SEMI-AUTOMATED SEARCH FOR MAXIMUM K_{eff} OF MULTI-CONSTITUENT SYSTEMS

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ABSTRACT

New maximum k_{eff} search options have been developed for SMORES – a prototypic analysis sequence recently developed for incorporation in the SCALE-5 code package. SMORES provides for an intelligent, semi-automatic search for the maximum k_{eff} of a given amount of specified fissile materials in combination with specified moderating/reflecting materials. SMORES will also search for the minimum critical mass. The new options developed are set to handle multi fuel and multi moderator/reflector constituents. The newly developed algorithms are illustrated for three types of problems, all involving search for the maximum possible k_{eff}. In two of the problems the mass of each of the two fissile materials is fixed. In another problem the total volume fraction of the two fissile materials is fixed. SMORES can be useful for determining margins of subcriticality and for other criticality safety applications.

1. INTRODUCTION

A new prototypic analysis sequence, referred to as SMORES (Standardized Computer Analyses for Licensing Evaluation), was recently developed for incorporation into the SCALE-5 code package[1]. SMORES provides for an intelligent, semi-automatic search for either the maximum k_{eff} of a given amount of specified fissile material, or the minimum critical mass. It is described in detail in Ref. [2] and [3]. SMORES can be used to determine margins of subcriticality by identifying the maximum value of the effective multiplication factor, k^m_{eff}, that can result from a given mass of a given fissile material when in combination with specified moderating and reflecting materials. The identification of k^m_{eff} is accomplished semi-automatically, using the optimization strategy of the SWAN code [4,5].

The present version of SMORES can address problems that have only one fissile constituent. The purpose of the present paper is to describe new maximum k_{eff} search algorithms developed for SMORES that can handle problems featuring two or more fissile materials along with one or more non-fissile material.

The theoretical foundation for the search for the optimal system composition, i.e., that system composition that yields maximum k_{eff} is described in references [2], [4] and [5]. In Sec. 2 we very briefly summarize the principles of this methodology. The structure of SMORES and optimization procedure are described in Sec. 3. Illustrations of the new multi-material optimization process are presented in Sections 4, 5 and 6. In Sec. 7 we discuss the status of SMORES and plans for its upgrade.

2. METHODOLOGY

2.1 REACTIVITY WORTH

The reactivity worth associated with the addition of a unit volume of material i into zone z, denoted as $E_i(z)$, is calculated by SMORES using the following expressions derived from first order perturbation theory[2, 5,6]:

$$E_i(z) = [-AC_i(z) + BC_i(z) + FC_i(z)/k_{eff}]/ NI \tag{1}$$

where

$$AC_i(z) = \int_z d\underline{r} \int dE \int d\underline{\Omega} [\Phi^+(\underline{r},E,\underline{\Omega}) \Sigma_{t,i}(E) \Phi(\underline{r},E,\underline{\Omega})], \tag{2}$$

$$BC_i(z) = \int_z d\underline{r} \int dE \int d\underline{\Omega} \int dE' \int d\underline{\Omega}' [\Phi^+(\underline{r},E',\underline{\Omega}') \Sigma_{s,i}(E \rightarrow E'; \Omega \rightarrow \underline{\Omega}') \Phi(\underline{r},E,\underline{\Omega})], \tag{3}$$

$$FC_i(z) = \int_z d\underline{r} \int dE' [\chi_i(E') \Phi^+(\underline{r},E')] \int dE [\nu_i \Sigma_{f,i}(E) \Phi(\underline{r},E)], \tag{4}$$

where $\int_z d\underline{r}$ denotes integration over the volume of zone z,

$$NI = \sum_i \int d\underline{r} \int dE' \chi_i(E') \Phi^+(\underline{r},E') \int dE\, \nu_i \Sigma_{f,i}(E) \Phi(\underline{r},E)]/ k_{eff}, \tag{5}$$

$$\Phi(\underline{r},E) = \int d\underline{\Omega}\ \Phi(\underline{r},E,\underline{\Omega}), \text{ and} \tag{6}$$

$$\Phi^+(\underline{r},E) = \int d\underline{\Omega}\ \Phi^+(\underline{r},E,\underline{\Omega})/4\pi. \tag{7}$$

In the above, $\Phi(\underline{r},E)$ is the scalar neutron flux and $\Phi^+(\underline{r},E)$ is the scalar adjoint or importance function. The fluxes and adjoint function to be used for calculating $E_i(z)$ are the solution of the k-eigenvalue form of the transport equation. The solution of these equations also yields the value of the eigenvalue k_{eff}. The spatial integral in Eq. (5) is carried over the entire system volume.

Usually the addition of a unit volume of a given constituent can take place only by removing from the system an equal volume of another "reference" constituent denoted by R. To account for this volume conservation condition we use the "equal volume replacement reactivity worth" (EVRRW) of material i in zone z, to be denoted as $\rho_{i,R}(z)$,

$$\rho_{i,R}(z) = - E_R(z) + E_i(z). \tag{8}$$

The EVRRW data provides the following information on the status of the system:

- How close the present system composition is to the optimal composition.
- Variation of the concentration of which system constituent would be most effective for increasing k_{eff}.
- What is the most effective way to vary the space dependent concentration of the most promising constituents.

2.2 OPTIMALITY CONDITION

The criterion for the optimum system is the uniformity, across the total number of zones (Z) that participate in the optimization, of the EVRRW $\rho_{i,R}(z)$ of constituent i. Specifically,

$$\rho_{i,R}(z) \quad \begin{cases} < \text{constant, for} \quad \psi_i(z) = {}^{\min}\psi_i(z) \\ = \text{constant, for } {}^{\min}\psi_i(z) \le \psi_i(z) \le {}^{\max}\psi_i(z) \\ > \text{constant, for} \quad \psi_i(z) = {}^{\max}\psi_i(z) \end{cases} \tag{9}$$

where $\psi_i(z)$ is the volume fraction of constituent i in zone z; ${}^{\min}\psi_i(z)$ is the minimum permissible volume fraction (usually 0) and ${}^{\max}\psi_i(z)$ is the maximum permissible volume fraction. This condition implies that, at the optimum, any permissible infinitesimal change in the concentration of the variable constituents should leave the system k_{eff} unchanged, provided that

$$0 \le {}^{\min}\psi_i(z) \le \psi_i(z) \le {}^{\max}\psi_i(z) \le 1.0. \tag{10}$$

Material conservation requires that

$$\sum_i \psi_i(z) = \text{constant} \le 1.0 \tag{11}$$

where the summation is over all the I constituents of variable concentration. If the summation is smaller than unity, (1.0 – constant) fraction of the volume of zone z is allocated for materials of fixed concentration. Examples for such materials are structural or coolant materials.

The volume fraction is used as a measure of concentration since SMORES is set to work with the macroscopic cross sections of the system constituents.

2.3 VARIATION OF COMPOSITION

The variation in the volume fraction of the i^{th} material in the n^{th} iteration is calculated from the expression:

$$dy_i^n(z) \equiv y_i^n(z) - y_i^{n-1}(z) = A_i^n \, Q_{e,i}^{n-1}(z) + B_i^n \, Q_{c,i}^{n-1}(z), \tag{12}$$

where the $Q_{x,i}(z)$ variables are the "effectiveness functions"; $Q_{e,i}(z)$ is $\rho_{i,R}(z)$ and $Q_{c,i}(z)$ is the mass of material i in zone z. For materials with no mass constraint the B_i coefficient is zero and there is no need to specify $Q_{c,i}$. A_i and B_i are coefficients that determine the amplitude of the volume fraction variation per iteration.

There are four major steps in the determination of the new density distribution: Determination of the A_i coefficients, determination of the B_i coefficients, the calculation of the new density distributions [Eq. (12)], and readjustment of the new density distributions if they have overflowed the specified density limits. For problems subjected to a constraint, as do most of the problems considered here, the value of the B_I coefficients are uniquely determined so as to satisfy the constraint condition. With this condition imposed, Eq. (12) can be worked out[2,6] into the following expression:

$$dy_i^n(z) = A_i^n \left[Q_{e,i}^{n-1}(z) - \frac{\int d\underline{r}\, Q_{c,i}^{n-1}(z)\, Q_{e,i}^{n-1}(z)}{\int d\underline{r}\, [Q_{c,i}^{n-1}(z)]^2} Q_{c,i}^{n-1}(z) \right]. \tag{13}$$

The A_i^n coefficients are calculated as follows:

$$A_i^n = a_i^n \Big/ \left[Q_{e,i}^{n-1}(z_m) - \frac{\int d\underline{r}\, Q_{c,i}^{n-1}(z)\, Q_{e,i}^{n-1}(z)}{\int d\underline{r}\, [Q_{c,i}^{n-1}(z)]^2} Q_{c,i}^{n-1}(z_m) \right], \qquad (14)$$

where z_m denotes the zone in which the volume fraction change will be the maximum (in absolute value) and a_i^n are input data.

3. SMORES STRUCTURE AND OPTIMIZATION PROCEDURE

The SMORES sequence consists of the following modules: BONAMI-S, NITAWL-III, CENTRM, PMC, ICE, XSDRNPM-S and SWIF.

Before starting the optimization process, a reference system is defined. This includes the core dimension and composition and reflector thickness and composition. The optimization process is iterative. SMORES calculates the EVRRW for all of the constituents and uses them to guide an automated redistribution of the system constituents so as to increase k_{eff} while keeping the imposed constraints and restraints. Then SMORES recalculates the flux, importance function and EVRRWs and does another iteration on the zone-wise distribution of the constituents. The sequence of iterations is terminated when either the optimization convergence criterion is met, or the maximum number of iterations specified by the user is reached.

The general sequence of steps for each iteration is as follows:

- Define the reference system composition, geometry and zones.
- Calculate self-shielded cross sections for each of the constituents in each of the zones. This is done using BONAMI-S and NITAWL-III or BONAMI-S, CENTRM and PMC. BONAMI performs resonance self-shielding calculations for materials having Bondarenko data, while NITAWL-III applies the Nordheim resonance self-shielding correction to materials having resonance parameters. CENTRM/PMC calculates fluxes using point-wise cross sections and generates flux-weighted multi-group cross sections.
- Use the functional module ICE to create from the self-shielded cross sections a macroscopic cross section library of the material mixtures considered as the zone constituents or candidate constituents.
- Using above cross-sections, use XSDRNPM-S to solve the forward and adjoint neutron transport equations of the system. This module performs the 1-D criticality calculation that provides the flux and importance function distributions across the system, as well as k_{eff} .
- Using the resulting fluxes, importance function, k_{eff} and self-shielded cross sections, use the SWIF functional module to calculate the user specified effectiveness functions. If the user requested effectiveness functions only, the sequence terminates. Otherwise, SWIF continues with the last step.
- Using the EVRRWs, SWIF calculates a zone-wise modified system composition and a new iteration starts.

4. ILLUSTRATION # 1 – CONSERVE MASS OF EACH FUEL CONSTITUENT

The system is spherical and consists of two fissile materials, $^{239}PuO_2$ and $^{241}PuO_2$, and water for the moderating and reflecting material. The inventory of each of the PuO_2 constituents is 297.622 gram and is to be kept fixed. Initially the two PuO_2 constituents are distributed uniformly over a 20 cm

radius core. Their volume fraction is 0.00075 each; water makes up the remainder 0.9985 fraction of the core volume. The core is surrounded by a 30 cm thick water reflector. The question is what is the maximum k_{eff} one can get by redistributing the given inventories of the system constituents and what is the corresponding optimal composition, i.e., the composition corresponding to the maximum k_{eff}. For the purpose of the optimization the system is divided into 2.5 cm thick zones (spherical shells); the material composition within each zone is assumed constant.

Figure 1 shows k_{eff} evolution with the number of SMORES iterations. It is seen that after 10 iterations k_{eff} got close to its maximum value but it took additional ~40 iterations to approach it asymptotic value. Figure 2 gives the optimal distribution of the two PuO_2 constituents. The volume fraction not taken by PuO_2 is taken by water. This composition gives the maximal k_{eff}. The peak k_{eff} is achieved when the ^{241}Pu is concentrated in the inner part of the core, peaking at the center, and when the ^{239}Pu is located in the core periphery. The evolution of ^{241}Pu towards its optimal distribution is illustrated in Figure 3. The total inventory of each of the fuel constituents is kept throughout the optimization process in the range between 297.621 grams and 297.622 grams.

Figure 4 shows the EVRRW of $^{241}PuO_2$ versus water for three selected iterations. Initially (iteration number 1), this reactivity worth (RW) is positive throughout the core and is larger the closer the zone is to the core center. This indicates that k_{eff} is expected to increase by transferring $^{241}PuO_2$ from the core periphery to the core center (conserving the $^{241}PuO_2$ inventory). This is, indeed, what SMORES is doing, as seen in Figure 3. Consider, next, the RW corresponding to iteration number 69. It is somewhat lower for the three outer zones. This suggests that we should keep transferring $^{241}PuO_2$ from the outer three zones to inner zones. However, at this point in the iteration process there is no more $^{241}PuO_2$ left in the outer three zones. In the inner zones where $^{241}PuO_2$ exists, the RW is pretty flat implying that we have an optimal or close to optimal concentration distribution. That this indeed is the case can also be inferred by comparing the RW in the inner three zones after iteration 70 with that after iteration 69; the RW goes down from above its value in zone 4 to below its value in zone 4. In iteration 80 (not shown in Fig. 4) the RW of zones 1 to 3 go up again above the RW of zone 4. This fluctuation is one of the indicators that the system is near its optimal composition. The amplitude of the fluctuations can be reduced and the problem may converge slightly better by reducing the amplitude of composition variation per iteration (An input specification option). Figure 5 tells a similar story for $^{239}PuO_2$. This fuel is concentrated in the outermost 3 zones of the core where the RWs are flat.

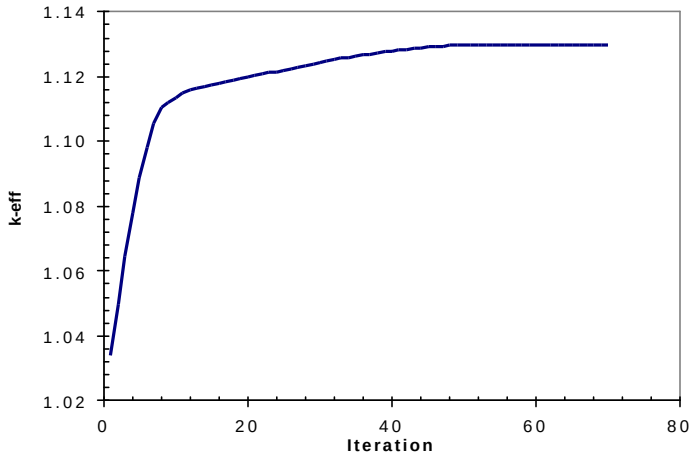

Fig. 1 k_{eff} evolution with number of iterations. Illustration # 1

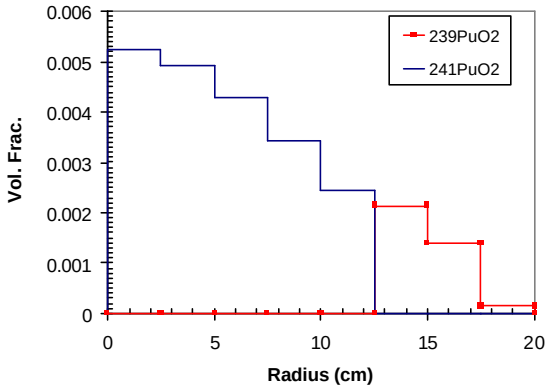

Fig. 2 Optimal distribution of $^{239}PuO_2$ and $^{241}PuO_2$ in Illustration # 1

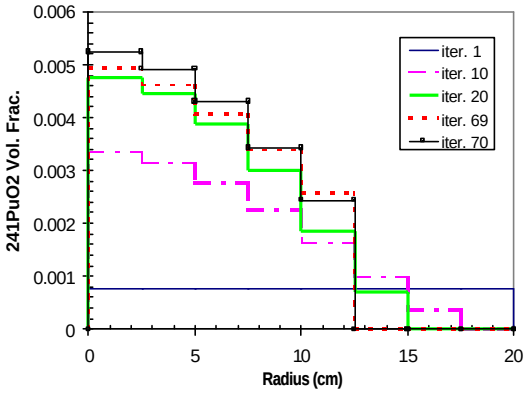

Fig. 3 Evolution of $^{241}PuO_2$ distribution to optimal. Illustration # 1

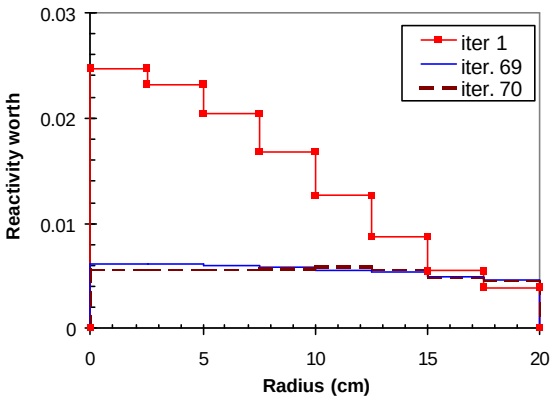

Fig. 4 Reactivity worth of $^{241}PuO_2$ versus H_2O for illustration #. 1

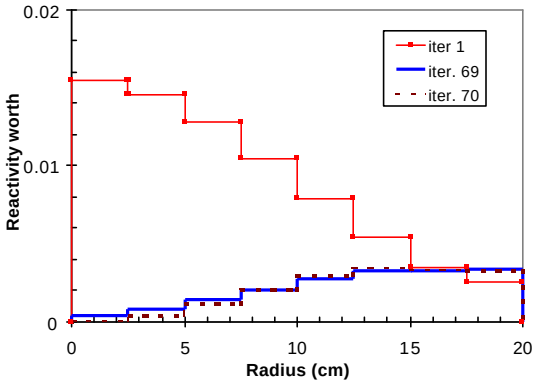

Fig. 5 Reactivity worth of $^{239}PuO_2$ versus H_2O for illustration # 1

5. ILLUSTRATION # 2 – CONSERVE TOTAL FUEL VOLUME

This illustration is similar to the previous one except that what is conserved is the total volume of the fissile materials and that $^{241}PuO_2$ is replaced by $^{233}UO_2$. Initially the $^{241}PuO_2$ and $^{233}UO_2$ each occupies 0.075% of the core volume. Their densities are assumed to be, respectively, 11.46 g/cm^3 and 10.75 g/cm^3. Figure 6 shows the evolution of k_{eff} from its initial value of 0.880 to its maximum value of 1.0328. Figure 7 shows the corresponding evolution of the total mass of each of the fuel constituents while figures 8 and 9 show the evolution of the space-dependent concentration of these fuel constituents. The optimal system has $^{239}PuO_2$ in the outer six zones only and $^{233}UO_2$ in the inner two zones only. The $^{239}PuO_2$ mass increased from 298 grams to 543 grams while the $^{233}UO_2$ mass was correspondingly reduced from 270 grams to 48.9 grams. The total fuel volume was conserved.

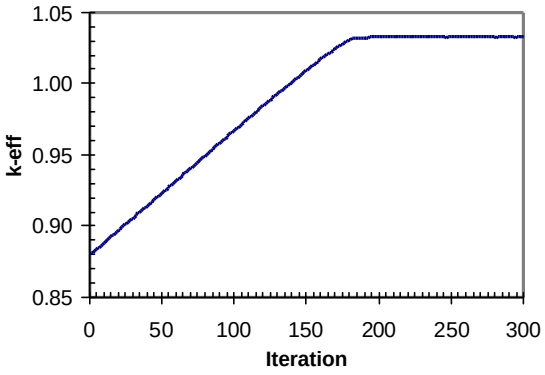

Fig. 6 Evolution of k_{eff}. Illustration # 2

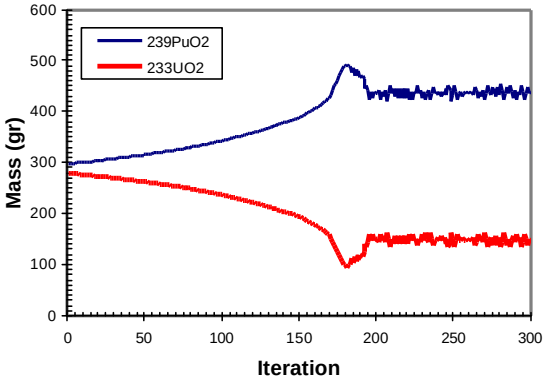

Fig. 7 Evolution of $^{239}PuO_2$ and ^{233}U mass. Illustration # 2

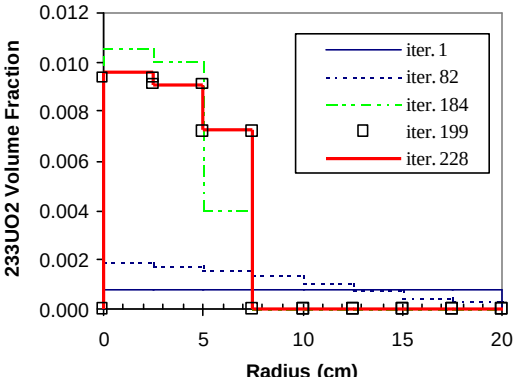

Fig. 8 Evolution of $^{233}UO_2$ distribution to optimal. Illustration # 2

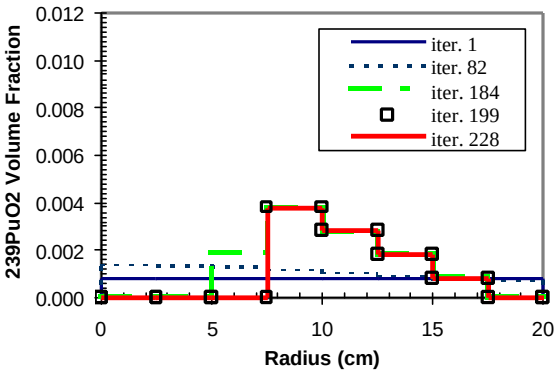

Fig. 9 Evolution of $^{239}PuO_2$ distribution to optimal. Illustration # 2

6. ILLUSTRATION # 3 – FOUR MATERIALS OF VARIABLE CONCENTRATION

This illustration is similar to Illustration # 1 except that there are two moderating – reflecting materials in addition to two fuel materials. The two fissile materials are 60% (by volume) $^{239}PuO_2$ + 40% $^{241}PuO_2$ and $^{233}UO_2$. The moderating/reflecting materials are polyethylene (Poly) and beryllium. The inventory of each of the two fuel constituents is to be kept constant. The inventory of Poly and Be can vary. Initially the 20 cm radius core has a uniform composition made of 0.075 volume % PuO_2 (297.622 g), 0.075% UO_2 (279.183 g), 19.85% Be (6138.06 g) and 80% Poly; it is surrounded by an effectively infinite water reflector. Four materials can vary their concentration within the 20 cm radius sphere: the 2 fuels, Be and Poly.

Figure 10 illustrates the k_{eff} evolution with iteration number while Figures 11 and 12 give the optimal system composition corresponding to iteration number 300. Also shown in the last two figures the composition corresponding to iteration number 141; it is seen to be very close to that of iteration 300. This is also implied from Figure 10 that shows that k_{eff} actually reached its peak value at about iteration 141. It is observed that the UO_2 is concentrated in the innermost four 2.5cm zones whereas the PuO_2 is concentrated in the next two zones; there is no fuel beyond 15 cm. Poly is the preferred moderator in the inner part of the core, roughly coinciding with the location of the PuO_2 whereas Be is the preferred moderator in the spherical shell between 10 and 15 cm. There is some overlap of Poly and Be in between 7.5 and 12.5 cm. Beryllium is the preferred reflecting material.

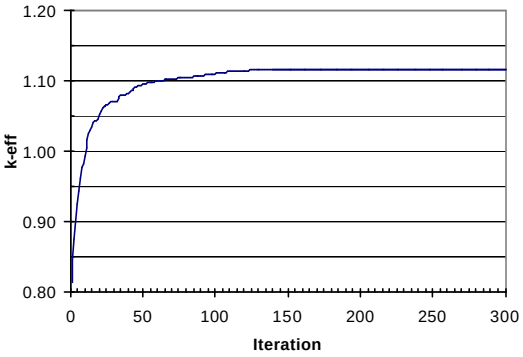

Fig. 10 k_{eff} evolution for Illustration # 3

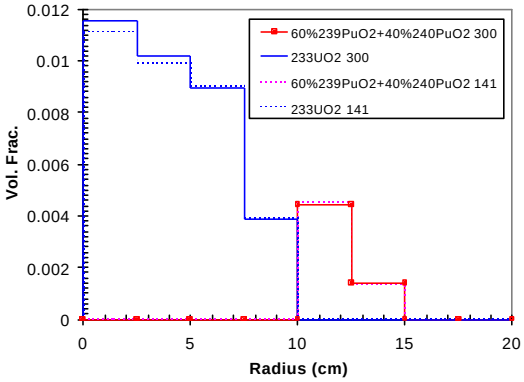

Fig. 11 Fuel distribution for Illustration # 3

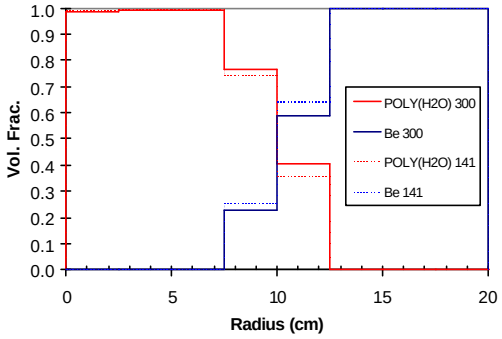

Fig. 12. Distribution of Poly and Be for Illustration # 3

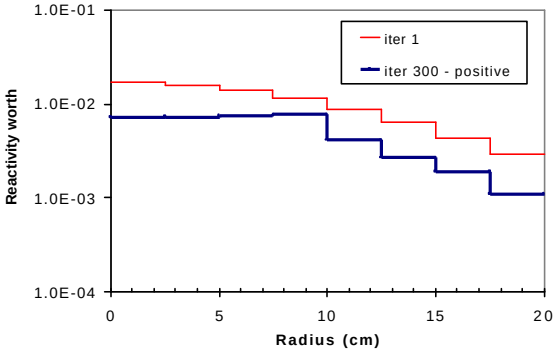

Fig. 13. Reactivity worth of $^{233}UO_2$ versus Be in Illustration #3

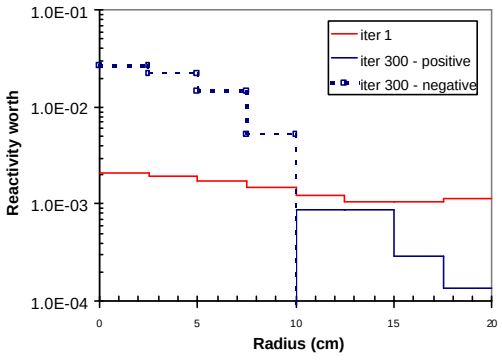

Fig. 14 Reactivity worth of PuO_2 versus Be for Illustration # 3

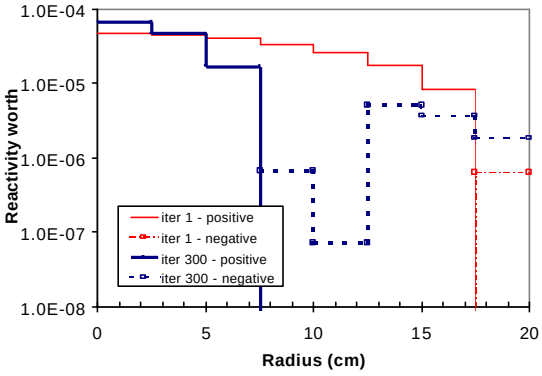

Fig. 15 Reactivity worth of Poly versus Be for Illustration # 3

How do we know that the above-described composition is indeed the optimal? For this we have to examine the RW distributions of Figures 13 to 15. Figure 13 shows that the RW for UO_2 is essentially flat over the innermost 10 cm of the core, where all the UO_2 is concentrated. The RW at outer zones is lower, but there is no UO_2 left in these zones to transfer to the higher RW zones. This implies that the UO_2 distribution is optimal. A similar story is being told by Figure 14; the RW of PuO_2 versus Be is flat in the annulus between 10 cm and 15 cm zones where all the PuO_2 is concentrated. Up to 10 cm the RW is negative and beyond 15 cm the RW is lower implying that transfer of PuO_2 from between 10 to 15 cm to elsewhere will result in a drop in k_{eff}. Figure 15 shows that beyond 12.5 cm, the RW of Poly versus Be is negative, implying that we do not want to replace the Be there by Poly. Replacing some Be by Poly in between 7.5 cm and 12.5 cm is expected to result in some increase in k_{eff}. However, the amplitude of the RW in that region is low so the effect on k_{eff} will be very small. If the Be concentration in these zones is increased at the expense of Poly, the RW would flip its sign from negative to positive (not shown in the figure). Such a flip would imply that we are near the peak k_{eff}.

7. DISCUSSION

The first version of SMORES to be released with SCALE 5 is set to search for maximum k_{eff} or minimum mass for systems having only one fissile material that is an optimization variable. The extension of the SMORES capability to search for maximum k_{eff} in multi-constituent problems reported in this work required development of more sophisticated algorithms for handling the change in material densities. The theoretical basis has not been changed. However, the efficiency of the optimization process, that is, the rate of convergence to the system composition giving maximum k_{eff}, strongly depends on the value used for the a_i^n coefficients [Eq. (14)]. Presently these values need to be specified by the user. Too small values may result in many iterations but smooth convergence. Too large values may cause oscillations that may lead to erroneous conclusions. The value of the coefficients need be selected such that the relative change in the concentration of the different constituents that participate in the optimization process will be of the same order of magnitude. In the future we are planning to automate the choice of the value of the a_i^n coefficients. This will make the optimization process fully automated.

Algorithms have been developed so far for the following types of multi-constituents optimization problems:

- Fixed mass of each of the constituents.
- Fixed mass of each of the fuel constituents.
- Fixed volume of all of the fixed constituents.
- Fixed volume fraction of all fuel constituents in each zone.

We have not developed algorithms yet for the direct search of the minimum fuel mass required for attaining a given value of k_{eff}. Such a capability is available in the present SMORES for problems that feature a single fuel constituent. Nevertheless, by applying SMORES to find the maximum k_{eff} corresponding to two or more fuel inventories, it is possible to find by interpolation or extrapolation the minimum mass corresponding to the desirable k_{eff}.

The search for the maximum k_{eff} described above assumes that the concentration of each of the constituents of variable concentration can vary continuously in each of the zones within the range specified by Eq. (10). We are presently developing new algorithms for search for maximum k_{eff} for problems in which the fuel is lumped into given volume zones and the variables are the location of the different fuel and moderator zones. These new algorithms do not need to use the a_i^n coefficients discussed above.

CONCLUSION

New maximum k_{eff} search options were successfully developed for SMORES – a prototypic analysis sequence recently developed and incorporated in the SCALE-5 code package. The new options developed are set to search for the maximum possible k_{eff} in problems having multi fuel and multi moderator/reflector constituents. Illustrations are given for three types of problems, all involving two fuel materials. SMORES can be useful for determining margins of subcriticality and for other criticality safety applications.

ACKNOWLEDGMENT

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