Time Dependent Neutronics for Laser Fusion Blanket and Materials Analysis

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F. Beranek and R.W. Conn

Fusion Technology Institute
University of Wisconsin
1500 Engineering Drive
Madison, WI 53706

http://fti.neep.wisc.edu

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Abstract

Time dependent neutronics studies are an important part of the analysis of a laser fusion system. It has been found that swelling may be less in metals undergoing a pulsed irradiation rather than steady irradition with an equivalent average wall loading. Analysis of the neutron pulse is thus necessary for accurate radiation damage work.

The differences between neutronics studies for a magnetic confinement fusion reactor (MCTR) and the inertially confined fusion reactor (ICTR) are discussed. It is shown that some of the calculational techniques used for the MCTR studies do not work for the ICTR. In particular, the discrete ordinates method for solving the time dependent transport equation often produced negative scalar fluxes. This problem can be attributed to the Legendre polynominal expansion used for the differential transfer cross sections. A new expansion method is discussed which retains the Legendre polynomial formalism yet results in positive fluxes.

Damage results are given for the preliminary SOLASE calculations which indicate extremely high instantaneous displacement rates are possible in this type of system. A peak displacement rate of 4.5 dpa/sec was calculated in SS 316 with a wall loading of .255 MJ/m^2/pulse.

I. Introduction

Neutronics is an integral part of any nuclear reactor system design. In fission reactors the concern is for the neutron multiplication factor and the material damage to the fuel assemblies and reactor vessel. Tritium breeding, neutron energy deposition, and material damage to the walls and structure of a reactor are the problems for fusion reactor systems. The calculation of the primary parameters can be accomplished using traditional steady state neutron transport codes such as ANISN.[1]

A new problem arises in inertially confined thermonuclear reactor (ICTR) systems because the time history of the neutron source dramatically affects the instantaneous damage rate even though the average damage rate to the structure in an ICTR is the same as that of an MCTR of equal wall loading. The rate at which the damage occurs in an ICTR is several orders of magnitude greater than in all other systems and may influence the choice of laser pulse repetition rate.[2] In particular, it has been shown that there is a temperature dependent pulse frequency threshold. If the system is pulsed at a rate lower than this limit, void growth is inhibited while a higher pulse rate allows void growth. The reason is that the very high instantaneous fluxes of the ICTR produce extremely high dpa rates (~1-10 dpa/s). The recombination rate between vacancies and interstitials is dependent on the product of their concentrations so the high dpa rates are followed by high recombination rates. The removal rate of vacancies to voids is only linearly proportional to the vacancy concentration (the void concentration remaining constant) so many of the vacancies will recombine with interstitials before migrating to voids. This causes the swelling to be less than that which is produced if the vacancies are produced over a longer time interval. Thus even though the average dpa rate is the same for equal wall loadings in the two fusion systems, the swelling in

the ICTR may be less. Only by performing time dependent neutronics studies can the damage rates be accurately evaluated. A time dependent neutron transport code, TDA, is being used for this purpose.[3]

II. Neutron Source

The energy and arrival time characteristics of the neutron source in an MCTR are well known. The fusion reactions producing the neutrons may be sustained for thousands of seconds. Since the plasma is relatively tenuous ($\sim 10^{14}/cm^3$), the neutrons have no collisions as they travel to the wall in an energy packet centered at an average of 14.1 MeV. The width of the packet is determined by the temperature of the fuel. The time of flight spreading of the packet due to the energy spread has no significance in the damage calculation since the time spread is on the order of nanoseconds, much less than the actual source duration time. The neutron slowing down time in the blanket is on the order of tens or hundreds of microseconds which again is much less than the source length. The neutronics of an MCTR are thus characterized as a steady state problem with a 14.1 MeV source. In performing a multigroup calculation for this problem, a fraction of the source neutrons may need to be placed in lower energy groups if the energy spread encompasses more than just the first group (Table I).

The source for an ICTR has a very different arrival time spectrum but a similar energy spectrum. In a pellet explosion, the outward directed velocity of the fuel adds another component to the spread of the energy spectrum. The full width at half maximum (fwhm) of the spectrum will be larger than the spread of the MCTR energy distribution in which the fuel temperature is the only mechanism causing the spread. If neutron collisions with the pellet debris are considered, the energy spectrum is slightly softer but presently the magnitude of this effect is unknown. The softening is dependent on the ρR of the pellet and the nature of the pellet explosion. A neutron energy spectrum from a pellet of $\rho R=5$ (neglecting neutron-fuel collisions) has been calculated to have a fwhm of 1.7 MeV about an average of 14.1 MeV.[4]

An important characteristic of the source is the time span over which it actually exists. This is determined by the period over which the fusion reactions occur. Typically this is on the order of 10-100 ps. The time of flight spreading of the pulse as it travels on the order of 5m to the first wall causes the time spectrum width to be 10 ns. This is greater than the actual source duration and so becomes the effective source width. Since this time is less than the neutron slowing down time in the blanket a pulsed neutron problem exists. The same total number of neutrons are present in this pulse as exist over a one second period in an MCTR (assuming equal energy release) but they all arrive over a 10 ns period in the ICTR. This produces the high instantaneous damage rates which are of interest to the material damage investigators.

III. Cross Section Expansion

Determination of the damage rates is accomplished by following the neutron pulse in time through the zones of interest. A time dependent discrete ordinates neutron transport code can be used to calculate these rates. However, serious problems arise in the calculation because large negative scalar fluxes appear as the pulse passes through the material zones. Variation of the spatial or time mesh has no corrective effect.

The source of the problem is the expansion of the cross section data in Legendre polynomials. The fit of a highly anisotropic differential cross section (which is peaked near $\mu=1$ and zero in a large portion of the remaining range of μ) with a third order polynomial is substantially in error for most scattering angles. Though the first few moments of the cross section are preserved, the cross sections for scattering through a majority of the angles are incorrect and often negative due to the oscillatory nature of the polynomial. Since in a discrete ordinates code only cross sections for scattering through certain specified angles are required, the cross section expansion by moment preservation is inadequate.

The most significant problem lies in the calculation of the first collided source. The procedure in TDA utilizes the source group in-group scattering cross section which is very anisotropic at 14 MeV. In addition, the external neutron source in this problem is extremely anisotropic being essentially a monodirectional beam normal to the surface. The anisotropic source and Legendre polynomial cross section expansion combine producing large negative angular fluxes which result in negative scalar fluxes at times after the uncollided and forward scattered fluxes leave the zone. It should be mentioned that if either the cross sections or the source are isotropic no negative scalar fluxes will appear.

A method is being developed to correctly compute the necessary cross sections using the Legendre polynomial formalism. This formalism is preserved since most neutronic computer codes are written to accept Legendre polynomial expansion coefficients. The new method calculates the coefficients in a manner which preserves the exact differential cross section rather than the cross section moments.

Let us digress briefly to review the scattering and source terms in the transport equation. The time dependent form of the neutron transport equation can be written as

$$\frac{\partial}{\partial t} vN(\vec{r},E,\vec{\Omega},t)+\vec{\nabla}\cdot\vec{\Omega}vN(\vec{r},E,\vec{\Omega},t)+\Sigma_t(\vec{r},E)vN(\vec{r},E,\vec{\Omega},t)$$

$$=\int\int v'\Sigma(\vec{r},E')f(\vec{r};E',\vec{\Omega}'\rightarrow E,\vec{\Omega})N(\vec{r},E',\vec{\Omega}',t)dE'd\vec{\Omega}'+q(\vec{r},E,\vec{\Omega},t)$$

where

$N(\vec{r},E,\vec{\Omega},t) \equiv$ neutron density,

$\Sigma(\vec{r},E')f(\vec{r};E',\vec{\Omega}'\rightarrow E,\vec{\Omega}) \equiv$ probability per unit path length of a neutron transferring from $(E',\vec{\Omega}')$ to $(E,\vec{\Omega})$ at $\vec{r}$,

$q(\vec{r},E,\vec{\Omega},t) \equiv$ external neutron source, and

$\Sigma_t \equiv$ macroscopic total cross section.

The scattering term is often expanded in a series of Legendre polynomials for easier numerical manipulation,

$$\Sigma(\vec{r},E')f(\vec{r};\ E',\vec{\Omega}'\rightarrow E,\vec{\Omega}) = \sum_{\ell=0}^{\infty} \frac{2\ell+1}{4\pi} \Sigma_\ell\ (\vec{r},E'\rightarrow E)\ P_\ell\ (\mu_o)$$

where $\mu_o=\vec{\Omega}\cdot\vec{\Omega}'$. The orthogonality property of Legendre polynomials is used in the traditional method of calculating the expansion coefficients as

$$\Sigma_\ell(\vec{r};\ E'\rightarrow E) = 2\pi \int_{-1}^{1} \Sigma(\vec{r},E')f(\vec{r};\ E'\rightarrow E,\mu_o)P_\ell(\mu_o)d\mu_o.$$

The $P_\ell(\mu_o)$ term is then expanded into a form more suitable for integration using the Addition Theorem for Legendre polynomials,

$$P_\ell(\mu_o)=P_\ell(\mu)P_\ell(\mu')+2\sum_{m=1}^{\ell} \frac{(\ell-m)!}{(\ell+m)!} P_\ell^m\ (\mu)\ P_\ell^m\ (\mu')\cos\ m\ (\phi'-\phi)$$

where the P_ℓ^m terms are the associated Legendre functions. Integration over ϕ' causes the second term to vanish resulting in the following scattering term,

$$\int_{-1}^{1} \sum_{g'=1}^{G} \sum_{\ell=0}^{\infty} \frac{2\ell+1}{2} \Sigma_\ell^{g'\to g} P_\ell(\mu) P_\ell(\mu') \Phi_{g'} d\mu'$$

where the multigroup approximation has been made. The discrete ordinates form of this term allows the angular integration to be represented by a summation,

$$\int_{-1}^{1} P_\ell(\mu')\Phi_{g'}(x,\mu',t)d\mu' \cong \sum_{i=1}^{N} \omega_i P_\ell(\mu_i)\Phi_{g'}(x,\mu_i,t)$$

with the μ_i representing the discrete direction cosines and the ω_i terms being the quadrature weights. The resulting expression is

$$\sum_{g'=1}^{G} \sum_{\ell=0}^{\infty} \frac{2\ell+1}{2} \Sigma_\ell^{g'\to g} P_\ell(\mu_i) \sum_{j=1}^{N} \omega_j P_\ell(\mu_j) \Phi_{g'}(x,\mu_j,t) \quad .$$

This represents the number of neutrons travelling in all directions and at all energies which are scattered into group g and angle μ_i.

Also included as a source of neutrons in this part of phase space is the external source (the first collided source) which is represented as

$$Q_{g'}(x,\mu_i,t) = \sum_{\ell=0}^{\infty} \frac{2\ell+1}{2} \Sigma_\ell^{g'\to g'} P_\ell(\mu_i) Q_{g'}(x,t)$$

when the uncollided flux is incident normal to the surface ($\mu_j=1$, $P_\ell(\mu_j)=1$). It has been shown elsewhere that a Legendre polynomial expansion of the in-group scattering cross section for any nuclide (replacing the upper limit of the ℓ summation in the above expression with a L for a P_L expansion) produces negative values for scattering into certain angles.[5] Positive values for scattering into directions which are impossible for a neutron to reach and remain in the same energy group are also created.

The basis for the new method of calculating the coefficients lies in the physical interpretation of the source terms in the transport equation. The Q_g term represents the probability that a neutron travelling normal to the surface in energy group g will scatter into the angular range represented by μ_i and remain in energy group g. This quantity can be calculated exactly for each μ_i and should be preserved by the expansion. Similarly, the scattering probability

between any two discrete angles should be preserved by the expansion. If this is done correctly, the total cross section is preserved as the first expansion coefficient as in the traditional method. However in the new method, the scattering between all angles and the first collided source will be accurately computed.

As a brief example, the equations for obtaining a set of S_2 coefficients is outlined. The following cross sections are preserved:

$$\sigma(1\rightarrow\mu_i): \quad i=1,2,3$$
$$\sigma(\mu_i\rightarrow\mu_i): \quad i=1,3$$
$$\sigma(\mu_i\rightarrow\mu_j): \quad i=1,j=2.$$

All other cross sections are equal to one of the above if the usual symmetry conditions ($\mu_i=-\mu_{N+1-i}$; $\mu_{N+1}=-1$) are observed. In order to obtain the expansion coefficients, the following equations must be solved:

$$\sigma(1\rightarrow\mu_1) = \sum_{\ell=0}^{5} \frac{2\ell+1}{2} P_\ell(\mu_1)\,\sigma_\ell \qquad \sigma(\mu_1\rightarrow\mu_1) = \sum_{\ell=0}^{5} \frac{2\ell+1}{2} P_\ell^2(\mu_1)\,\sigma_\ell$$

$$\sigma(1\rightarrow\mu_2) = \sum_{\ell=0}^{5} \frac{2\ell+1}{2} P_\ell(\mu_2)\,\sigma_\ell \qquad \sigma(\mu_3\rightarrow\mu_3) = \sum_{\ell=0}^{5} \frac{2\ell+1}{2} P_\ell^2(\mu_3)\,\sigma_\ell$$

$$\sigma(1\rightarrow\mu_3) = \sum_{\ell=0}^{5} \frac{2\ell+1}{2} P_\ell(\mu_3)\,\sigma_\ell \qquad \sigma(\mu_1\rightarrow\mu_2) = \sum_{\ell=0}^{5} \frac{2\ell+1}{2} P_\ell(\mu_1)P_\ell(\mu_2)\,\sigma_\ell.$$

This technique allows accurate results to be obtained without recourse to modification of the code. It only requires the alteration of the data library.

There are some drawbacks to this technique. The new expansion requires a larger order Legendre polynomial expansion than is normally used. In previous work a P_3 expansion had been found to be adequate. However in the new method, the expansion order is determined by the quadrature order. An S_N calculation requires a $P_{\left(\frac{N(N+6)+4}{4}\right)}$ fit for complete accuracy. A P_N fit for an S_N calculation

suffices if only the first collided flux is to be computed exactly. It has been found that this correction reduces the magnitude of the error but does not eliminate it entirely. Thus larger data libraries must be constructed to allow for the larger number of expansion coefficients.

Another disadvantage of this method is that the cross section expansion order is determined by the quadrature order. Thus, different data sets must be used for different order S_N calculations. This does not increase the cost of a calculation but requires the storage of several data sets and may prove more serious upon implementation of various options which are to be added to the code and are discussed shortly.

IV. Code Efficiency

The present code, TDA, consumes a relatively large amount of computer time while performing a calculation. Two hours and forty minutes of CPU time is consumed on a UNIVAC 1110 system for a problem with 130 time steps simulating a neutron pulse slowing down for 10 μs using an S_4-P_3 model. An S_4 model is a very crude approach to this problem considering the anisotropy of the source but it is conjectured that an S_8 calculation would consume almost 5 hours. Therefore another goal of the research at the University of Wisconsin is the development of techniques that would reduce the time required for a calculation.

One method is to allow an energy dependent quadrature order. At low energies the flux and cross sections are nearly isotropic. Thus there is no reason to require an S_8 formulation at these energies merely because the high energy flux is very anisotropic. The ability to perform a high order S_N calculation at high energies and switch to a lower order as the energy decreases is a very important asset. This option is presently being investigated.

An anticipated problem is that of the changing Legendre expansion order if this option is implemented with the new expansion method. Several data sets must then be used. One would then want to construct a data set for the particular calculation using the appropriate cross sections from each library. This would be compiled before the transport calculation and used as data for the program.

V. Results

The cross section expansion modification outlined earlier has been implemented for the in-group scattering cross sections of the first energy group and for the nuclides used in the preliminary Solase blanket (Fig. I). The blanket consists of a spherical shell with an inner diameter of 10 m. The innermost portion of the shell contains a 1.5 cm thick graphite liner of normal density supported such that the back of the liner is 1 cm from the first wall. The first structural wall is composed of a bank of stainless steel pipes (O.D.=1cm; I.D.= .8cm) and can be represented for neutronics purposes by homogenizing the zone creating a 1 cm region of stainless steel with a density factor of 0.36. This wall is followed by a breeding zone of Li_2O, He and a small amount of structure. In an effort to save computer time, the breeding zone is not extended to its actual dimensions. Since the damage to the liner and first wall are the main concerns, the blanket extends only 20 cm with appropriate albedos entered to account for backscattering.

The damage results correspond to a 100 MJ microexplosion and a peak neutron wall loading of .255 MJ/m^2/pulse. The damage rates initially follow the shape of the pulse which is expected since this is the highest flux the region receives. An interesting result is that although the peak displacement rate for SS316 is about 4.5 dpa/sec and for graphite is 2.7 dpa/sec, the total number of displacements per pulse is about the same (figs. II-V). This is because the displacement cross sections for stainless steel at high energies are almost twice as high as those for graphite while the opposite is true at lower energies and suggests that caution should be exercised in using steady state (or cumulative) results to project possible peak rates.

Acknowledgement

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VI. References

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2. N. Ghoniem and G. L. Kulcinski, "Void Growth Kinetics Under an Irradiation Pulse," Nuclear Engineering Department Report UWFDM-138, University of Wisconsin (October 1975).

3. S. A. Dupree, et al., "Time Dependent Neutron and Photon Transport Calculations Using the Method of Discrete Ordinates," Joint Los Alamos Scientific Laboratory - Oak Ridge National Laboratory Report LA-4557 (ORNL-4662) (1971).

4. Geoffrey Shuy, private communication.

5. F. Beranek, "Time Dependent Neutronics Studies for Inertial Confinement Reactor Systems," Thesis Proposal at University of Wisconsin (March 1977).

Tables and Figures

Table 1

Neutron 25 Energy Group Structure in eV

Group	Group Limits E(Top)	E(Low)	E(Mid Point)
1	1.4918 (+7)	1.3499 (+7)	1.4208 (+7)
2	1.3499 (+7)	1.2214 (+7)	1.2856 (+7)
3	1.2214 (+7)	1.1052 (+7)	1.1633 (+7)
4	1.1052 (+7)	1.0000 (+7)	1.0526 (+7)
5	1.0000 (+7)	9.0484 (+6)	9.5242 (+6)
6	9.0484 (+6)	8.1873 (+6)	8.6178 (+6)
7	8.1873 (+6)	7.4082 (+6)	7.7979 (+6)
8	7.4082 (+6)	6.7032 (+6)	7.0557 (+6)
9	6.7032 (+6)	6.0653 (+6)	6.3843 (+6)
10	6.0653 (+6)	5.4881 (+6)	5.7787 (+6)
11	5.4881 (+6)	4.4933 (+6)	4.9907 (+6)
12	4.4933 (+6)	3.6788 (+6)	4.0860 (+6)
13	3.6788 (+6)	3.0119 (+6)	3.3453 (+6)
14	3.0119 (+6)	2.4660 (+6)	2.7390 (+6)
15	2.4660 (+6)	1.3534 (+6)	1.9097 (+6)
16	1.3534 (+6)	7.4274 (+5)	1.0481 (+6)
17	7.4274 (+5)	4.0762 (+5)	5.7518 (+5)
18	4.0762 (+5)	1.6573 (+5)	2.8667 (+5)
19	1.6573 (+5)	3.1828 (+4)	9.8779 (+4)
20	3.1828 (+4)	3.3546 (+3)	1.7591 (+4)
21	3.3546 (+3)	3.5358 (+2)	1.8541 (+3)
22	3.5358 (+2)	3.7267 (+1)	1.9542 (+2)
23	3.7267 (+1)	3.9279 (+0)	2.0597 (+1)
24	3.9279 (+0)	4.1399 (-1)	2.1718 (+0)
25	4.1399 (-1)	2.200 (-2)	2.1800 (-1)

Table I (cont.)

Gamma-Ray 21 Energy Group Structure in MeV

Group	Group Limits E(Top)	E(Low)	E(Mid Point)
1	14.00	12.00	13.00
2	12.00	10.00	11.00
3	10.00	8.00	9.00
4	8.00	7.50	7.75
5	7.50	7.00	7.25
6	7.00	6.50	6.75
7	6.50	6.00	6.25
8	6.00	5.75	5.875
9	5.75	5.00	5.375
10	5.00	4.50	4.75
11	4.50	4.00	4.25
12	4.00	3.50	3.75
13	3.50	3.00	3.25
14	3.00	2.50	2.75
15	2.50	2.00	2.25
16	2.00	1.50	1.75
17	1.50	1.00	1.25
18	1.00	0.40	0.70
19	0.40	0.20	0.30
20	0.20	0.10	0.15
21	0.10	0.001	0.0505

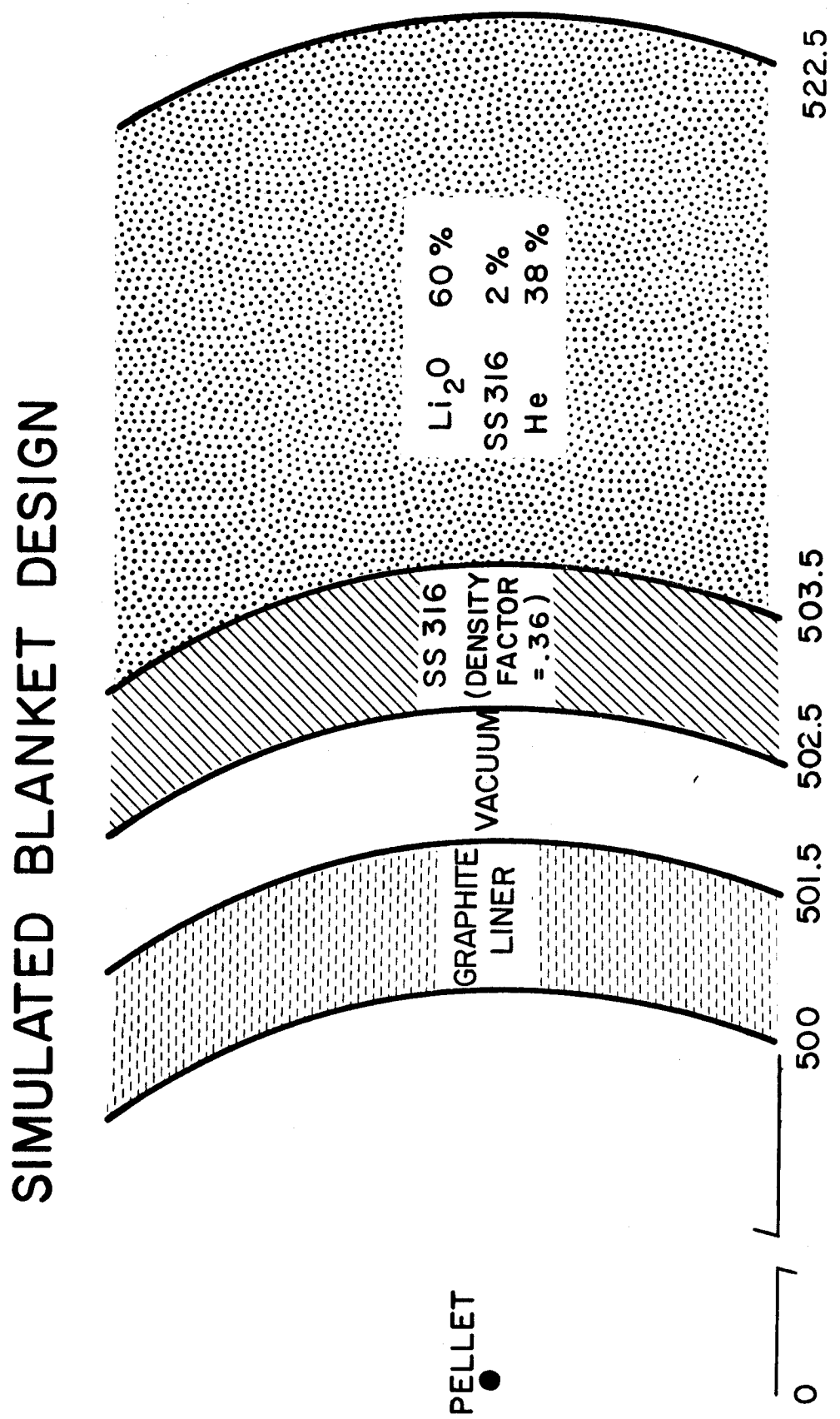
SIMULATED BLANKET DESIGN
PELLET
0
500
501.5
502.5
503.5
522.5
GRAPHITE LINER
VACUUM
SS 316 (DENSITY FACTOR = .36)
Li_2O 60 %
SS 316 2 %
He 38 %

FIGURE I

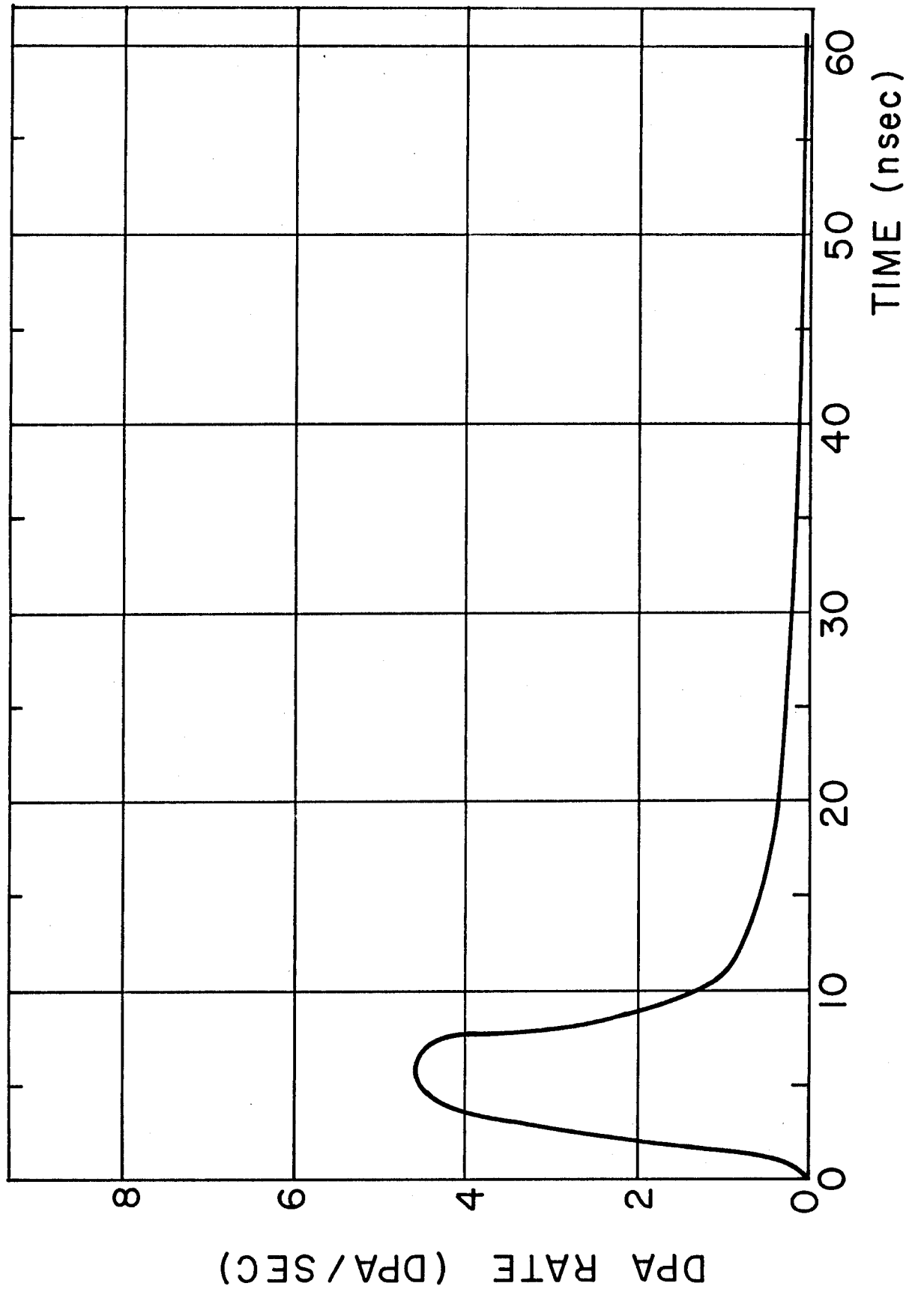
DPA RATE (DPA/SEC)
0
2
4
6
8
0
10
20
30
40
50
60
TIME (nsec)
DPA RATE IN 316 SS VS TIME
FOR UWICTR

FIGURE II

CUMULATIVE DPA IN SS 316 VS. TIME
NORMALIZED TO
5.2×10^{-8}

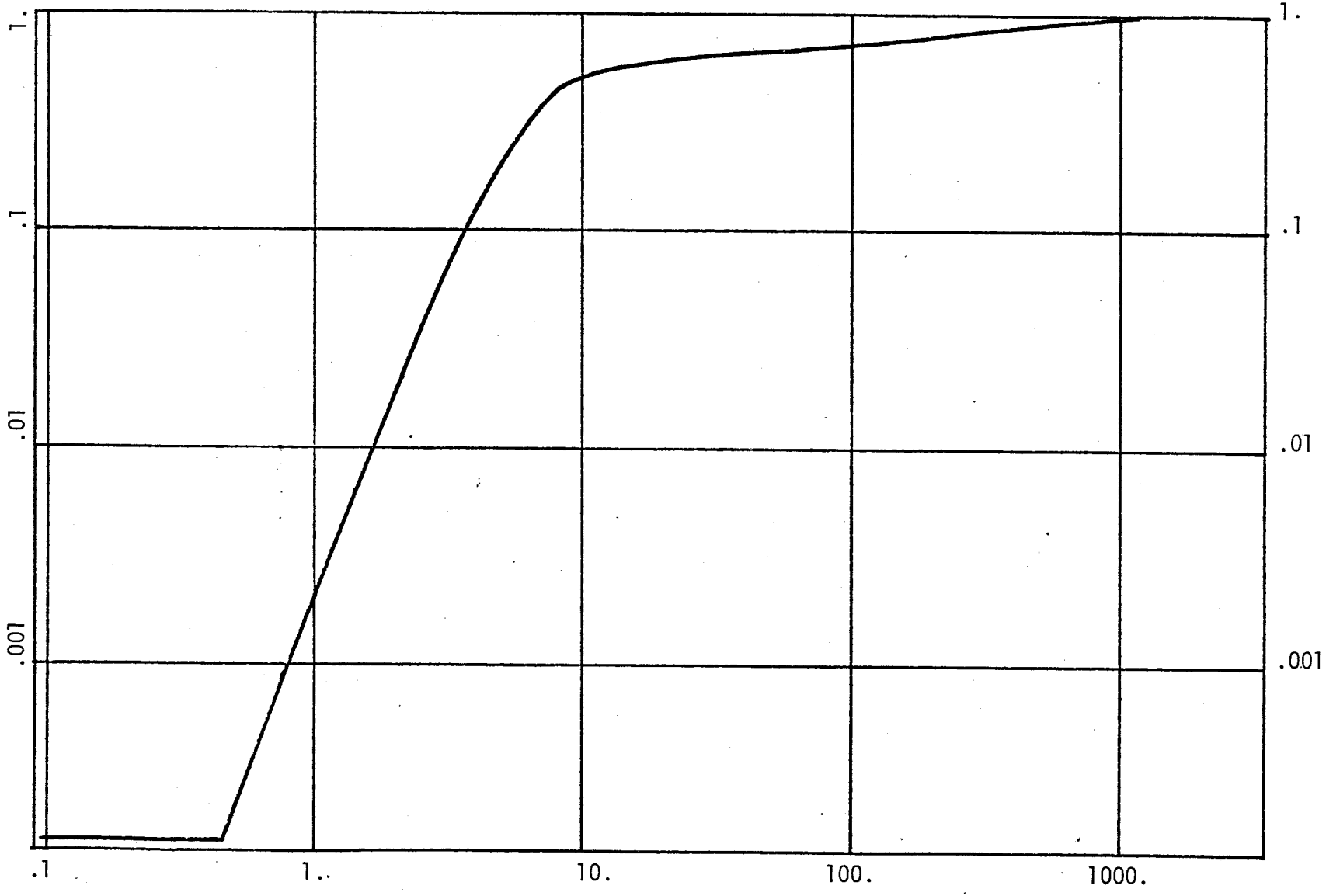

FIGURE III

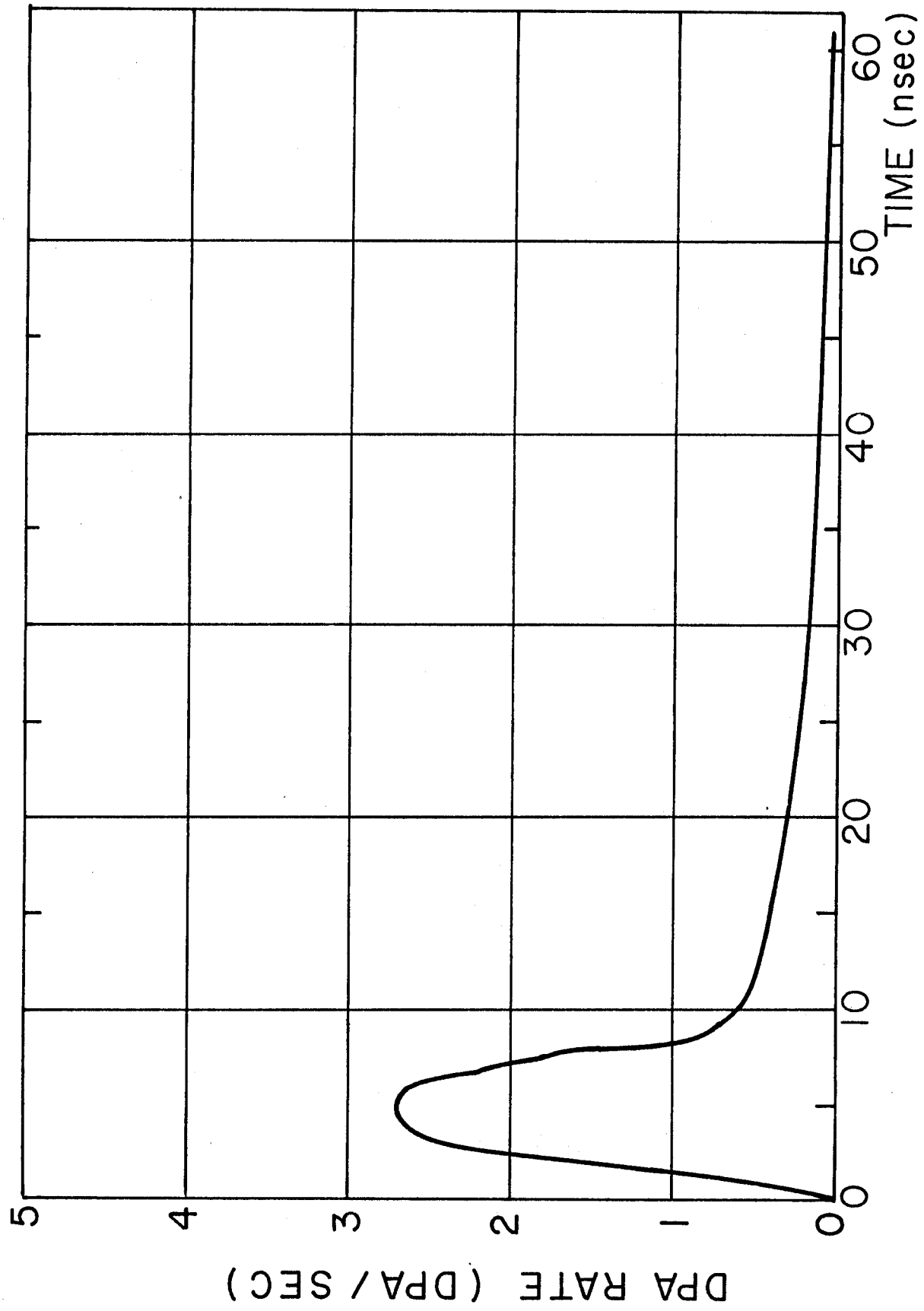
DPA RATE (DPA / SEC)
0
1
2
3
4
5
0
10
20
30
40
50
60
TIME (nsec)
DPA RATE IN GRAPHITE VS TIME
FOR UWICTR

FIGURE IV

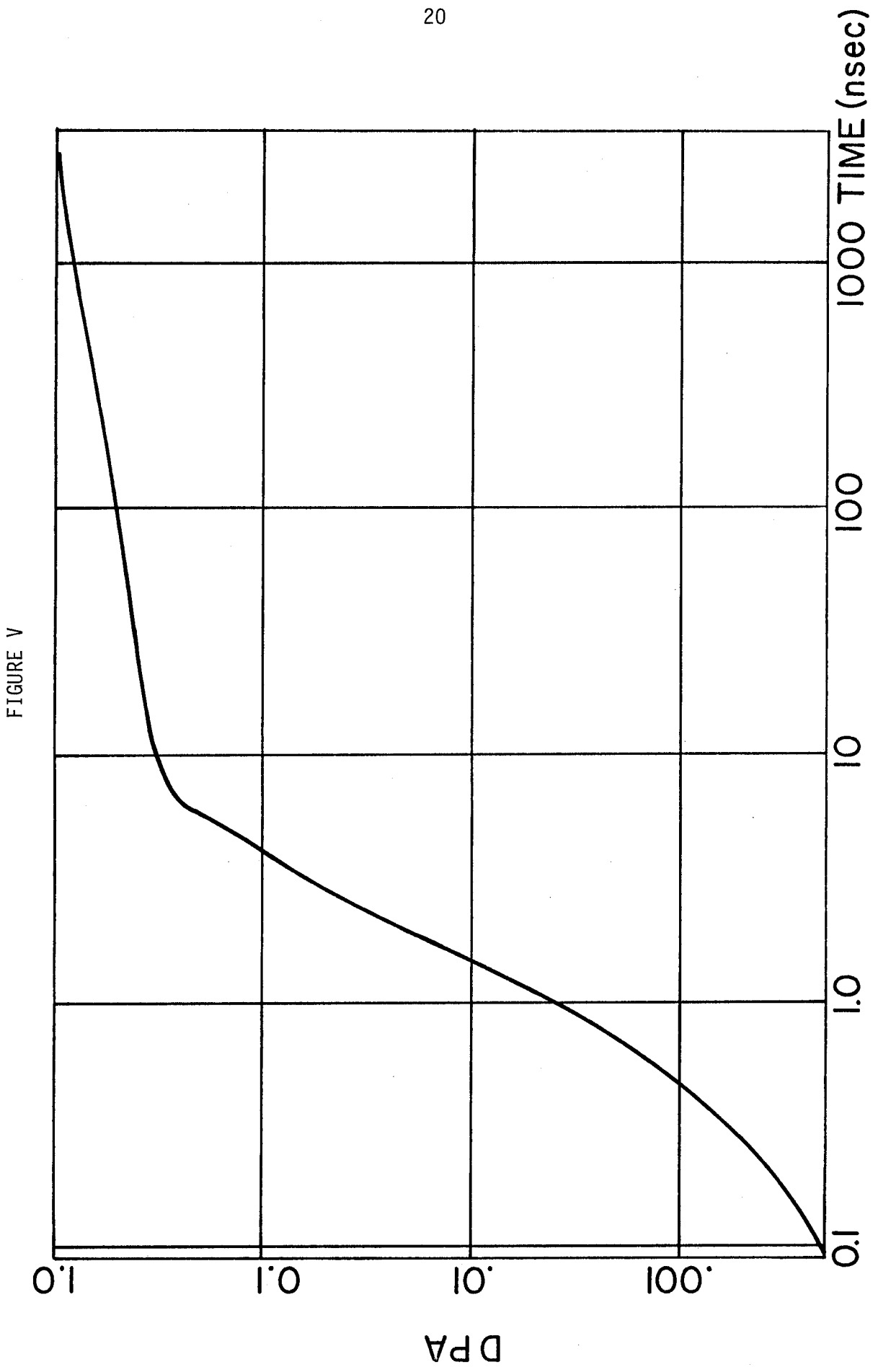
DPA
1.0
0.1
.01
.001
0.1
1.0
10
100
1000 TIME (nsec)
CUMULATIVE DPA IN GRAPHITE VS TIME
NORMALIZED TO TOTAL OF 5.19 x 10^-8

FIGURE V

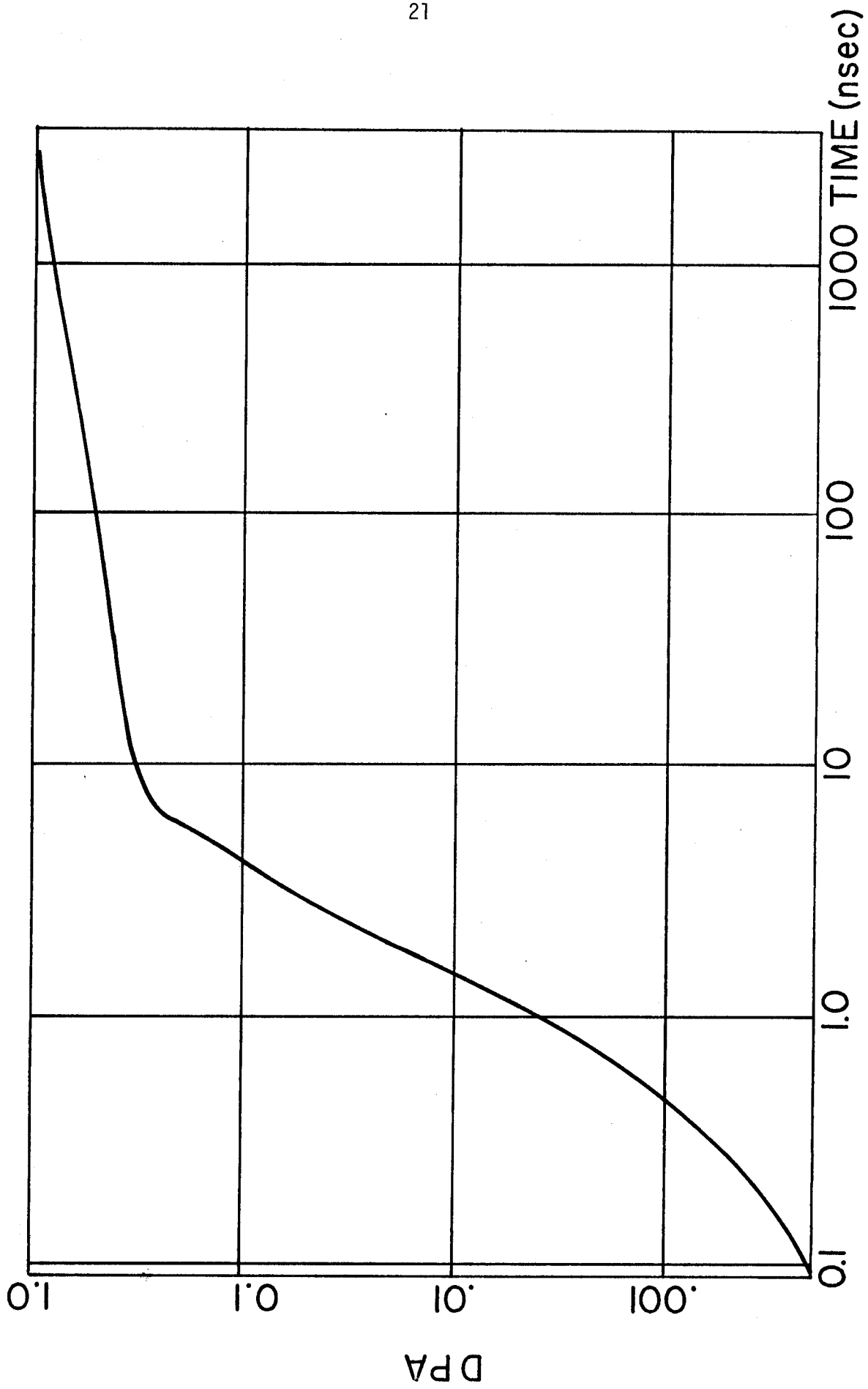
DPA
1.0
0.1
.01
.001
0.1
1.0
10
100
1000 TIME (nsec)
CUMULATIVE DPA IN GRAPHITE VS TIME
NORMALIZED TO TOTAL OF 5.19 x 10⁻⁸

FIGURE VI