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NEW MAXIMUM K_{eff} SEARCH OTIONS FOR "SMORES"

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ABSTRACT

New semi-automatic search options for maximum k_{eff} of systems having a given number of fixed composition fuel elements were successfully developed for SMORES – a new prototypic analysis sequence of SCALE-5.0. They are useful for identifying that distance between the fuel elements that will result in maximum k_{eff}. The new optimization algorithms were tested by applying them to identify the maximum k_{eff} thermal systems could have when made of a given number of fixed composition fuel elements, a moderator and a reflector. It was found that the optimal systems generally feature non-uniform spacing of the fuel elements – the optimal spacing tends to increase from the center towards the reflector. The spacing non-uniformity depends on the combination of moderator and reflector materials, on the number of fuel elements in the system and on the reflector thickness. The general trend is increasing spacing width with reduction in the number of fuel slabs and with reduction in reflector thickness. Particularly large can be the spacing of the outermost to the next-to-outermost fuel elements when using very low absorbing moderator, such as graphite, along with a relatively absorbing reflector such as water. When using a thick low absorbing reflector, such as graphite, the spacing of the fuel elements is nearly uniform and only slightly larger than the optimal spacing in an infinite lattice. Otherwise the optimal spacing can be significantly larger than the optimal infinite lattice spacing.

Key Words: Maximum k_{eff}; Optimization; SMORES; SCALE-5.0

1. INTRODUCTION

A new prototypic analysis sequence, SMORES (Scale Material Optimization and REplacement Sequence), was recently developed for incorporation into the SCALE-5.0 code package [1,2] to provide the criticality-safety community improved capability for determining margins of subcriticality. SMORES provides for a semi-automatic search for either the maximum k_{eff} of a given amount of specified fissile material, k^{m}_{eff}, or the minimum critical mass (MCM). Presently SMORES is limited to one-dimensional systems.

The optimization process is iterative and guided by Equal Volume Replacement Reactivity Worth (EVRRW) traverses calculated using first order perturbation theory. An EVRRW of material i with respect to reference material I is the reactivity effect of replacing a cubic centimeter of material i by the same volume of material I. Illustration of the optimization capabilities of the presently available SMORES can be found in references [1] to [5].

Several k^m_{eff} or MCM search methods can be executed by the presently available SMORES sequence. All of them are based on the change of composition of zones of a given dimension. At the outset of the optimization problem the user specifies the type of materials to be considered as constituents of each zone and their initial volume fraction. The concentration of these constituents is uniform across the zone. One or more of the constituents may have a fixed concentration in the zone and the volume fractions of the rest are the optimization design variables. The optimization process searches for that combination of the variable constituent volume fractions over all the system zones that include variable concentration constituents that will maximize k_{eff} (or minimize the critical mass for a given k_{eff}).

Recently we investigated 5 new strategies for search for optimal geometries of fixed composition zones. We refer to these strategies as the (1) "in-out" search; (2) "out-in" search; (3) "effectiveness difference" search; (4) "effectiveness gradient" search and (5) "moderator thickness" search. The purpose of this paper is to briefly describe these strategies, referred to by the general term of "geometric optimization" and to illustrate the application of the latter three; they were found the more useful new strategies.

2. GEOMETRIC OPTIMIZATION METHODS DESCRIPTION

2.1. General

The part of the system to be optimized is divided into NZ zones. These NZ zones are usually followed by a reflector region of a fixed composition and thickness. Each zone is of a fixed composition. NF ($\leq$NZ) of the zones contain fuel. The other NM = NZ – NF zones contain non fuel constituents; typically a moderating material. The question addressed is how many moderating zones should be placed in-between fuel zones and, possibly, beyond the outermost fuel zone, so as to maximize k_{eff}. Of the five optimization algorithms tried, four involve gradual interchange of fuel and moderator zones; they are described in Section 2.2. The fifth algorithm is based on optimization of the volume of the moderator in-between each two fuel zones; it is described in Section 2.3. Illustrations of the applicability of the last three algorithms, particularly of the fifth one, are presented in Section 3.

2.2. Fuel/Moderator Interchanging Algorithms

All four fuel/moderator interchanging algorithms are guided by the EVRRW pertaining to the replacement of the moderator by fuel in the zones adjacent to the fuel zones. Two EVRRW values are calculated for each fuel zone; one pertaining to the moderator zone on the inner side of the fuel zone, W_{in}, and the other pertaining to the moderator zone on the other side, W_{out}. The EVRRW values are calculated based on first-order perturbation theory [1,2]. The algorithms differ in the way the set of EVRRW values is used to guide the iterative optimization process.

1. *"In-out" search* Starting from the outermost fuel zone, the driver of the optimization process compares W_{in} and W_{out}. If $W_{in} < W_{out}$, the composition of the fuel zone and of the moderator zone on its outer side is interchanged; that is, the fuel zone is moved to the adjacent zone on the outer side. The interchange is done with the adjacent inner

moderator zone when $W_{in} > W_{out}$. This process is repeated iteratively until the relative magnitude of W_{in} and W_{out} is reversed. When this happens, the process is applied to the next fuel zone – the one having closest proximity to the previously handled. This iterative process continues until the optimal location of the innermost fuel zone is determined. Then the process is repeated all over again for an additional iteration, starting from the outermost fuel zone, until convergence.

The convergence test is done as follows: for a given iteration the value of k_{eff} of the configuration arrived at in this iteration is compared against the k_{eff} values from all previous iterations. If it is the largest, an additional iteration is undertaken. Next, it is checked whether the present configuration had already been visited in a previous iteration. If it had been, a configuration change is made guided by the second-to-the-maximum value of the weight-function (EVRRW) and the above described procedure is repeated. If no new configuration of larger k_{eff} can be found, the largest k_{eff} configuration is taken to be the optimal configuration and the iterations are terminated.

2. *“Out-in” search* This algorithm is very similar to the “in-out” algorithm except that the optimal fuel zone location search process starts from the inner-most rather than the outer-most fuel zone.

3. *“effectiveness difference” search (MAXKL option)* Rather than marching from the outermost fuel zone inward or from the innermost fuel zone outward, this option selects the order of fuel zones relocation by the magnitude of the EVRRW; the fuel zone having the largest EVRRW is treated first. There are 2*NF such EVRRW values.

4. *“effectiveness gradient” search (MAXKLG option)* This algorithm is similar to the previous one except that the order of fuel zones relocation is guided by the EVRRW gradients; that is, by the magnitude of the difference (gradient) between the EVRRW of the moderator versus fuel in the zones adjacent (right and left) to each fuel zone. There are NF such values.

2.3. Moderator Width Optimization Algorithm

This algorithm uses a moderator composition optimization process that is translated into a moderator width variation. Each moderator zone is assigned a couple of constituents: the moderating material itself and a “void” material – a material having negligible cross sections. The initial moderator material density is set to be X times the nominal density and the initial volume fraction of this material is set at 1/X, so as to preserve the initial inventory of the actual moderating material. The rest of the volume fraction, (1-1/X) is filled with the void. The code is searching for that volume fraction in each of the NM moderating zones that will maximize k_{eff}. This is a well established optimization option of SMORES [1,2,3]. After the optimal values of all the NC volume fractions are found, the width of each of the moderating zones is adjusted so that it will contain the optimal quantity of the moderating material when at nominal density, while completely eliminating the “void” material.

For one-dimensional slab geometry problem, no additional iterations are required. However, for cylindrical or spherical problems, the thickness of each of the fuel zones need be adjusted for problems requiring conservation of the fuel inventory. After adjusting the fuel zone width to conserve the fuel inventory, the moderator width optimization process is repeated. Convergence is usually achieved in few iterations.

3. ILLUSTRATIONS

3.1. Effectiveness Difference and Effectiveness Gradient Search

As an illustration of Options 3 and 4 optimization procedures consider the following problem: a slab geometry core having half thickness of 19.75 cm that is reflected by 20 cm thick water and is subjected to a reflective boundary condition on the left (system center) and vacuum boundary condition on the right. The core is divided into 0.5 cm thick zones. The innermost zone has a half width of 0.25 cm (making the effective slab width 0.5 cm). There are a total of 40 zones in the core. Each of these zones is made of either 100% volume fraction $^{239}PuO_2$ or water. The initial composition is water in all the core except in NF=3 zones arbitrarily defined to be between 6.75 to 7.25, 11.75 to 12.25 and 16.75 to 17.25 cm (zones # 15, 25 and 35) that contain $^{239}PuO_2$.

Figure 1 shows the k_{eff} evolution with iteration while Figures 2 and 3 show the corresponding evolution of the location of the 3 fuel slabs as obtained using Options 3 and 4. Both options converged to the same maximum value of k^m_{eff} = 1.5468 but Option 4 converges considerably smoother and faster – within 44 iterations versus 117 iterations of Option 3. The value of k^m_{eff} was reached in, respectively, iterations 42 and 112. The optimal fuel locations arrived at by the two options is zones 5, 12 and 20. However, a brute-force calculation of all possible permutations of the three fuel zone locations (9880 possibilities in total!) gives a slightly higher value of 1.548 for the absolutely maximum k_{eff} value. It is achieved when the fuel zones are shifted one interval to the left; i.e., they are located in zones 4, 11 and 19. It is concluded that Options 3 and 4 may be “stuck” in a local optimum, although the k_{eff} of this configuration is only slightly smaller than the absolutely maximum k_{eff} configuration. By repeating the optimization process starting with different initial conditions, it might be possible to avoid the local optimum. It is also observed that the optimal spacing between the fuel slabs is non-uniform. We’ll elaborate on this phenomenon later.

Options 3 and 4 were also applied to the optimization of a problem that is similar to that described above but having spherical rather than slab geometry. The k_{eff} evolution with iterations is illustrated in Figure 4. Both options get to the same optimal configuration in which the fuel is located in zones 22, 31 and 40. The corresponding maximum k_{eff} value is 1.2434. As in the slab problem, Option 4 gets smoother and sooner – within 19 iterations versus 45 iterations of the MAXKL option.

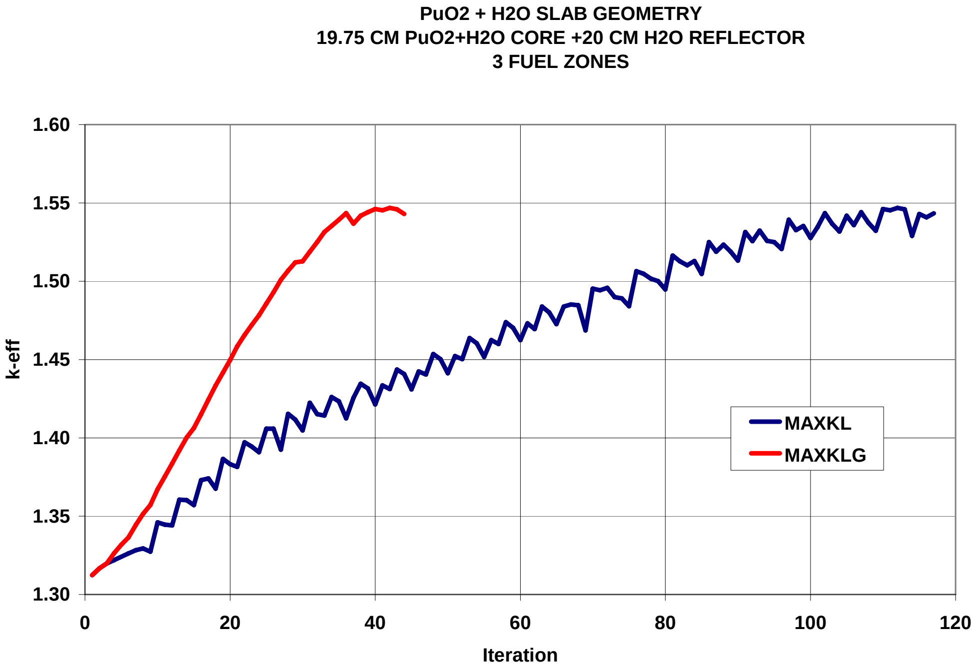

Figure 1. k_{eff} evolution in a 3-fuel slabs geometric optimization problem using Option 3 (MAXKL) and Option 4 (MAXKLG)

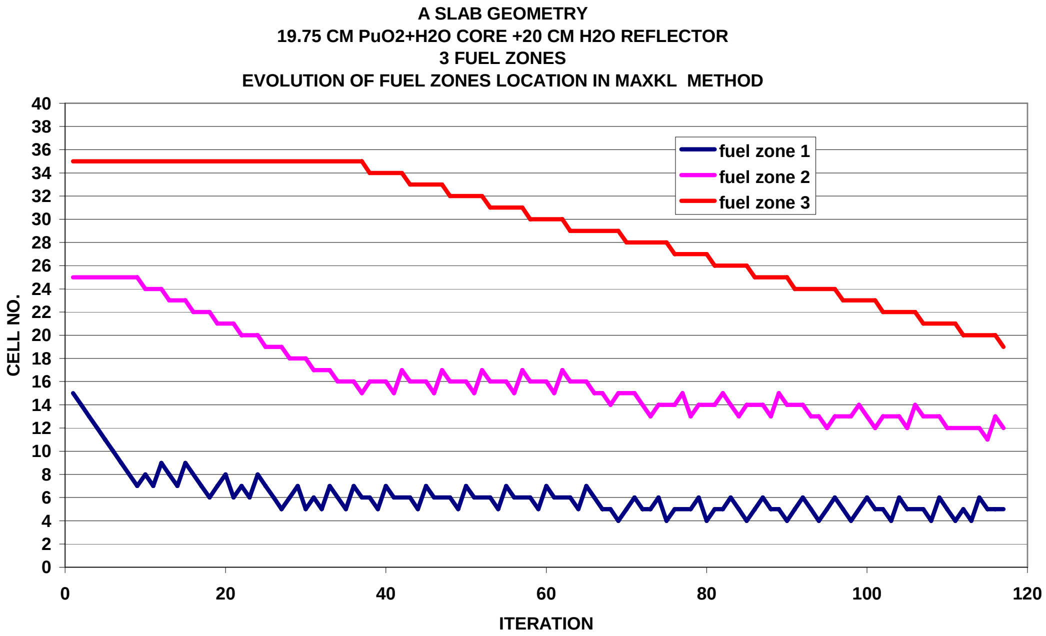

Figure 2. Evolution of location of fuel zones with iteration using MAXKL option

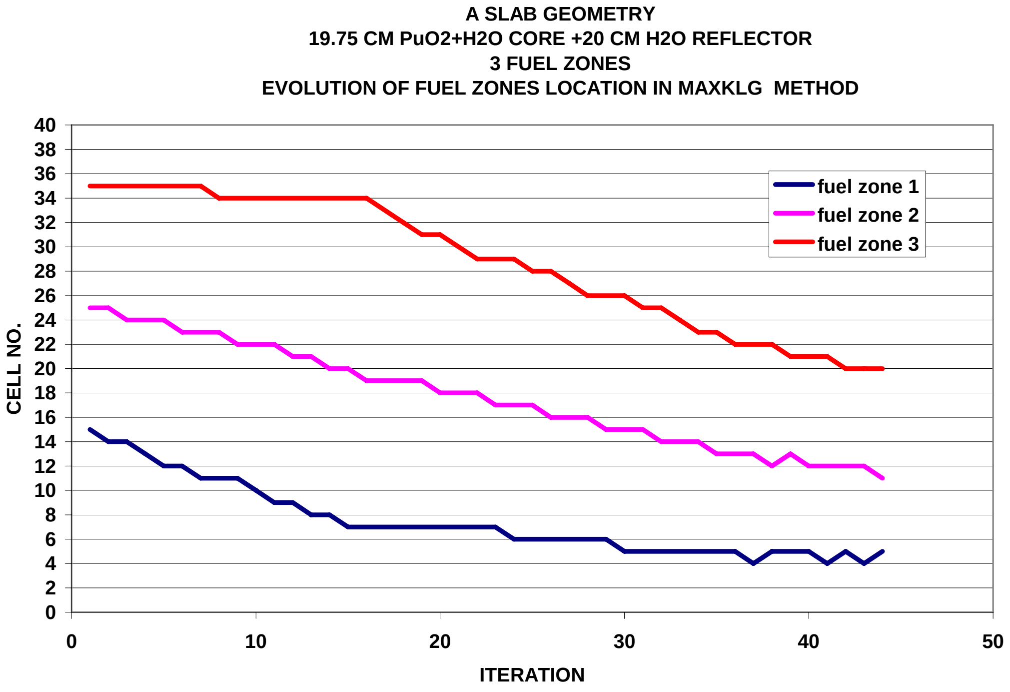

Figure 3. Evolution of location of fuel zones with iteration using MAXKLG option

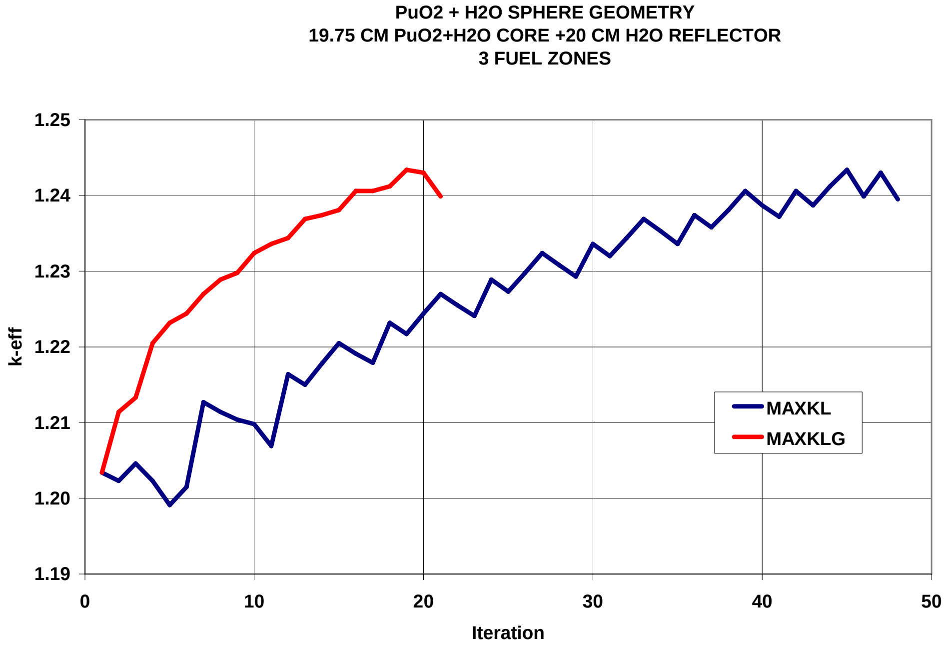

Figure 4. k_{eff} evolution in a 3-fuel slabs geometric optimization problem using Option 3 (MAXKL) and Option 4 (MAXKLG)

3.2. Moderator Width Optimization Search

3.2.1. Section 3.1 problem

Applying the moderator width optimization algorithm to the first (slab) illustration addressed in Section 3.1 resulted in a maximum k_{eff} of 1.54948; even higher than in the brute-force approach. Table I compares the optimal results obtained with the different approaches. It is observed that the moderator width optimization places the first two fuel slabs in-between the optimal locations identified by the other two methods, while the third slab location is close to that set by Options 3 and 4. Figure 5 compares the k_{eff} evolution of the three methods; the moderator width optimization convergences significantly faster.

Table I. Comparison of Optimal Systems Arrived at Using Different Search Approaches

Parameter	**Option 3 or 4 optimization**	**Brute-force search**	**Moderator-width optimization**
k_{eff}	1.5468	1.5488	1.5495
Location of fuel slab #			
1	1.75 - 2.25	1.25 - 1.75	1.556 - 2.056
2	5.25 - 5.75	4.75 - 5.25	5.079 - 5.579
3	9.25 - 9.75	8.75 - 9.25	9.257 - 9.757

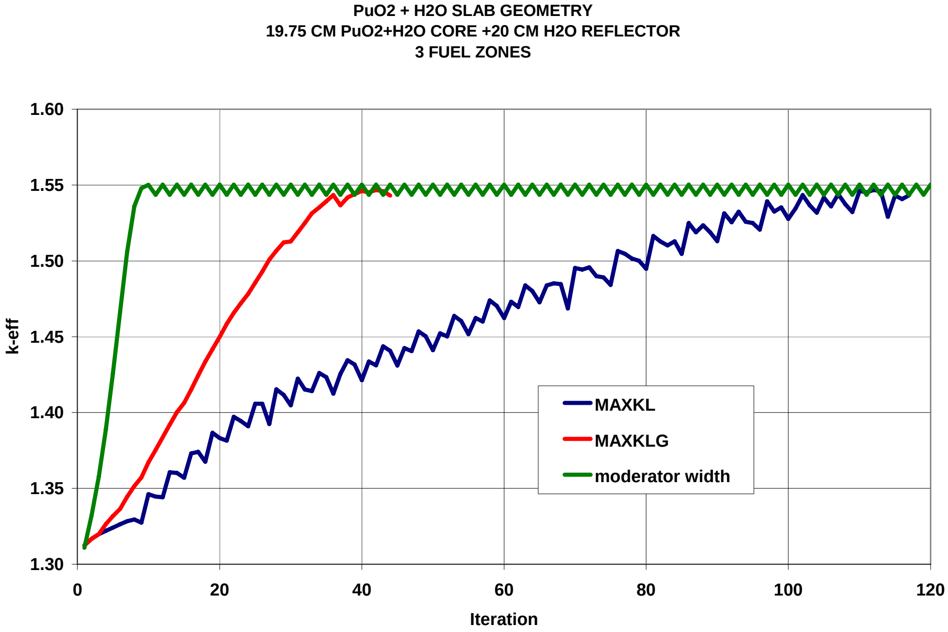

Figure 5. k_{eff} evolution in a 3-fuel slabs geometric optimization problem using Option 3 (MAXKL) and Option 4 (MAXKLG)

3.2.2 Water moderator and water reflector

As another illustration of the moderator-width optimization algorithm developed for SMORES, consider the following simplified one-dimensional slab problem: Find the location of 13 fuel slabs in water that will give the maximum k_{eff}, when the system is reflected by 20 cm water. The fuel is 5% enriched uranium dioxide that is 0.8 cm thick and has 0.1 cm aluminum clad. The optimization variables are the optimal distance between the given composition and dimension fuel slabs. The convergence criterion on the water density was set at 1%.

The convergence of this option was significantly faster than that of the Effectiveness Difference and Effectiveness Gradient search algorithms illustrated in Section 3.1. The optimal distance between the fuel slabs was found to gradually increase from 2.05 cm near the center up to 3.20 cm between the outermost two fuel slabs as follows: 2.05, 2.06, 2.15, 2.28, 2.50 and 3.20 cm. The corresponding k^{m}_{eff} is 1.3894. For comparison, when imposing a requirement for equal distance between all the fuel slabs, the optimal distance is 2.20 cm and the corresponding k_{eff} is 1.3855. The optimal distance between identical fuel slabs in an infinite lattice is 1.46 cm and the corresponding k_∞ is 1.5742.

Comparing the neutron balance between the two finite cases it was found that the leakage probability from the system having optimal non-uniform spacing is smaller – 9.89% versus 10.95% from the uniform spacing system. This difference is partially compensated by enhanced parasitic neutron capture in the water of the non-uniform spacing system – 11.16% versus 10.18%. The net effect is a 0.08% gain in k_{eff}.

3.2.3. Water moderator and graphite reflector

Consider the problem of Section 3.2.2 but with graphite replacing water as the reflector. Table II compares the optimal water moderator width and corresponding k_{eff} for water and graphite reflectors of different thickness.

Table II. Sensitivity of Water Moderator Width Distribution on Reflector Type and Thickness

Reflector		**k_{eff}**	**Water moderator width (cm)**					
Type	**Thickness(cm)**		**1st**	**2nd**	**3rd**	**4th**	**5th**	**6th**
H_2O	1	1.3580	2.15	2.19	2.29	2.51	3.03	5.85
H_2O	5	1.3801	2.07	2.10	2.18	2.33	2.64	3.57
H_2O	20	1.3894	2.05	2.06	2.15	2.28	2.50	3.20
C	25	1.4778	1.76	1.76	1.77	1.79	1.83	1.93
C	50	1.5168	1.65	1.65	1.65	1.66	1.68	1.71
C	100	1.5323	1.60	1.60	1.60	1.60	1.61	1.62

It is observed that the optimal spacing between fuel slabs is generally smaller, and of a smaller spread, when using a graphite reflector. For very thick graphite reflector (100 cm) the spacing is almost uniform; significantly more uniform than for an effectively “infinite” (20 cm) water reflector. This is due to the fact that a smaller fraction of the neutrons that leak into the reflector get lost when using the thick graphite reflector. Thus, the optimal spacing between the fuel slabs is close to the spacing in an infinite lattice (1.46 cm). As the graphite reflector becomes thinner and, therefore, leakier, the spacing between the fuel slabs increases as does the difference in spacing between the outermost and the innermost two fuel slabs (1.93 cm versus 1.76 cm for 25 cm thick graphite reflector). This effect is more pronounced in case of a thin water reflector.

Table III illustrates the sensitivity of the fuel slab spacing to the number of fuel slabs in the system. The last entry in each raw denotes the optimal water layer thickness between the outer fuel slab and the graphite reflector. The general trend is increasing spacing with reduction in the number of fuel slabs and with reduction in reflector thickness. For small reflector thickness some water is called for in-between the outermost fuel slab and the graphite reflector. This water helps in slowing down the fast neutrons.

Table III. Sensitivity of Fuel Slab Spacing on Number of Fuel Slabs in Graphite Reflected Water-Moderated Systems

Number fuel slabs	Reflector thickness (cm)	Water moderator width (cm)						
		1st	2nd	3rd	4th	5th	6th	7th
3	**25**	2.50	0.55					
5	**25**	2.18	2.20	0.37				
9	**25**	1.90	1.91	1.94	1.96	0.19		
13	**25**	1.76	1.76	1.77	1.79	1.83	1.93	0.08
3	**100**	1.99	0.00					
5	**100**	1.77	1.77	0.00				
9	**100**	1.65	1.65	1.68	1.68	0.00		
13	**100**	1.60	1.60	1.60	1.60	1.61	1.62	0.00

3.2.4. Graphite moderator and water reflector

This illustration is done for a problem similar to that defined in Section 3.2.3 but interchanging the role of water and graphite – the graphite is used as the moderator and the water as the reflector. The reflector is 20 cm thick water. The number and composition of fuel slabs are the same. The fuel slabs were initially spaced 10 cm apart.

Figure 6 shows k_{eff} evolution with number of iterations while Figure 5 shows the evolution of the graphite zone widths. The maximum k_{eff} value of 1.62471 was arrived at in iteration number 202. The corresponding optimal spacings are, going from the center of the system outward, 30.23, 31.06, 31.36, 32.30, 34.92 and 103.36 cm. As in the case with water moderator and reflector considered In Section 3.2.2, the moderator width keeps increasing as the reflector region is approached. But the increase in the outermost moderator zone thickness, that is, of the spacing between the outermost fuel slabs is by far more pronounced when graphite is used for the moderator. This is due to the fact that the fission neutrons “age” is significantly larger in graphite while the graphite macroscopic absorption cross section for thermal neutrons is significantly smaller than that of water. By displacing the outermost fuel plate outwardly and adding graphite moderator, the core becomes effectively of a larger dimensions and the neutron leakage probability is reduced more than the parasitic capture in graphite increases. The slow convergence of the outer graphite moderator thickness, as evidenced from the insert to Figure 6 and from Figure 7, is due to the relatively low sensitivity of k_{eff} to this variable, when the value of this variable is close to the optimum.

If the spacing between the same number of identical fuel slabs is to be constant, the optimal graphite width is found to be 32.6 cm and the resulting k_{eff} is 1.6191. The optimal infinite uniform lattice is 30.2 cm and the maximum k_∞ is 1.6488.

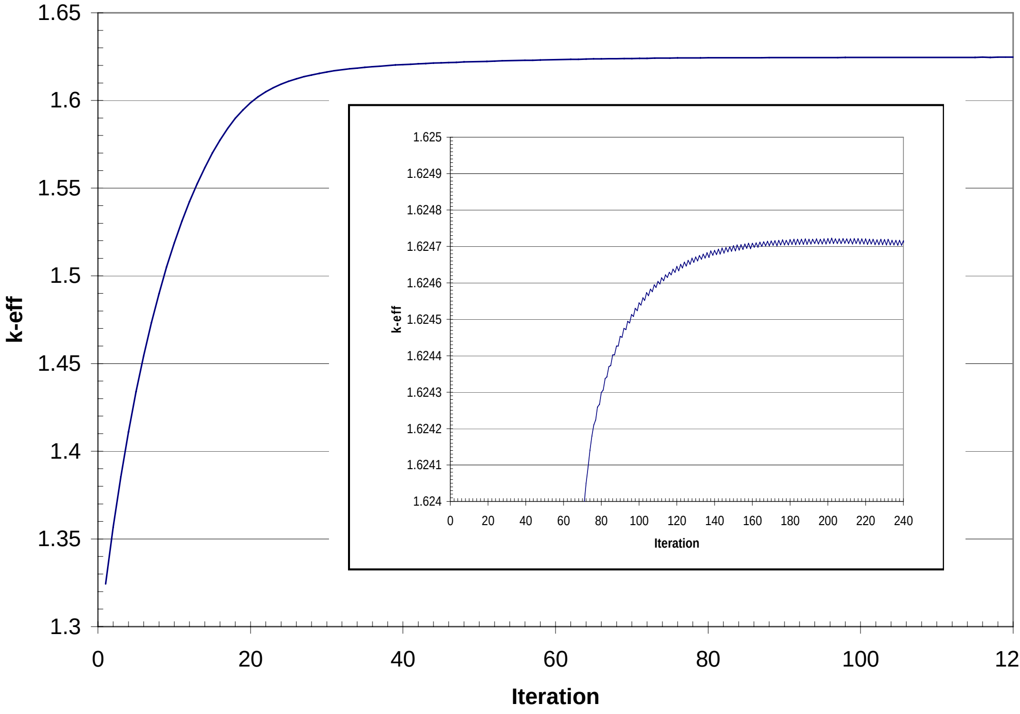

Figure 6. k_{eff} evolution with number of iteration for the graphite-moderated, water-reflected illustration

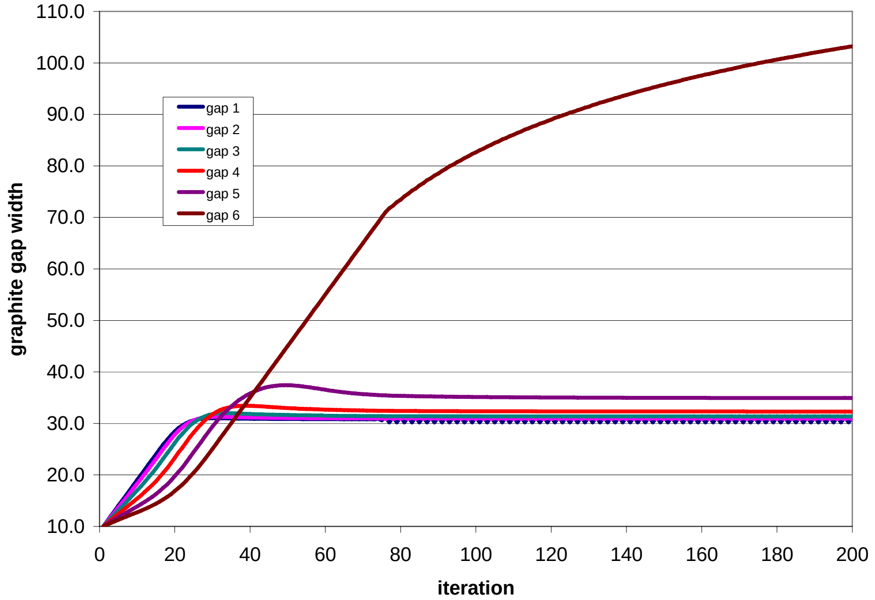

Figure 7. Graphite moderator zone-width evolution with number of iteration for the graphite-moderated, water-reflected illustration

3.2.4. Water moderated and reflected cylindrical system

Consider a one-dimensional cylindrical system having four fuel elements made of 5% enriched UO_2 and clad by zirconium. A 0.5 cm in radius fuel rod clad with 0.05cm thick zirconium is located at the system center. The other three fuel elements are in the form of cylindrical shells the volume of which correspond to the volumes of which are, respectively, 6, 12 and 18 times of the central fuel rod volume. Each of these fuel annuli is wrapped by a Zr clad that is of equal thickness on the inside and outside. The clad-to-fuel volume ratio in each annulus is as of the central fuel rod. A 1cm wide shell containing uniformly “mixed” water and vacuum is introduced between adjacent fuel elements. The water is taken to have 10 times its nominal density but occupies only 0.1 of the zone volume fraction. There is a 20 cm thick water reflector beyond the outermost fuel element. Vacuum boundary conditions are applied at the reflector outer boundary.

The search for optimal moderator width is done using SCALE 4.0. Figure 8 shows the moderator width evolution with outer iterations. After a given outer iteration, within which the search is for the optimal water volume fraction of fixed width zones, the width of all the zones, including the fuel and clad zones, are adjusted so as to conserve the optimal amount of moderator arrived at and the nominal mass of fuel and clad. As in the case of slab problems, the moderator width increases towards the reflector. The value of k_{eff} increased from 0.537 for the initial system to 0.732 for the optimal system.

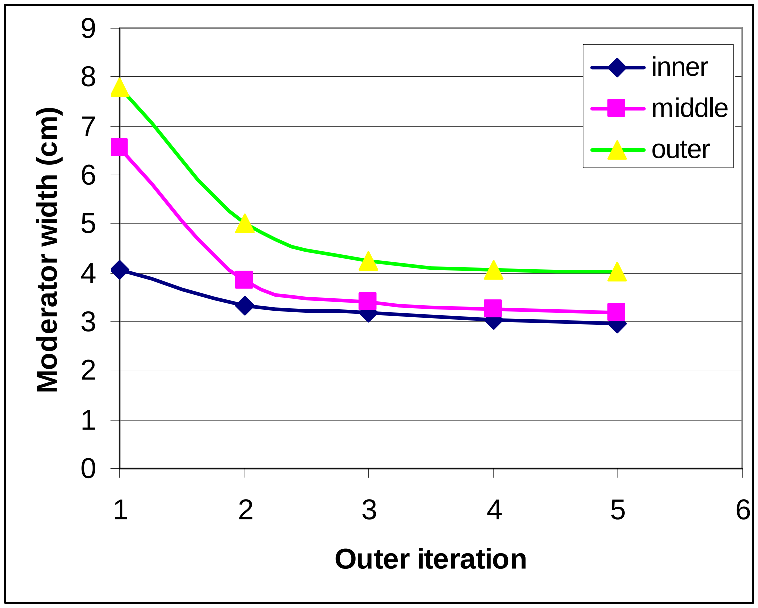

Figure 8. Water moderator zone-width evolution for the water moderated and reflected cylindrical problem

4. DISCUSSION

The new Geometric Optimization capability developed for SMORES could be of help to the criticality safety community. By applying this new capability to find the maximum k_{eff} value a given number of fuel elements of a given composition can provide when in combination with a given moderating and reflecting materials, one can set a limit on the maximum number of fuel elements one can safely handle, while imposing the minimum practical safety margin. Using a brute-force trial-and-error kind approach to search for the optimal spacing between the fuel elements can be a very time consuming effort and may not be practical when the numbers of fuel elements to be handled is large.

Presently the new optimization capability is restricted to one-dimensional systems. However, the methodology developed can be applied to two-dimensional and three-dimensional systems. The Moderator Width (actually density) approach to optimization appears to be the most practical to implement for multi-dimensional system optimization.

5. CONCLUSIONS

New maximum k_{eff} search options for systems having a given number of fixed composition fuel elements were successfully developed for SMORES. They are useful for identifying that distance between the fuel elements that will result in maximum k_{eff}. The most effective option is based on the moderator width search. Relative to the other Geometric Optimization algorithms developed in this work it converges faster, is not stuck in local maxima, and is not restricted to placing the fuel zones within user defined zone boundaries. However, it is not convenient to apply to systems of fixed outer dimensions.

The maximum k_{eff} thermal systems made of a given number of fixed composition fuel elements, a moderator and reflector features a non-uniform spacing of the fuel elements – the optimal spacing tends to increase from the center towards the reflector. The spacing non-uniformity increases k_{eff} by, primarily, reducing the neutron leakage probability.

The spacing non-uniformity depends on the combination of moderator and reflector materials, on the number of fuel elements in the system and on the reflector thickness. The general trend is increasing spacing width with reduction in the number of fuel slabs and with reduction in reflector thickness. Particularly large can be the spacing of the outermost to the next-to-outermost fuel elements when using very low absorbing moderator, such as graphite, heavy-water and beryllium, along with a relatively strong absorbing reflector such as water. When using a thick low absorbing reflector, such as graphite, the spacing of the fuel elements is nearly uniform and only slightly larger than the optimal spacing in an infinite lattice. Otherwise the optimal spacing can be significantly larger than the optimal infinite lattice spacing. Some of these conclusions are illustrated in Figure 9.

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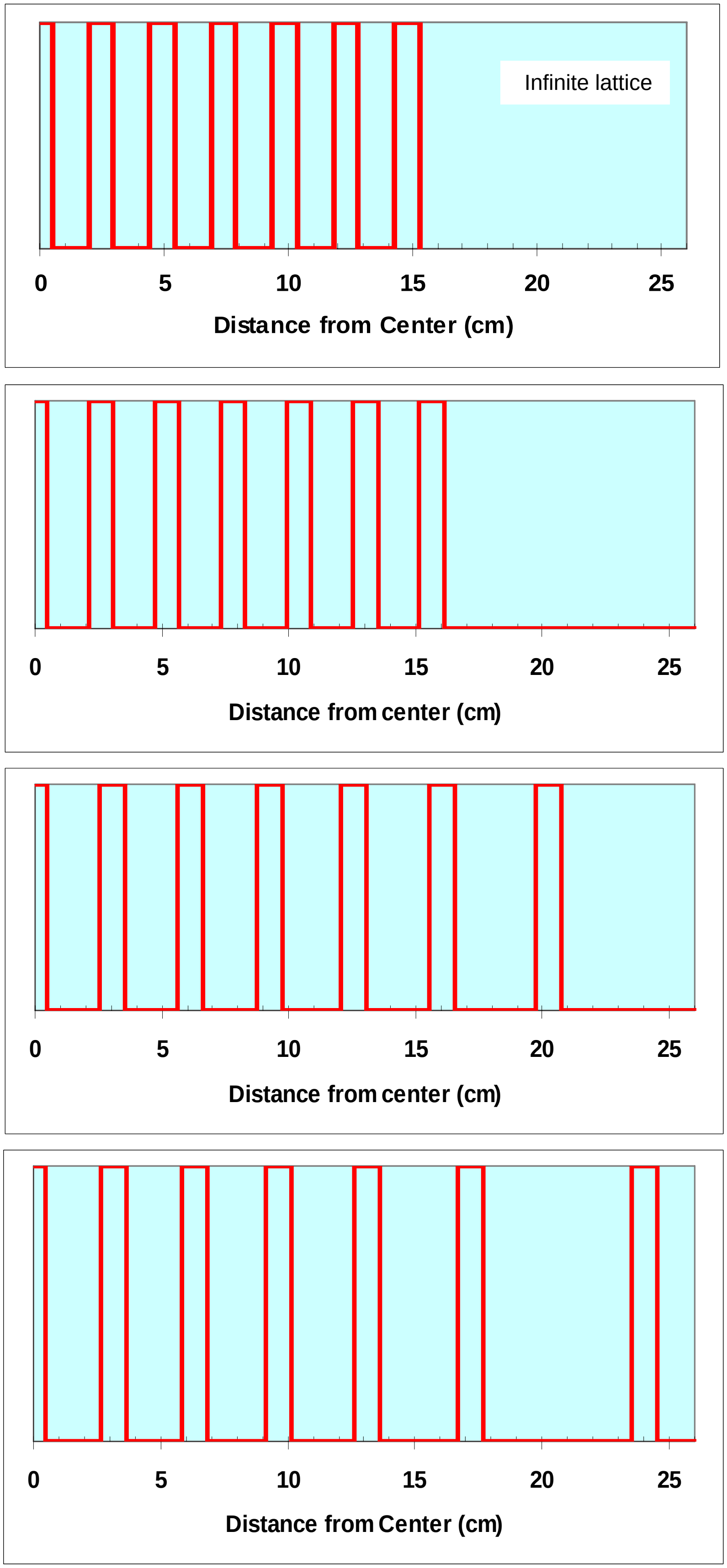

Mod	Reflector		k
Type	type	thickness	,
H_2O	None	N/A	1.5742
H_2O	C	100	1.5323
H_2O	H_2O	20	1.3894
H_2O	H_2O	1	1.3580

Figure 9. Comparison of optimal water moderated slab systems having 13 fuel elements