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VALIDITY OF HANSEN-ROACH CROSS SECTIONS IN LOW-ENRICHED URANIUM SYSTEMS

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ABSTRACT

Within the nuclear criticality safety community, the Hansen-Roach 16 group cross section set has been the "standard" for use in k_{eff} calculations over the past 30 years. Yet even with its widespread acceptance, there are still questions about its validity and adequacy, about the proper procedure for calculating the potential scattering cross section, σ_p, for uranium and plutonium, and about the concept of resonance self shielding and its impact on cross sections. This paper attempts to address these questions. It provides a brief background on the Hansen-Roach cross sections. Next is presented a review of resonances in cross sections, self shielding of these resonances, and the use of σ_p to characterize resonance self shielding. Three prescriptions for calculating σ_p are given. Finally, results of several calculations of k_{eff} on low-enriched uranium systems are provided to confirm the validity of the Hansen-Roach cross sections when applied to such systems.

BACKGROUND

The sets of multigroup neutron cross section data known as the Hansen-Roach cross sections were first formally presented in late 1961 as both six- and sixteen-group cross sections for fast and intermediate critical assemblies [1]. The six-group cross sections were for the study of fast neutron critical assemblies, and the sixteen-group cross-sections were for intermediate neutron critical assemblies. In the sixteen-group data the top five energy groups were identical to the top five groups of the six-group set. In September, 1963, a second report was issued containing six-, sixteen-, eighteen-, twenty four-, and twenty five-group cross sections [2]. These cross section sets were designed for reactor calculations with neutron energies ranging from fast to thermal. In all these sets the top five energy groups were the same. It is in Ref. 2 that "revised" cross sections for ^{235}U and ^{238}U were presented for the sixteen-group cross sections. The eighteen-, twenty four-, and twenty five-group specifications provided more energy groups in the epithermal and thermal energy ranges relative to the sixteen-group specification and thus would have been expected to be more suitable for thermal neutron systems. However, only the sixteen-group cross sections have survived the nearly three decades of use, and these have become known as the Hansen-Roach cross sections. Taking only the "revised" cross sections for ^{235}U and ^{238}U, the data tabulated in Ref. 2 covers 108 "nuclides." These 108 "nuclides" actually represent only 31 different elements and isotopes. The difference is that many of the nuclides represent cross section sets for the same fissionable isotope but for differing resonance absorption treatments. The isotopes of ^{233}U, ^{235}U, ^{238}U, ^{239}Pu, and ^{240}Pu have such multiple cross section sets.

Up to this point, things seem to be fairly clear regarding the history of the Hansen-Roach library, but such is not actually the case. In the early 1960's multigroup neutronics computer codes for perfoming calculations were beginning to come of age. Since the codes required cross section data, the 16 group Hansen-Roach library was quickly acquired and accepted by those doing criticality safety analyses. Numerous versions of the library began to appear as users began adding data for additional nuclides for their own needs. Even within the 1960's the genealogy of some of these libraries was difficult to track down. Today there are a number of data sets which bear the label "Hansen-Roach" library, and their origins and quality assurance/validation are obscure. However, there are three prevalent sets which are widely used: one used at Los Alamos which tracks the data in Ref. 2.; one used with KENO [3] and which is called the AMPX working library; and the library attached to the SCALE/CSAS code system [4]. The Hansen-Roach AMPX working library and the SCALE/CSAS library seem to be derived from similar parentage through Oak Ridge National Laboratory although it should be noted that a recent notice was issued concerning problems with the AMPX working library [5]. It appears that the LANL library and the SCALE/CSAS library can be used with reasonable confidence.

Even though the sixteen-group cross sections were not originally designed to span the complete energy range of critical assembly types, they have done a remarkable job of providing good calculational predictions of k_{eff} for virtually all types of critical assemblies and systems, *when the proper fissionable "nuclide" is used.*

RESONANCE SELF-SHIELDING AND THE CALCULATION OF σ_p

One of the major problems that seems to arise from the use of the Hansen-Roach cross sections stems from the existence of multiple sets of cross sections for the fissionable isotopes ^{233}U, ^{235}U, ^{238}U, ^{239}Pu, and ^{240}Pu. For example, there are 13 sets of cross sections for the isotope ^{235}U. The presence of these multiple sets of data for a given isotope causes much confusion for many users of the library. In most other cross section libraries there is only one set of data for each isotope. In those cases where multiple sets are provided, there is usually a temperature associated with each set to identify the set. For the Hansen-Roach library, however, the different sets are not due to temperature differences but, instead, are to properly account for "resonance self shielding" of the fissionable isotopes in different mixtures of fissionable absorbers and neutron-moderating material. While it is not within the scope of this paper to present the theory of resonance absorption, a few words are helpful to provide some level of understanding of the need for, and importance of, the multiple sets of cross sections. Although much of the following applies equally well to elements and isotopes other than the fissionable isotopes of uranium and plutonium, for purposes of this paper the presentation will be specifically focused on these latter two elements.

Principles of Resonance Absorption and Self Shielding

For neutron energies between, say, 0.1 eV and 3 keV, the absorption cross section of the isotopes of uranium and plutonium varies markedly in a series of sharp, narrow (in energy), very pronounced "resonances." Most of the absorption of neutrons in this energy range takes place in these resonances. These resonances are frequently only about 0.1 eV in width, may have peak amplitudes of thousands of barns, and are separated from one another by about 20 eV. This pronounced resonance structure in the neutron-energy-dependent cross section leads

to a corresponding fine energy structure in the neutron flux. In general, there will be a dip in the neutron flux at the energy and the location where there is a strong absorption resonance.

Now, the vast majority of neutrons produced by fission are born with energies greater than 50 keV; that is, they are born with energies well above the resonance energy range. For neutrons to acquire energies where they can see the resonances of uranium and plutonium, they must be slowed down, or moderated, from their birth energies by means of scattering collisions. For practical purposes, such moderation requires that relatively low atomic weight material (a moderator) must be present in addition to fissionable material. For example, unreflected systems of uranium or plutonium metal have virtually no neutrons with energies below about 10 keV and ordinary criticality calculations for these systems are not sensitive to the existence of resonances. If moderating material is present, the overall neutron flux energy spectrum in the eV - keV range varies as 1/E to good approximation. Superimposed on this overall energy shape are the local flux dips resulting from the resonances in the fissionable material or "absorber". If a flux dip due to a strong resonance is "felt" by a resonance at a lower energy, then the neutron absorption in the latter resonance will be less than would have occurred if the higher energy resonance had not been present simply because the neutron flux that "sees" the second resonance is reduced by the first resonance. In other words, the second (and third, and fourth, etc.) resonance "downstream" from the first resonance may be somewhat shielded by the first resonance. This phenomenon is called *resonance self shielding*. The greatest absorption by the resonances will occur when there is no resonance self shielding. The degree to which self shielding affects the overall neutron absorption in resonances depends strongly on the amount of scattering (moderation) present in the absorber-moderator mixture, or, conversely, on the amount of absorption present in the mixture, that is, the degree of "dilution" of the resonance-absorbing isotope in the moderator. The dilution of the resonance-absorbing isotope is measured by the ratio of the moderator macroscopic scattering cross section to the atom density of the particular resonance-absorbing fuel isotope in question. This ratio is referred to as the *potential scattering cross section* for that resonance-absorbing isotope. It follows, then, that the greatest absorption by the resonances (per absorber atom) will occur when the absorbing isotope is "infinitely" dilute with an enormously large potential scattering cross section so that there is no resonance self shielding. The least amount of absorption by the resonances per absorber atom will occur with the least possible dilution (a potential scattering cross section of zero) where resonance self shielding is a maximum. *Note that each resonance-absorbing isotope in the mixture will have its own unique potential scattering cross section.*

In generating multigroup cross sections, it is necessary to determine the average cross section for an element or isotope over the energy range of a given energy group. In averaging the absorption cross section of a resonance absorbing isotope over an energy range encompassing many resonances, therefore, the average cross section is dependent on the potential scattering cross section for that isotope *in that mixture*. Thus, to generate a general library which can be used for all types of mixtures of resonance-absorbing material with varying degrees of moderation, it is necessary to generate multiple cross section sets for each resonance-absorbing isotope; one set for each characteristic mixture type. This is precisely what the Hansen Roach library contains - multiple sets of cross sections which encompass the full range of isotope-moderator types. The range of mixture-types is characterized by the potential scattering cross section parameter for the resonance-absorbing isotopes of uranium and plutonium. The use of the proper set of cross sections for the fissionable isotopes is very important; indeed, for

low-enriched moderated systems, it is *essential!*

It is noted that the multiple sets of cross sections in the Hansen-Roach library are for *room temperature* materials. Temperature effects, most notably in the Doppler broadening of the resonances, are not accounted for.

Calculating σ_p

The remaining issue in the proper use of the Hansen-Roach cross sections is the determination of the potential scattering cross section, σ_p, for each of the extant fissionable isotopes in the system to be analyzed. The basic definition of this quantity was provided without further explanation on page 6 of Ref. 2 where it is stated "The notation SIG P, or SIGMA P, specifies a scattering cross section per absorber atom for neutrons:

$$\sigma_p \equiv \frac{\Sigma_s(\text{moderator})}{N\,(\text{atomic density of absorber atoms})}" \tag{1}$$

The definition of "moderator" has caused some differences in the way σ_p has been calculated. Three basic prescriptions used to calculate σ_p use different definitions of "moderator": (1) the KENO, or SCALE/CSAS, prescription found in Ref. 3, (2) the Hopper-Renier prescription [6], and (3) the Hansen-McLaughlin prescription. To the authors' knowledge, the third prescription has not previously been published even thought it has been in use for three decades.

All three prescriptions for calculating σ_p for fissionable isotope "x" can be cast in a common generic form:

$$\sigma_{p,x} = \frac{1}{N_x}\sum_{i=1}^{M}(WF)_i N_i \sigma_{s,i} \tag{2}$$

where:
N_x is the atom density of fissionable isotope x,
M is the number of nuclides in the mixture
N_i is the atom density of nuclide i in the mixture,
$\sigma_{s,i}$ is the average scattering cross section in the resonance region for nuclide i in the mixture,
WF_i is a weighting factor for nuclide i in the mixture, different for each prescription.

SCALE/CSAS:

$$WF_i = 1.0, \quad \text{for all } i \tag{3}$$

Hopper-Renier:

$$WF_i = \frac{1 + \frac{(A_i-1)^2}{2A_i}\ln\left[\frac{A_i-1}{A_i+1}\right]}{(0.14474)[\ln(1000)]}, \quad \text{for all } i \tag{4}$$

Hansen-McLaughlin:

$$\begin{aligned} WF_i &= 1.0, \quad A_i \le 15, \\ &= 0.5, \quad A_i = 16, \\ &= 0.0, \quad A_i > 16. \end{aligned} \tag{5}$$

In Eqs. (4) and (5), A_i is the atomic weight of nuclide i.

The third prescription is that suggested by Gordon Hansen and Thomas McLaughlin as being appropriate for use with the Hansen-Roach library. It has the advantage of being simple to use since only the light nuclides (hydrogen through oxygen) are considered to be moderators.

Sensitivity of k_{eff} on σ_p Used

The value of σ_p calculated for a given system is strongly dependent on the enrichment of the fuel and on the H/X atom density ratio where X denotes the fissionable isotope in a mixture containing hydrogen. Generally, the value of σ_p is only weakly dependent on the prescription used to calculate it. Since the Hansen-Roach library only has cross sections for selected values of σ_p, it is probable that the calculated σ_p will fall between available values. The accepted procedure in such a case is to linearly apportion the cross sections between the two available library values. For example, suppose a σ_p for ^{238}U with an atom density of 0.04 is calculated to be 550. The library contains cross sections for σ_p's of 400 (u238-6r) and 600 (u238-7r). Thus, one could model the actual ^{238}U with u238-6r at an atom density of 0.01 plus u238-7r at an atom density of 0.03. For many applications it is not necessary to go to such fine detail as just described but instead to simply use the nuclide in the library whose σ_p lies closest to the calculated σ_p. The main point is to use library data for σ_p close to the calculated σ_p. This is especially true for low-enriched uranium solutions as is dramatically shown in Figure 1. The actual system used for this figure is 5 weight percent enriched uranium in a critical bare infinitely long cylinder of UO_2F_2 solution with a $H/^{235}U$ ratio of 500 The calculated σ_p for the ^{238}U is about 550. Plotted in the figure is the k_{eff} as a function of the Hansen-Roach ^{238}U nuclide used for the different σ_p's available in the library. Note that if "infinitely dilute" ^{238}U is erroneously used, a k_{eff} of 0.73 results – a grossly nonconservative value. Conversely, if metallic

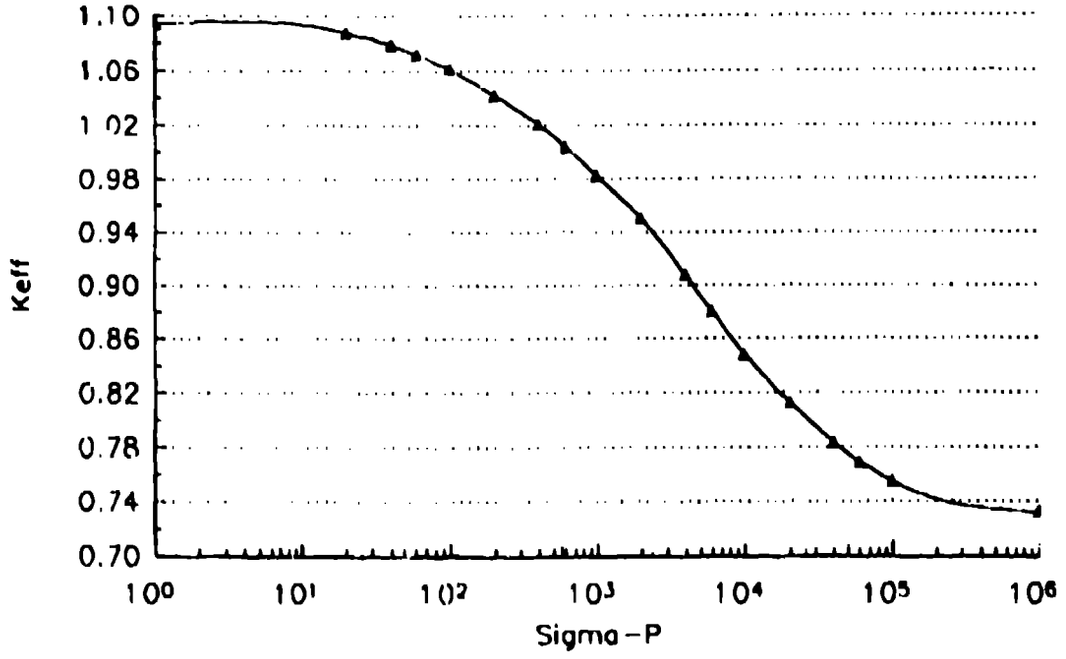

Fig. 1. Variation in k_{eff} with Different ^{238}U σ_p for a Critical System of $U(5)O_2F_2$ Solution

^{238}U cross sections are used erroneously, a value of k_{eff} of 1.09 results – a large overestimate of k_{eff}. Finally, note that using the ^{238}U with σ_p of 600 (close to the calculated value of 550) results in a k_{eff} very near to unity. Thus, the proper selection of the ^{238}U based on σ_p from the Hansen-Roach library is *essential* for low-enriched uranium solution calculations.

It is logical to ask if the proper selection of the fissile ^{235}U nuclide based on σ_p is equally important. Generally, the answer is no. The reason for this is that with the fissile isotopes resonance self shielding affects both fission and capture resonances. Since these two processes compete with one another in their effect on k_{eff}, there tends to be a cancelling effect. The net result is a much lesser degree of sensitivity on k_{eff} when different fissile nuclide cross section sets are used from the Hansen-Roach library. Nevertheless, it is still wise to use the σ_p parameter to select the correct self shielded cross section set for both fissile and fissionable isotopes.

Validity of Hansen-Roach Sets with Low-Enriched Uranium

For fast neutron systems, there are few complaints about the validity of the Hansen-Roach 16 group cross sections for calculating k_{eff}. The reason for this is simply that resonance self shielding effects are minimal in fast systems since there are few neutrons with energies in the resonance energy range. However, there appear to be misconceptions or uncertainties on the usefulness and validity of the Hansen-Roach 16 group cross section sets when applied to low-enriched uranium, well-moderated systems. Choi, et al [7] reported that when the cross sections were used in such a system, " substantial errors resulted." Admittedly, the authors went on to say that better results could be obtained using a lower resonance absorption ^{238}U cross section set, but they do not make it clear that *it is necessary to use the correct* ^{238}U based on a proper σ_p for the system. Similar statements and general misunderstandings regarding the selection of the proper ^{238}U cross section set are not uncommon. It is our feeling that the primary source of error in applying the Hansen-Roach cross sections to low-enriched uranium, well-moderated systems is due to an unclear understanding of σ_p and its impact on the correct modeling of such systems.

To check the validity of the library with low-enriched uranium, well-moderated systems, several criticals were evaluated using TWODANT [8] and KENO V.a with the Hansen-Roach 16 group library. These criticals are from Johnson and Cronin [9] and apply to $U(4.9)O_2F_2$ solutions in cylinders. k_{eff} values are shown in Tables I and II for different $H/^{235}U$ ratios using the three different prescriptions for σ_p.

These results show "exact" agreement (within statistics) between the TWODANT discrete ordinates code and the KENO Va Monte Carlo code. All of the calculated k_{eff}'s give a close prediction of criticality. Additional review of the validation literature on the subject of low-enriched uranium systems [10],[11], indicates that about 48 different critical systems have been analyzed using the Hansen-Roach library. In both Ref. 10 and 11, the k_{eff}'s were within 3% of unity and the judgment was that these low-enriched systems could be used to validate both codes and cross section libraries. Their results together with our calculations confirm that when a standard prescription method for calculating σ_p is used to select the correct self shielded cross section set, the Hansen-Roach cross sections are valid for use with low-enriched uranium, well-moderated systems.

TABLE I. k_{eff} from TWODANT

$H/^{235}U$	SCALE/CSAS	Hopper-Renier	Hansen-McLaughlin
524	0.986	0.991	0.989
643	0.994	0.997	0.996
735	0.997	1.000	0.999
994*	0.991	0.992	0.992

TABLE II. k_{eff} from KENO Va

$H/^{235}U$	SCALE/CSAS	Hopper-Renier	Hansen-McLaughlin
524	0.987±0.005	0.987±0.005	0.988±0.005
643	0.997±0.005	0.995±0.005	1.001±0.004
735	0.995±0.004	1.000±0.004	1.000±0.004
994*	0.993±0.003	0.992±0.003	0.986±0.003

* a "near-critical" experiment

SUMMARY

We have presented a background history of the Hansen-Roach 16 group cross sections together with an explanation of the existence of, and need for, multiple sets of cross sections for the fissionable isotopes of uranium and plutonium. These multiple sets are necessary to provide for differences in resonance self shielding as a function of the potential scattering cross section, σ_p, for the fissile isotope in a moderating mixture. Three prescriptions for calculating σ_p were presented. Results indicate that very little difference occurs among k_{eff} calculations using any of the three prescriptions. Similarly, we found excellent agreement between results from discrete ordinates and Monte Carlo codes. We also showed that if no prescription is used, or if the uranium/plutonium cross section is selected at random, very large errors (25% or larger) in k_{eff} can occur. However, results indicate that with the proper use of σ_p to predict resonance self shielding effects, the Hansen-Roach cross sections are valid for use with low-enriched uranium systems with varying degrees of moderation.

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