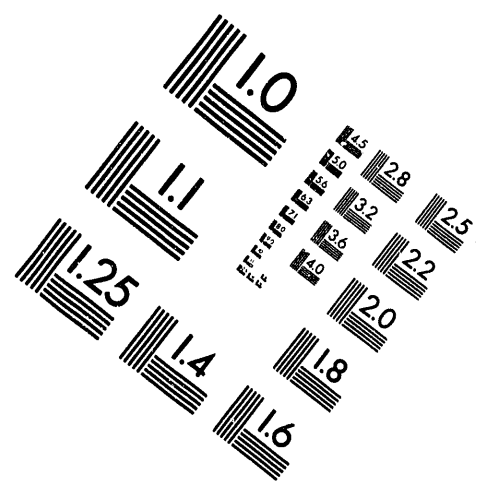
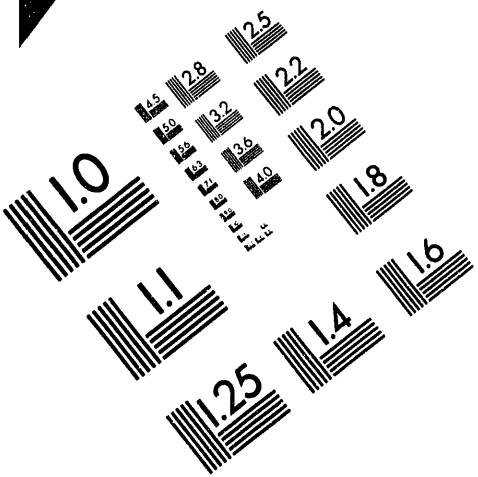




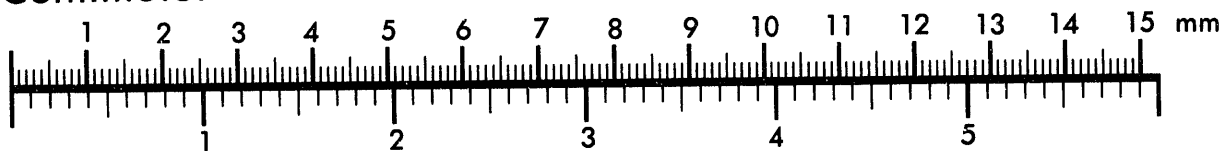
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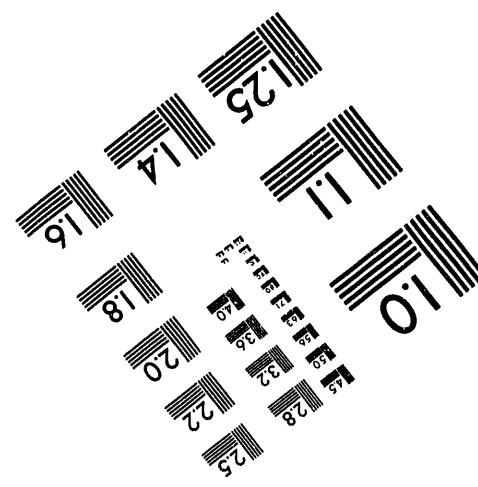
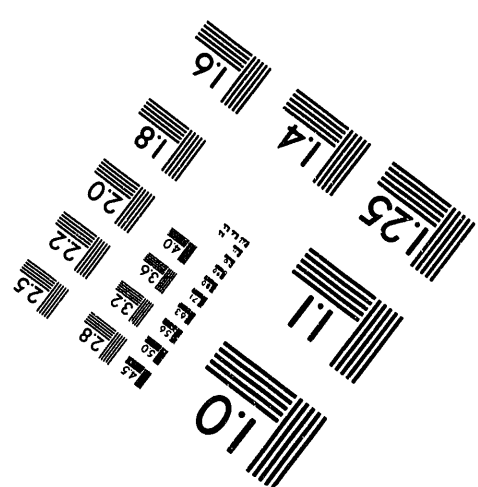
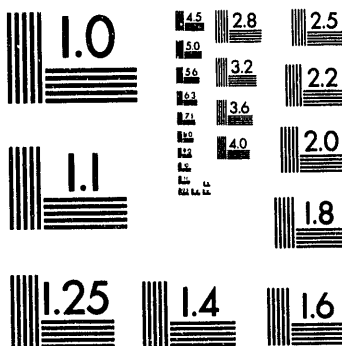
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GENERATION OF NEUTRONIC THERMAL DATA IN SUPPORT OF SPACE NUCLEAR PROPULSION*

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Abstract

The scattering kernel data for ${}^7\text{LiH}$ have been generated for the first time in the temperature range 50-1000 K. This is based on a phonon distribution function derived from both experimental data and theoretical calculations. A detailed study of the variation of the moderator temperature coefficient $\alpha_m(T)$ with temperature, T , is carried out for a typical space nuclear reactor of the particle bed type. It is established that the moderator temperature coefficient due to chemical binding effects follows the relationship $\alpha_m(T) = C F_v(H)^{1.6} T^{-1.65}$ where $F_v(H)$ is the volume fraction of bound solid hydrogen and C is a normalization constant which depends on the moderator capture thermal cross section. The value 1.65 is to be compared with 1.54 ± 0.06 derived in a previous study where water scattering kernels are applied. For control and safety reasons, a minimization of this positive component temperature coefficient can be most effective by operating the moderator at high temperatures. Advantages of this approach are outlined. In addition, suggestions are made to render the overall temperature coefficient negative.

INTRODUCTION

The thermophysical properties of lithium hydride (${}^7\text{LiH}$), particularly small density (0.775 g/cc), high melting point (961 K) and relatively high hydrogen atomic number density makes it an attractive material for use as a neutron moderator and shield (for LiH) in space nuclear thermal propulsion. However, the unavailability of neutronic cross section data in the thermal energy range for ${}^7\text{LiH}$ necessitated the generation of the relevant data which is required in criticality studies and for the determination of temperature-dependent feedback coefficients in the moderator and fuel regions.

GENERATION OF THE SCATTERING KERNEL DATA

The phonon frequency distribution function of ${}^7\text{LiH}$, derived from experimental data (Zemlyanov et al. 1965, Woods et al. 1960, Plekhanov and Altukhov 1985, and Brodsky and Burnstein 1967) as well as theoretical calculations (Verble et al. 1968 and Jaswall and Hardy 1968) is shown in Figure 1. One interesting feature of this phonon spectrum is the presence of an energy gap between 0.062 and 0.074 eV separating the acoustical and optical phonon modes. This phonon spectrum, evaluated in the present study, is utilized in GASKET calculations (Koppel and Houston 1978) to determine the scattering matrix elements $S(\alpha, \beta)$, the Debye-Waller integrals and the effective temperatures in the temperature range 50-1200 K for two cases using the full strength of the acoustic component as well as one in which it is reduced by 28. These results are summarized in Table 1 and are compared with similar results for the $\text{ZrH}_{1.85}$. Subsequently, the calculated $S(\alpha, \beta)$ values were cast in an ENDF format in order to be processed by the NJOY Code (McFarlane et al. 1982) which produces files for the MCNP Library. This code computes the incoherent and coherent energy dependent scattering cross sections as well as probability distributions. Figure 2 presents the incoherent cross section results determined for the first time in the present investigation for cryogenic as well as high temperatures ($T=50, 100, 300, 400, 600$ K). For neutron energies above 0.3 eV, the incoherent neutron cross sections coalesce to the free scattering cross section of hydrogen, 20.49 b (Mughabghab et al. 1981).

MODERATOR TEMPERATURE COEFFICIENT

The present results are incorporated in the Monte Carlo neutron and photon (MCNP) library and tests have been carried out to access the magnitude and temperature dependence of the moderator temperature coefficient

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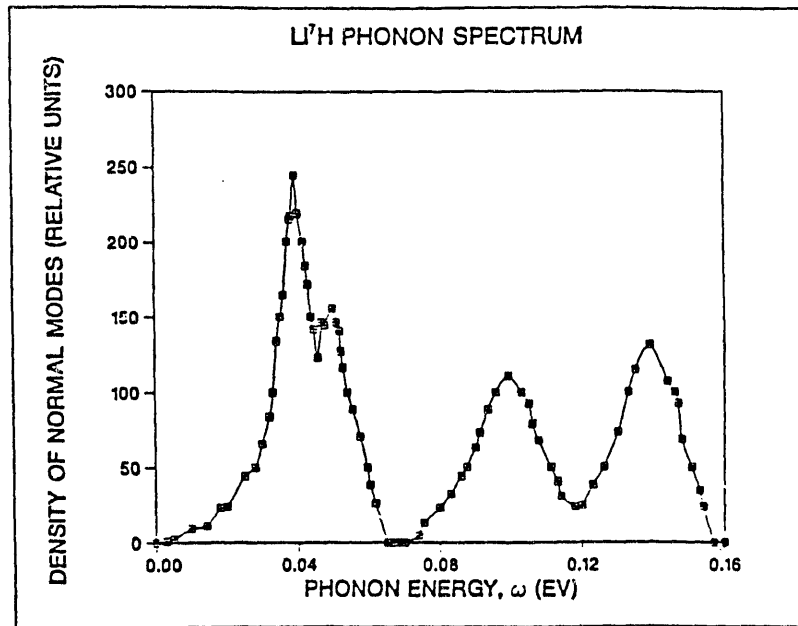


FIGURE 1. The Evaluated ⁷LiH Phonon Frequency Distributions Employed in the GASKET Calculations.

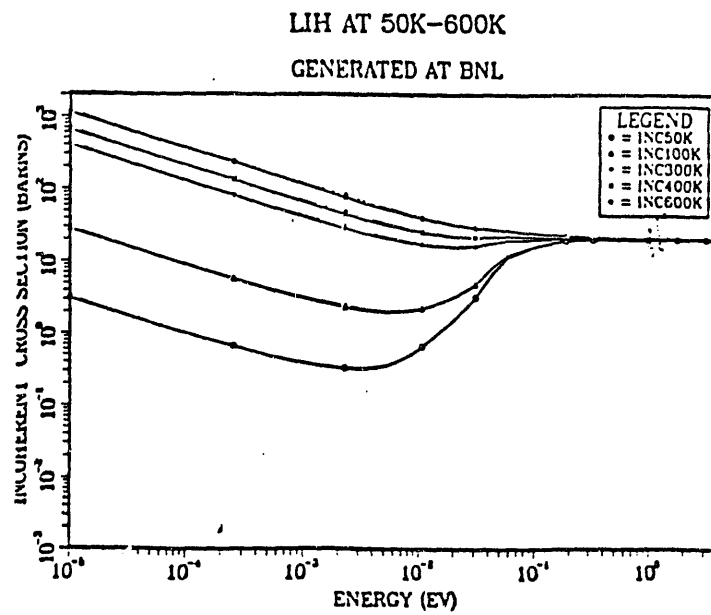


Figure 2. The Incoherent Cross Sections of ⁷LiH as Computed by GASKET and Based on the Phonon Frequency Distribution of Figure 1.

for typical nuclear space reactors with lithium hydride moderators. A particle bed reactor design (Ludewig et al. 1989) with a pitch of 12 cm, height 60 cm, 19 fuel elements with a total fuel volume of 30 liters, side as well as top and bottom beryllium reflectors (10 cm each) is considered.

TABLE 1. Debye-Waller Integrals and Effective Temperatures for H in ${}^7\text{LiH}$ and $\text{ZrH}_{1.85}$.

Temperature (K)	Integral (${}^7\text{LiH}$) ^a (eV ⁻¹)	T _{eff} (${}^7\text{LiH}$) ^a (K)	Integral (${}^7\text{LiH}$) ^b (eV ⁻¹)	T _{eff} (${}^7\text{LiH}$) (K)	Integral ($\text{ZrH}_{1.85}$) (eV ⁻¹)	T _{eff} ($\text{ZrH}_{1.85}$) (K)
50	17.68	481.5	9.31	674.1		
100	18.92	484.1	9.40	674.4		
200	23.84	507.1	9.77	683.6		
300	29.81	546.5	10.39	694.1	8.48	806.8
400	37.35	607.6	11.31	727.4	9.09	830.0
500	44.83	676.6	12.54	779.9	9.82	868.4
600	52.53	753.4	13.76	836.3	10.67	920.1
800	68.29	921.9	16.84	988.2	12.64	981.8

^aFull acoustic phonon component

^bReduced acoustic phonon component

For the purpose of this study the reactivity temperature coefficient is maximized in order that it be determined more easily by the Monte Carlo method. A ${}^7\text{LiH}$ moderator with a maximum volume fraction of 85% and 15% coolant channels is assumed. A cross sectional view of this reactor as generated by the MCNP code is depicted in Figure 3.

The reactivity temperature coefficient of the moderator is determined by the relationship

$$\alpha_m(T) = \frac{\Delta K}{K\Delta T} \quad (1)$$

where ΔK is the change in the neutron multiplication factor corresponding to a change, ΔT , in the moderator temperature as reflected in the temperature dependence of $S(\alpha, \beta)$. To achieve highly accurate statistical results, the neutron multiplication factor for each of the calculations require one million neutron histories. The temperature dependent moderator coefficients thus determined are represented in Figure 4 and are compared with the power law $\alpha_m(T) = AT^n$ established previously (Mughabghab et al. 1990a) from similar analysis. The present results show that the $\alpha_m(T)$ due to binding effects is always positive for a heterogenous reactor and decreases with temperature. This is caused by shifts in the thermal part of the neutron spectrum to higher energies in the moderator region, which results in smaller capture in the hydrogen, and subsequent increase in the multiplication factor.

To assess the effect of the volume fraction of the solid hydrogen moderator on the temperature coefficient, the same reactor design but with 75% and 50% volume fractions ${}^7\text{LiH}$ in the moderator is studied. The results are described in Figure 5. From the present as well as previous results (Mughabghab et al. 1990b) the following dependence for the moderator temperature coefficient is deduced.

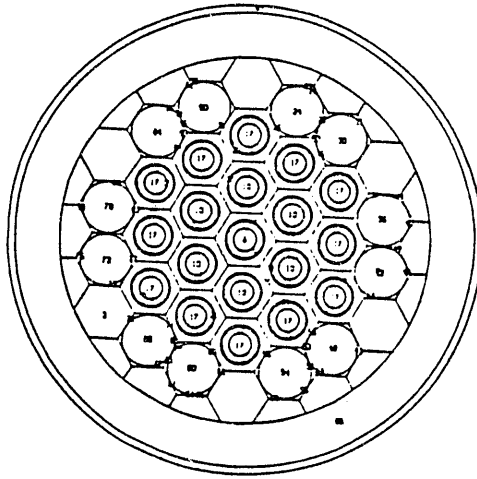


Figure 3. A Cross Sectional View of a Small Nuclear Space Reactor with 19 Fuel Elements as Generated by the Code MCNP.

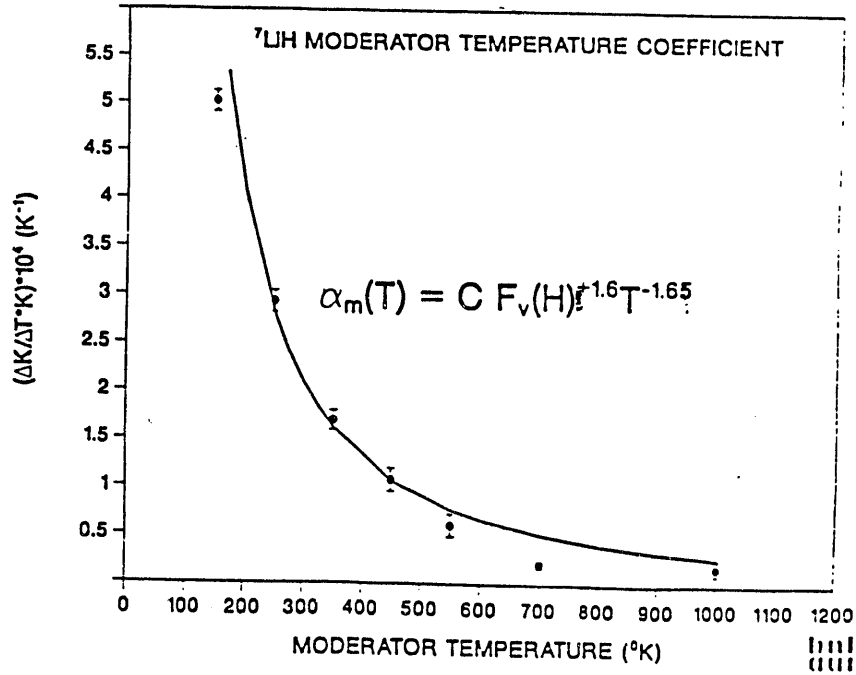


Figure 4. The Reactivity Temperature Coefficient as a Function of the Temperature and a Least Squares Fit to the MCNP Results.

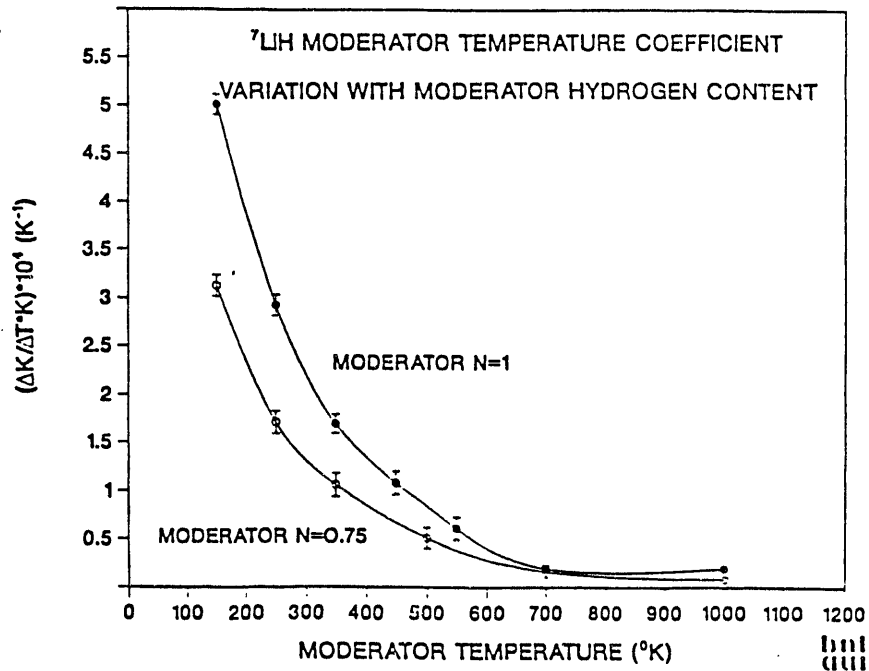


FIGURE 5. The Dependence of the Temperature Coefficient on Volume Fractions of ${}^7\text{LiH}$.

$$\alpha_m(T) = C F_v(H)^{1.6} T^{-1.65} \quad (2)$$

where $F_v(H)$ is the volume fraction of the solid hydrogen moderator and C is a normalizing constant which depends on the thermal capture cross section of the particular moderator under consideration.

With the aid of the four factor formula, it can be shown that, under the assumption of no change in the fission rate with temperature, the C in Equation 2 is related to the Maxwellian average capture cross section of the moderator (Mughabghab 1990a). The temperature power -1.65 compares well with a value $-1.54, \pm 0.04$ determined previously (Mughabghab 1990b) for a water moderated reactor design.

The positive component of the temperature coefficient due to chemical binding effects can be counteracted by several methods:

1. Reduction of the solid hydrogenous solid moderator,
2. Replacement by a moderator with a smaller thermal cross section such as D , ${}^9\text{Be}$, ${}^{11}\text{B}$, ${}^{12}\text{C}$ (Mughabghab 1981),
3. Operation of the moderator at a high temperature such as 800 K (Figure 5)
4. A change in moderator density due to expansion, and
5. Combination of the above four methods.

An application of these methods as illustrated in Figure 6 where a fraction of the ${}^7\text{LiH}$ is replaced by Be . The two curves at $T = 300$ and 800 K coalesce at about 50% volume fraction for Be indicating a negligible temperature coefficient for the moderator at that value.

Method 3 provides negative temperature coefficient for some moderators. For ${}^7\text{LiH}$ moderator, density changes of 20% from 800 K to 1000 K results in a large negative reactivity if a mechanism of expansion for the ${}^7\text{LiH}$ out of the moderator region is allowed similar to a pressurized boiling water reactor. A preliminary estimate of negative activity of 2.5% in this temperature range is achieved for this reactor design.

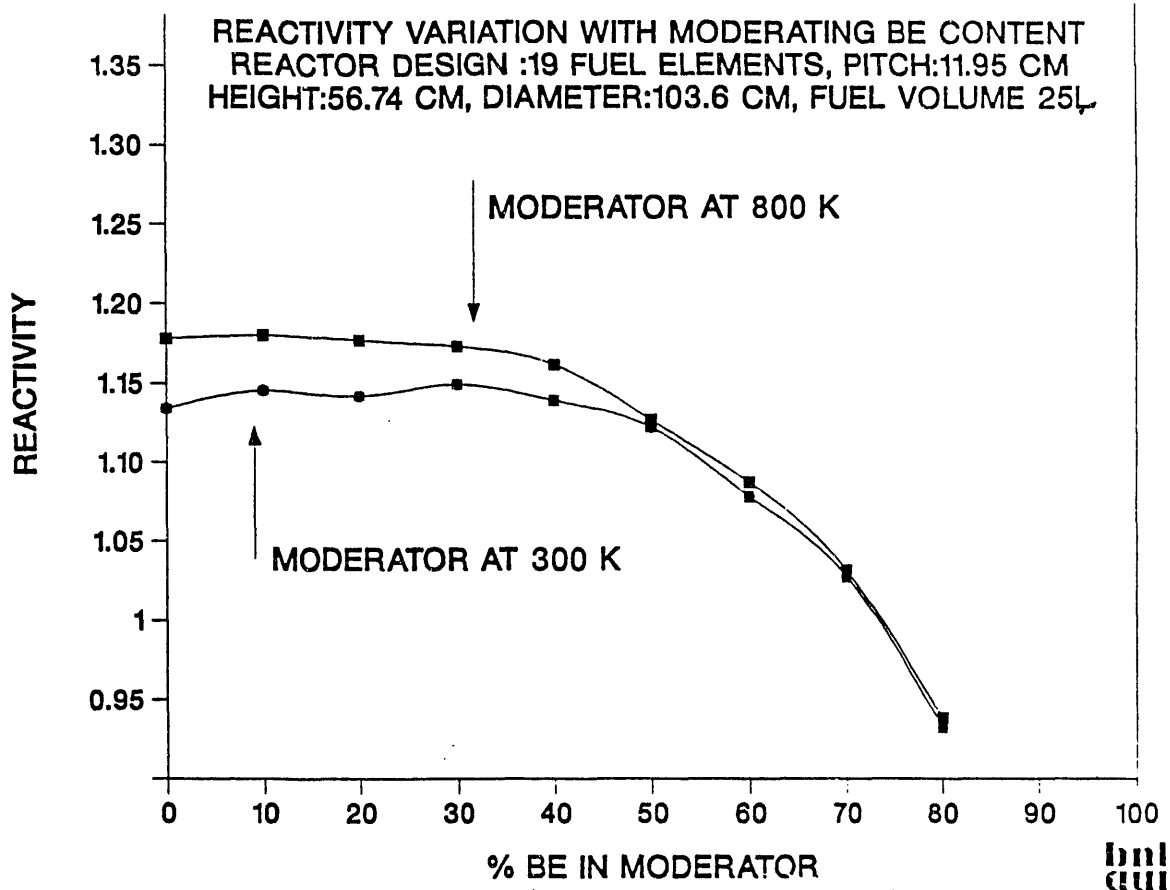


FIGURE 6. Reactivity Variation with Moderating Be Content for $T = 300$ and 800 K

The sensitivity of the temperature coefficient to the strength of the acoustic component of the phonon frequency distribution is under study and will be reported elsewhere.

Finally, the present results will be benchmarked in the future against the measured neutron spectra leaking from various LiH slabs (Verbinski 1967) where the neutron spectra at very low neutron energies are sensitive to molecular binding effect of hydrogen in lithium.

However, to fully validate the present results, differential temperature dependent neutron cross section measurements as a function of neutron energy are needed.

CONCLUSIONS

The ${}^7\text{LiH}$ kernels in the temperature range 50 to 1000 K have been generated and applied in a Monte Carlo transport calculations. The reactivity temperature coefficient in this temperature range have been determined and a relationship have been developed for it (Equation 2). Various methods for the reduction of the positive component of the moderator temperature coefficient are outlined.

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