LA-8047-T
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A Statistical Model Investigation of Nuclear Fission

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Post Office Box 1663 Los Alamos, New Mexico 87545

This thesis was accepted by the University of Wisconsin, Madison, Wisconsin, in partial fulfillment of the requirements for the degree of Doctor of Philosophy in Nuclear Engineering. It is the independent work of the author and has not been edited by the Technical Information staff.

UNITED STATES
DEPARTMENT OF ENERGY
CONTRACT W-7405-ENG. 36

LA-8047-T
Thesis

UC-34c
Issued: October 1979

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by

Richard Edwin Pepping

ABSTRACT

To assist in the improvement of fission product yield data libraries, the statistical theory of fission has been investigated. Calculation of the theory employs a recent nuclear mass formula and nuclear density of states expression. Yields computed with a simple statement of the theory do not give satisfactory results. A slowly varying empirical parameter is introduced to improve agreement between measured and calculated yields. The parameter is interpreted as the spacing between the tips of the fragments at the instant of scission or as the length of a neck in the fissioning nucleus immediately prior to scission. With this spacing parameter semi-quantitative agreement is obtained between calculated and measured mass chain yields for six cases investigated, $^{233}U(n_{th},f)$, $^{235}U(n_{th},f)$, $^{239}Pu(n_{th},f)$, $^{235}U(n+14,f)$, $^{238}U(n+14,f)$, and $^{252}Cf(sf)$. An indication of the source of mass asymmetry in fission is presented.

The model developed predicts a mass and energy dependence of some of the parameters of models currently in use in data generation. A procedure for the estimation of the fission product yields for an arbitrary fissioning system is proposed.

INTRODUCTION

Reliable nuclear data is required for both civilian and military applications of nuclear energy. In reactor operation, fission product buildup affects reactivity and fuel burnup through neutron absorption. The fission products themselves are sources of decay heat which must be taken into account in the design of safety systems. After leaving the reactor, shielding and cooling requirements of the spent fuel again demand that the composition be known in order to insure safe handling. In some cases of importance accurate measurements have been made to determine these sources. For less frequent fission events and for less well measured fissioning systems, modeling has been employed to estimate the yields of the various fission products. It is the object of this work to improve upon the method of yield estimation through the use of a reasonable physical model.

In selecting a model for use here, there are basically two schools of thought. By computing from first principles the dynamic behavior of a heavy nucleus as it proceeds from its original state to two fission fragments one may expect to understand the entire fission process in addition to understanding the probability of the formation of a given pair of fission fragments, the fission fragment yield. Such a calculation is possible, in principle, but is tedious and prohibitively expensive in practice. Alternatively, one may make a simplifying assumption that renders the exact details of the fission process of little importance and concentrates

upon the fission yields. Such a simplifying assumption would be to assume that the entire process is statistical, completely determined by the properties of the final state. This assumption appears to have been first made by Fong.[1]

That the fission process may indeed be statistical is indicated by examining the available data on fission yields. The distributions of product mass vary slowly between fissioning systems, differences which appear being understood through simple conservation laws. The mass yields also vary slowly with particle energy in particle-induced fission. Again, the final state appears to be the important factor in determining yields.

The application of statistical models to the fission process is not a new idea. Fong[1] presented the idea over 20 years ago and has written prolifically on the subject since then. More recently, calculations have been presented by other authors.[2,3] Most recently, Wilkins, et al.[4] gave an extensive treatment of the topic giving qualitative agreement with observations of many fissioning systems. It shall be the object of this work to investigate the statistical model to determine its validity in a quantitative sense for possible use in improving fission product data libraries.

As an aid to the reader, the following is a brief guide to the organization of the presentation that follows. The fission process is briefly reviewed in order to qualitatively describe the process and establish some of the language to be used to describe it. The theory is then cast quantitatively to demonstrate the

nature of the assumptions necessary to make the theory calculable. It should be kept in mind that a large number of things must be assumed, any one of which, if in error, is of sufficient consequence to change any conclusions dramatically. Given a set of assumptions, a number of things may be computed, in addition to the yields, as diagnostics and are discussed in the section "The Yield and Its Moments." Following this section, three sets of assumptions to be used in calculations are described and motivation given for their selection. After specifying some expressions necessary to the evaluation in the section titled "The Densities," the calculation may proceed.

The first yield calculation is performed for several reasons. It employs the density expression most similar to the other statistical model evaluations mentioned and gives historical continuity to this work. It also allows some experimentation with the masses and single-particle energy treatments. Most importantly, it is used to demonstrate the equivalence of two of the sets of assumptions, thereby simplifying the calculation. This particular calculation is performed with extreme computational care in order to insure that none of the conclusions made are the results of numerical artifacts.

Having become somewhat more at ease with the calculation and the various input quantities, a new density expression is introduced, a feature which, along with the mass formula, sets this

work apart from previous calculations. With this expression and the mass formula the model is completely free of adhoc parameters other than those explicitly appearing. After establishing the computational technique to be used with the new density, a set of sample yields is computed and discussed.

To obtain quantitative agreement, some parameterization is necessary in order to achieve overall agreement between measured and computed values of the chain-yields, prompt neutron number, total gamma energies, and total kinetic energy. In describing independent yields, the model employed when data is poorly known requires the use of some empirically determined parameters. Working backward, one may extract the values of these parameters from both the published yields and calculated yields. Comparing these values reveals some small differences. Possible reasons for these discrepancies are discussed.

Finally, observations of potential practical use by way of simple models and scaling relations are discussed. The various physical models necessary for the calculation are briefly discussed in several appendices. Any one of these subjects is, by itself, deserving of a thorough treatment. The appendices, however, describe only the features necessary for this calculation and their methods of implementation.

FISSION REVIEW

If one examines the familiar plot of binding energy per nucleon for stable nuclei,[5] it may be seen that nuclei near mass number 60

are most tightly bound with about 8.5 MeV of binding energy per nucleon. With increasing mass number the binding energy per nucleon decreases. For a sufficiently heavy nucleus it may then be energetically favorable for the nucleus to split into two lighter nuclei. To do this the heavy nucleus must deform and elongate to such a degree that the repulsive Coulomb force is sufficient to overcome the attractive nuclear force. At this point, the nucleus may split, or fission, rather than return to its ground state shape.

In order to describe the nucleus as it elongates, one must be able to describe its behavior as it proceeds along some trajectory in a multi-dimensional space of shape coordinates. Shapes that have been useful in describing the behavior specify such general quantities as elongation, mass asymmetry, axial asymmetry, and neck formation of the deformed nucleus. Initially, the heavy nucleus may resist deformation such that an elongation of its shape is accompanied by the increase in the potential energy of the system. At larger deformations the potential energy may actually begin to decrease, a manifestation of shell effects in the deformed nucleus. These shell effects depend strongly upon the shape of the nucleus. In the multidimensional shape space the potential energy surface may have many local maxima and minima. The minima are associated with so called shape-isomerism in heavy nuclei, metastable states of the deformed nucleus. At some point the Coulomb repulsion becomes sufficiently strong that it overcomes the nuclear attraction. The nuclear potential energy then decreases with further elongation. In general, any of the local

maxima define saddle-points in the potential energy. In the discussion that follows, the term "saddle-point" shall be used to refer to that shape at which the Coulomb repulsion and nuclear attraction exactly cancel.

As the nucleus proceeds beyond the saddle-point deformation, the shape may begin to resemble that of a dumbell with two lobes, the nascent fragments, connected by a neck. The Coulomb force may drive the elongation further until the nuclear restoring force is no longer able to hold the system together. The neck snaps and fission occurs. At this instant, called the scission-point, the system consists of two separate nuclei.

During the descent from saddle to scission the fragments may accelerate in the Coulomb field such that at the scission-point the fragments possess some translational kinetic energy associated with the motion of their centers of mass. Depending upon the exact nature of the descent and snap, they may also be rotating and their shapes vibrating. Beyond the scission-point the fragments may further accelerate in the Coulomb field. The energy associated with translational kinetic energy at the scission-point and the energy obtained from the Coulomb repulsion may be measured in the lab as the fragment total kinetic energy. The energy associated with rotation, shape vibration and deformation, and any internal excitation gained during the descent provides energy for prompt neutron and gamma ray emission. The distinction shall be made between fission <u>fragments</u> and fission <u>products</u>, the fragments being

the two nuclei immediately following scission and the products resulting after prompt neutron emission from the fragments.

THE THEORY

During the descent from saddle to scission, the nuclear shape is driven to further elongation, the nascent fragments acquiring translational kinetic energy, under the influence of Coulomb repulsion. Depending upon the nature of the nuclear Hamiltonian, the collective degrees of freedom may be coupled to internal degrees of freedom such that the collective motion is damped, some of the energy gained during the descent being converted into internal heat. At the scission-point an amount of energy, G, is released,

$$G = M^{*} - m_1 - m_2 - C$$

Here, M^{*} is the mass of the fissioning nucleus, m_i is the mass of the i^{th} fragment, and C is the Coulomb interaction energy. As a result of the strong Coulomb repulsion, the fragments may be deformed such that their masses are increased by the amount D relative to the ground-states values, m_{io}. Denoting collectively by $\vec{\alpha}$ any parameters assumed to describe the fragments' geometry at scission, G may be written,

$$G(\vec{\alpha}) = M^{*} - m_{1o} - m_{2o} - D_1(\vec{\alpha}) - D_2(\vec{\alpha}) - C(\vec{\alpha}) \quad .$$

This energy may appear as fragment excitation energy or rotational,

vibrational, and translational kinetic energy. Energies associated with rotation and vibration are neglected, justification of which is offered in Appendix C. The energy at the scission-point is assumed to be partitioned between intrinsic degrees of freedom, or heat, and collective translational kinetic energy degrees of freedom.

Formally, the decay width is given by the Fermi Golden Rule,[6]

$$\Gamma(A,Z,\vec{\alpha}) = |\langle f|H_{fiss}|i\rangle|^2 \rho(G) \quad ,$$

Here, A and Z specify the mass and charge of the light fragment, the mass and charge of the heavy fragment given by conservation laws, H_{fiss} is the perturbing Hamiltonian causing the decay, $|i\rangle$ denotes the initial state, the fissioning nucleus, and $|f\rangle$ denotes the final state, two fragments of specified mass, charge, and any other parameters, $\vec{\alpha}$, assumed to describe the scission configuration. Herein lies the problem.

Specification of the mass and charge division alone does not adequately describe the scission-point. Until the $\vec{\alpha}$-parameters are given, the calculation can not begin. These parameters are given by H_{fiss}, making it an extremely important quantity. This may be illustrated with regard to the nuclear shapes by assuming the phase-space density to be given by a constant temperature Boltzman expression,

$$\rho(G) = \exp(G/T) \quad ,$$

and H_{fiss} to be a constant for all possible final states. The most probable scission configuration is that for which G is a maximum. Wilets[7] has determined this configuration, in the limit of the liquid-drop behavior, to be two infinitely long nuclear needles of vanishing diameter. In a real nucleus, this limit is not attainable. The conclusion is similar, however, that the overriding factor is the Coulomb energy driving the shape to one of extreme elongation, a shape that may be attained with sufficiently many degrees of freedom.

For more modest deformations of the fragments another problem arises. The energy, G, to be partitioned must be positive. It has been suggested[1] that at the scission-point the fragments are tangent. Even for the largest deformations which the mass formula allows (Appendix A), positive values of G can not be obtained without introducing a spacing parameter, δ, to be interpreted as the distance between the tips of the fragments. Introduction of this parameter allows the Coulomb energy to be reduced sufficiently to allow positive values of G. As the parameter increases, G increases such that the most probable scission configuration corresponds to fragments at infinite separation with $C = D_1 = D_2 = 0$.

It would then appear that the nature of H_{fiss} is quite important since it is the only factor remaining which can prohibit these configurations so strongly favored through the phase-space term. Proceeding from first principles, one must then compute the behavior of the fissioning system as it descends from the saddle-

point to the scission-point, the end of the fission process, keeping track of all energies, coordinates, and quantum numbers. Having determined the scission-point shapes, separations, matrix elements, and energy partition, an important quantity to be discussed later, for all possible final states, the phase-space term may be computed for each and the yield of a given mass and charge given by integrating over the uninteresting variables.

The descent has only been calculated for a few nuclei, and then only in the context of a simplified model. Rather than attempt to solve this problem here, the Golden Rule shall be used with existing fission product yield data[8] to view the fission process in hope that the nature of H_{fiss} may be extracted. Clouding this view will be other assumptions and model limitations necessary to make the calculation possible.

THE YIELD AND ITS MOMENTS

It shall be assumed that, apart from determining the scission-point energy partitions and shapes, the matrix element is a constant. The shapes are presumed to be given by some distribution, $f(\vec{\alpha})$. The yield of a given fragment charge and mass is then proportional to the sum over $\vec{\alpha}$ of the decay widths,

$$y(A,Z) \propto \sum_{\vec{\alpha}} f(\vec{\alpha}) \cdot \Gamma(A,Z,\vec{\alpha}) = \sum_{\vec{\alpha}} \rho\,[G(\vec{\alpha})] \cdot f(\vec{\alpha}) \quad ,$$

with the definition,

$$I_y(A,Z) = \sum_{\vec{\alpha}} \rho[G(\vec{\alpha})] \cdot f(\vec{\alpha}) \quad .$$

The yield is given by normalizing,

$$y(A,Z) = \frac{I_y(A,Z)}{\sum_{A,Z} I_y(A,Z)} \quad .$$

To evaluate $\rho[G(\vec{\alpha})]$, thermal equilibrium shall be assumed between the intrinsic degrees of freedom and the collective translational kinetic energy degrees of freedom. Supressing the $\vec{\alpha}$ argument,

$$\rho(G) = \int_0^G \rho(k) \int_0^{G-k} \rho_1(E_1)\rho_2(E_2=G-k-E_1)\,dE_1\,dk \quad ,$$

where $\rho(k)$ is the density of states of translational kinetic energy, k, and $\rho_i(E_i)$ is the density of states of the i^{th} fragment at excitation energy E_i.

In addition to the yield integral, two moments of interest shall be computed,

$$I_E(A,Z) = \sum_{\vec{\alpha}} f(\vec{\alpha}) \int_0^G \rho(k) \int_0^{G-k} E_1 \rho_1(E_1)\rho_2(G-k-E_1)\,dE_1\,dk \quad ,$$

$$I_k(A,Z) = \sum_{\vec{\alpha}} f(\vec{\alpha}) \int_0^G k\rho(k) \int_0^{G-k} \rho_1(E_1)\rho_2(G-k-E_1)\,dE_1\,dk \quad .$$

With respect to the $\vec{\alpha}$-parameters, weighted averages may be computed for any quantity, Q,

$$I_Q(A,Z) = \sum_{\vec{\alpha}} Q(\vec{\alpha}) \cdot f(\vec{\alpha}) \cdot \rho[G(\vec{\alpha})] \quad .$$

Then the average value of any quantity is given by

$$\langle Q \rangle = \frac{I_Q(A,Z)}{I_y(A,Z)} \quad .$$

Of particular interest are the quantities $\langle D \rangle$, $\langle C \rangle$, $\langle k \rangle$, $\langle E_1 \rangle$, and $\langle E_2 \rangle = \langle G \rangle - \langle k \rangle - \langle E_1 \rangle$.

These moments may be used as checks on the various parameters and assumptions. For example, after normalization, the moments, $\langle k \rangle$, $\langle C \rangle$, $\langle E_i \rangle$, and $\langle D_i \rangle$ may be compared to experimental values of the total fragment kinetic energy, $\langle TKE \rangle$, and the decay energy for prompt neutron and gamma ray emission, X_i,

$$\langle C \rangle + \langle k \rangle = \langle TKE \rangle \quad ,$$

$$\langle D_i \rangle + \langle E_i \rangle = \langle X_i \rangle \quad .$$

With a table of neutron separation energies, an upper bound on the number of prompt neutrons may be determined from X_i.

In making comparisons between measured and computed yields, some of the terminology that shall be used is as follows:

1) Independent yield: the A and Z dependent yield, y(A,Z).

2) Mass-chain yield, mass yield, or chain-yield: the yield of a given mass, independent of charge,

$$y(A) = \sum_{Z} y(A,Z) \quad .$$

3) Charge yield: the yield of a given charge, independent of mass,

$$y(Z) = \sum_{A} y(A,Z) \quad .$$

Energies and diagnostic terms weighted by the independent yields and summed are referred to as integral values.

Within a fixed mass chain, the independent yields may be devided by the chain yield to form the fractional independent yield, fiy(A,Z),

$$fiy(A,Z) = \frac{y(A,Z)}{y(A)}$$

THE SCISSION CONFIGURATION

Before the calculation can begin, the parameters, $\vec{\alpha}$, describing the scission configuration must be specified. Since the fragments are neutron-rich, unstable, and highly deformed, experimental knowledge of their masses is not available. A mass formula must then be used to estimate the mass and its shape dependence. Seeger and Howard[9] give such a formula, described in Appendix A, with two parameters specifying the shape. These are the Nilsson parameters, ε and ε_4, used to describe the single-particle potential well of the nucleus. They describe axially symmetric shapes, only. Some

of the shapes considered are shown in Figure 1. Approximate values of the coefficients of a collective radial expansion in Legendre Polynomials corresponding to these shapes appear in Table 1. The charge is assumed to be uniformly distributed throughout the nuclear mass. Only multipoles of even order appear in a multipole expansion of the Coulomb interaction energy since only even order multipoles appear in nuclear potential. The scission configuration is then specified by four shape parameters and the spacing parameter, δ, which shall initially be held constant for all masses, charges, and shapes.

The distribution of shape parameters, $f(\vec{\alpha})$, is given by H_{fiss}. As an example of such a distribution, it has been proposed that the fissioning nucleus is extremely dissipative and that the descent from saddle to scission is so slow as to be quasi-static. If this is the case, it is argued,[1] the nucleus may follow a minimum potential energy trajectory on its way to scission. The energy release, G, is equivalent to the negative of the potential energy. Then a consistent method exists to define a scission-point configuration, which shall be called the GMAX configuration,

$f(\vec{\alpha}) = 1.$ $\quad G(\vec{\alpha})$ = maximum

$f(\vec{\alpha}) = 0.$ $\quad$ all other $\vec{\alpha}$.

More detailed investigations of the behavior of viscous liquid-drops reveal that the presence of high viscosity causes the trajectory to deviate considerably from that of minimum potential energy for the case of symmetric mass splits. It may then be anticipated that the view of the scission-point may be somewhat obscured

by computing yields at the GMAX shapes. Two other shape distributions, $f(\vec{\alpha})$, shall also be considered. Within the space of allowed shape combinations in the fragments, the yield integrals may be evaluated at all points and a yield surface determined for a given A and Z. Assuming $f(\vec{\alpha}) = 1.$ for all $\vec{\alpha}$, the yield is given by summing over all $\vec{\alpha}$, defining the SUM method. Having the yield surface, the shape combination at which it takes on maximum value defines the YMAX configuration and the YMAX shape distribution,

$$f(\vec{\alpha}) = 1. \qquad \rho[G(\vec{\alpha})] = \text{maximum} \quad ,$$

$$f(\vec{\alpha}) = 0. \qquad \text{all other } \vec{\alpha} \quad .$$

The interest in these three configurations may be seen in the following. Assume for the time being a constant temperature form for the phase-space term,

$$\rho(G) = \exp(G/T) \quad ,$$

The yield surface peaks at the GMAX configuration and may be approximated as a Gaussian about this point. The SUM method is then approximately the integration of a Gaussian, the result of which is the product of the peak value, the GMAX value, and a width parameter. To the extent that the yield surface is approximately Gaussian and the width parameter smoothly varying with mass and charge, the GMAX and SUM yields are identical, the width parameter entering as an overall constant which drops out of the yield expression upon normalization. Comparison of the two yields should indicate the validity of these assumptions.

In fact, the phase-space term is not of a constant temperature form. In addition to the G-dependence single-particle terms in the fragments affect the yield. It is for this reason that the YMAX yield is greater than that of the GMAX yield. Again, the SUM yield may be compared with the YMAX yield to test the validity of the assumption of Gaussian behavior about the YMAX configuration and the smoothness of the width parameter.

A practical problem arises with the YMAX and SUM yields, namely that the yield integrals must be evaluated at all combinations of the shape parameters. When possible, this is done. In the larger shape space ultimately to be considered, this is too tedious and a restricted area in the vicinity of GMAX is explored to find the YMAX configuration. The SUM method is too expensive to be applied in this case.

THE DENSITIES

A. The Kinetic Energy Density

The density of linear momentum states for a two-particle system of reduced mass, μ, in a volume, V, is given by,

$$\rho(k) = \frac{d}{dk} N(k) \quad ,$$

where k is the translational kinetic energy and N(k) is the total number of translational states of kinetic energy less than or equal to k,

$$N(k) = \frac{V}{h^3} \int_0^{p_{max}} d^3p$$

$$= \frac{4\pi V}{3h^3} p^3_{max}$$

$$= \frac{4\pi V}{3h^3} (2\mu k)^{3/2}$$

Hence,

$$\rho(k) = \frac{4\pi V}{h^3}\sqrt{2\mu^3 k}$$

The reduced mass of the two particles of approximate mass A_1 and A_2 is

$$\mu = \frac{A_1 A_2}{A_1 + A_2} \text{ mass units} \quad .$$

As only proportionalities are important, the expression used for $\rho(k)$ is taken as.

$$\rho(k) = \sqrt{(A_1 A_2)^3 k} \quad .$$

In later cases, the A_1 and A_2 terms are dropped, these being slowly varying quantities.

B. The Nuclear State Density

The density of states for a nucleus of N neutrons and Z protons at excitation energy E is formally defined as the inverse Laplace transform of the partition function, $\Omega(\alpha_N, \alpha_Z, E)$, for the system,

$$\rho(N,Z,E) = \frac{1}{(2\pi i)^3} \oint\oint\oint \exp[\Omega(\alpha_N, \alpha_Z, \beta) - \alpha_N N - \alpha_Z Z + \beta E] \, d\alpha_N d\alpha_Z d\beta \quad .$$

The partition function is computed separately for the neutron and proton systems,

$$\Omega(\alpha_N,\alpha_Z,\beta) = \Omega_N(\alpha_N,\beta) + \Omega_Z(\alpha_Z,\beta) \quad .$$

The contour integral may be well approximated at reasonable excitation energies by the saddle-point method,

$$\rho = \frac{e^S}{(2\pi)^{3/2} D^{1/2}} \quad ,$$

where S is the entropy,

$$S = \Omega - \alpha_N N - \alpha_Z Z + \beta E \quad ,$$

and D is the 3x3 determinant of the matrix of second derivatives of Ω with respect to α_N, α_Z, and β. Through the saddle-point approximation, the quantities α and β take on the identities of the chemical potential and reciprocal temperature of the system. All quantities are to be evaluated at the saddle-point, defined by the location of the peak of the integrand,

$$N = \frac{\partial\Omega}{\partial\alpha_N} \qquad Z = \frac{\partial\Omega}{\partial\alpha_Z} \qquad E = -\frac{\partial\Omega}{\partial\beta} \quad .$$

The partition function has been determined for a system of Fermions with a residual pairing interaction by Sano and Yamasaki.[11] Densities computed with this partition function have been investigated by Moretto[12] and Huizenga, et al.,[13-15] and are the basis for yields computed later. The formalism and its implementation are described in Appendix D.

By assuming the single-particle states to be uniformly spaced an analytical density expression may be obtained. The expression was first proposed by Bethe[16] and was later modified by several others[17-21] in order to improve agreement between predicted and measured neutron resonance spacings. The form of the density in the constant spacing limit is given by

$$\rho(E) = \frac{\sqrt{\pi}}{12} \frac{\exp(2\sqrt{aU})}{a^{1/4} U^{5/4}} ,$$

where U is the excitation energy and a is the "density parameter". It is upon the density parameter that effort has been concentrated since it allows the introduction of empiricism to account for the shortcomings of the constant single-particle spacing assumption. This expression is described in Appendix E.

The analytical expression is significant since it was the only expression available before fast electronic computers allowed the implementation of the more realistic method proposed by Moretto and Huizenga. It is still in use[22] and has been used by Fong to compute fission product yields.[1] Yields based on both methods will be presented in this work.

A SAMPLE YIELD CALCULATION BASED ON AN ANALYTICAL DENSITY FORMULA

As an example of the method of evaluation, yields are computed for $^{235}U(n_{th},f)$ assuming the nuclear density of states expression to be given by the analytical expression of Gilbert and Cameron.[17] This formula is discussed at length in Appendix E. The expression is written in two pieces and describes the density of states at

excitation energy, E,

$$\rho_H(E) = \frac{\sqrt{\pi}}{12} \frac{\exp(2\sqrt{aU})}{a^{1/4} U^{5/4}} \qquad E > E_x$$

$$\rho_L(E) = \frac{1}{T} \exp\left(\frac{E-E_o}{T}\right) \qquad E < E_x$$

The subscripts, L and H, refer to the value of E relative to a transition energy, E_x, L (low) for energies less than E_x and H (high) for energies above E_x. The two formulas are required to join smoothly at E_x, a condition which defines the two parameters appearing, T, the temperature, and E_o,

$$\frac{1}{T} = \sqrt{\frac{a}{U}}\Bigg|_{E_x} - \frac{5}{4U}\Bigg|_{E_x}$$

$$E_o = E_x - T \log [T \rho_H(E_x)] \quad .$$

The excitation energy in the high excitation energy form is written as U and is related to the excitation energy argument, E, by

$$E = U + P \quad .$$

P is the pairing energy of the nucleus. This particular statement accounts for the fact that there is a residual interaction, pairing, in the ground state of the nucleus. Its effect is to cause an overall shift of the energy axis. The transition energy, E_x, is actually given in terms of U_x,

$$U_x = E_x - P$$

where

$$U_x = 2.5 + 150/A$$

This result was determined empirically by Gilbert and Cameron.[17] The fit expression reproduces the data to approximately ± 200 keV. As shown in Appendices E and F, use of this formula also requires a single-particle shell energy, S, which enters through a, the density parameter. The density parameter is usually the object to be modeled when using this formula, as discussed in Appendix F.

Depending upon the value of E relative to the cross-over energy, E_x, three types of integrals are encountered in the yield calculation,

$$I_1 = \int k^{n/2} \int E^m \rho_L^{(i)}(E) \rho_L^{(j)}(G-k-E)\, dE\, dk$$

$$I_2 = \int k^{n/2} \int E^m \rho_L^{(i)}(E) \rho_H^{(j)}(G-k-E)\, dE\, dk$$

$$I_3 = \int k^{n/2} \int E^m \rho_H^{(i)}(E) \rho_H^{(j)}(G-k-E)\, dE\, dk \quad ,$$

where, for the yield, n = 1, m = 0, for the mement, $\langle I_E \rangle$, n = 1, m = 1, and for the moment $\langle I_k \rangle$, n = 3, m = 0. The subscripts refer to the form of the Gilbert and Cameron density, low excitation (L) or high excitation (H), and the superscripts index the single-particle parameters appropriate to that fission fragment. I_1 may be evaluated analytically. The order of integration in I_2 may be reversed and one integration performed analytically, the second

integration performed numerically. Both integrations in I_3 must be performed numerically.

For this first example, it is desired that the integrals be evaluated sufficiently accurately that numerical errors may confidently be ignored. Any choice of computational method must satisfy this requirement. To determine the method of numerical evaluation of the integrals, fragment data were scanned to determine extreme and median values of the energies, S, P, E_x, and T. Test cases were then chosen and the integrals evaluated by a standard adaptive Newton-Cotes Quadrature Rule[23] with a relative computational error of 10^{-9}. These same test integrals were then evaluated using Gauss-Legendre and Gauss-Laguerre Quadrature Rules[23] and compared to the Newton-Cotes values. Ultimately, combinations of 12-point Gauss-Legendre and Gauss-Laguerre Rules were chosen giving values that deviated by less than 7 parts in 10^4 from those of the Newton-Cotes. The Gauss Quadrature Rules are generally faster than the Newton-Cotes Rule making them more desirable.

Modeling of the density parameter, $\underline{a}$, is discussed in Appendix F. For this example, simple model forms shall be used. The model itself accompanies a set of single-particle shell and pairing energies, S and P, and is of the form,

$$a/A = p_1 - p_2 S \quad ,$$

where A is the mass number and p_1 and p_2 are constants. An older set of single-particle energies is that of Cook et al.[18] Values of p_1 and p_2 they give are

$p_1 = 0.120$

$p_2 = 0.00917$.

In order to compute the mass formula of Appendix A, S, and P values are again calculated, the results differing from those of Cook. Determining a model for the density parameter based upon these values gives,

$p_1 = 0.1624$

$p_2 = 0.0131$.

As mentioned in the Appendix A, the standard deviation of the computed and measured masses using the mass formula is about 700 keV. This is a rather large error on a term which appears in an exponential. The Garvey-Kelson recursion relations[24] give standard deviations between computed and measured masses of only 157 keV, but the relations do not give the deformation dependence of the mass. One may envision a mass formula which gives a ground-state mass according to Garvey-Kelson and a shape dependence according to the mass formula of Appendix A. While the two mass expressions differ by less than 2 MeV, on the average, it shall be shown that the effect upon the yields computed is quite pronounced. of the possible combinations of single-particle energies and masses, three combinations have been selected,

1) S and P values and ground-state masses taken from the mass formula of Appendix A.
2) Cook S and P values and Garvey-Kelson ground-state masses.
3) Garvey-Kelson ground-state masses and S and P values taken from the mass formula of Appendix A.

As with the Garvey-Kelson masses, the mass formula of Appendix A is used to determine the deformation dependence of the Cook shell and pairing energies. For all of these cases, a constant value of the spacing parameter, δ, was chosen with $\delta = 3$ fm. Also in this example, fragment shape degrees of freedom were restricted somewhat by not allowing ε_4 to vary freely. The shapes allowed were those of Figure 1 with ε_4 assuming the value for a given ε corresponding to the midline of the grid, i.e., ε_4 usually equal to zero.

The integrals must be evaluated at every combination of the shape parameters in each fragment. The YMAX configuration is that combination of shapes at which the yield integral is maximum and the GMAX configuration is that combination which maximizes G, which may be determined prior to actual evaluation of the integrals. At each point in the space of shape parameters, the energies essential to G, the Coulomb energy, the masses, the shell and pairing energies, must be computed. These may be recorded as diagnostics. Other quantities recorded for later reference are such things as the scission-point elongation of the fragments, the deformation energies, the parameters of the density of states expression, T, E_x, and E_o, or any combination of any of these quantities deemed of interest. The computed yields provide the weighting function for computing averages of these quantities. Of particular interest are two quantities averaged over all charges and masses, the total kinetic energy (TKE) of the fragments and the energy appearing in

prompt de-excitation, <D> + <E>. Assuming a simple neutron emission model, described in Appendix J, an estimate is made of the number of prompt neutrons, ν_p, and prompt gamma energy, E_γ. Experimental values of these quantities are[25]

$\nu_p = 2.40$

$E_\gamma = 6.96$ MeV

TKE = 169.6 MeV .

The yields obtained for each of the three cases for the GMAX, YMAX, and SUM methods are shown in Figures 2-10. For reference, the chain yields from ENDF/B[8] for this reaction are shown in Figure 11. The total kinetic energies, prompt neutron numbers, and total gamma energy appear in Table 2. Overall agreement is reasonable, the prompt neutron number being a little too high. This may be a result of the fact that the computed chain yield, the weight function for computing these averages, is displaced somewhat from the measured mass-chain yield.

Regarding the mass yield plots, the location of the fragment mass peaks seems least sensitive to the choice of masses and single-particle energies. The peaks are determined by the quantity,

$$G - P_1 - P_2$$

since, in the saddle-point approximation, the yield integral is proportional to

$$\exp[2\sqrt{(a_1 + a_2)(G-P_1-P_2)}]$$

where a_1 and a_2 are constants. The plot in Figures 12 shows

this quantity for the case of S and P values and masses as given by Seeger. The source of the peak is the shell correction term to the binding energy, shown in Figure 13.

Experimentally[8] the mass distribution rises smoothly to mass 90, is fairly flat from mass 90-100, peaking at 95, and drops into a valley about symetric mass splits. The ratio of the yields at mass 95 and 118 is about 600. The computed mass peaks are then 5 to 6 units too close to symmetry as compared to data. Still, the results are encouraging in light of the simplicity of the model.

The valley is well defined for yields computed assuming that the ground-state masses are given by the Garvey-Kelson formula. However, the Seeger mass formula, of Appendix A, gives a much more shallow valley in the YMAX and SUM cases and a third peak in the GMAX case. This serves as an illustration of the sensitivity of the calculation to the input quantities. As a general rule, it is not advisable to correct one mass formula with another. Since only the Seeger formula allows direct evaluation of the mass of nuclei in shapes other than that of the ground-state and has been tested for agreement with neutron-rich mass measurements in a few cases, as discussed in Appendix A, it is more desirable. It should not be surprising, however, if mass asymmetric yields are not easily achieved.

As mentioned in previous discussion, the hope here is to demonstrate the equivalence of either the YMAX or GMAX methods with the SUM method. The chain yield plots are qualitatively similar,

especially the results of the SUM and YMAX methods. The SUM method is dominated by the YMAX term, by definition. The variables over which the sum is performed are the shape variables describing the fragments at the scission-point so that the yield may be seen as a surface in the shape variables. If this surface is sharply peaked at the YMAX configuration, the SUM method may be seen as an integration over a sharply peaked surface. To the extent that this surface is Gaussian, the result is the YMAX value multiplied by some term typical of the width of the Gaussian. To the extent that the width variable is a constant or a slowly varying quantity between fragments, this term drops out of the yield expression upon normalization. The extent to which the YMAX and SUM yields are the same is then a measure of the constancy of this width parameter. There is one complicating factor.

The space of allowed shapes is somewhat limited in that in all of the three cases considered, the GMAX shape required that the heavy fragment assume the shape of maximum prolateness. The YMAX case had a prolatness corresponding to about 0.1 less than maximum value of ϵ, i.e., $\epsilon \simeq 0.6$ for GMAX vs $\epsilon \simeq 0.5$ for YMAX. With the distribution peaked so close to the edge of the shape grid, there may be some terms missing in the SUM method, all of the major contributing terms not appearing within the space of allowed shapes (Figure 1).

The problem may be cast somewhat more quantitatively in the following. Denoting by α the fractional elongation of the symmetry axis of the fragment relative to that of spherical fragment, the

effect upon the G energy of an elongation is given by the relationships,

$$D \propto \alpha^2 \qquad C \propto 1/R \qquad R \propto R_o \alpha \qquad R_o = r_o A^{1/3} \qquad r_o = 1.2254 \text{ fm}$$

where R is the fragment center-to-center distance. About the GMAX configuration, G is approximately parabolic in the α variables for each fragment, α_{light} and α_{heavy}. Then

$$G(\alpha) \simeq G_{max} + \sum_{\substack{i = light, \\ heavy}} \frac{1}{2}\left(\frac{\partial^2 G}{\partial \alpha_i^2}\right)_o (\alpha_i - \alpha_{o,i})^2$$

$$\simeq G_{max} - \left\{ \frac{D_{light}}{\alpha_{o,light}^2} + C\left[\frac{R_{o,light}}{R}\right]^2 \right\} (\alpha_{light} - \alpha_{o,light})^2$$

$$- \left\{ \frac{D_{heavy}}{\alpha_{o,heavy}^2} + C\left[\frac{R_{o,heavy}}{R}\right]^2 \right\} (\alpha_{heavy} - \alpha_{o,\,heavy})^2$$

From the average values of the yields computed, the necessary quantities are C = 166 MeV, R = 19 fm, D_{light} = 2 MeV, D_{heavy} = 15.5 MeV, A_{light} = 102, and A_{heavy} = 134. These values are representative of the three cases. Then,

$$G \simeq G_{max} - \left(\frac{\alpha_{light} - \alpha_{o,light}}{0.153}\right)^2 - \left(\frac{\alpha_{heavy} - \alpha_{o,heavy}}{0.093}\right)^2$$

In terms of the α-coordinates, the space of allowed shapes is limited to values of $\alpha \leq 0.43$. For the YMAX case, the average values are $\alpha \simeq 0.3$ in both fragments. To the extent that the width of the

SUM distribution about the YMAX configuration is measured by the values of the second derivatives of G about GMAX, the edge of the grid is too close to assure inclusion of all of the dominant contributing terms in the SUM method. Errors may be introduced into the YMAX and SUM comparisons as a result of this also. Comparison of the computed mass-chain yields between the YMAX and SUM results shows values in error by a multiplicative factor of 1.57 on the average with extreme values of 0.6 and 3.1 for the three cases considered. This type of error is compatible with those anticipated based upon limitations of the shape grid. The YMAX yield may then be assumed to be typical of the SUM yield, maximum error being a multiplicative $3^{\pm 1}$.

YIELD CALCULATIONS BASED ON THE MORETTO DENSITY FORMULA

To evaluate the yield and interest moments, three integrals must be evaluated,

$$I_y = \int_0^G \int_0^{G-k} k^{1/2} \rho_1(E_1) \rho_2(G-k-E_1)\, dE_1 dk$$

$$I_E = \int_0^G \int_0^{G-k} E_1 k^{1/2} \rho_1(E_1) \rho_2(G-k-E_1)\, dE_1 dk$$

$$I_k = \int_0^G \int_0^{G-k} k^{3/2} \rho_1(E_1) \rho_2(G-k-E_1)\, dE_1 dk \quad .$$

Integral I_y is the unnormalized yield, I_E is the excitation energy moment, and I_k is the translational kinetic energy moment. The

quantities in the integrands are $\rho_i(E_i)$, the density of states of the i^{th} fragment at excitation energy E_i, G, the energy released at the scission point, and k, the prescission translational kinetic energy. In this case, $\rho(E)$ is assumed to be given by the Moretto density expression[12] developed in Appendix D. By this method the thermodynamic functions necessary to determine the density of states are evaluated as sums over realistic single-particle states. In Appendix D, spline fits are determined to the required functions in terms of the temperature, T, of the excited nucleus. Recall the definition,

$$\beta_i = \frac{1}{T_i} = \frac{d\ell n \rho_i(E_i)}{dE_i}$$

Having these analytical expressions, the integrals may be evaluated employing the numerical techniques used to evaluate the integrals over the analytical density expressions. However, with little loss of accuracy, these integrals may be evaluated by the saddle-point technique. Very simply, this means that the integrand is approximated as a Gaussian completely described by a width and a peak value. The integration limits are extended to $\pm \infty$ with the following expression resulting,

$$I = \iint f(x,y)dx\ dy = 2\pi f(x_o,y_o)\ \frac{1}{D^{1/2}} \quad .$$

D is the determinant of 2^{nd} partial derivatives of $\ell n\ [f(x,y)]$

evaluated at the saddle-point, $x_o y_o$. The saddle-point is defined by the solutions to

$$\frac{\partial \ell nf}{\partial x} = 0 \qquad \frac{\partial \ell nf}{\partial y} = 0 \quad .$$

Applying these conditions to the yield integral, I_y, the following equations must be solved

$$T_1(E_{1o}) = T_2(E_{2o})$$

$$k_o = 0.5T_{1o}$$

$$G - k_o - E_{1o}(T_1) - E_{2o}(T_2) = 0 \quad .$$

The second derivatives are, denoting $f_y = \ell n[k^{1/2}\rho_1\rho_2]$

$$\frac{\partial^2 f_y}{\partial k^2} = \frac{-1}{2k_o^2} + \left.\frac{\partial \beta_2}{\partial E_2}\right|_o \qquad \frac{\partial^2 f_y}{\partial E_1^2} = \left.\frac{\partial \beta_1}{\partial E_1}\right|_o + \left.\frac{\partial \beta_2}{\partial E_2}\right|_o$$

$$\frac{\partial^2 f_y}{\partial k \partial E_1} = \left.\frac{\partial \beta_2}{\partial E_2}\right|_o \quad .$$

Since $E_i = E_i(\beta \text{ only})$, $\frac{\partial \beta_i}{\partial E_i} = \frac{d\beta_i}{dE_i}$. Hence, in addition to the splines determined in Appendix D, splines are also needed for $E_i(T_i)$ and $\frac{d\beta_i}{dE_i}$. This derivative was computed exactly, but it was found that the spline approximation to $E_i(T_i)$ was so good that the spline itself could be differentiated to give this quantity with better than 1% agreement to the exact evaluation.

For the integral, I_E, the saddle-point is given by

$$T_2 = (E_1 T_1)/(E_1 + T_1)$$

$$k_o = 0.5 T_2$$

$$G - k_o - E_1(T_1) - E_2(T_2) = 0 \quad .$$

Letting $f_E = \ell n[E_1 k^{1/2} \rho_1 \rho_2]$, the second derivatives are

$$\frac{\partial^2 f_E}{\partial k^2} = \frac{-1}{2k_o^2} + \frac{\partial \beta_2}{\partial E_2}\bigg|_o \qquad \frac{\partial^2 f_E}{\partial E_1 \partial k} = \frac{\partial \beta_2}{\partial E_2}\bigg|_o$$

$$\frac{\partial^2 f_E}{\partial E_1^2} = \frac{-1}{E_{1o}^2} + \frac{\partial \beta_1}{\partial E_1}\bigg|_o + \frac{\partial \beta_2}{\partial E_2}\bigg|_o$$

For the integral I_k, the saddle-point is given by

$$T_1 = T_2$$

$$k_o = 1.5\ T_1$$

$$G - k_o - E_1(T_1) - E_2(T_2) = 0 \quad .$$

Letting $f_k = \ell n[k^{3/2} \rho_1 \rho_2]$, the second derivatives are

$$\frac{\partial^2 f_k}{\partial k^2} = \frac{-3}{2k_o^2} + \frac{\partial \beta_2}{\partial E_2}\bigg|_o \qquad \frac{\partial^2 f_k}{\partial E_1^2} = \frac{\partial \beta_1}{\partial E_1}\bigg|_o + \frac{\partial \beta_2}{\partial E_2}\bigg|_o$$

$$\frac{\partial^2 f_k}{\partial E_1 \partial k} = \frac{\partial \beta_2}{\partial E_2}\bigg|_o \quad .$$

Hence, the saddle-point approximation yields simple plug-in formulas by which all integrals may be evaluated. The accuracy of the approximation must be determined.

To test the validity of the saddle-point approximation, assume the density of the states to be given by

$$\rho(E) = \exp\left(2\sqrt{aE}\right) .$$

For this experiment, the a-parameter shall be assumed to be given by

$$a = A/9.5\ \text{MeV}^{-1}$$

where A is the mass number, and empirically observed result[26]. To span the range of values anticipated, values of A_1 assumed were A_1 = 75, 95, and 118 with A_2 given by 236 - A_1. The integrals were evaluated using a standard 7-point Newton-Cotes Quadrature Rule[23] and the results compared to the saddle-point approximation for values of G ranging from 1 to 65 MeV. The Newton-Cotes evaluation was carried out to a relative computational error of 10^{-4}. The approximation for I_y reproduced the Newton-Cotes value to within 25% at 1 MeV, the error dropping to 2% at 5 MeV and increasing monotonically to 10% at G = 65 MeV. This monotonic error indicates a small systematic error in the saddle-point approximation, but its smallness make the expression acceptable. In the case of the integral, I_E, the saddle-point expression reproduced the Newton-Cotes values very well with an error of 5% at 1 MeV and a monotonically decreasing error with increasing G. The k-moment integral, I_k, was consistently low by about 10% relative to the Newton-Cotes value.

The small value of k predicted by this theory, $k \simeq 1$ MeV, makes this error of little consequence.

A SAMPLE YIELD BASED ON THE MORETTO DENSITY FORMULA

Consider the prediction of yields for the reaction $^{235}U(n_{th},f)$ using the spline fit expressions for the thermodynamic functions required to evaluate the density of states expression according to the Moretto prescription[12] (Appendix D). As an example, assume the spacing parameter, δ, to be a constant for all mass and charge splits, $\delta = 3$ fm, and allow both shapes of freedom, ε and ε_4 in each fragment. Two cases are considered, described previously, the GMAX and YMAX cases. The YMAX method is modified somewhat by requiring the YMAX configuration to lie in the vicinity of the GMAX configuration. This is done by exploring the shape combinations about GMAX until the local maximum is found. This is necessary due to the size of the space of possible shape combinations. With 39 shapes possible in each fragment, there are 39 x 39 combinations for which the yield integral would have to be evaluated. This is simply too expensive. Recall that the interest in the YMAX configuration comes from the possibility that single-particle effects may displace the centroid of the shape distribution from that expected by assuming a minimum potential energy configuration. Masses are taken from the Seeger and Howard[9] mass formula. There are no explicit single-particle energies, S or P.

In Figure 14, the GMAX and YMAX yields are shown. Both yields rise rapidly to about mass 90 and then more slowly toward symmetry.

The GMAX shows a local minimum at mass 102. Both yields favor even mass numbers. The energy to be partitioned is shown for both cases in Figure 15. The behavior is similar to the yield with the obvious pairing effect. The source of the GMAX dip in the yield at mass 102 is apparent in the GMAX G. The dip is suggested in the YMAX G but is totally absent in the YMAX yield. To explain this, the effect of single-particle corrections upon the density of states must be investigated. In the YMAX case, the single-particle shell correction energies for the fragments sum to -1.5 MeV in the vicinity of mass 102 whereas the same energies sum to +0.5 MeV in the GMAX case. This may be understood in the context of the analytical density formulation, namely, that the nuclei with the smaller shell corrections have the larger level densities.

This calculation was repeated for 6 values of δ such that the yield and configuration parameters were scanned through values of $1 \text{ fm} \leq \delta \leq 7 \text{ fm}$. Similar yields were obtained and, based on this fact alone, it is concluded that the statistical model of fission based on the assumption of fixed scission-point tip-to-tip separation is not very good. One point is noteworthy and has implications regarding the analytical density formulation. In Figure 16 are plotted the values of the spectrum averaged values of the single-particle shell energies for the fragment (light) and compliment (heavy). These plots seem to support the observation of Gilbert and Cameron[17] regarding the effect of the shell correction energy upon the density.

A caveat is in order here. In computing the YMAX and GMAX yields, the shapes of the fragments at the scission-point was recorded. For the earlier yield calculation based on the analytical density model, mention was made of the fact that the scission configuration usually occurred at maximum values of the ε shape parameter, $\varepsilon = 0.6$. In the case of yields based on the Moretto density with two shape degrees of freedom, ε and ε_4, the problem with ε is diminished. However, the values of ε_4 now assume the prolate maximum (see Figure 1). It would be a tedious but straightforward process to extend the space of allowed shapes in the ε_4 degree of freedom. To do so, however, would be to admit some rather unphysical shapes, shown in Figure 17, with surface ripples and sharp corners. Looking at the fragment elongations for the two cases in this yield example, α_{light} and α_{heavy},

	$\alpha_{,light}$	$\alpha_{,heavy}$
GMAX	0.504	0.494
YMAX	0.441	0.504

With both ε and ε_4 degrees of freedom available, the maximum elongation is 0.613. In the case of ε only varying, the maximum elongation is 0.432 (Appendix H and Table 1). It may be seen that while the maximum value of ε was not attained, a greater elongation was attained. This is a manifestation of the effect described in the discussion of the scission configuration: as more shape degrees of freedom are added to the collective shape description, the GMAX configuration assumes shapes of greater elongation until, with

infinitely many degrees of freedom, the shape is that of an infinitely long needle.[7] Of course, before that limit is attained, the description of the nucleus via the mass formula breaks down completely.

SEMIQUANTITATIVE AGREEMENT

The yields computed for fixed values of δ bear little resemblance to experimental data. The yield integrals are quite sensitive to δ through the energy release, G. Allowing δ to become a free variable depending upon such things as mass, charge, and incident neutron energy, it may be possible to parameterize the yield in terms of δ in a way which varies smoothly between fissioning systems.

In any comparison made between computed scission-point yields and measured fission product yields, a treatment of prompt neutron emission is necessary. The emission of prompt neutrons appears to be post-scission phenomenon, the neutrons emitted from highly excited fission fragments. Models have been developed to treat the general problem of the decay of highly excited nuclei. These are, in general, too expensive considering the large number of nuclei for which such calculations would be performed. Two simple treatments are presented in Appendix J. These are proposed as methods of estimation of the number of prompt neutrons which may be emitted from the fragments.

To further minimize the effect of prompt neutrons, a parameterization is attempted in terms of the fragment charge. While

the charge yield is not affected by the emission of prompt neutrons, it may be affected by any beta-decay contamination in the data. That such contamination may be present is indicated by the fact that the yield for a given charge is not necessarily equal to that of the complimentary charge in the accepted data set.[8] In the absence of better information, the yield of a given fragment charge is assumed to be the average of the yields of that charge and its compliment.

Yields are computed, y_c, for all masses and charges for seven values of δ, 1 fm $\leq \delta \leq$ 7 fm, giving a set of $y_c(A,Z,\delta)$. These values are then lumped according to charge to give the charge yield, $y_c(Z,\delta)$,

$$y_c(Z,\delta) = \sum_A y_c(A,Z,\delta) \quad .$$

For a given Z, $\log[y_c(Z,\delta)]$ is a smooth function of δ allowing cubic spline interpolation for intermediate values. Assuming some δ_o and Z_o, the solution of

$$\frac{y_c(Z,\delta)}{y_d(Z)} = \frac{y_c(Z_o,\delta_o)}{y_d(Z_o)} \quad ,$$

for all Z, where y_d is the measured (data) yield of a given charge, gives a family of $\delta(Z;Z_o,\delta_o)$ which reproduces the charge yields. To make the final comparison, the logarithms of the computed yields, $y_c(A,Z,\delta)$, are also interpolated using cubic splines in δ. Figure

18 shows the smooth behavior of both charge and independent yields integrals.

As an example, yields for $^{235}U(n_{th},f)$ were computed for both the YMAX and GMAX cases for seven values of δ. Assuming $Z_o = 46$ and $\delta_o = 2$ fm, the family of $\delta(Z)$ shown in Figure 19 results. Using these $\delta(Z)$, the yields were redetermined and are shown in Figures 20 and 21. The two treatments of prompt neutrons described in Appendix J give the final fission product yields shown in Figures 22 and 23. In general, the YMAX yields are smoother and more satisfactory than the GMAX yields and the simple cascade treatment of prompt neutrons is better than the 2T model. Small discrepancies in the computed and measured charge yields, Figure 21, are apparent. This is due to the fact that, in spite of the smooth behavior predicted in Figure 18, the computed yield has some small discontinuous variation as G, increasing with δ, allows other terms to "turn on" and contribute to the total charge yield.

Other integral quantities are of interest here, the total number of prompt neutrons, ν_p, and the total energy available for gamma-ray emission, E_γ, computed from the two neutron models, the prescission kinetic energy, k, the Coulomb energy at the scission point, C, and the average cooling energy, the total energy of de-excitation taken away by emitting a neutron, E_{cool},

	CASCADE		2T	
	GMAX	YMAX	GMAX	YMAX
γ_p	3.96	4.21	3.52	3.77
E_γ	5.43	5.01	7.66	7.41
E_{cool}	7.32	7.45	7.70	7.72
k	1.42	1.38	1.42	1.38
C	158.	157.	158.	157.

All energies are given in MeV. Energy accounting is very good with ν_p x cooling + E_γ, the energy in prompt de-excitation channels, agreeing to within 0.5 MeV for the two neutron treatments for both the YMAX and GMAX cases. Again, the Simple Cascade Model prompt neutron treatment fission product spectra (Figure 23) agrees better with the experimental yields. The total number of prompt neutrons for this case is high by about 1.5 while the total gamma energy is only about 1 MeV low. It then appears that the total fragment excitation energy is high by 10-12 MeV, rather than improperly distributed, on the average, between neutron and gamma decay. Note also that the total fragment kinetic energy, k + C, is low by about 10 MeV.

Up to this point it has been assumed that all of the energy, G, is to be partitioned. From this example, however, it appears that 10 MeV or so of the G energy should be constrained to remain in the translational kinetic energy degree of freedom, i.e., $G = k_o + E_1 + E_2 + k$, with $k_o \approx 10$ MeV. Then $G - k_o$ is the energy to be partitioned. Note that the postulated slow, quasi-static descent from saddle-to-scission[1] is incompatible with the apparent

requirement of a high prescission kinetic energy to achieve overall agreement with experimental observation. A scission configuration which nearly satisfies experimental observed values of the total fragment excitation energy, translational kinetic energy, and yield distribution may be achieved by carefully choosing an amount of energy to be shifted into a constant k_o coupled with the $\delta(Z)$ determination.

In the process of determining the $\delta(Z)$, the energies relevant to determining any energy to be shifted into k_o may also be determined as functions of Z and $\delta(Z)$ and interpolated with cubic splines in δ. The energies of interest are G, the energy released at the scission-point, the scission-point Coulomb energy, C, and the scission-point energy of deformation, D. All quantities used are the spectrum-averaged values. Assuming $Z_o = 46$ and examining these energies as functions of the value of δ_o, the following results are obtained from the GMAX case:

δ_o	<G>	<C>	<D>
2	21.9	158.	14.03
3	32.2	152.	9.57
4	41.6	145.	7.16
5	49.4	138.	6.40
6	56.9	133.	4.36
7	63.3	129.	3.06

All energies are in MeV. For the case of $\delta_o = 2$ fm, the GMAX yield gives $\nu_p = 3.96$ and an average neutron cooling energy of 7.32

MeV/neutron. For this case, the value, <G> = 21.9 MeV, yielded 6 or 7 charges for each mass, similar to ENDF/B.[8] This value may be taken as a lower bound on <G> with lower values giving to few charges. The prompt neutron yield is governed by the sum of the excitation and deformation energies, <E> + <D>. For the purpose of this exercise, it shall be assumed that <E> $\simeq$ <G> since <k> is generally small. The value of ν_p is high by about 1.5 in the δ_o = 2 fm case.[8] At 7.32 MeV cooling energy, the indication is that <G> + <D> is high by about 1.5 x 7.32 MeV $\simeq$ 11.0 MeV. The amount of energy necessary for the desired number of prompt neutrons is then about (21.9 + 14.03) - 11.0 $\simeq$ 25.0 MeV. By increasing the value of δ_o, the energy, G, in excess of about 22.0 MeV may be arbitrarily moved into the prescission kinetic energy degree of freedom and, after adding the Coulomb energy, compared to the experimental value. At the same time, the sum of the deformation energy and G may be compared to the value needed for the prompt neutrons and gammas, 25.0 MeV. Defining the energy which may be shifted, Δ, as

$$\Delta = \langle G \rangle - 21.9 \text{ MeV} \quad ,$$

the total kinetic energy is given by <k> + <C> + Δ. The energy for prompt neutrons and gammas is <E> + <D> = <G> + <D> - <k> - Δ $\simeq$ <G> + <D> - Δ . The following results are obtained:

δ_o	Δ	$\langle C \rangle + \Delta$	$\langle G \rangle + \langle D \rangle - \Delta$
3	10.3	162.3	31.47
4	19.7	164.7	29.06
5	27.5	165.5	28.03
6	35.0	168.0	26.26
7	41.4	170.4	24.96

Recalling the k is of the order of 1 MeV and that the gamma ray energy was low by about 1 MeV, some δ_o between 5 and 6 fm should give acceptable results.

Assuming $\delta_o = 5$ fm and $Z_o = 46$, the computed G-energy is arbitrarily shifted by 27.5 MeV. The yield integrals are evaluated at 5, 6, and 7 fm and quadratic splines used to interpolate intermediate values of δ. Fitting gives the family of $\delta(Z)$ shown in Figure 24. Using these values, the yields were recomputed. In Figures 25 and 26 the fragment mass and charge distributions resulting are shown. Assuming the simple cascade treatment (Appendix J) of the prompt neutrons, the fission-product distribution shown in Figure 27 results. Again, YMAX yields are somewhat better than GMAX yields.

Energy accounting may be performed. The spectrum averaged energies of interest are

	GMAX	YMAX
ν_{pl}	1.223	1.067
ν_{ph}	1.586	1.948
$E_{\gamma l}$	2.338	2.230
$E_{\gamma h}$	2.412	2.890
$cool_l$	7.401	7.427
$cool_h$	7.073	7.162
C	141.3	139.4
k	28.33	28.28

Again, energies are in MeV. Where appropriate, the terms are listed separately for the light(l) and heavy(h) fragment. Experimental values are available[8,25] for ν_p, E_γ, and total kinetic energy, $\overline{TKE}$, a bar over the quantity denoting an experimental value,

$\overline{\nu}_p$ = 2.40

$\overline{E}_\gamma$ = 6.96 MeV

$\overline{TKE}$ = 169.6 Mev

The computed number of neutrons is high and the gamma energy low. With the average cooling energy available for each emitted neutron, ΔE_ν may be defined,

$$(\nu_{pl} + \nu_{ph} - \overline{\nu}_p) \times \left[\frac{\nu_{pl} \times Cool_l + \nu_{ph} \times Cool_h}{\nu_{pl} + \nu_{ph}} \right] = \Delta E_\nu \quad .$$

Here, ΔE_ν is the estimate of the excess excitation energy in the neutron decay channel. For the gamma decay channel, a similar