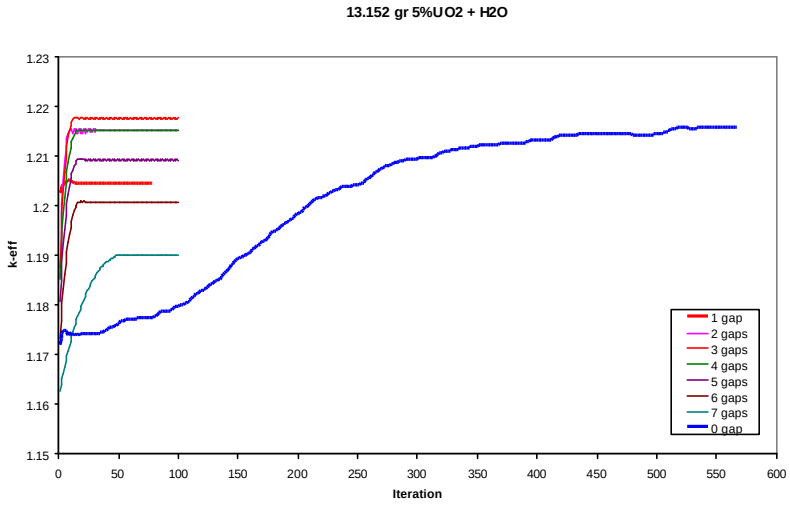


**Fig. 5** Maximum $k_{eff}$ SMORES converged to starting with different initial composition and 0.25 cm zones. "0 gap" corresponds to homogeneous initial composition.

Is found that the brute-force application of SMORES underestimated the peak $k_{eff}$ by about 0.2%. It is also found that the peak $k_{eff}$ obtained using 0.25 cm thick zones is lower than that obtained using 0.1 cm thick zones by approximately 14%. This is probably due to the less than optimal water to fuel ratio arrived at using the thicker fuel zones.

### 2.3 Effect of Density Amplitude Change per Iteration

The irregular spacing of the fuel lumps SMORES arrives at when starting with a homogeneous composition is expected to depend on the amplitude of density change per iteration; the larger the density change per iteration the more likely it is to have irregularity in the distance between fuel lumps. A set of numerical experiments was done to check the sensitivity of the degree of irregularity and of number of iterations required for convergence on the "acoef" input parameter of SMORES; these are the input parameters that determine the amplitude of density change per iteration.

The system considered has 12.987 g $UO_2$ per $cm^2$ of slab area and is divided into 0.5 cm thick zones (0.25 cm thick central half-zone). The outer core radius is 19.75 cm and the initial fuel distribution is uniform homogenous 6% volume fraction. The system was "brute-force" optimized using either one of four different density amplitude changes: the "acoef" values selected for the optimization were 0.001, 0.006, 0.030 and 0.150.

Figure 6 compares the $k_{eff}$ evolution using the four different "acoef" values whereas Figures 7 through 10 show the lumped distribution SMORES converged to. Figure 6 shows that the larger is "acoef" the convergence to the peak $k_{eff}$ takes a smaller number of iterations. However, for large "acoef" values (acoef = 0.150) the approach to the peak $k_{eff}$ is oscillatory rather than smooth monotonic, and the peak $k_{eff}$ value is smaller than the absolute maximum. This is because use of a too large "acoef" may result in highly irregular lattice pitch as shown, for example, in Figure 10 (Compare versus Figure 7).

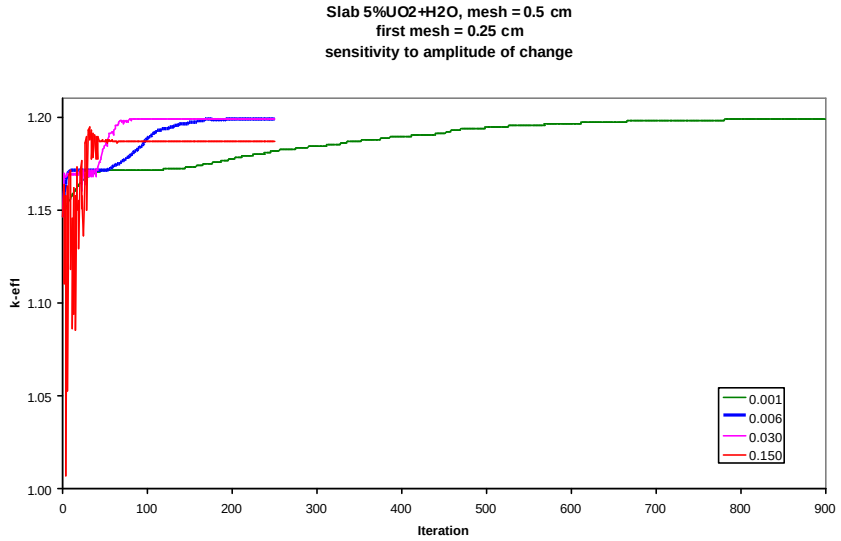


**Fig. 6** Evolution of $k_{eff}$ using either one of four different "acoef" values. Slab problem using 0.5 cm zones

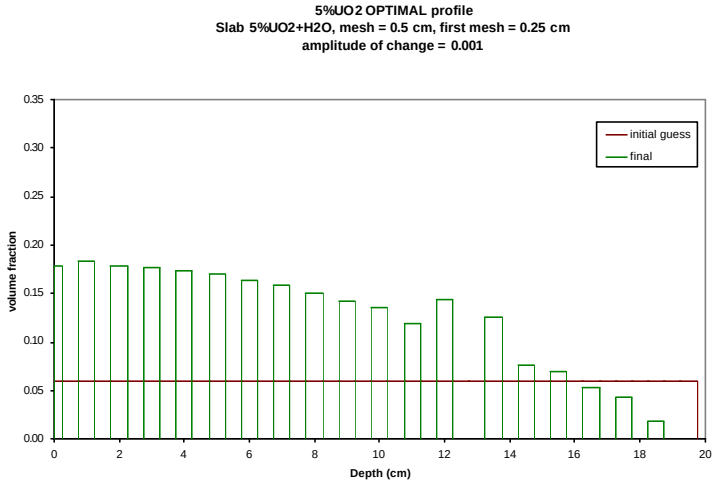


**Fig. 7** Optimal lumped profile arrived at using "acoef" of 0.001

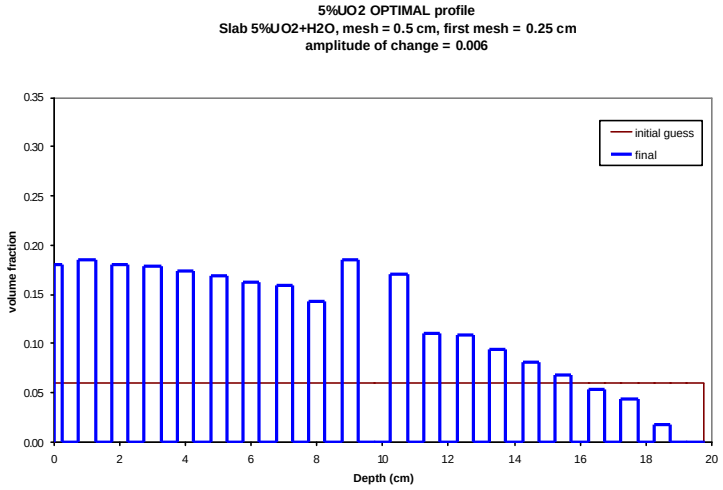


**Fig. 8** Optimal lumped profile arrived at using "acoef" of 0.006

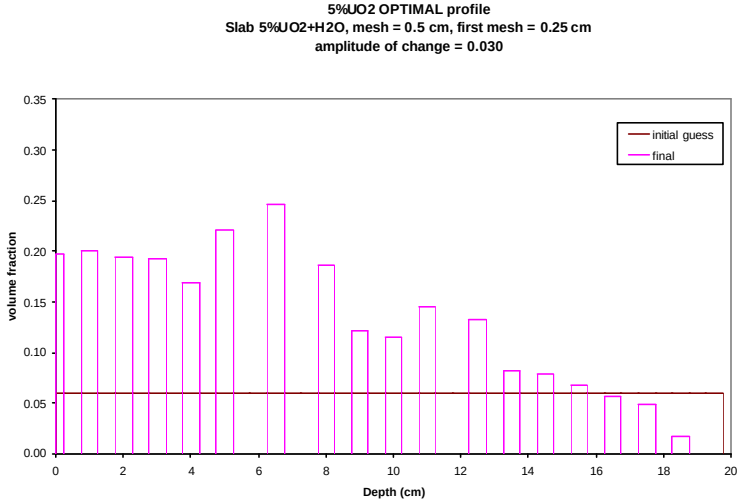


**Fig. 9** Optimal lumped profile arrived at using "acoef" of 0.030

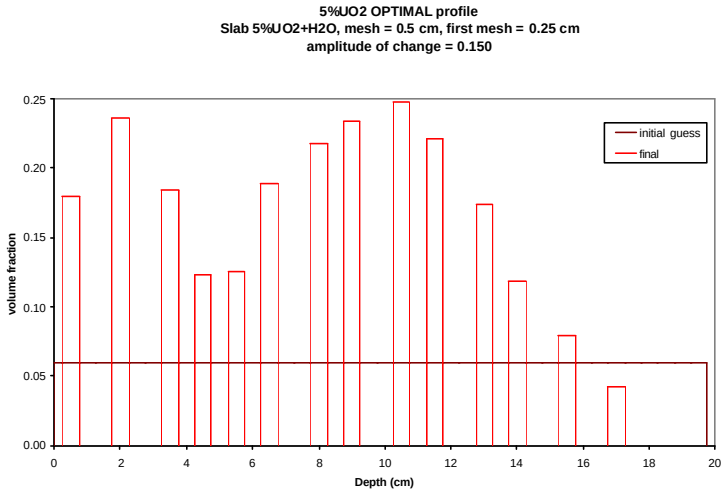


**Fig. 10** Optimal lumped profile arrived at using "acoef" of 0.15

## 2.4 Lumped Initial Composition with Floating Fuel Zones

In the studies reported upon in the above two sections the fuel containing zones were pre-defined. In this section we investigate the ability of SMORES to vary the number and location of fuel lumps when starting from a non-optimal lumped composition. The system considered is that defined in Section 2.1 but the core is divided into 0.25 cm thick zones except for the central zone that is 0.5 cm thick. The initial composition has the fuel volume fraction alternating between 11% and 1%.

Figure 11 shows the $k_{eff}$ evolution with the number of iterations while Figure 12 shows the optimal composition SMORES arrived at. It is found that SMORES can modify the width of the water gaps between fuel lumps when starting with off-optimal gaps. The optimal lumped composition SMORES arrived at has nearly equal water gap widths between the fuel lumps; its $k_{eff}$ is very close to the absolutely maximum attainable using 0.25 cm wide zones (Fig. 5).

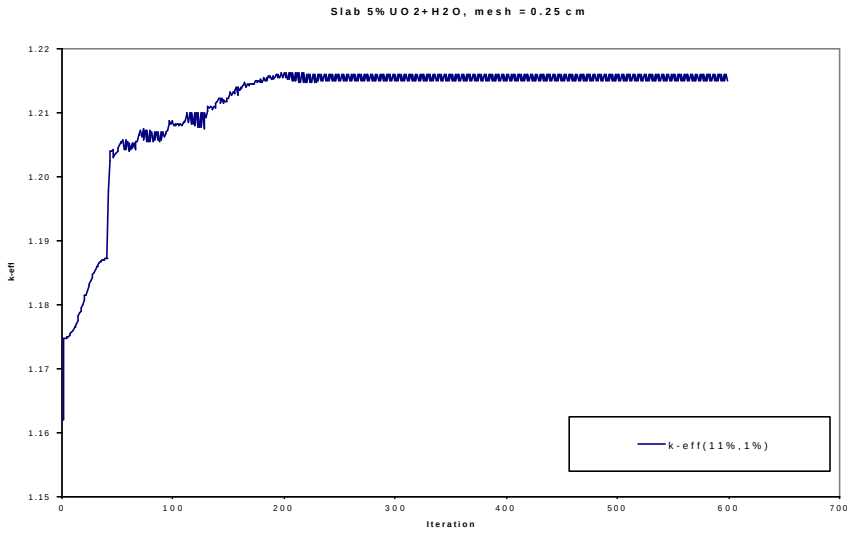


**Fig. 11** $k_{eff}$ evolution in slab system optimization starting from a lumped fuel composition having alternating zones volume fraction of 11% and 1%

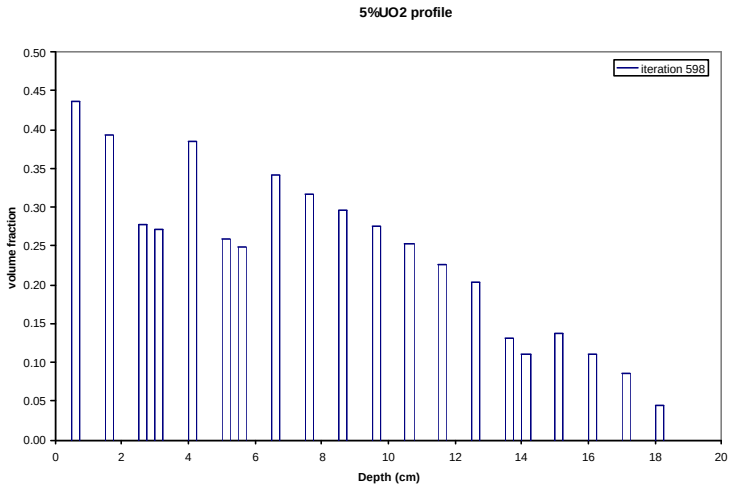


**Fig. 12** Optimal composition arrived at starting from alternate $11^{v}/_{o}$ - $1^{v}/_{o}$ fuel zones

## 3. Conclusions

SMORES is capable of identifying nearly optimal lumped composition of cores fueled with low enriched fuel the $k_{eff}$ of which can increase by increasing the resonance self shielding. The near optimal composition can be identified starting from either homogeneous or non-optimally lumped composition. The deviation of the converged lumped composition from the absolutely optimal depends on the amplitude of density change per iteration (the "acoef" parameter) in addition to the initial composition. Large density changes per iteration may impair convergence and result in far from optimal lumped composition.

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