**THEORETICAL PHYSICS DIVISION
ANNUAL REPORT
January-December 1975
Volume 1**

T. Wainwright

B. Tarter

MASTER

January 20, 1976

Prepared for U.S. Energy Research & Development
Administration under contract No. W-7405-Eng-48

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INTRODUCTION

The Theoretical Physics Division supports research that spans a broad range of pure and applied physics. This first annual T-Division report covers (in Vol. 1) the Division's unclassified research during the 1975 calendar year; classified research is described in a second volume. Since most of the Division's activities in 1975 were funded by ERDA's Division of Military Applications, research devoted to direct and indirect or long-range support of nuclear weapons development is emphasized. Recently, the Division has increased its participation in other Laboratory programs funded by ERDA. It has also been able to broaden its research activities by involvement in programs funded by other government agencies — and plans to do more such reimbursable work. In this way the Division will try to remain as versatile as possible so as to continue to meet the demands of the weapons program while providing the Laboratory with a broad enough research base to respond rapidly and effectively to new programs.

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1. ATOMIC, MOLECULAR, AND NUCLEAR PHYSICS

Introduction

The Division's work in atomic, molecular, and nuclear physics support the weapons program primarily through the maintenance of atomic and nuclear data libraries and through the determination of photon and neutron cross sections. Research in these areas of physics also is fundamental to various reimbursable contracts and other Laboratory programs; for example, the x-ray laser studies were funded by the Advanced Research Projects Agency, the nuclear

theory effort aids the Laboratory's experimental nuclear physics program, and the work on molecular photodissociation is relevant to certain isotope separation schemes. In addition, most of the topics discussed here currently are under investigation in universities, so that this work provides a strong and mutually beneficial source of interaction between Laboratory physicists and academic researchers.

Opacities

THE HOPE CODE

Over the past several years we have developed a general code, HOPE, which can compute the equation of state, frequency-dependent photon absorption coefficients, and mean radiative and conductive opacities, for a single element at nearly arbitrary temperature and density. During the past year the code has been expanded to allow calculations for mixtures of up to ten elements. HOPE, and the mixture version, HOPE-S, are now the standard opacity production codes for the Laboratory. Here, we briefly describe the basic physics contained in HOPE, discuss the recent work involved in its extension to mixtures, and indicate the areas in which further effort is still needed.

To calculate the transport of energy by photons, one needs to know their material absorption coefficient. This coefficient can be written as

$$K_{\nu} = \sum_{i,j} N_i \sigma_{ij}(\nu)/\rho.$$

where N_i is the number of atoms in quantum state i , ρ is the density, and $\sigma_{ij}(\nu)$ is the cross section for absorbing a photon of frequency ν in the transition

from state i to j . Once K_{ν} is known, the mean radiative opacity, K_R , is obtained by averaging it over frequency. The total opacity is then computed by reciprocally adding the radiative opacity and the opacity due to electron thermal conduction.

A major physics advance in HOPE is the self-consistent quantum mechanical determination of an atomic potential, from which the N_i and $\sigma_{ij}(\nu)$ can be computed. The starting point in the code is a Thomas-Fermi-Dirac statistical routine, which provides a good first guess for the potential. The relativistic Schrödinger equation is then solved in this potential for the single electron energy levels and wave functions. These wave functions are used to obtain an improved potential and the procedure is continued iteratively until self-consistency is achieved. It is then straightforward to compute the N_i , the equation of state, and other thermodynamic quantities of interest.¹⁻¹

The absorption cross sections, $\sigma_{ij}(\nu)$, are due to an array of processes: bound-bound transitions (line absorption), bound-free absorption (photoionization), free-free absorption (inverse bremsstrahlung),

Compton scattering, and pair production. HOPE's calculation of these quantities includes the following sophisticated features:

- Direct in-line calculation of bound-bound and bound-free cross sections
- Density dependence of absorption cross sections
- Fully relativistic treatment of Compton scattering
- Inclusion of electron impact, Stark, statistical, Doppler, and natural broadening in determining the line shape

The first and second items are particularly significant because they provide cross sections obtained from a self-consistent potential rather than from simple formulas as is done in most other codes.^{1-2,1-3} The density effects can be quite pronounced, as shown in Figs. 1-1 and 1-2, where we have plotted oscillator strengths (proportional to the bound-bound cross section) and photoionization cross sections for two illustrative cases. During the last year, a great deal of effort has been spent on the line broadening problem because lines can be the dominant contributor to the opacity in many regimes of interest. The current approach is to add the broadening due to electron impacts, natural damping, and the Stark effect, to form

Fig. 1-1. Oscillator strengths for various atomic transitions in cold aluminum plotted as a function of matter density. The reference density, ρ_0 , is 2.7 g/cm^3 .

Fig. 1-2. Photoionization cross sections of cesium at a temperature of 1 kV plotted as a function of photon energy. The cross sections are in units of the square of the Bohr radius ($a_0^2 = 2.801 \times 10^{-17} \text{ cm}^2$) and the photon energy in atomic units (1 a.u. = 0.0272 keV). The various curves refer to densities ρ equal to: — ρ_0 ; ρ_0 ; - - - $0.1\rho_0$, where $\rho_0 = 2.7 \text{ g/cm}^3$.

a Lorentz profile, and to convolve this into a Voigt profile with the Gaussian broadening due to statistical fluctuations and the Doppler effect.

Another major recent project has been the extension of HOPE to the calculation of opacities for mixtures of elements. This is accomplished by first obtaining a self-consistent equation of state for all constituents of the mixture, and using the resulting potential as an input to HOPE. HOPE then computes the individual absorption cross sections for each element, superposes them, and averages over frequency to obtain the total mixture opacity. The code has been checked extensively, and appears to be in sufficiently good shape for use in a production mode, although a number of test problems are still being run to check various aspects of the code. Unfortunately, the computer time requirements are substantial (5 to 20 min per point in a complicated mixture), so that this poses a severe restriction on such work.

An obvious question with regard to HOPE is whether its improved and relatively complex physics has led to any significant changes in opacities compared

with those computed by other codes. Some specific cases are considered in the classified companion volume of this report, but the HOPE numbers can be substantially different (factors of two or three) from other codes in the low temperature region (T less than a few hundred volts), and in isolated regimes for high Z materials at low density and moderately high temperature. In addition to its intrinsically better physics, a further measure of confidence in the code is provided by its ability to successfully calculate a variety of other atomic physics quantities, such as resonances in photoionization and photodetachment, Auger and radiative widths, and fluorescence yields.

The principal areas of future work on HOPE are:

- Systematic analysis and documentation of HOPE opacities and comparison with opacities computed by other codes
- Improvements in the line broadening and electron conduction calculations
- Completion and testing of the mixture version of the code
- Development of a production system for routinely generating and making available both mean opacities and frequency-dependent absorption coefficients

OTHER OPACITY CODES AND THE EQUATION OF STATE LIBRARY

In addition to the major development effort on the HOPE code, the Division maintains two older opacity codes and is working on several special purpose codes. A function related to our general opacity work is the production and maintenance of the equation of state library, in which equation of state and opacity data is tabulated in a form appropriate for use in radiation flow, hydrodynamics codes. Here, we briefly describe the status of these projects.

HANK

HANK¹⁻⁴ is a general purpose equation of state and opacity code, which provides reasonably accurate results for single elements or mixtures whose temperature is greater than a few electron volts. We have added the effects of electron thermal conduction to HANK, so that calculations of the radiative, conductive, and total opacity are now available. Although HANK is not as accurate as HOPE or some of the codes available elsewhere, it has the great virtues of speed and ease of usage (a typical problem can be set up and run in less than a minute from any teletype). In addition, it is sufficiently accurate that parameter studies are both easy and useful. If one wishes to determine the effects of an impurity on the

opacity, or find out which material is most appropriate in a given experimental situation, then HANK is an ideal investigative tool. Consequently, we plan to maintain the code, and comparisons between it and other codes will continue to be made to better define its accuracy.

CHAINJ

CHAINJ^{1-5,1-6} is a code originally developed at the Rand Corporation; most of the early opacities used at the Laboratory were obtained from it. Recently, it has been debugged and placed in operation on our computer system. Although somewhat difficult to run and relatively inaccurate at temperatures less than a few hundred electron volts, it provides useful insight into the line broadening problem for high- Z materials and, as such, it remains a useful research tool.

STOP

STOP is a code designed to calculate the opacity of relatively light elements ($Z \lesssim 26$), particularly at low to moderate densities. Instead of employing the concept of an average atom (a nucleus surrounded by a fractional number of bound electrons) as do HOPE, HANK, CHAINJ, and most other codes, it treats all

possible ionic states of a given element. In addition, it utilizes the extensive literature of atomic physics calculations on light elements rather than generating the data by prescription. The equation of state part of STOP has been completed, and the opacity part of the code is nearly finished. What now remains is to add the considerable body of atomic data needed to carry out realistic calculations. When this is accomplished, it should be an important special purpose code, as well as an ideal research tool to use in conjunction with HOPE.

Electron Thermal Conduction

Current prescriptions in our codes for the opacity resulting from electron thermal conduction treat only electron-ion interactions, and ignore correlations and other many body effects. The pioneering work of Hubbard and Lampe¹⁻⁷ several years ago led to a code that included electron-electron terms and some provision for correlations in computing the conductive opacity. During the last year we have acquired this code, and are currently trying to make it operational on our system. When this becomes a reality, we will incorporate the results into our opacity codes and also make the code available for general usage. Compared with simpler treatments, the main changes in the conductivity occur for very low Z elements at high densities, a regime of considerable importance for laser fusion.

Equation of State Library

The equation of state library contains material properties—pressure, energy, and opacity for a variety of materials as a function of temperature (T) and density (ρ).¹⁻⁸ Input data, generated theoretically, phenomenologically, or experimentally, are fit by the COMPLEX code in the form

$$Q = \sum_{i,j=0}^2 a_{ij} \rho^i T^j,$$

where Q is the quantity being fitted. For an array of "boxes" in the ρ , T plane the coefficients a_{ij} are tabulated; they allow a user to compute the appropriate material property or its derivatives.

During the past year two long-standing problems with the library system have been at least partially resolved. Because of the volume of information involved and the frequent addition or deletion of tables, it has always been difficult to make up-to-date compilations of the library easily available. A conversion to microfilm is now nearly completed, and should soon make it easy for a user to obtain current equation of state data. A second problem has been the relatively poor documentation of the sources and accuracy of the data. Although this is still contingent upon the individual providing the input, a substantive effort is being made in this regard, and all new tables will be prefaced by a page such as that shown in Fig. 1-3.

Nonequilibrium Plasmas

ATOMIC PROCESSES IN VERY DENSE PLASMAS

To achieve laser-induced nuclear fusion we need to understand atomic phenomena in plasmas of very high density (electron concentration $N_e > 10^{18} \text{ cm}^{-3}$). A principal reason for this is the potential utility of ionic spectral lines for diagnosing laser-heated plasmas, which most often are not in local thermodynamic

equilibrium. With regard to atomic processes, these plasmas can differ in three important respects from nonequilibrium plasmas of lower densities.

- Three-body reactions can be very rapid
- Rates of many transitions induced by collisions

(a) SPECIFICATIONS FOR EOS 46, AIR

INFORMATION FOR THE FOLLOWING FUNCTION TABLES :
PRESSURE AND ENERGY

DATA ORIGINATOR :

H. GRABOSKE H-DIVISION THEORETICAL EOS GROUP ULL

DATA GENERATED SEPT. 1975

DATA AUTHORIZED BY H-DIVISION THEORETICAL EOS GROUP ULL

RANGE OF APPLICABILITY :

RHO(GM/CC) : 1.000E+01 TO 1.500E+01

T(KEV) : 1.500E-01 TO 3.000E+01

COMMENTS :

THIS DATA BASE ACCURATELY REPRODUCES THE DETAILED NBS
IDEAL GAS DISSOCIATION-IONIZATION PHYSICS CURRENTLY USED AS
THE TABULAR AIR EOS. OVER THESE NBS TEMPERATURES WHERE
THIS APPROXIMATION IS VALID. FOR HIGHER DENSITIES AND BOTH
LOWER AND HIGHER TEMPERATURES, IT INCLUDES LENSE MOLECULAR
AND ATOMIC INTERACTIONS, THE LENSE PARTIALLY IONIZED
COULOMB PLASMA, AND THE VERY DENSE METALLIC COULOMB FLUID.

DATA SOURCES

REFERENCES :

JOINT-169 : A NEW EOS FOR AIR H. GRABOSKE 9-16-75

(b) SPECIFICATIONS FOR EOS 46, AIR

INFORMATION FOR THE FOLLOWING FUNCTION TABLES :

OPACITY

DATA ORIGINATOR :

A. MERTS LASL AND D. BARFIELD LASL

DATA GENERATED 1974

DATA AUTHORIZED BY B. TAPFER THEORETICAL PHYSICS DIVISION

RANGE OF APPLICABILITY :

RHO(GM/CC) : 1.293E+09 TO 1.292E+02

T(KEV) : 2.370E+05 TO 2.000E+01

COMMENTS :

THIS TABLE REPRESENTS AN AMALGAMATION OF THE STANDARD
LOW-Z LASL CODE MOOP (WHICH INCLUDES SOME MOLECULES) AND A
LOW-T MOLECULAR CODE ABSO WHICH LASL ACQUIRED FROM AFNL.
THE FORMER CODE EXTENDS DOWN TO 2 EV, THE LATTER UP TO 1.9
EV. UNFORTUNATELY THE CODES CAN DIFFER BY ENORMOUS FACTORS
(10 TO 100) AT THEIR POINT OF NEAR OVERLAP. LASL SUGGESTS NO
SIMPLE RESOLUTION OF THE INCONSISTENCY. WE HAVE BASICALLY
USED LINEAR INTERPOLATION OF ABSO FROM T=1.5 EV TO JOIN
THE 2 EV MOOP DATA. OBVIOUSLY SIGNIFICANT UNCERTAINTY STILL
EXISTS NEAR 1 EV BUT THE NEW TABLE SHOULD STILL BE A
SUBSTANTIAL IMPROVEMENT OVER THE PREVIOUS ONES.

DATA SOURCES

CODE :

MOOP A. MERTS LASL AND ABSO D. BARFIELD LASL

DATA :

CARD DECKS OF MOOP AND ABSO OUTPUT

Fig. 13. Example of the documentation which is now provided with new tables in the equation of state library.

can exceed allowed radiative rates for the same transitions

- The interparticle spacing, $N^{-1/3}$, can be so small that atomic systems are significantly perturbed by neighboring (charged) particles. Such particles manifest their presence by screening Coulomb interactions within the plasma. For the most part, the first two problems can be treated straightforwardly; however, the third requires additional theoretical work, since realistic many-body calculations are still difficult, even for individual atoms.

Two simple models¹⁻⁹ have been developed to approximate the effects of plasma screening – the Debye-Hückel (DH) model, which is obtained in the high temperature/low density limit, and the ion-sphere (IS) model, which is obtained in the low temperature/high density limit. In these two limiting cases, the potential that binds an electron to a nucleus of charge Z is

$$V_{DH} = -(Z/r) \exp(-r/D), \quad (1-1)$$

where D is the Debye length of the plasma; in the second, it is

$$V_{IS} = -(Z/r) + [(Z-1)/(2R_0)] [3 - (r/R_0)^2],$$

$$r \leq R_0, \quad (1-2)$$

where the ion-sphere radius R_0 is defined by the equation $4/3 \pi R_0^3 N_e = Z-1$. Stewart and Pyatt¹⁻¹⁰ have shown that the two models are in fact compatible: the Debye-Hückel model is appropriate at large distances from the nucleus, whereas the ion-sphere model is appropriate near the nucleus.

Weisheit and Shore¹⁻¹¹ recently demonstrated that the elimination in dense plasmas of long-range Coulomb interactions markedly affects certain bound-bound and bound-free photoabsorption processes. Within the past year the effects of plasma screening on other atomic processes also have been investigated.

Recombination

The general problem of electron-ion recombination in dense plasmas is complicated by the fact that radiative, dielectronic, and three-body processes all contribute to the total rate of recombination, but the total rate is not simply the sum of these separate recombination processes. This is because dielectronic and three-body recombinations preferentially populate highly excited states of the recombined system, and these states themselves are rapidly mixed and ionized by collisions. Moreover, at high densities many excited states are removed by plasma screening, which depresses the continuum. Therefore, the net rate of recombination must be found by solving the coupled set of first-order equations that describe the time-rate-of-change in the density (N_i) of each state of recombined ions.

$$\frac{dN_i}{dt} = N_e N_e R(i) + \sum_j N_j N_e Q(j,i), \quad (1-3)$$

where $N_e Q(j,i)$ and $N_e R(i)$ are, respectively, the probabilities (s^{-1}) of the transition $j \rightarrow i$ and of recombination (radiative + dielectronic + 3-body) directly to state i , N_e is the density of recombining ions, and the summation ranges over all bound states. (Here, the term $Q(j,i)$ is negative and represents the probability of transition from state i to all other states.)

Numerical studies¹⁻¹² of recombination in dense plasmas yield several interesting results.

- Depression of the continuum by plasma screening does not significantly inhibit the total recombination rate of ions of charge Z unless the plasma temperature (K) and density satisfy the inequality $N_e > 10^{14} Z T \text{ cm}^{-3}$.

- At densities in excess of 10^{18} cm^{-3} , only the lowest few ($\lesssim 20$) bound states need to be included in Eq. 1-3. This is illustrated in Table 1-1, which lists both the total recombination rate coefficient, $R_2(\text{cm}^3 \text{ s}^{-1})$, for one-electron sodium ions ($Z = 10$)

Table 1-1. Net recombination rate coefficient R_2 (cm^3s^{-1}) of He^+ ions of charge $Z = 10$. The number in brackets below each entry is the highest bound state that must be considered in order to obtain the total rate; if starred, it is also the uppermost bound state of the ion.

$T_e, ^\circ\text{K}$ \ $N_e (\text{cm}^{-3})$	10^{18}	10^{20}	10^{21}	10^{22}	10^{23}
10^6	$4 \cdot 38 - 12$ [22]	$7 \cdot 13 - 12$ [22*]	$1 \cdot 25 - 11$ [12*]	$3 \cdot 32 - 11$ [7*]	$7 \cdot 31 - 11$ [3*]
10^7	$6 \cdot 65 - 13$ [19]	$6 \cdot 43 - 13$ [10]	$6 \cdot 44 - 12$ [7]	$6 \cdot 70 - 13$ [7]	$7 \cdot 51 - 13$ [7*]
10^8	$7 \cdot 07 - 14$ [23]	$6 \cdot 57 - 14$ [18]	$6 \cdot 51 - 14$ [12]	$6 \cdot 26 - 14$ [8]	$6 \cdot 16 - 14$ [5]

and the highest bound state that need be considered to obtain a coefficient within 1% of the correct value.

• The two-step process of dielectronic recombination can be interrupted by collisions involving the intermediate, autoionizing states. Certain collisions enhance the dielectronic rate by collisionally stabilizing these states, but many collisions tend to reduce the rate of dielectronic recombination by ionizing the doubly-excited, autoionizing states before they stabilize themselves. Although these processes have a marginal influence on the total rate of recombination (at the densities at which they occur, radiative and three-body recombinations are dominant), they do have important consequences for plasma diagnostics: Radiative transitions that stabilize autoionizing levels of the $(Z-1)$ times ionized atom produce satellite lines on the long-wavelength side of resonance lines of the Z -time ionized atom. Gabriel¹⁻³ assumed that the dielectronic process is uninterrupted by collisions and then argued that the ratio, $I_s^{(Z-1)+}/I_0^{Z+}$, of a given satellite-line intensity to that of the adjacent resonance line is only a function of temperature, varying approximately as

$$[I_s^{(Z-1)+}/I_0^{Z+}] \propto T^{-1} \quad (1-4)$$

However, collisions in dense plasmas reduce these ratios, thereby introducing a density dependence as

well. This is shown in Table 1-2, again for the case of recombining sodium ions, $\text{Na}^{+10} + e \rightarrow \text{Na}^{+9} + \text{photon}$, the photon producing one of the first three ($n = 2, 3, 4$) satellites of the Na^{+10} Lyman- α line. There is a strong Z -dependence for this collisional quenching, which evidently has been seen in the spectra of dense laser plasmas.¹⁻¹⁴

Spectral Line Profiles

Lines arising from one-electron ions in plasmas exhibit linear Stark broadening because of the dipole interaction between the radiating ion and perturbing particles. At high densities, inhomogeneities (quadrupole term) in the plasma microfield are known

Table 1-2. Factors by which the intensity ratios $I_s(n)/I_0$ for He-like satellites of the Na^{+10} Lyman- α line are suppressed due to collisional ionization of autoionizing levels of Na^{+9} .

$T_e, ^\circ\text{K}$	n	$N_e (\text{cm}^{-3}) = 10^{20}$	10^{21}	10^{22}	10^{23}
1×10^6	2	1.00	1.00	0.99	0.84
	3	1.00	0.98	0.75	0.70
	4	0.99	0.87	0.32	0 ^a
10×10^6	2	1.00	0.98	0.80	0.30
	3	0.99	0.91	0.49	0.09
	4	0.98	0.83	0.31	0.04

^aState removed by continuum lowering.

to cause detectable asymmetries in these Stark profiles. Now plasma screening of the Coulomb interaction that binds the radiator (Eqs. 1-1 and 1-2) lifts the orbital-angular-momentum degeneracy that exists for isolated hydrogenic systems, and produces additional broadening and asymmetry.¹⁻¹⁵ Lyman- α Stark patterns that include this screening effect are shown in Figs. 1-4 and 1-5, for Be^{+3} and Ne^{+9} ions in homogeneous plasmas of different ion densities N_p . The ion-sphere potential was employed in these calculations because only the potential near the nucleus is important in this problem. Furthermore, the plasma microfield was taken to be that produced by the "nearest neighbor" ion, which was separated from the radiating ion by a distance equal to R_0 , the

Fig. 1-4. Lyman- α Stark pattern for a homogeneous beryllium (Be IV) plasma at two different ion densities. The linear Stark half-width Δ_d is the unit of energy, and the crosses (+) indicate the Lyman- α fine structure components' positions and intensities in the low-density limit. Full and dashed lines show results obtained with and without taking into account the effect of plasma screening on the radiating electron. The zero-point of energy is the position of the unperturbed Lyman- α -line position, and the direction of increasing transition energy is to the right.

Fig. 1-5. As in Fig. 1-4, for a homogeneous neon (NeX) plasma.

ion-sphere radius. The dipole and quadrupole widths Δ_d and Δ_q (in atomic units) of the ionic Lyman- α line are given in Table 1-3 for this specialized case, as are the ion-sphere and fine-structure splittings Δ_{IS} , and Δ_{fs} (also in atomic units) of the Be^{+3} and Ne^{+9} ($n = 2$) levels. In this instance *only* one has $\Delta_{fs} = \Delta_q$; this is not true in general.

The results may be readily understood by comparing the relative magnitudes of the four widths Δ_d , Δ_q , Δ_{fs} , and Δ_{IS} . When Δ_d is the largest width, as in the Be plasma -- both densities and the Ne plasma at the higher density, then the familiar Stark pattern emerges. However, when $\Delta_{fs} \approx \Delta_d$ then the two lines, arising from the mixed states of total angular momentum $j = 1/2$, appear far to the left (i.e., the red) of the $j = 3/2$ components. In this case, which occurs for the Ne plasma at the lower density, the splitting of the two former states is determined by the electric field of perturbing ions, and that of the latter two states, by the gradient of the electric field.

Table 1-3 also lists the intensity ratios, I_B/I_R , of the blue and red components of the mixed $j = 1/2$ states, computed with (IS) and without (no IS) the ion-sphere screening. This screening increases the ratio I_B/I_R , so the asymmetry of the Lyman- α line is enhanced or reduced depending upon whether I_B/I_R (no IS) is larger or smaller than unity. This, in turn, depends on whether Δ_{fs} is larger or smaller than $|\Delta_q|$.

Table 1-3. Energy and asymmetry parameters, in atomic units, for Lyman- α lines arising in dense plasmas

Plasma	Plasma ion density (N_p), cm^{-3}	Δ_{fs}	$\Delta_{IS} = -\Delta_q$	Δ_d	I_B/I_R (IS)	I_B/I_R (no IS)
Be	10^{20}	4.26 (-4)	6.98 (-5)	3.53 (-3)	1.063	1.042
	10^{22}	4.26 (-4)	6.98 (-3)	7.60 (-2)	0.9156	0.8354
Ne	10^{21}	1.66 (-2)	3.35 (-4)	1.97 (-2)	1.612	1.586
	10^{23}	1.66 (-2)	2.35 (-2)	4.23 (-1)	0.9486	0.8765

These calculations can be used to show that the overall result of plasma screening is to reduce the asymmetry less in the far wings of the Lyman- α line than in the near wings, which is just the type of effect needed to bring about better agreement between measured and computed profiles.¹⁻¹⁶

Spectra of Two-Electron Ions

Spectral line intensities of two-electron, helium-like ions are a very useful plasma diagnostic tool. This is because of the proximity of allowed, intercombination,

and forbidden lines arising from the states $(1sn\ell)$, and also because these ions predominate throughout a wide range of plasma conditions. At high densities the relative intensities of these lines are strongly affected both by the trapping of resonance-line radiation and by recombination processes. The effects of these phenomena on certain line intensity ratios were investigated by means of the computer code used in the recombination studies discussed above.¹⁻¹⁷ In order to do this, it was argued that even in extremely transient laser-plasmas, consecutive ionization stages

Fig. 1-6. Silicon line intensity ratios at $T = 6.8 \times 10^6$ K. The different curves, which are for an optically thin plasma, dimension $l = 0$ [---], and for plasmas of dimensions $l = 10 \mu\text{m}$ [—], and $l = 30 \mu\text{m}$ [...], demonstrate the marked effect of opacity.

are approximately in coronal equilibrium, collisional ionizations being balanced by radiative recombinations. Then, resonant-photon trapping was treated by employing the concept of an "escape probability", $P_e(i,j)$, which is the fraction of photons emitted in the transition $i \rightarrow j$ that eventually escape the plasma. Thus, each radiative transition probability, $A(i,j)$, included in Eq. (1-3) is reduced,

$$A(i,j) \rightarrow P_e(i,j) A(i,j); \quad (1-5)$$

as is the corresponding line intensity,

$$\begin{aligned} I(i,j) &\rightarrow P_e(i,j) I(i,j) \\ &= P_e(i,j) N_j A(i,j) h\nu_{ij}. \end{aligned} \quad (1-6)$$

The escape probability P_e is a sensitive function of the line opacity.

Figures 1-6 and 1-7, show intensity ratios for selected lines of Si^{12} ions in very dense plasmas at $T = 6.3 \times 10^6$ °K, the temperature at which one- and two-electron Si ions are equally abundant (assuming coronal equilibrium). It is obvious that opacity and recombination effects can produce order-of-magnitude changes in the intensity ratios for these strong lines. Calculations such as these have been used to interpret x-ray spectra produced by irradiating thin SiO_2 shells with the high-power Janus laser system at LLL. The plasma conditions inferred from this analysis are in harmony with elaborate computer simulations of the entire hydrodynamic/radiative-transfer problem.

Fig. 1-7. Silicon line intensity ratios at $T_e = 6.3 \times 10^6$ K. The solid curves are the same as those shown in Fig. 3. The dashed curves show results obtained neglecting recombinations and cascades from higher states. A plasma dimension of $\lambda = 10$ μm was assumed for all computations.

The theoretical part of the joint ARPA-ERDA x-ray laser program has had three main goals:

- Construction of numerical codes that include all relevant processes and can be used to design an x-ray laser experiment
- Development of a scheme for achieving laser action at wavelengths $\lambda < 100 \text{ \AA}$ using high-power lasers as pumping sources
- Development of techniques for interpreting x-ray line spectra from dense laser produced plasmas

The first part of this program is essentially complete. Table 1-4 summarizes the atomic processes that are now included in numerical codes for calculating atomic level populations. These codes can be used in conjunction with the LASNEX code, which calculates density and electron temperature as a function of space and time in a laser-produced plasma. Our original nonequilibrium code, XSNQ, included the first five processes listed in Table 1-4. A good deal of our time this past year has been spent in debugging this code and improving its accuracy for calculating excited state populations. In addition, while this code

is adequate for calculating level populations in nearly fully stripped plasmas, it cannot be used for "cool" plasmas where Auger processes are important. Consequently, we have written a new program, RAMA, which calculates the populations of low-lying levels in dense plasmas taking into account Auger and electron collisional processes as well as the effects of continuum lowering. This code is described in more detail in Ref. 1-18, and is now being used to study x-ray laser schemes based on photoionization of inner shell levels. By combining these codes with the LASNEX code, we can find whether irradiation of a given target with a high-power laser pulse will lead to desired population inversion densities in the x-ray laser "medium" part of the target.

The second part of the program, development of x-ray laser schemes, has concentrated on producing population inversions by either allowing a small laser-heated fiber to expand¹⁻¹⁸ or exposing a cold medium to an intense flash of x rays. Our main efforts so far have focused on defining the theoretical problems that must be solved.

Table 1-4. Atomic processes included in rate equation codes

Process	Formula	Beginning of project	Now
Radiative decay	$X(p) \rightarrow X(q) + \gamma$	Yes	Yes
Radiative recombination	$X^+ + e \rightarrow X(q) + \gamma$	Yes	Yes
Electron collisional excitation	$e + X(p) \rightarrow e + X(q)$	Yes	Yes
Electron collisional ionization	$e + X(p) \rightarrow e + e + X^+$	Yes	Yes
Electron collisional recombination	$e + e + X^+ \rightarrow e + X(p)$	Yes	Yes
Auger ionization	$X(p,q) \rightarrow X^+ + e$	No	Yes
Dielectronic resonance capture	$e + X^+ \rightarrow X(p,q)$	No	Yes
Dielectronic radiative decay	$X(p,q) \rightarrow X(q) + \gamma$	No	Yes
Electron collisional transition	$e + X(p,q) \rightarrow e + X(p,r)$	No	Yes
Electron collisional ionization	$e + X(p,q) \rightarrow e + e + X^+$	No	Yes
Electron collisional transition involving autoionizing states			
Electron collisional ionization of autoionizing states			

For example, the work carried out this past year on expanding plasmas has led to a much better understanding of the conditions needed to produce population inversions, particularly with regard to constraints on expansion rates and initial temperatures and densities. Armed with this better understanding of the conditions required to produce population inversions, we are now carrying out calculations that should show when hydrodynamic expansion of a supersonically heated fiber can lead to laser action for the $n = 3$ to $n = 2$ transition. So far, the calculations suggest that the highest Z element for which this is practical is aluminum ($Z = 13$). Figure 1-8 shows the results of preliminary calculations of the ratio of the width δ of the region over which significant population inversions exist in an expanding aluminum plasma divided by $\sqrt{\lambda/\alpha}$ where α is the mean gain at wavelength λ . This quantity must be greater than unity in order to produce laser action. We have not yet found the optimum initial conditions for aluminum, but our calculations indicate that this element is near the limit where hydrodynamic expansion alone can lead to laser action. Production of $n = 3$ to $n = 2$ population inversions in higher Z materials would require faster expansion or cooling than can be achieved hydrodynamically. Such cooling might be achieved

Fig. 1-8. The ratio $\delta\sqrt{\lambda/\alpha}$ plotted as a function of radius.

radiatively, but it does not appear that achievement of x-ray laser action by such a means is very practical in the near future. It may be possible, however, to achieve laser action in the soft x-ray region by allowing a thin fiber of low Z material to hydrodynamically expand after being heated with a high-power laser pulse. However, we are no longer pursuing this approach as our first priority because prospects are not good for extending this approach to usefully small wavelengths.

At the present time exposure of an initially cold material to an intense x-ray flash appears to be the most promising approach to laser action at wavelengths less than 50 Å. As first pointed out by Duguay and Rentzepris,¹⁻¹⁹ the ejection of electrons from inner shells of atoms by photoionization is a straightforward way of creating inner shell vacancies. If the pumping x-ray source is intense enough and has the right spectral shape then one could produce population inversions. The main problem with this approach is that the upper laser level in a cold material will be rapidly destroyed by the Auger effect. Elton¹⁻²⁰ has pointed out, however, that for $Z \lesssim 20$ the Auger decay of the upper level leads to a level that is sufficiently shifted in energy that it will not contribute to resonant absorption. Furthermore, some elements, such as sulfur, have the property that an L-vacancy state decays more rapidly than the K-vacancy state can radiatively decay. Thus, one might hope to achieve "quasi-cw" laser operation on K_{α} transitions in these elements. We have studied this problem in detail.¹⁻²¹ When one takes into account the heating of the medium due to Auger processes and electron collisions, then positive gain for any particular line only lasts about 10 fs. This means that the rise time for the x-ray pumping source must be on the order of 10^{-14} s. When one takes into account the high pumping powers that would be required (at least 10^{12} W), one sees that realization of a pumping source with the required characteristics is probably well beyond the capabilities of present day technology. Although the pumping powers required are available from high-power infrared

lasers now existing or under construction, the rise time of the high-power pulses from these lasers cannot be made much shorter than 10 ps. Either some method for significantly compressing laser pulses must be developed or some scheme for lengthening the lifetime of states with positive gain must be found.

Recently, we carried out an initial study¹⁻²² of the possibility of obtaining laser action in a multistage photoionization scheme in which the outer electrons were removed, leaving a hydrogen-like or helium-like ion in an inverted state. Removal of the outer electrons eliminates the large decrease in the lifetime of excited states due to the Auger effect. By operating at much smaller densities (perhaps gaseous rather than solid densities) than previously discussed, one might hope to reduce the rate of destruction of excited states by

electron collisions. The price paid for operating at reduced densities is that the gain length becomes much longer. This means that the energy needed to pump the system must be correspondingly greater.

Simple estimates suggest that laser pulse energies that will soon be available should be adequate to pump the K_{α} transition for low Z elements. Furthermore, laser pulse rise times on the order of 10 ps would be adequate to energize the x-ray radiator which converts the laser light into pumping x rays. Thus, lasers under construction at the Laboratory might be adequate as pumping sources for multistate photoionization schemes. We are currently studying these schemes, as well as designs for targets that convert the incident laser pulse into an x-ray pulse with the intensity, spectrum, and rise time required to pump the x-ray laser medium.

CORONAL PLASMAS

A coronal plasma is one in which the ionization structure is determined by balancing collisional ionizations against radiative and dielectronic recombinations.^{1-23,1-24} Thus, the radiation and particle densities must be low enough so that photoionization and three-body recombinations are relatively unimportant processes. Such a plasma has the characteristic that its equation of state and emission properties are essentially independent of density, and can be computed simply by specifying the temperature. For elements of low to moderate atomic number, $1 \leq Z \lesssim 26$, these conditions will prevail for temperatures greater than a few electron volts and densities less than about 10^{18} particles per cubic centimeter.

Such plasmas are of practical importance because of their inhibiting effect on the temperature achieved by a potential fusion system. Radiative emission from minor plasma constituents can be the dominant energy loss mechanism, so that small amounts of wall material or other impurities can severely degrade the

performance of the system. This is particularly serious for many low density, magnetic confinement schemes, such as Tokamaks. During the last year we have carried out calculations of the losses expected from some of the impurities present in such devices.

In Fig. 1-9 we have plotted the radiative losses from iron as a function of temperature for $0.1 \lesssim T < 20$ keV. The strong emission at low temperatures ($T \approx 0.1$ keV) and the secondary maximum near one kilovolt both arise from atomic transitions in which no change of principal quantum occurs; such transitions have generally been ignored in our higher density plasma codes. In Table 1-5 we list the fractional impurity concentration at which the impurity losses from oxygen, silicon, and iron are equal to those from hydrogen, usually the main component of a fusion plasma. Obviously, even a small amount of contaminant can overwhelm the losses from hydrogen, and in our early calculations of plasma energy losses were based on the assumption of a pure hydrogen plasma.

Fig. 1-9. Radiative losses from iron under conditions of coronal equilibrium plotted as a function of plasma temperature.

Table 1-5. Fractional impurity concentration at which impurity and hydrogen radiative losses are equal

T, keV	Oxygen	Silicon	Iron
0.1	7×10^{-4}	8×10^{-6}	3×10^{-6}
0.2	2×10^{-4}	3×10^{-5}	5×10^{-6}
0.5	1×10^{-3}	2×10^{-4}	1×10^{-5}
1.0	4×10^{-3}	2×10^{-4}	1×10^{-5}
2.0	7×10^{-3}	5×10^{-4}	1×10^{-4}
5.0	1×10^{-2}	1×10^{-3}	2×10^{-4}
10.0	1×10^{-2}	3×10^{-3}	4×10^{-4}
20.0	1×10^{-2}	3×10^{-3}	6×10^{-4}

Radiative losses from higher Z materials, such as molybdenum, are also of practical interest, but an accurate computation of those losses requires much more atomic data and modeling capability than is presently available. During the next year we hope to be able to carry out such calculations for at least a few such elements, and to develop scaling laws which are approximately valid for all elements.

Atomic and Molecular Physics

RELATIVISTIC HARTREE-FOCK CALCULATIONS

In recent years numerous experiments have been performed to observe transitions involving highly excited ions. Excitations accompanying nuclear transformations and ionizations by electrons and x rays have been joined by high-energy ion collisions and high-temperature plasmas as sources for the observation of fluorescent x-rays or Auger electrons. Theoretical calculations which yield the spectroscopic assignments for the observed radiation and the rates for the decay modes are important not only for predicting the rates of production, but also as an aid in interpreting the experimental results.

During the last year, existing computer programs were modified to calculate the energy levels and radiative decay rates of arbitrary ionic multiplet states.

Relativistic Hartree-Fock codes previously used in such calculations assume an average occupation of each partially filled subshell.¹⁻²⁵ However, this is an accurate description of the ionic states only when there is no more than a single vacancy or electron in addition to all completely occupied subshells. The extension to arbitrary multiplet states was accomplished by using as basis states coupled, single-particle, Hartree-Fock wave functions. The matrix of the Hamiltonian operator, which includes both electric and magnetic interactions among the electrons, was then diagonalized to obtain the energy eigenvalues and eigenfunctions. Subsequently, rates for the emission of x rays in transitions between eigenstates were calculated using the relativistic version of the transition operator.

Different versions of the code have recently been applied to a number of specific problems. Using the Hartree-Fock model with the Slater approximation for exchange, we computed the photoionization cross sections of neutral atoms at the energies of magnesium and aluminum K_{α} characteristic radiation, 1254 and 1487 eV, respectively.¹⁻²⁶ An explicit treatment of the multiplet states was used to calculate energy levels

and transition rates of helium-like ions, for comparison with observations of x-ray emission by laser-produced plasmas.^{1-9,1-27} Calculations of energies and rates were also performed and compared with the x-rays from iodine ions used in a beam foil experiment at Kansas State,¹⁻²⁸ and with x-rays from chlorine ions used in collision experiments performed at the Laboratory.¹⁻²⁹

MOLECULAR PHOTODISSOCIATION

The primary motivation for our work on photodissociation is for the purpose of proposing, evaluating and improving laser isotope separation methods. Laser isotope separation schemes under development use an isotope selective photoexcitation followed by an energy selective photodissociation or photoionization. One (or both) of these stages uses an inefficient visible or ultraviolet laser. The efficient lasers, like CO_2 or CO, are in the infrared. Recent experiments at Los Alamos and in the Soviet Union have used infrared lasers to achieve isotope selective dissociation of light molecules. Their dissociation energy far exceeds the energy of a single photon. Thus, the photodissociation mechanism, although incompletely understood, is assumed to be a succession of one-photon excitations (transitions between real energy levels close to resonance with the incident light) and multiphoton excitations (transitions between real nonresonant levels through intermediate virtual energy levels). Radiationless transitions can also intervene. We study these processes in order to apply them to photoseparation of molecules with heavier atoms.

We consider the irradiation of molecules with a given set of energy levels and transition matrix elements between these levels. We ask whether photodissociation is possible and seek to determine its efficiency in the face of competing side reactions. We will then seek conditions for optimum photodissociation. Our approach to the problem is based on a quantum mechanical solution, rather than the simpler but cruder rate equation or perturbation

theory treatments. These alternatives cannot yield population inversions among the levels; the fully quantum mechanical treatment can. Such inversions can greatly improve the overall efficiency of photodissociation. Thus, we want conditions when perturbation theory and rate equation treatments are invalid.

Perturbation theory fails when the pulse duration exceeds the characteristic time (Rabi period) $\tau_R = \lambda^{-n} \omega^{-1}$, where n is the number of photons in the transition, $\lambda = e_0 \bar{d} / \hbar \omega_L$; e_0 and ω_L are the amplitude and frequency of the laser pulse; and $\bar{d}$ is a characteristic transition dipole matrix element. The rate equation treatment is inadequate when the spontaneous radiative lifetime and the mean collision time exceed τ_R . Transitions between levels are then called coherent. For $\omega_L \sim 10^{14}$ Hz and $\bar{d} \sim 0.01$ D, $\tau_R = (10^{-8} I^{1/2})^n \times 10^{-14}$ s, where I is the laser intensity in W/cm^2 . When $I \sim 10^{10}$ W/cm^2 , the one- and two-photon Rabi period are 10^{-11} and 10^{-8} s, while the three-photon time is 10^{-5} s. Thus, conditions for one- and two-photon coherent resonant excitations are attainable.

We have developed a multiple-time-scale (MTS) perturbation theory, which is applicable to the general situation described above, avoids the secularities and other failures of conventional perturbation theory, and agrees with numerical calculations on model systems. We have successfully applied it to studies of monochromatic photoexcitation of an N -level system, demonstrating two-photon Rabi oscillations and

optical Stark shifts, and to Doppler-free two-photon complete passage using chirped pulses. Our future objectives include:

- An application of the N-level work to specific molecules of increasing complexity, hoping to gain some understanding of the existing experiments on the dissociation of SF_6 by a CO_2 laser. We also hope to propose and evaluate methods for isotope-selective multiphoton dissociation of UF_6 .

Nuclear Theory

During the past year, work has been carried out on a variety of topics in nuclear physics, ranging from completion of an effective method of calculating inelastic neutron cross sections to initial studies on a new approach to *ab initio* fission cross sections. Here, we will describe some of the more significant results.

Inelastic Cross Sections

One of the complications in attempting to theoretically deduce inelastic neutron (n,n') cross sections is that the target nucleus is a "soft object"; that is, it is altered by the presence of the incident neutron in a highly nonlinear way that varies with the target nucleus, the particular level being excited, and the energy of the incident neutron. Experimental nuclear physicists have at their disposal several different probes: protons, alpha particles, photons, and electrons; neutrons are rarely used because of experimental difficulties. However, at the Laboratory, one is predominately interested in neutrons. Our major recent accomplishment is the application of a theoretical model to synthesize the information from proton, alpha particle, and electromagnetic experiments to deduce the inelastic neutron cross sections for the excitation of the most important transitions over the neutron energy range relevant to Laboratory programs.^{1,30,32} In those cases where

- An extension of the MTS theory to include continuum as well as bound levels. This will permit the systematic treatment of photoionization and photodissociation.

- Inclusion of the multiple-time scale approximations in the analysis of coherent photoexcitations in the general theory of propagation of intense light through complex media.

- Application of coherent multiphoton infrared photoexcitation to development of efficient visible and ultraviolet lasers.

experimental data are available, the agreement is excellent.^{1,33}

For each nucleus in Table 1-6, we have listed the type of nucleon transition (due to valence neutrons,

Table 1-6. Comparison of β_{pp}/β_{em} with theory

Nucleus	Type	c_{eff}	β_{pp}/β_{em}		Experiment
			NPSM	OPSM	
⁴⁴ Ca	n	1.49	1.28	1.08	1.13
		1.95	1.28	1.05	
⁵⁰ Ti	p	1.55	0.67	0.75	0.83
⁵² Cr	p	1.92	0.692	0.805	0.74
⁵⁴ Fe	p	1.93	0.72	0.83	0.86
⁵⁸ Ni	n	1.90	1.35	1.19	1.07
⁶⁰ Ni	n	1.34	1.30	1.12	1.09
⁶² Ni	n	0.91	1.27	1.17	1.19
⁶⁴ Ni	n	0.97	1.24	1.12	1.04
⁸⁸ Sr	p	1.65	0.66		.75
⁹⁰ Zr	p	2.4	0.67		0.95
⁹² Mo	p	1.9	0.69		0.91
¹¹² Sn	n	0.72	1.26	1.22	1.17
¹¹⁴ Sn	n	0.79	1.24	1.17	1.13
¹¹⁶ Sn	n	0.72	1.20	1.18	1.13
¹¹⁸ Sn	n	0.75	1.20	1.15	1.16
¹²⁰ Sn	n	0.73	1.19	1.14	1.06
¹²² Sn	n	0.84	1.17	1.09	0.95
¹²⁴ Sn	n	0.89	1.16	1.06	1.00
¹³⁸ Ba	p	1.79	0.63	0.73	0.58

n or protons, p), the effective charge of the valence nucleons for the transition, and the values of β_{pp}/β_{em} obtained from a no parameter schematic model (NPSM), a one parameter schematic model (OPSM), and from experiment. β_{pp} is a parameter proportional to the strength of the inelastic transition for excitation by protons, and β_{em} is the same quantity for electromagnetic excitation. From our theory one can then calculate β_{nn} , the desired quantity for inelastic excitation by neutrons. Extensions and refinements of the theory, in addition to the calculation of the parameters necessary for cross section calculations, are in progress.

Fission Theory

The recent advent of several existing and proposed heavy ion accelerators has spurred theoretical interest in methods of calculating the properties of heavy ion reactions.¹⁻³⁴ The knowledge inferred from these studies is directly applicable to fundamental calculations of fission processes. In collaboration with individuals at several other laboratories, we are engaged in as microscopic an approach to these processes as

nuclear theory and available computer facilities permit. This approach is called Time Dependent Hartree Fock (TDHF) and consists in following the time evolution of the "best" antisymmetrized product wave function representing the nuclear system. This implies not only following in time all of the individual wave functions, but also treating the nuclear interactions in a time-dependent self-consistent way. In this model one uses a form of an effective nuclear potential, which has been tested over several years and fitted to many known ground state properties of nuclei. In testing and developing the theory for low energy (2 to 100 MeV/nucleon) ion-ion reactions, one has access to a regime intrinsically simpler than a large fissioning nucleus and more accessible to detailed experimental verification. An understanding of the phenomena occurring in these reactions can then be applied to the inverse process, namely fission. It is also possible that one may gain insight into the formation of exotic nuclear species.¹⁻³⁵ Because of the formidable technical difficulties, present work is limited to one and two dimensional systems with a considerable degree of symmetry, but we believe these restrictions can eventually be relaxed.

Physical Data

Our work on physical data consists of two closely related functions. The first is the compilation (Refs. 1-36 through 1-42), evaluation (Refs. 1-43 through 1-46), and dissemination of nuclear data for weapons design, diagnostics output, and effects calculations. The second function is the development and maintenance of data-oriented Monte Carlo neutronics and photonics codes.¹⁻⁴⁷ Because of the large computational requirements associated with such codes, their proper design is connected in a very intimate manner with the accuracy and completeness of the available data. Thus, we have found it highly desirable to maintain a close relationship between

those who collect and process nuclear data and those who design Monte Carlo codes that use these data. This is especially important since our evaluated data library is constantly being improved as new experimental data become available, and the Monte Carlo codes can take advantage of this circumstance only if they can be modified to keep pace with the experimental situation. Thus, we can easily make changes and improvements in the Monte Carlo codes and in the data used by these codes, test the results against our standardized series of benchmark integral experiments, and then quickly disseminate the results and codes to all parts of the Laboratory.

To accomplish these functions, we have emphasized five areas:

- Libraries of available microscopic experimental data and of data from integral or bulk measurements are maintained.

- Processed sets of "evaluated data", constructed from the raw material of the experimental library, are maintained and continuously improved. (Fig. 1-10 shows recent evaluated cross sections for V^{51} .) In developing these sets, the uses for which they are

Fig. 1-10. Various evaluated neutron-induced cross sections for ^{51}V from the ENDL library plotted as a function of neutron energy.

intended must be kept in mind to avoid either over- or under-specification of the data.

- Computational facilities are provided for processing the evaluated data sets in the forms required by the various Laboratory neutronics codes.¹⁻⁴⁸ This involves the calculation of sets of groups-averaged cross sections, transfer matrices, and related quantities required by the neutronics codes.

- Monte Carlo neutronics and photonics codes are developed, tested for accuracy and efficiency (including some tests against similar codes developed at other laboratories), and made available to the users.

- The evaluated data sets are checked by comparing them against the available integral experiments, using the Monte Carlo codes. The integral experiments consist mainly of pulsed-sphere experiments and critical assembly data. (See Fig. 1-11.) During the past year work was carried out in each of these areas and will be discussed below.

Cross Section Libraries

The LLL Experimental Cross Section Information Library (ECSIL) is widely used for the evaluation of neutron cross section information, not only here but also at Los Alamos and several other ERDA-funded installations. Several years ago an arrangement was made with the National Neutron Cross Section Center at Brookhaven National Laboratory to supply us with the experimental data that are forwarded to them by the other three major neutron cross section centers at Saclay, France; Vienna, Austria; and Obninsk, U.S.S.R. Having the data supplied to us routinely eliminates the need for a literature search on our part. During the past year a new automatic translating routine was developed and debugged. This has eliminated a major bottleneck in the processing of experimental data for entry into the ECSIL system. During the last three months over 400,000 data points were converted, checked for error, and entered into the library.

The current ECSIL system contains only cross sections for neutron-induced interactions. The Oak Ridge Charged Particle Center maintains a similar

library for charged particle induced interactions. Because of possible future Laboratory applications requiring charged particle data, an ECSIL format has been designed to allow cross section data for any incident and emerging particle to be entered into the system. Arrangements have been made to obtain copies periodically of the charged particle bibliographic and data files. The bibliographic file is routinely permuted into the required order and distributed at LLL. These listings are now widely used for a variety of applications. Documentation has also been produced for a substantial fraction of the LLL Evaluated Nuclear Data Library (ENDL).¹⁻⁴⁵

Evaluated Data

We carried out three cooperative efforts in producing evaluated data. In collaboration with Hubbell of the National Bureau of Standards, Viegele and Briggs of Kaman Nuclear, and Brown and Cramer of Los Alamos, a set of evaluated data for cold-photon cross sections for coherent and incoherent scattering for all elements from $Z = 1$ to $Z = 100$ were produced. For years there has been a cooperative arrangement with A. B. Smith and his colleagues at Argonne National Laboratory to produce joint evaluations. During the past year evaluations of neutron cross sections for Nickel and ^{238}U have been carried out. In cooperation with McCrosson at the Savannah River Laboratory, new evaluations were produced for three trans-plutonium isotopes of interest. At low energies these evaluations were based on data from reactors at Savannah River, while the high energy numbers were derived from techniques commonly used at this Laboratory.

Because of the importance of the $\text{Be}(n,2n)$ reaction in many applications, the representation of this reaction was investigated at some length. The nuclear levels in Be^9 through which the $n,2n$ reaction proceeds are very wide. To test the significance of the width of the levels, a wide level representation was introduced into the evaluated library system to see whether a better agreement could be obtained with

Fig. 1-11. Comparison of experimental and calculated neutron spectrum after the passage of 14 MeV neutrons through a 4.8 mean-free-path thick iron sphere. The plot shows the ratio of the counting rates obtained with and without the iron target. Calculations were done with TART using the ENDL evaluated nuclear data.

the emission spectrum measured with the LLL pulse sphere. We found that the more detailed representation improved the agreement only marginally, but increased the running time of the Monte Carlo calculations by 15%. Consequently, we decided to continue to use the narrow level representation.

Monte Carlo Codes

Seven production codes based on the Monte Carlo method are currently being maintained and modified

to meet users needs: TART, TART-H, TART-M, TORTE, TARTNP, HUCKFINN, and TORTEEP. Of these codes the most widely used and most recent is TARTNP. Documentation of this code has been completed. During the past year, features changed or added to TARTNP included generalized planes, spectral reflection from a generalized plane, expanded post-processing capabilities. Various modifications to TARTNP resulted in decreasing the computational machine time by about 10%. In addition, we have

helped incorporate various parts of our Monte Carlo codes into several major weapon design code subroutines.

During the past year there has been a revival of interest in calculating the neutron cross sections of configurations in which low-energy-neutron interactions are important. In such systems, it is important to include Doppler-broadening in neutron and charged particle cross sections, and we have completed work on a stable scheme that is capable of constructing accurate Doppler-broadened cross sections. The problem of resonance self-shielding was addressed by constructing a library of cross section probability tables from the entire ENDL library for the TART multigroup library. During this process a library of Bondarenko self-shielded cross sections was also constructed for that TART library.

Future Activities

Over the next several years we plan activities in a number of areas:

- Continuing and updating the library of experimental neutron cross section information
- Completing documentation of the evaluated library
- Producing new evaluations for about ten transplutonium isotopes
- Improving the input specifications and other aspects of the Monte Carlo codes to make them easier to use.
- Providing an upgraded library of activation cross sections for applications in the field of peaceful nuclear explosives.

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2. LASER FUSION, PROPAGATION, AND EFFECTS

Introduction

This section describes the activities and progress of the division in laser-related research. This work has been supported almost entirely by outside reimbursable contracts or by laser projects within the laboratory itself and has been concentrated in the following general areas:

- Laser fusion. Basic requirements and limitations of laser fusion have been explored.
- Laser propagation. One of the most important questions that must be answered in evaluating high-energy laser systems is whether the laser energy can be transmitted to the target without serious beam degradation. The division has a continuing program for supplying the Army and Navy with propagation codes for carrying out this type of systems evaluation. Additional theoretical laser propagation research has been devoted to: (1) the problem of calculating small-scale self-focusing in realistic laser systems such as the Y-Program Cyclops laser; (2) the stability of laser beams propagating in magnetically confined

cylindrical plasma columns; and (3) the possibility of using lasers to create low-density channels in the atmosphere.

- Laser effects. The presence of a normal atmosphere can significantly alter the nature of the interaction between an intense laser beam and a target by creating laser-supported absorption waves, which travel back up the laser beam. Pressures created at the target surface by a backward-moving detonation wave can become a potent damage mechanism, as has been determined in a 3-year ARPA-funded theoretical study. Additional work has been carried out to determine the response of high-explosive materials to laser radiation. This work has been in support of a Laboratory program to investigate high-power lasers as antimissile weapons.

- Miscellaneous laser physics. A theory has been derived for predicting the energy extraction from a CO₂ laser as a function of the duration and fluence of the input pulse.

Laser Fusion: Basic Requirements and Limitations

Introduction

A central problem of laser-driven pellet fusion is achievement of the very large thermonuclear energy gain necessary to compensate for the low efficiency of short-pulse lasers and of the fuel-compression process. To achieve the required energy gain with the least amount of laser-pulse energy, a small amount of thermonuclear fuel must be highly compressed; its inertial confinement, measured by its ρR product, must attain a large, specified value. This minimum energy and required ρR product can be estimated by considering a simple model of the ignition and burn

of the compressed fuel.²⁻¹ It is found that isentropic fuel compression at near-minimum entropy is needed to avoid excessive laser-pulse energy requirements.

An elementary treatment of the hydrodynamics of isentropic compression shows that the ρR product that can be achieved is proportional to the square root of the peak hydrodynamic power expended.²⁻² A more detailed consideration of the pellet ablation process²⁻³ shows that this square-root relation also applies, approximately, to the peak laser power absorbed by the pellet, the coefficient of proportionality being an increasing function of the pellet aspect ratio (inner

radius divided by wall thickness). Thus there is a motivation to employ thin hollow shells, rather than the solid DT spheres originally proposed,²⁻⁴ to reduce the peak laser-pulse power required to drive the implosion.

It is expected, however, that fluid instabilities of the Rayleigh-Taylor type will limit the thinness of the shell that can be employed and therefore limit the reduction in peak power that can be achieved by this means. Exact results for the linear Rayleigh-Taylor instability problem have been obtained for the case of homogeneous, isentropic compression and have been used to evaluate this limitation.

Overall, it seems that the requirements for laser fusion based on fusion alone will be very difficult to achieve and that laser fusion reactors will be based on the "hybrid" concept of fusion-fission, at least for the near future.

Required Pellet Gain

The basic energy-balance equation of a power plant based on laser-driven pellet fusion is

$$\epsilon_{\text{He}} f_e \epsilon_{\text{eL}} G_P = 1, \quad (2-1)$$

where ϵ_{He} is the conversion efficiency of heat into electricity, f_e is the fraction of the total electric power generated that is supplied to the laser, ϵ_{eL} is the efficiency of the laser in converting its electrical input to light output absorbed by the target pellet, and G_P is the pellet gain; i.e., the ratio of thermonuclear energy produced to the light energy absorbed by the pellet. A typical set of values for these factors might be: $\epsilon_{\text{He}} = 0.4$, $f_e = 0.25$, $\epsilon_{\text{eL}} = 0.05$, $G_P = 200$.²⁻⁵

It is useful to write the pellet gain, G_P , as

$$G_P = \epsilon_{\text{LF}} G_F, \quad (2-2)$$

where ϵ_{LF} is the fraction of absorbed laser light converted into internal energy by highly compressing the core of thermonuclear fuel (DT) at the instant of fuel ignition. A typical value for ϵ_{LF} is 0.05,²⁻⁵ so

that a fuel gain, G_F , of 4000 would be required to achieve a pellet gain of 200.

Required Inertial Confinement

The inertial confinement necessary to achieve the large pellet gains required for laser fusion can be evaluated by means of a simple model.²⁻¹ The model used is that of a uniformly compressed pellet of DT ignited by a small, hot, central "spark." The spark is specified to be large enough and hot enough to ignite the remainder of the compressed fuel via an out-going thermonuclear detonation.

The fuel gain (G_F) is shown in Figs. 2-1 and 2-2 as a function of the inertial confinement parameter (H_F) denoting the ρR of the compressed fuel for a sequence of values of the internal energy (W_F) supplied to the compressed core ranging from 50 J to 50 kJ. If ϵ_{LF} equals 0.05, this corresponds to laser-pulse energies, $W_L (= W_F/\epsilon_{\text{LF}})$, ranging from 1 kJ to 1 MJ.

Fig. 2-1. Fuel-gain (G_F) vs inertial confinement parameter (H_F) for fuel-energies (W_F) of 50, 160, 500, 1600, 5000, 16000, and 50000 J, assuming minimum entropy compression ($\alpha = 1$).

Fig. 2-2. Same as Fig. 2-1 but with $\alpha = 2$. (Twice as much work must be done to achieve the same compression η .)

Figure 2-1 applies to the most favorable case, that of minimum-entropy compression ($\alpha = 1$). Figure 2-2 applies when twice as much work ($\alpha = 2$) must be done to achieve the same compression. Inspection of Figs. 2-1 and 2-2 shows that H_F must amount to 2-3 g/cm² if fuel gains of several thousand are to be realized.

Required Laser-Pulse Energy

Inspection of Figs. 2-1 and 2-2 also shows that laser-pulse energies of 100 to 800 kJ are necessary if a pellet gain as large as 200 is to be achieved, again assuming the efficiency (ϵ_{LF}) to be 5%. The scaling of the least laser-pulse energy (W_L) required to achieve a desired pellet gain (G_P), in terms of the principal factors describing the implosion and burn of the fuel, is found to be²⁻¹

$$W_L^* \propto \alpha^3 (G_P/q_{DT})^{12/5} H_B^{9/5} A_S^{2/5} / \epsilon_{LF}^{17/5}, \quad (2-3)$$

where

$$H_B = 8M_i/\alpha \geq 7 \text{ g/cm}^2 \quad (2-4)$$

$$\sigma = \langle \sigma_{DT} \rangle / c_s \quad (2-5)$$

$$A_S = T_S(\text{eV}) [H_S(\text{g/cm}^2)]^3 / 540 \geq 1. \quad (2-6)$$

Here, M_i is the average ion mass, c_s is the isothermal speed of sound in DT, $\langle \sigma_{DT} \rangle$ is the Maxwell-averaged DT cross section, and q_{DT} is the energy of the DT fusion reaction. T_S and H_S are the temperature and ρR of the central ignition spark, respectively.

We note that the laser-pulse energy is a strong function of everything except the size (A_S) of the ignition spark. In particular, the cubic dependence on α and the greater-than-cubic dependence on ϵ_{LF} demonstrate the importance of achieving near-minimum-entropy compression at high compression efficiency.

We also note that the strong (twelve-fifths power) dependence of laser-pulse energy on pellet gain, together with the anticipated difficulty of achieving the large pellet gain needed for practical power production based purely on fusion, suggest that the laser fusion-fission or hybrid option²⁻⁶ is especially attractive.

The value of the confinement parameter H_F^* that minimizes the required laser-pulse energy scales as

$$H_F^* \propto (H_B^{3/4} A_S G_P / q_{DT} \epsilon_{LF})^{4/15}. \quad (2-7)$$

It is a far less sensitive function of the implosion parameters than is the laser-pulse energy itself.

Required Laser-Pulse Power

It is easily shown that the mechanical power (P_M) required to homogeneously and isentropically compress an ideal ($\gamma = 5/3$) gas is proportional to the square of the ρR product achieved by the compression. This relationship can be shown by noting that the internal energy (W_F) of the gas being compressed,

$$W_I = 2\pi\rho R^3 c_s^2, \quad (2-8)$$

doubles in a time τ proportional to the sound transit time

$$\tau \propto R/c_s. \quad (2-9)$$

The mechanical power supplied is then given by the proportionalities,

$$P_M = W_I/\tau \propto \rho R^2 c_s^3 = (c^3/\rho)(\rho R)^2. \quad (2-10)$$

However, the factor (c^3/ρ) appearing on the right of Eq. (2-10) is constant along an isentrope, so that

$$P_M \propto \alpha^{3/2}(\rho R)^2. \quad (2-11)$$

If, in addition, we assume that the efficiency with which laser energy can be converted into compressive work does not depend significantly on the ρR product achieved, we may write the proportionality above in terms of the laser power P_L as

$$P_L \propto \alpha^{3/2}(\rho R)^2. \quad (2-12)$$

A more detailed treatment that takes into account the nature of the pellet-ablation process leads to the closely similar result:

$$P_L \propto \alpha^{7/6}(\rho R)^{11/6}. \quad (2-13)$$

Combining this result with that of Eq. (2-7), and identifying H_F^* with ρR , we obtain the scaling relation for laser-pulse peak power P_L^* ,

$$P_L^* \sim \alpha^{7/6} (H_B^{3/4} A_S G_p / q_D T \epsilon_{LF})^{1/2}. \quad (2-14)$$

We note that the required laser-pulse peak power is a far less sensitive function of the implosion and burn parameters than is the laser-pulse energy.

The coefficient of proportionality relating P_L and $H_F^{11/6}$ depends on the aspect ratio (ξ_u) of the

unablated portion of the imploded shell, i.e., the aspect ratio of the *payload* of the ablation-driver rocket. A semianalytical result, obtained by a best-fit to detailed computer runs of imploded shells with a wide range of aspect ratios (including solid spheres), is^{2,3}

$$P_L \text{ (TW)} = \{160/\Omega\} [H_F \text{ (g/cm}^2\text{)}]^{11/6}, \quad (2-15)$$

where

$$\Omega = \sqrt{1 + 3\xi_u^2} \quad (2-16)$$

A solid sphere is characterized by $\Omega = 1$. The Ω has, therefore, the physical significance of the factor by which the peak laser power can be reduced (by imploding hollow shells with aspect ratio $\xi_u (\neq 0)$ instead of solid pellets).

Substituting the value of 2.5 to 3 g/cm² for H_F into Eq. (2-15), we obtain for the absorbed laser power required to implode a solid pellet:

$$P_L = 900 \text{ to } 1200 \text{ TW}. \quad (2-17)$$

If we assume that nonlinear optical effects limit the output of the laser to 3×10^9 W per square centimeter of laser output aperture, it follows that the required output aperture is

$$A_L = 30 \text{ to } 40 \text{ m}^2, \quad (2-18)$$

which corresponds to about 1000 beams 20 cm in diameter. If hollow shells are imploded instead of solid pellets, it appears that these power and aperture requirements will be reduced by a factor of 5 to 10.

We see that there is considerable advantage in imploding hollow shells instead of solid pellets. Not only is the peak power requirement reduced (by the factor Ω), but the intensity of the absorbed light will be lower, leading to reduced excitation of nonlinear optical effects and plasma instabilities, and improved corona-core coupling. However, we expect that the

minimum feasible shell thickness will be limited by the growth of fluid instabilities during implosion.

Required Shell Thickness

The amplitude of a surface perturbation of a homogeneously and isentropically imploded shell increases, due to Rayleigh-Taylor instability growth, by the factor²⁻³

$$\Gamma_v = \frac{\cosh(\sqrt{\ell} \chi) - \beta^{2v} \cos(\sqrt{\ell} \chi)}{1 - \beta^{2v}}, \quad (2-19)$$

where

$$\chi = \cosh^{-1} \eta^{1/3}, \quad \beta = R_{10}/R_{20}. \quad (2-20)$$

η is the compression of the shell, and β (< 1) is the ratio of the inner and outer shell radii. The surface perturbation is described by the spherical harmonic $Y_{\ell m}(\theta, \phi)$. Equation (2-20) reduces to the following simple form for large values of η and ℓ ,

$$\Gamma_v \approx \frac{1}{2} (8\eta)^{\sqrt{\ell}/3} \quad (\beta^{2v} \ll 1, \eta \gg 1). \quad (2-21)$$

Application of these results to the question of shell break-up leads to the following limit on the shell aspect ratio ξ_u

$$\xi_u < [3 \ell n(5 \epsilon_0)/\ell n \eta]^2 - 1. \quad (2-22)$$

and on the peak power reduction factor Ω

$$\Omega < 3\sqrt{3} [\ell n(5 \epsilon_0)/\ell n \eta]^{1/2}. \quad (2-23)$$

where ϵ_0 is the initial fractional surface perturbation amplitude $\delta R_{20}/R_{20}$. If $\eta = 10^4$, and $\epsilon_0 = 2 \times 10^{-5}$, for example, then ξ_u must be less than 8 to avoid shell break-up, and Ω can therefore not exceed 5. (Since η and ϵ_0 enter Eqs. (2-22) and (2-23) only logarithmically, these results are relatively insensitive to the values of η and ϵ_0 chosen.)

We conclude that the initial aspect ratio of the unablated or "payload" portion of the shell cannot exceed about ten, which implies a less than ten-fold reduction in peak laser power as compared with the peak laser power required to implode solid spheres to the same density.

In obtaining these results we have not taken into account the effects of ablation, viscosity, heat diffusion, or finite density gradient at the fluid surface, each of which will tend to decrease the growth rate of the shorter wavelength modes. This omission appears to be crudely justified by two-dimensional computer simulations of isentropically imploded shells that include the above-named effects.²⁻⁷ Such simulations exhibit growth rates amounting to 50 to 100% of the Rayleigh-Taylor values for wavelengths considered here ($\ell \lesssim 10$).

Laser Propagation

TIME-DEPENDENT PROPAGATION OF HIGH-ENERGY LASER BEAMS THROUGH THE ATMOSPHERE

The thermal blooming of intense laser beams in the atmosphere is well understood for steady-state conditions and wind velocities substantially below sound speed.^{2-8,2-9} There is also reasonably good understanding of the time-dependent blooming of single, short, axially symmetric pulses.²⁻¹⁰⁻²⁻¹² There

remain, however, a number of categories of high-energy-propagation problems for which understanding is either incomplete or only beginning. Among these are the following:

- Propagation in the presence of transonic and supersonic winds brought about by beam slewing

Table 2-1. Basic outline of four-dimensional propagation code

Variables	x, y, z, t where x, y are transverse coordinates and z is axial displacement.
Form of propagation equation	Scalar wave equation in parabolic approximation $2ik \frac{\partial E}{\partial z} = \nabla_{\perp}^2 E + k^2(n^2 - 1)E,$
Method of solving propagation equation	Symmetrized split operator, finite Fourier series, fast Fourier transform (FFT) algorithm $E^{n+1} = e^{\frac{i\Delta z}{4k} \nabla_{\perp}^2} e^{-\frac{i\Delta z}{2k} \chi} e^{\frac{i\Delta z}{4k} \nabla_{\perp}^2} E^n$ $\chi = k^2(n^2 - 1).$
Hydrodynamics for steady-state problems	Uses exact solution to linear hydrodynamic equations, Fourier method for $M < 1$. Characteristic method for $M > 1$. Solves $v \frac{\partial \rho_1}{\partial x} + \rho_0 \nabla_{\perp} \cdot v_1 = 0$ $\rho_0 v \frac{\partial v_1}{\partial x} + \nabla_{\perp} p_1 = 0$ $v \frac{\partial}{\partial x} (p_1 - c_s^2 \rho_1) = (\gamma - 1) \alpha I.$
Transonic slewing	Steady-state calculation valid for all Mach numbers except $M \approx 1$. Code can be used arbitrarily close to $M = 1$.
Treatment of stagnation zone problems	Time-dependent isobaric approximation. Transient succession of steady-state density changes; i.e., solves $\frac{\partial \rho_1}{\partial t} + v \frac{\partial \rho_1}{\partial x} = - \left(\frac{\gamma - 1}{c_s^2} \right) \alpha I.$
Treatment of multipulse density changes and blooming	Density changes resulting from previous pulses in train calculated with isobaric approximation. Density changes resulting from the same pulse calculated using acoustic equations and assumption of triangular pulse shape.
Method of calculating density change for individual pulse in train	Takes two-dimensional Fourier transform of $\frac{\alpha \tilde{I}}{c_s^2} \frac{t_p}{2} \left\{ 1 - \frac{\sin^2 \left[\frac{1}{2} c_s (k_x^2 + k_y^2)^{1/2} t_p \right]}{\left[\frac{1}{2} c_s (k_x^2 + k_y^2)^{1/2} t_p \right]^2} \right\}$ where $\tilde{I}$ is Fourier transform of intensity and t_p is the time duration of each pulse. Source aperture should be softened when using this code provision.

Table 2-1 (continued)

Treatment of steady-state multipulse blooming	Previous pulses in train are assumed to be periodic replications of the current pulse. Pulse self-blooming effects are self-consistently included.
Treatment of turbulence	Uses phase-screen realization of Bradley and Brown with Von Karman spectrum. Phase screens can be selected either to be independent of time or to move with the wind.
Treatment of lens optics	Uses $\frac{1}{z_f} = \frac{1}{z_T} + \frac{1}{z_L}$ where z_f is the desired lens focal length, z_T is the lens focal length that is compensated for by a lens transformation, and z_L is the lens focal length used explicitly in calculation.
Adaptive lens transformation	Applicable to cw or steady-state multipulse problems. Removes quadratic phase and tilt from beam profile at each z step. Phase is chosen by variational principle.
Modeling of nondiffraction limited behavior	Either spherical aberration or a random phase screen can be employed
Scenario capability	Moving laser platform, moving target, and arbitrary wind direction, all coplanar. Capable of following target over fixed linear trajectory. Resulting wind can be function of time as well as z .
Treatment of multiline emission effects	Required only for long propagation paths. It is assumed that the field distribution at the source is the same for every emission wavelength; z -dependent weighted cross section can then be calculated.
Code output	Isointensity, isodensity, isophase and spectrum contours. Intensity averaged over contours. Plots of intensity, phase, density, spatial spectrum along specific directions, etc., at specific times. Plots of peak intensity and average intensity vs time.
Numerical capacity when used with CDC 7600 and restricted to internal memory (large and small core)	Spatial mesh, 64×64 , 35 sampling times, no restriction on number of axial space increments.
Problem zoning features	Number of space increments in x and y directions must be equal and expressible as a power of two.
Selection of z step	Propagation path can be broken up into segments each having separate data. In particular, z step can be different for each segment. The code can also be allowed to choose its own z step based on the maximum allowable transverse phase gradient.
Problem running time on CDC 7600 computer	The running time will vary with edit frequency and other problem conditions. However, a reasonable average is 0.9 s per z step per time step for a 64×64 mesh.

- Propagation through "dead" or stagnation zones, where the wind velocity goes to zero

- Propagation of multi-pulse trains

The solution of propagation problems in the above-mentioned categories requires either a more general treatment of steady-state hydrodynamics than has hitherto been used, or a time-dependent -- sometimes referred to as a "four-dimensional" -- approach to the solution of the propagation problem as a whole. The time-dependent treatment is essential for treating problems in the second and third categories.

A general time-dependent three-space-dimensional propagation code has been developed that is capable

of treating the above phenomena. This work has been supported by ARPA, the Navy, and the Army and is part of a continuing project to supply the Department of Defense with the propagation codes that will be used in the evaluation of its High-Energy Laser (HEL) program.

This code is capable of treating the propagation of high-energy laser beams through the atmosphere and includes the effects of horizontal wind and turbulence for most situations of interest. Possible cases are propagation of cw beams through stagnation zones, multipulse propagation (including the self-consistent treatment of pulse self-blooming), and propagation involving transonic slewing. The solution of the

Fig. 2-3. Evolution with time of multipulse isointensity contours resulting from propagation through a stagnation zone half-way to target (a) 100 pulses per second.

Maxwell wave equation in Fresnel approximation is obtained by means of a discrete Fourier transform method, which, surprisingly, gives excellent results for diffraction problems. The latter provide a stringent test for the accuracy of any solution method. Considerable use is also made of discrete Fourier transform methods in solving the hydrodynamic equations. The treatment of turbulence is based on the generation of random phase screens at each calculation step along the propagation path. In a time-dependent calculation, the random phase screens can either be made to move with the wind at a given propagation position or generated anew for each successive time. The code is equipped with a general scenario routine

involving a moving laser platform as well as a target. This routine allows the code to treat an effective transverse wind velocity that varies with time as well as axial position. Thus, it is possible to take into account the motion of the stagnation point in treating the propagation of beams through stagnation zones. The code is equipped with extensive editing facilities, which generate various averages, contour plots, and plots of quantities of interest as a function of time.

The capabilities of the code as well as the methods used are summarized in Table 2-1. For a more complete description of the code the reader is referred to Ref. 2-13.

Fig. 2-3. Evolution with time of multipulse isointensity contours resulting from propagation through a stagnation zone half-way to target (b) 10 pulses per second.

Figures 2-3a and 2-3b show the time evolution of laser isointensity profiles on target calculated for a multipulse laser beam that has been propagated through a stagnation zone that lies half-way to the target. The time-averaged aperture power of the laser is 60 kW, the range to target

is 2.5 km, and the wavelength is 10.6 μm . All scenario dynamics including the motion of the laser, target, and stagnation point have been taken into account. The seriousness of thermal blooming associated with stagnation zones is clearly evident.

SIMULATION OF SMALL SCALE SELF-FOCUSING IN HIGH-POWER GLASS LASERS

Introduction

Nonlinear self-focusing of laser beams in glass can, under certain conditions, damage glass laser amplifiers through whole beam self-focusing.²⁻¹⁴ More often, however, self-focusing leads to beam deterioration and even breakup or small scale self-focusing by amplifying tiny random imperfections in the beam wave front. This phenomenon was first examined in a linearized analysis of the optical propagation equation by Bespalov and Talanov,²⁻¹⁵ who likened the effect to an "optical Taylor instability." In the Bespalov-Talanov theory, one assumes that the laser beam field amplitude can be represented in the form

$$e = e_0 + e \cdot \exp(iK \cdot r + hz). \quad (2-24)$$

It can then be shown that the gain h depends on the beam intensity I_0 , the refractive index n , the optical disturbance wave number K , and the nonlinear optical coefficient n_2 :

$$h = K \sqrt{\frac{n_2 4\pi I_0}{cn^2} - \frac{K^2}{4k^2}}. \quad (2-25)$$

Unfortunately, this simple theory is valid only for simple nonamplifying slabs of nonlinear material. A real laser system with amplifying disks, Faraday rotators, lenses, spatial filters, and air gaps can only be described by a detailed computer model.

The FLAC code solves the following Helmholtz

equation in Fresnel approximation for such a detailed laser system.

$$\nabla_T^2 E - 2ik \left(\frac{\partial}{\partial z} - \frac{g}{2} \right) E + \frac{2n_2}{n} k^2 |E|^2 E = 0. \quad (2-26)$$

The solution of Eq. (2-26) is based on a finite Fourier series representation and the fast Fourier transform (FFT) algorithm. This method is ideally suited to the study of the growth of individual Fourier components — such as given in Eq. (2-75) — since one only needs to propagate a δ -function disturbance through the entire system and then compare the output and the input Fourier spectra.

A Simplified Bespalov-Talanov Theory for a Medium with Gain

For a strong background plane wave plus a weak plane wave perturbation propagating at an angle θ to the strong wave, Eq. (2-26) can be linearized in the weak beam amplitude. After converting to the unitless Bespalov-Talanov coordinates²⁻¹⁵ $(\bar{x}, \bar{y}, \bar{z}) = (kx, ky, kz)$, $h = g/k$, $E = E\sqrt{2n_2/n} \exp(h\bar{z}/2)$, we obtain $\nabla_T^2 E - 2i \frac{\partial}{\partial \bar{z}} E + |E|^2 \exp(h\bar{z}) = 0$. The linearized equation is obtained by means of the ansatz $E = (E_0 + e) \exp[-i(\exp(h\bar{z}) - 1)|E_0|^2/(2h)]$, where e satisfies

$$\nabla_T^2 e - 2i \frac{\partial}{\partial \bar{z}} e + 2E_0^2 e^{h\bar{z}} \text{Re}(e) = 0. \quad (2-27)$$

For $e = \tilde{e} \cos(k\theta x) = (\tilde{e}_1 + i\tilde{e}_2) \cos(\theta \bar{x})$, Eq. (2-27) becomes the simultaneous pair of ordinary differential equations:

$$\frac{d}{d\bar{z}} \begin{pmatrix} \tilde{e}_1 \\ \tilde{e}_2 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 0 & -\theta^2 \\ \theta^2 - 2E_0^2 e^{h\bar{z}} & 0 \end{pmatrix} \begin{pmatrix} \tilde{e}_1 \\ \tilde{e}_2 \end{pmatrix} \quad (2-28)$$

In the following section some results of a simple numerical solution to Eq. (2-28) will be presented.

Trenholme²⁻¹⁶ has examined the behavior of $\ln[|\tilde{e}(1)/\tilde{e}(0)|]$, maximized with respect to the phase angle of $\tilde{e}(0)$ for some simple systems. This maximum we shall refer to as the "maximum total ripple gain." This number seems to be the best measure currently in use for the rate of beam deterioration due to a specific Fourier component. Even this definition, however, has at least two limitations. First, for systems with air spaces, there are some weak beam angles for which $|\tilde{e}(z)|$ is larger in planes prior to the output plane than in the output plane itself. For such systems $|\tilde{e}(z)/\tilde{e}(0)|$ should be maximized over both $\bar{z}$ and the phase angle of $\tilde{e}(0)$, which is a very unwieldy procedure. Second, in the neighborhood of $\theta = 0$ the maximum total ripple gain doesn't account for the fact that in any real laser system there is not enough propagation distance in linear ($n_2 = 0$) elements to convert phase ripple to amplitude ripple.

To illustrate some of the properties of the maximum total ripple gain we have calculated this quantity as a function of the weak beam angle θ for a slab of glass ($n = 1.567$, $n_2 = 1.73 \times 10^{-13}$) for various values of the total amplifier gain, and an output intensity of 20 GW/cm^2 . The results for a 30-cm slab are shown in Fig. 2-4. The main difference between ripple spectra and the simple Bessel-Talanov gain spectrum is that the former have a nonzero limit as $\theta \rightarrow 0$. The small weak beam angle ($\theta \approx 0$) portion of the ripple gain spectrum can pass through a spatial filter, but there are two reasons why the small θ portion of the spectrum is less damaging than the large θ portion. First, most of the ripple near $\theta = 0$ is phase

ripple, which does not damage optical components, although it can degrade the focal plane characteristics of the laser beam. Second, the unfilterable $\theta \approx 0$ modes grow more slowly with the length of glass in the system than do modes with large θ . In the limit $\theta \rightarrow 0$ one can show that the maximum total ripple gain is given by

$$R_g = \ln[B + \sqrt{1 + B^2}],$$

where

$$B = 8\pi^2 n_2 / (nc\lambda) \int_0^L I(z) dz$$

Fig. 2-4. Maximum total ripple gain as a function of normalized wave number in a 30-cm slab of ED-4 glass ($n = 1.567$, $n_2 = 1.73 \times 10^{-13}$) for an output intensity of 20 GW/cm^2 .

is the "break-up" integral and all quantities are measured in c.g.s. units. For constant $I(z)$, the maximum total ripple gain for any θ is $R_g \cong B$. Thus, the more nonlinear material there is in the beam path, the smaller is the fraction of the ripple gain spectrum near $\theta = 0$.

For the initial condition of pure amplitude ripple ($\text{Im}[e(0)] = 0$), the results of a cross-check of the FLAC code and the ODE code are shown in Fig. 2-5. The values of $\ln[|\text{Re}(\tilde{e}(1))/\tilde{R}(\tilde{e}(0))|]$, calculated with FLAC, agree with the solid curves, which were obtained from the ODE code. All the FLAC calculations were done with $n_2 = 1.73 \times 10^{-13}$ esu,

Fig. 2-5. A comparison of the amplitude ripple gain generated by FLAC with the results of an independent ODE code. The beam was passed through a 30-cm slab of ED-4 glass and had an output intensity of 20 GW/cm².

$n = 1.5667$, and $I(1) = 20 \text{ GW} \cdot \text{cm}^2$ ($2 \times 10^{17} \text{ ergs/cm}^2$). We used a z -step size of 0.25 cm (except for the point $G = 2$, $\theta = 0.004$ where a 0.125 cm step was used) and an FFT mesh of 32 points spaced 1/8 of a ripple wavelength apart.

Because the ripple gain is sensitive to the initial ripple phase ($\tan^{-1} [\tilde{e}_2(0)/\tilde{e}_1(0)]$), any code that examines ripple growth should allow arbitrary initial phase angles to be examined. We have recently added this capability to FLAC; by running the two input phase angles -0 and $\pi/2$ — and displaying the complex ripple amplitude for each, one can examine the output for an arbitrary input phase angle in the linear growth regime by an elementary application of the superposition principle.

Calculation of Ripple Gain for the CYCLOPS Laser Using the FLAC Code

The ripple gain spectrum for the LLL CYCLOPS laser has been calculated using the FLAC code and the results are displayed in Fig. 2-6. In the calculation, an initially diverging beam was assumed to be

Fig. 2-6. Ripple gain vs wave number for CYCLOPS laser, starting from beam apodizer and proceeding through B modules.

propagated from the apodizing aperture through three rod amplifiers, two A-disk modules, a telescope, three B modules, and various optical elements such as Faraday rotators, polarizers, and a Pockel cell. The gain curve in Fig. 2-6 is always bounded by the value of

the B integral, which is 4.0. A significant feature of this spectrum is the relatively large gain values below the 9-cm^{-1} cut off of a spatial filter that consists of a $300\text{-}\mu\text{m}$ -diam pinhole in the focal plane of a 1-m focal length lens.

SELF-TRAPPING OF A LASER BEAM IN A CYLINDRICAL PLASMA COLUMN

The availability of high-power $10.6\text{ }\mu\text{m}$ CO_2 lasers has created interest in the scheme, proposed by Dawson *et al.*,²⁻¹⁷ for heating a magnetically confined underdense plasma column to kilovolt temperatures with a propagating laser beam. End losses and long absorption lengths at high temperatures require a very long plasma column and hence the propagation of the heating laser beam over considerable distances. Steinhauer and Ahlstrom²⁻¹⁸ have shown, using geometric optics, that a trapped wave-guide or "light-pipe" mode (a mode characterized by periodic focusing and defocusing) results from an electron distribution with an on-axis minimum. Such a favorable density distribution can be created by the expansion of a laser-heated plasma.

Since the laser beam, by heating the plasma, creates its own density profile, the propagation becomes a nonlinear phenomenon, and there is no assurance that it will be stable. In media possessing an intensity-dependent refractive index, or a cubic nonlinearity, for example, catastrophic self-focusing can result in a collapse of the beam limited only by the onset of stimulated scattering processes or nonlinear absorption. An additional complication in the plasma column case is that the electron density at a given instant of time depends on the preceding history of the medium and the laser pulse. A time-dependent self-consistent treatment of both the beam propagation and the medium hydrodynamics is therefore required in order to correctly predict the behavior of the laser beam.

Calculations of this type have been performed and

the results demonstrate that the propagation of a laser beam in an initially uniform plasma can result in the formation of a filament with alternate focusing and defocusing of the beam in a manner suggestive of a wave-guide or light-pipe mode. To our knowledge, this is the first self-consistent theoretical demonstration of stable beam trapping in a plasma column.

The underlying physical model is described by Eqs. 2-29 through 2-35 below, which are based upon the assumptions of cylindrical symmetry, charge neutrality, negligible axial hydrodynamic flow, and a two-temperature MHD description of the plasma.

$$\frac{\partial N}{\partial t} + \frac{1}{r} \frac{\partial}{\partial r} (Nur) = 0, \quad (2-29)$$

$$\begin{aligned} \frac{\partial}{\partial t} (Nu) + \frac{1}{r} \frac{\partial}{\partial r} (Nu^2 r) = & -\frac{1}{M} \frac{\partial}{\partial r} \\ & \times \left(P_e + P_h + \frac{B^2}{8\pi} + Q \right), \end{aligned} \quad (2-30)$$

$$\begin{aligned} \frac{\partial W_e}{\partial t} + \frac{1}{r} \frac{\partial}{\partial r} [u(W_e + P_e)] = & \sigma n |E|^2 \\ & + \frac{1}{r} \frac{\partial}{\partial r} \left(r K_e \frac{\partial T_e}{\partial r} \right) \\ & - (3/2)n \frac{(kT_e - kT_h)}{\tau_{eh}} \\ & + \partial \left(\frac{c}{4\pi} \frac{\partial B}{\partial t} \right)^2 - \frac{u}{8\pi} \frac{\partial B^2}{\partial r}. \end{aligned} \quad (2-31)$$

$$\frac{\partial W_h}{\partial t} + \frac{1}{r} \frac{\partial}{\partial r} [u(W_h + P_h + Q)] = (3/2)n \times \frac{(kT_e - kT_h)}{\tau_{eh}} + \frac{1}{r} \frac{\partial}{\partial r} \left(r K_h \frac{\partial T_h}{\partial r} \right), \quad (2.32)$$

$$\frac{\partial n}{\partial t} + \frac{1}{r} \frac{\partial}{\partial r} (nur) = \alpha n(N - n) - \beta n^3, \quad (2.33)$$

$$\frac{\partial B}{\partial t} + \frac{1}{r} \frac{\partial}{\partial r} (Bur) = \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{c^2}{4\pi} \frac{\partial B}{\partial r} \right), \quad (2.34)$$

$$\frac{\partial E}{\partial z} + \frac{i}{2k} \nabla^2 E = -\frac{\sigma n E}{2} (1 + i\omega\tau). \quad (2.35)$$

Here t is measured with reference to the time of arrival of the front of the pulse at axial position z , N and n are the heavy particle (ion plus atom) and electron number densities, u is the radial fluid velocity, and Q is an artificial viscosity. The variables, r , W , K , T represent the partial pressure, energy density (internal plus kinetic), thermal conductivity, and temperature of electrons or heavy particles, according to whether they bear the subscript e or h , respectively.

Equation (2.34) for the solenoidal magnetic field contains both convective and diffusion terms; Eq. (2.35) is Maxwell's wave equation in Fresnel approximation, where E is expressed in units such that $|E|^2$ represents intensity. The absorption is due to inverse bremsstrahlung, where the cross section is given by

$$\sigma = \frac{k}{n_c} \frac{\omega\tau}{1 + (\omega\tau)^2}. \quad (2.36)$$

Here k and ω are the wave number and circular frequency for the light, n_c is the critical electron density, and τ is the electron collision time.²⁻¹⁹ The transverse conductivities K and the electron-ion relaxation time τ_{eh} are given by Spitzer.²⁻²⁰ Equation (2.33) for the electron number density

includes the effects (not required here) of collisional ionization and three-body recombination with coefficients α and β , respectively.²⁻²¹

Figures 2-7-2-9 refer to the case of a Gaussian beam with an $1/e$ intensity radius of $100 \mu\text{m}$ incident on an initially uniform hydrogenic plasma with a density of $5.38 \times 10^{17}/\text{cm}^3$ and a temperature of 2 eV . A uniform plasma was chosen so that beam trapping would result solely from the self action of the laser beam. The laser pulse was chosen to be Gaussian in time with a $1/e$ full width of 1 ns . The wavelength was taken to be $10.6 \mu\text{m}$. For this example, the magnetic field was turned off. Other cases run with a magnetic field showed no qualitative differences.

In Fig. 2-7 the half-power radius - defined as the radius of a circle through which one half of the total instantaneous beam power flows - is plotted as a

Fig. 2-7. Variation of the beam half-power radius with propagation distance for several times in the pulse. The leading edge ($t = 0$) diffracts freely while the trailing edge ($t = 2 \text{ ns}$) focuses twice. Varying degrees of trapping occur for other time values.

function of propagation distance for various times in the pulse history. Stable trapping in a waveguide or light pipe mode is clearly evident near the end of the pulse. At earlier times the self-focusing action of the electron density well, resulting from hydrodynamic

Fig. 2-8. Temporal variation of the half-power radius of the laser pulse as it passes an axial position z . a) $z = 3.5$ mm. Before the first focus, the minimum beam waist is at the end of the pulse where focusing is strongest. b) $z = 6.0$ mm. After the rear of the pulse passes through its focus and begins to diverge, the minimum beam waist moves forward into the pulse. c) $z = 14.0$ m. At the second focus, the rear of the pulse once again exhibits the minimum radius. The original minimum has moved to the center of the pulse.

Fig. 2-9. Axial laser intensity at $z \approx 17$ mm with distinct hump on the trailing edge. This feature is correlated with the variation in half-power radius shown in Fig. 2-8c.

motion, reduces the diffractive spreading of the beam. With the passage of time, the electron density well deepens and the self-focusing effect becomes stronger, finally resulting in trapping with the formation of multiple foci. By the end of the propagation path shown, 75% of the original pulse energy has been absorbed. This absorption of the beam makes the electron density trough shallower at a given retarded time t and consequently the trapping weaker with increasing z . This effect, and perhaps tunneling through the sides of the trough, lead to wider and wider excursions of the beam radius.

The behavior of the half-power radius as a function of retarded time for three different axial positions is displayed in Fig. 2-8. Figure 2-8c shows that focusing is occurring near the center and at the rear of the pulse with defocusing taking place in between. This behavior leads to a double hump in the on-axis intensity variation with time (Fig. 2-9). With the occurrence of more "bounces" as z increases, the number of humps can be expected to grow. Similar behavior of the on-axis intensity is known to occur during transient

self-focusing in a medium with a cubic optical nonlinearity, when the relaxation time of the field-induced refractive index change is comparable to or longer than the laser pulse duration.^{2-22,2-23} For this case an undulating dependence of half-power radius on z , which correlates with the humps in the on-axis intensity distribution, has been calculated in Ref. 2-22 and inferred in Ref. 2-23. This behavior can similarly be explained by an alternate focusing and defocusing of the beam within the confines of a self-trapped filament. There is, however, no evidence that the transverse size of the filament formed stabilizes before some other nonlinear effect sets in.^{2-22,2-23}

In the present case, the variation with propagation distance z of the half-power radius for the end of the pulse is given with good accuracy up to the first focus by

$$[R(z)/R(0)]^2 = 1 + [(kba^2)^2 - 1] \sin^2 bz. \quad (2-37)$$

Equation (2-37) can be derived from Eq. (2-35) by assuming that the beam is initially Gaussian with $1/e$ intensity radius a and that it propagates in an axially constant parabolic electron density distribution, defined by

$$\frac{n(r,t) - n(0,t)}{n_c} = (br)^2. \quad (2-38)$$

Here $n(r,t)$ refers to the position $z = 0$. The position of the first focus and the half-power radius of the beam at the first focus – given by Eqs. (2-37) and (2-38) – are compared with the results of detailed numerical calculations (Table 2-2). Beyond the first focus, Eqs. (2-37) and (2-38) cease to be applicable. The effect of including a magnetic field in the calculation is to confine the electron density depression closer to the z -axis and, hence, to bring the foci closer together.

In summary, a laser beam will form a stable self-trapped filament in an initially uniform plasma without the imposition of an initial favorable electron density distribution. Such self-trapped filaments exhibit similarities to those encountered during transient self-focusing in a medium with a cubic optical nonlinearity when the relaxation time for the field – dependent refractive index change is comparable to or longer than the pulse duration. The multiple focusing behavior of the filament in a plasma column is also qualitatively similar to that encountered when a beam propagates through an axially uniform parabolic density distribution, but it is more complicated because of the time-dependent interaction between the electron distribution and the propagating beam.

Table 2.2. Comparison of numerical calculations with Eq. (2-37) for position of first focus and beam radius at the rear of the pulse. The values of b are derived from computed electron density profiles at $z = 0$. In these runs, $I_{\max} = 10^{10}$ W/cm², $t_{\text{pulse}} = 1$ ns, $n(0) = 5.35 \times 10^{17}$ /cm³ and $T_e(0) = T_h(0) = 2$ eV.

Initial 1/e radius, μm	Magnetic field, kg	Eq. 2-37		Numerical calculation	
		Position 1st focus, mm	1/2 power radius, μm	Position 1st focus, mm	1/2 power radius, μm
50	0	1.80	31	1.85	31
50	10	1.57	26	1.50	24
100	0	3.97	34	4.00	33
100	10	3.60	32	3.50	30

Progress toward testing the feasibility of heating a long column of magnetically confined underdense plasma to kilovolt temperatures with a propagating laser beam has given rise to a number of interesting propagation problems. Because of the very strong refractive effect of plasmas, and the long propagation paths contemplated, the understanding of such phenomena is essential.

Kidder has suggested that scattering from fluctuations due to periodic focusing in the waveguide formed by laser heating might lead to loss of the beam. The present paper shows that fluctuations near the wavelength associated with periodic focusing cause an exponential growth in the radius of a Gaussian beam, even in an infinite trapping well.

Consider a plasma in which the refractive index varies quadratically transverse to the laser axis. In Fresnel approximation, the wave equation for the laser field E is

$$\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial E}{\partial r} \right) - (K\alpha)^2 h(z) E = -2Ki \frac{\partial E}{\partial z}, \quad (2-39)$$

which corresponds to the electron density profile

$$\frac{n(r,z) - n_0}{n_c - n_0} = (\alpha)^2 h(z). \quad (2-40)$$

In the above, $n(r,z)$ is the electron number density, n_0 the axial density, n_c the critical density at which the laser frequency equals the plasma frequency, K the laser wavenumber corresponding to density n_0 , and $h(z)$ is, for now, an unspecified function of z .

We assume a Gaussian solution for E in the form

$$E = E_0 [\sigma_0/g(z)] \exp[-r^2 f(z)/2\sigma_0^2]. \quad (2-41)$$

Here, σ_0 is the intensity $1/e$ radius, and $f(z)$ and $g(z)$

are complex scaling functions of z with initial conditions of $f(0) = 1$ and $g(0) = \sigma_0$, respectively.

A simple equation for the complex width g can be derived:

$$\frac{d^2 g}{dz^2} + \alpha^2 h(z) g = 0 \quad (2-42)$$

with initial conditions

$$g(0) = \sigma_0 \text{ and } (dg/dz)_0 = i/K\sigma_0. \quad (2-43)$$

Thus, the radius of the propagating beam is determined by a simple oscillator equation. Equation (2-42) is similar to the ray equation of geometric optics; the important difference is that the complex function g includes the effect of diffraction. Two simple examples will serve to demonstrate the usefulness of Eq. (2-42). First, consider the case $\alpha = 0$; i.e., free diffraction. Equations (2-42) and (2-43) then lead to

$$g = \sigma_0 \left(1 + \frac{iz}{K\sigma_0^2} \right), \quad (2-44)$$

so the Gaussian width $\sigma(z)$ is, as expected, given by

$$\sigma^2(z) = g g^* = \sigma_0^2 [1 + (z/K\sigma_0^2)^2]. \quad (2-45)$$

As a second example, consider $h(z) \equiv 1$; i.e., propagation in an axially uniform waveguide. Then

$$g = \sigma_0 (\cos \alpha z + \frac{i}{K\sigma_0^2 \alpha} \sin \alpha z), \quad (2-46)$$

and

$$\sigma^2(z) = \sigma_0^2 [1 + [(K\alpha\sigma_0^2)^2 - 1] \sin^2 \alpha z]. \quad (2-47)$$

In this case, the beam radius oscillates between maximum and minimum values whose geometric mean is the width of the fundamental mode, $(K\alpha)^{1/2}$.

The object of the present paper is to determine the effect on the oscillating solution – given in Eq. (2-46) – of a small periodic variation in the strength of the well. Such a variation might be caused by either a nonuniform axial magnetic field or by the variations in laser heating rate accompanying the focusing and defocusing of the beam described by Eq. (2-46). We shall take

$$h(z) = 1 + \epsilon \cos \beta z, \quad (2-48)$$

in which case Eq. (2-42) becomes

$$\frac{d^2 g}{dz^2} + \alpha^2(1 + \epsilon \cos \beta z) g = 0. \quad (2-49)$$

Equation (2-49) is Mathieu's equation and has both stable and unstable solutions depending on the values of α/β and ϵ . The important point for us is that, for ϵ finite, the solution for $\beta = 2\alpha$ is unstable. This is just the frequency one would expect for density fluctuations resulting from variations in laser heating.

The growth rate of the above solution can be substantial, the maximum value being $\epsilon\alpha/4$ at $\beta = 2\alpha$. In terms of the distance to the first "bounce" ($z_f = \pi/2\alpha$), the minimum e-folding length L_e is

$$L_e^{\min} = (8/\pi\epsilon) z_f. \quad (2-50)$$

In Fig. 2-10, the e-folding length is shown as a function of $\beta/2\alpha$ for perturbation amplitudes of 5 and

Fig. 2-10. The exponential growth of the beam radius as characterized by the e-folding radius, L_e . The growth is given here – in units of the focusing distance (z_f) – as a function of frequency offset for two values of the perturbation amplitude. The limits of the unstable region for the two cases are indicated by the dashed vertical lines.

10%. Since a typical value of z_f is a few cm, such perturbations could be disastrous for propagation over long distances.

In conclusion, it has been shown that small axial perturbations of density near the wavelength associated with beam focusing can cause unstable growth of the laser beam radius. This instability might have serious implications for the laser-heated solenoid as a fusion device; therefore, a self-consistent treatment of the coupled nonlinear problem over long distances would be useful.

CREATION OF REDUCED DENSITY CHANNELS IN AIR BY LASER BREAKDOWN

It has been suggested²⁻²⁴ that reduced density channels in air may be created by laser breakdown.

Subsequently it was experimentally demonstrated that the transmission of an electron beam through air could

be enhanced by the reduced density.²⁻²⁴ The absorption of laser energy ionizes and heats the air, which then expands. Simple arguments based on ideal blast wave theory and adiabatic expansion suggest that the central density of such a channel might decrease by at least an order of magnitude in a time of the order of 1 μ s.

To investigate the feasibility of such "channel digging," we have made some preliminary calculations with the LIP code - developed to model laser breakdown and the heating of hydrogenic plasmas contained in solenoids. The code assumes an initial neutral gas at room temperature and calculates the absorption of laser energy, avalanche ionization, and subsequent expansion.

Two basic questions need to be answered about channel digging: How much laser energy must be absorbed per unit path length to create the desired density reduction and channel size? Is it possible to propagate one or more laser pulses over enough distance to bring about the energy absorption necessary for channel formation?

Preliminary calculations have dealt with spatially and temporally Gaussian laser pulses that have a duration of several tens of nanoseconds and a wavelength of 10.6 μ m. The expansion of the hot plasma resulting from breakdown was followed for tens of microseconds. These calculations indicate that it is possible to reduce the on-axis air density to a few percent of normal density (see Fig. 2-11). The channel formed, however, never attains a practical length, since the critical density plasma created by breakdown absorbs the laser pulse over a distance of a few wavelengths. A critical density plasma can be avoided by using shorter wavelength lasers (e.g., Nd or ruby).

Fig. 2-11. Air density as a function of radius for various times in laser breakdown pulse. The minimum density in the channel reaches 3% of normal.

Even though the absorption length can be increased by a couple of orders of magnitude with these shorter wavelengths, the absorption length still remains impractically small.

Two alternative methods of laser-induced channel formation are currently being investigated. These involve aerosol-induced breakdown and heating by selective molecular absorption. Both methods can substantially reduce the required total laser energy absorption per unit path length. In any case, an additional constraint must be placed on the laser pulse duration to avoid substantial thermal blooming. The laser energy should be deposited in a time short in comparison with an acoustic transit time across the laser beam.

LIGHT PROPAGATION IN A PLANE STRATIFIED PLASMA

The absorption of light by a plane stratified plasma decreases sharply as the angle of incidence

increases.²⁻²⁵ Therefore, if this angle is not small enough, too much laser energy may be reflected by

the plasma surrounding an irradiated laser-fusion pellet.

Analytical solutions of the wave equation in a plane stratified medium have been obtained for only a few profiles of the plasma density.²⁻²⁶ Corresponding geometric optics analyses are similarly limited and involve the integration of underdense absorption coefficients that display an unrealistic singularity at the critical surface. Asymptotic approximations of the complicated wave optics solutions can lead to reflection coefficients that are more than 20% less than the geometric optics results.²⁻²⁷ To resolve some of these questions we have developed a code²⁻²⁸ that accurately integrates the wave equation with a plane stratified plasma for a general density distribution and an arbitrary angle of incidence.

The reflection and transmission of a plane wave are computed as a function of the angle of incidence θ into the stratified medium. The polarization of the electric vector is assumed to be perpendicular to the plane of incidence, and changes in the plasma density profile due to the influence of the light wave are neglected. Thus, if $\epsilon(z)$ denotes the effective permittivity of the plasma, the complex amplitude u of a plane wave satisfies the equation

$$\frac{d^2 u}{dz^2} + \frac{\omega^2}{c^2} [\epsilon(z) - \sin^2 \theta] u = 0, \quad (2-51)$$

where ω and c are the angular frequency and vacuum velocity of the wave. The stratified layer is assumed to have thickness ℓ and to lie between a vacuum and a constant dielectric medium. The density profile between the vacuum and the dielectric is

$$\rho(z) = \rho_c \left(\frac{z}{D} \right)^a \quad 0 \leq z \leq \ell, \quad (2-52)$$

where D is the distance into the critical surface, ρ_c is the electron density at the critical surface and $0 \leq \epsilon \leq 40$. Other profiles could easily be implemented. A plane wave with unit amplitude is assumed to propagate into the dielectric, and Eq. (2-51) is

integrated backwards to the vacuum in order to compute reflection and transmission coefficients.

If we consider a fully ionized two-fluid plasma with infinitely heavy fixed ions that scatter mobile electrons, then the effective permittivity could have the form²⁻²⁹

$$\epsilon(z) = 1 - \frac{\omega_p^2(z)}{\omega^2} \left[1 + i \frac{\nu(z)}{\omega} \right]^{-1}, \quad \text{where } i = \sqrt{-1}. \quad (2-53)$$

In Eq. (2-53), ω_p^2 represents the square of the local plasma frequency

$$\omega_p^2(z) = \frac{4\pi e^2 \rho(z)}{m}, \quad (2-54)$$

where m , e , and $\rho(z)$ are the electronic mass, charge, and local density, respectively; and $\nu(z)$ represents the local electron-ion collision frequency

$$\nu(z) = \frac{4}{3} \left(\frac{2\pi}{m} \right)^{1/2} \frac{Z e^4 \rho}{(kT)^{3/2}} \ln \Lambda(\omega), \quad (2-55)$$

where Z is the average number of electron charges per ion, k is Boltzmann's constant, T is the electron temperature in degrees Kelvin, and $\ln \Lambda$ is the Coulomb logarithm. The code actually uses Dawson and Oberman's more accurate model²⁻³⁰ for $\epsilon(z)$. Such usage only changes the complex plasma impedance by a small percentage. Equation (2-53) is not expanded in accordance with the inequality $\nu \ll \omega$; so the effective absorption coefficient does not have the factor $(1 - \omega_p^2/\omega^2)^{-1/2}$, which is singular at the critical surface.

The geometric optics analysis of a linear layer with an effective absorption coefficient having this singularity yields the reflection coefficient

$$R(\theta) = \exp(-2\sigma \cos^5 \theta), \quad (2-56)$$

where σ is an optical thickness parameter.²⁻²⁵ Figure 2-12 contrasts the wave-optics results obtained

(a)

(c)

(b)

Fig. 2-12. Calculated wave optics reflection coefficients (solid curves) and geometric optics reflection coefficients vs angle of incidence. (a) $\sigma = 0.05$, (b) $\sigma = 0.5$, (c) $\sigma = 5.0$.

from Eqs. (2-53) through (2-55) with a linear density profile. The close agreement at large optical thicknesses also contradicts the conclusions of another study,²⁻³¹ whose integrating packages for the wave equation are probably not accurate enough for large optical thicknesses.

If we also consider polarization in the plane of incidence, then we find that the electric field is singular where the effective permittivity for normal incidence vanishes. This unphysical singularity can be avoided if our analysis incorporates a more realistic, quasihydrodynamic, plane stratified model²⁻²⁶ that accounts for electron thermal motion and the generation of collective plasma oscillations. Our code can readily be refined to integrate the more complex system of ordinary differential equations, but its model for absorption by inverse bremsstrahlung is not appropriate for anomalous absorptive processes in high-power laser-fusion systems.

from Eq. (2-56). The largest differences are found at intermediate values of the optical thickness. The normally incident difference at $\sigma = 0.5$ is much less than the aforementioned 20% disagreement with asymptotic wave-optics estimates, which were obtained

Laser Effects

A STUDY OF EFFICIENT IMPULSE DELIVERY AND PLATE RUPTURE BY LASER-SUPPORTED DETONATION WAVES

Introduction

When a pulse from a sufficiently high-powered laser is directed at a solid target in an atmosphere, a laser-supported detonation (LSD) wave is ignited at the target surface and travels away from the target. The hot plasma produced by this LSD wave delivers an impulse to the target which may cause it to rupture or crack. To design a laser to damage a given target, we need to relate this impulse both to the beam parameters (such as intensity, pulse length, and spot size) and to the target parameters (thickness, area, material properties, and failure mode). We have made the pressure relaxation time much less than the target response time so that we can treat the plasma expansion and the target failure as separate problems. We have combined simple physical models with computer simulations to develop scaling laws linking the beam and target parameters when the energy in the laser pulse is converted into target damage in the most efficient manner.^{2-32,2-33}

Model of Impulse Delivery by LSD-produced Plasma

When a laser beam of radius R and intensity I_0 ignites an LSD wave at the target surface, a pressure of $P_{DW} \approx 10$ to 1000 MPa is created in the detonation wave (Fig. 2-13). This pressure quickly moves away from the target, leaving a steady pressure, $P_{ID} \approx 1/3 P_{DW}$, behind it until a relaxation wave relieves it (see Fig. 2-1).

The laser pulse time can be obtained from the hydrodynamic relaxation time. The characteristic times are the radial relaxation time $\tau_R = R/C_J$, where C_J is the Chapman-Jouguet sound speed and the axial relaxation time $\tau_z = \tau_p + D\tau_p/C_J = \tau_p (2 + 1/\gamma)$ where D is the detonation velocity.

The efficiency with which impulse is delivered to the target is measured by the coupling coefficient; i.e., the impulse I divided by the pulse energy E . To optimize I/E we choose τ_p so that $\tau_z = \tau_R$, thus minimizing the beam energy without sacrificing too

Fig. 2-13. Plasma geometry.

Fig. 2-14. Surface pressure at beam center vs time for various pulse lengths (LASNEX).

much pressure loading at the center of the target. Calling this pulse length τ_{opt} , we find that $\tau_{opt} = \gamma/2\gamma + 1 \tau_R = 0.351 \tau_R$ for $\gamma = 1.18$.

The relaxation behavior of $p(r,t)$ at $r = 0$ predicted by the above analysis was verified by LASNEX calculations²⁻³² (see Fig. 2-14). The initial pressure peak represents the detonation wave when it is directly on the target surface.

The impulse delivered to the target by an optimized pulse can now be written

$$I = f P_{ID} A_s a_R, \quad (2-57)$$

where $A_s = \pi R^2$ is the spot area and f is a blast scaling parameter > 1 that takes into account the additional impulse due to plasma expansion.

Computer calculations of f give values that depend on τ_p and also on whether we consider only I_s , the impulse delivered over the beam spot, or I_T , the total impulse applied to an infinite target. Typical values for f are 1.75 for spot loading and 15.3 for total loading when $\tau_p = \tau_{opt}$.²⁻³²

The total impulse exceeds the spot impulse by a factor of approximately ten, as shown in Fig. 2-15 for

pulses of various lengths. However the important quantity for damage is shown in Sec. 3 to be impulse intensity: i.e., impulse divided by area. To determine the plasma area as a function of time we have found that a hemispherical blast wave formula is in good agreement with LASNEX results.²⁻³² Hence, if we calculate I/A for spot and total loading, we find that $(I/A)_{spot}$ is $1/6$ of $(I/A)_{total}$ by a factor of 6 or more.²⁻³² Furthermore, spot loading can be shown to deliver an impulse most efficiently when the beam radius is made equal to the target radius. We will now consider a simple model of the target that will tell us the minimum impulse required to rupture it.

Model of Plate Deflection and Rupture Under Impulsive Loading

As a model for LSD impulse damage, we consider a simply supported thin circular plate of radius a and thickness T (see Fig. 2-16), to which we apply a uniform pressure pulse for a time that is short compared to the plate's response time. Figure 2-17 shows that the plate deflects such that the maximum deflection h depends on the applied impulse. Calculations and experiments have shown that the deflected shape at the time of rupture is approximately conical but that it has a rounded tip, which we approximate with a parabola.

Fig. 2-15. Spot and total impulse vs pulse length.

The deflection h at the center can be obtained by equating the kinetic energy due to the impulsive loading to the strain energy of plastic deformation. By equating these two energies and setting $R = a$, we get

Fig. 2-16. Target geometry.

Fig. 2-17. Deflected slope of a circular diaphragm under impulsive load.

$$\frac{h}{a} = \frac{1}{T\sqrt{2k_1}\sigma_0\rho} \frac{1}{\pi Ra}, \quad (2-58)$$

where k_1 is a dimensionless geometric factor, σ_0 is the yield stress, ρ is the plate density, and A is the plate area, showing that the deflection divided by the radius is expected to be a linear function of $1/A$. Experimental confirmation of Eq. (2-58) can be found in the work of Florence,²⁻³⁴ who subjected simply supported circular plates to uniform explosive loading and measured the permanent deformation. His results, reproduced in Fig. 2-18, show a linear dependence of h/a on $1/A$ for deflections up to $h/a = 0.32$ for aluminum.

Calculations with the finite element code NONSAP²⁻³⁵ and the finite difference code HEMP²⁻³⁶ are in good agreement with the data shown in Fig. 2-18.

Having established the validity of Eq. (2-18) we now apply it to determine the minimum impulse $I_{\min}$ required to rupture the plate. For this purpose we need to calculate the critical deflection $h_{\max}$ at which

Fig. 2-18. Impulses per unit area vs central deflection for aluminum (6061-T6).

rupture begins. This can be done through the application of the von Mises failure criterion, which relates the general state of stress and strain in a body to the properties of a simple tension test.

A calculation of the strain distribution in the deflected plate shows that

$$\frac{h_{\max}}{a} = \sqrt{\frac{\epsilon_f}{2k_2}}, \quad (2-59)$$

where k_2 is another dimensionless geometrical factor and ϵ_f is the strain at failure in a simple tension test.

Substituting $h_{\max}$ into Eq. (2-58) we obtain the minimum impulse required for rupture; for the pressure acting over the entire plate we have $R = a$ and

$$I_{\min} = K\pi RaT = KAT, \quad (2-60)$$

where $K = \sqrt{k_1/k_2} \epsilon_f \rho_0$. Note that the constant depends only on the material properties of the plate. We see that the impulse $I_{\min}$ required to rupture the plate is directly proportional to its volume. Typical values of K are 3.2 and 13.4 Ktsp/mm for aluminum and steel respectively.²⁻³²

In Fig. 2-19 we show the deflection and yielding (as calculated by the HEMP code)²⁻³⁶ of an aluminum plate with $R = 10$ cm, $a = 15$ cm, $t = 3$ mm. According to Eq. (2-60) we should need $(15/10)(3.2)(3) = 14.4$ ktsp to rupture the plate; the

Fig. 2-19. HEMP code results for an impulsively loaded plate.

Fig. 2-20. Impulse per spot area required for rupture of circular aluminum plate vs plate thickness (HEMP calculation).

calculation shows breakage with 14.7 ktsp. At maximum deflection $h_{\max}/a = 0.28$. This is in good agreement with Eq. (2-59), which predicts $h_{\max}/a = 0.27$. Figure 2-20 shows other HEMP results for $R/a = 2/3$. These results are in good agreement with Eq. (2-60).

Optimized Laser Design Curves

A pulsed laser beam of the type we have been describing is characterized by three parameters (i_0 , τ_p , and R), which determine other beam properties such as pulse energy, $E = I_0 \pi R^2 \tau_p$, and momentum, I . Similarly, three parameters are sufficient to describe our circular thin-plate targets: T , a , and K .

These six parameters are subject to four constraints:

- Pulse optimization: $\tau_p = \tau_{opt}$
- Equal radii: $R = a$
- Impulse to rupture: $I_{\min} = K\pi a^2 T$
- Equal impulses: $I = I_{\min}$

When these conditions are imposed, the laser beam parameters required to rupture a given target are completely determined by any two of the six beam and target parameters. For example, choosing I_0 and τ_p as the independent parameters, we obtain²⁻³²

$$R = c_1 I_0^{1/3} \tau_p \cdot \frac{I_s}{A_s} = c_2 I_0^{2/3} \tau_p \cdot \frac{E}{A_s} = I_0 \tau_p, \quad (2-61)$$

where

$$A_s \equiv \pi R^2, \quad c_1 = 13.20 \left(\frac{0.00125}{\rho_0} \right)^{1/3},$$

$$c_2 = 0.08461 (\rho_0 / 0.00125)^{1/3} f, \quad f \approx 1.5. \quad (2-62)$$

(in cgs units) when $\gamma = 1.18$.

In Figs. 2-21 through 2-24 we present graphs relating beam parameters and target parameters for intensities in the range $I_0 = 10^6$ – 10^9 W/cm².

Thus far, all results quoted have been independent of wavelength. Wavelength, however, is an important parameter when determining whether laser energy can be propagated to the target in the first place. For dirty

air at sea level, the breakdown threshold for 10.6- μ m radiation may be as low as 5×10^6 W/cm². Unless this threshold can be increased substantially through the use of precursor pulses, the values in Table 2-3 are of academic interest at the aforementioned wavelength — a shorter wavelength pulsed device will be required.

Fig. 2-22. Beam radius vs beam intensity for various values of aluminum plate thickness for optimized pulses in normal density air.

Fig. 2-21. Total impulse/area vs pulse energy for various values of beam intensity for optimized pulses in normal density air.

Fig. 2-23. Maximum rupturable plate thickness (aluminum and stainless steel) vs pulse energy for various values of beam intensity for optimized pulses in normal density air.

Table 2-3. Optimized laser beam parameters yielding $I_s/A_s = 10^4$ taps at

I_0 , W/cm ²	τ_p , μ s	E, MJ	R, cm	I_s 10 ⁶ dyne-s	I_s/E , taps J/cm ²	E/A_s , J/cm ²
10^7	73	4.4	44.7	62.8	14.3	697
10^8	15.7	2.1	20.7	13.5	6.3	1582
10^9	3.4	1	9.6	2.9	2.9	3453

We also observe that, for a target of given area, $\tau_p \propto T^{-1}$, $I_0 \propto T^3$, $E \propto T^2$; whereas for a given thickness $\tau_p \propto A$, $I_0 \propto A^{-3/2}$, $E \propto A^{-1/2}$. Thus, increasing the target thickness increases the energy requirements rapidly, whereas increasing the target area increases the pulse time but decreases the energy required.

The scaling of the laser parameters with ambient density (ρ_0) is determined by Eq. (2-62), which shows that $c_1 \propto \rho^{-1/3}$, $c_2 \propto \rho^{1/3}$. Thus, if I_0 and I_s/A_s are taken as independent parameters, we find that $\tau_p \propto \rho^{-1/3}$, $R \propto \rho^{-2/3}$, $E \propto \rho^{-5/3}$. The pulse energy (E) increases rapidly as ρ_0 is decreased; i.e., at higher altitudes. We see that the energy requirements at higher altitudes are greatly increased, while at the same time the coupling coefficient is reduced and the beam size increased. Thus, damage by LSD waves will be less feasible at high altitudes.

Fig. 2-24. Total impulse/area vs beam radius for various values of beam intensity for optimized pulses in normal density air.

IGNITION OF HIGH-EXPLOSIVES BY LASER PULSES

The response of high-explosive (HE) materials to laser radiation has been studied theoretically as part of a program of research on the potential of high-power lasers as antimissile weapons.

In the study²⁻³⁷ two distinct regimes of laser pulse duration (τ_p and flux density I_0) are identified in which the elementary physical pictures of the laser-target interaction are quite different. It is shown

that relatively low intensity, long duration pulses ($I_0 \lesssim 1$ kW/cm², $\tau_p \lesssim 1$ ms) can cause thermal initiation of the HE, whereas high intensity, short duration pulses (e.g., $I_0 \sim 50$ GW/cm², $\tau_p \sim 100$ ns) are capable of producing shock initiation.

For the thermal initiation regime the problem is modeled as one of transient heat conduction in one dimension in the presence of a self-heating (chemical

Table 2-4. Ignition times vs laser flux density

PETN		TNT		HMX	
t^* , s	I_0 , kW/cm ²	t^* , s	I_0 , kW/cm ²	t^* , s	I_0 , kW/cm ²
$(4.3)10^{-6}$	18.6	$(2.0)10^{-4}$	3.54	$(8.1)10^{-4}$	1.10
$(1.2)10^{-5}$	10.7	0.036	0.176	$(1.5)10^{-3}$	0.791
$(3.9)10^{-4}$	1.55	0.32	0.051	$(5.3)10^{-3}$	0.396
0.013	0.226	0.94	0.027	0.041	0.129
0.85	0.022	1.83	0.019	0.27	0.046

reaction) term. The following analytical formulas are obtained for a threshold flux density (I^*) and an ignition time (t^*), such that for a given value of $I_0 < I^*$, the onset of thermal runaway is predicted to occur at time $t^*(I_0)$, but for I_0 above I^* the rapid removal of material by laser-induced vaporization can preclude thermal initiation.

$$(t^*)^{1/2} \exp \left\{ -\frac{E/R}{(qI_0^2 t^*)^{1/2} + T_a} \right\} = \frac{(q)^{1/2} C I_0}{2QZ} \quad (2-63)$$

$$I^* = \frac{2QZT_v}{Cq}^{1/2} \exp \left\{ -\frac{E/R}{2[T_v + T_a]} \right\} \quad (2-64)$$

The parameters Q , Z , and E represent the heat of decomposition, frequency factor, and activation energy, respectively. C is the specific heat of the HE, T_v its vaporization temperature, and T_a is a reference (ambient) temperature value. R is the gas constant; the quantity $q = (1.26) \alpha^2 / (K\rho C)$, where α is the surface absorptivity, K is the thermal conductivity, and ρ is the density of the HE. Values of t^* and I^* for several HE's of interest are given in Tables 2-4 and 2-5.

Figure 2-25 shows the predicted variation of surface temperature with time for the case of PETN explosive illuminated by a step-function laser pulse. The figure indicates that thermal runaway in the sample precedes the onset of surface vaporization so long as $I_0 < I^*$.

Table 2-5. Critical flux density levels

HE material	I^* , kW/cm ²
PETN	18.6
RDX	1.9
HMX	1.1
TNT	0.051

In the impulse or shock initiation regime the physics of the problem is dominated by a shielding plasma that forms over the target surface; i.e., the blow-off vapor, which in the thermal initiation regime, is relatively cool, un-ionized, and transparent to the laser beam, is hot, ionized, and highly absorbing in this high-intensity case. For the purpose of making a coarse theoretical estimate, a self-regulating-ablation (SRA) model is adopted by which one can derive estimates of the pressure (P) exerted on the target surface as a function of the laser parameters, I_0 , τ_p . This information is then coupled with a " $P^2\tau$ " ignition criterion for HE's to determine the combinations of I_0 and τ_p that can produce shock initiation. The shock initiation condition is found to be

$$[\tau_p(\text{ns})]^{3/4} [I_0(\text{GW/cm}^2)]^{3/2} \geq 17[P^2(\text{kb})\tau(\mu\text{s})]_{\text{min}} \quad (2-65)$$

The right-hand side is of order 10^4 for explosives of interest; e.g., if $\tau_p = 100$ ns we need $I_0 \cong 50$ GW/cm².

In the near future it is expected that T-Division experiments can be performed to test these predictions. Earlier experiments in the thermal

initiation regime^{2,38} appear to be beyond the scope of the one-dimensional theory; impulse initiation experiments have yet to be tried.

Fig. 2-25. Growth of PETN surface temperature in time under exposure to a step-function laser pulse with flux density I_0 .

The normalization factor τ_θ is defined by

$$\tau_\theta = \theta^2 / (qI^2), \quad \theta \equiv \frac{E/R}{\ln(QZ/C)} - T_a$$

(In the absence of chemical heating τ_θ is the time required for the surface to reach the temperature θ .)

A short-duration CO₂ laser pulse propagating in a high-pressure amplifier is capable of extracting stored energy on several different time scales. The excited molecules of the amplifying medium possess "reservoirs" of rotational and vibrational energy, in addition to the immediately accessible energy stored on a given transition resonant with the pulse. A theory has been derived to predict the energy extraction as a function of the width, τ_p (ns), and fluence level, E_{in} (J/cm²), of the input pulse.²⁻³⁹

The range of effects one can expect is gauged by the parameters τ_p/τ_r , τ_p/τ_{vv} , and E_{in}/E_{sat} , where τ_r and τ_{vv} represent characteristic times for rotational and intramode vibrational-vibrational (V-V) energy transfer. E_{sat} is a characteristic saturation level for the input fluence, and is given by

$$E_{sat} \equiv (h\nu_{uv}/2\sigma) e^{-\alpha_0 L},$$

where ν_{uv} is the resonant frequency, σ is the

Fig. 2-26. Limiting curves for a CO₂ amplifier. The curves 2LS, RR, and V-V refer respectively to the limits $\tau_p/\tau_r \ll 1$, $\tau_p/\tau_r \gg 1$ with, when only rotational coupling is included, and $\tau_p/\tau_r \gg 1$ when both rotational and intramode V-V energy transfer is included. The indicated abscissa points have values in the ratio

$$E_3:E_2:E_1 = \gamma(M+1):(M+1):1.$$

Fig. 2-27. Comparison of theory with experiment.²⁻⁴²

electromagnetic absorption cross section, α_0 is the small signal gain of the amplifier, and L is amplifier length.

When the pulse duration is so short that $\tau_p / \tau_r \ll 1$, the rotational and vibrational energy transfers do not have time to occur during the pulse-molecule interaction. The amplifying medium then acts like a two-level system.²⁻⁴⁰ The amount of energy the pulse

can extract from the medium is governed by the initial value of the population inversion $[n^u(0) - n^l(0)]$ of the upper (u) and lower (l) vibrational-rotational levels directly involved in the laser transition. In the opposite extreme, when the input pulse duration is quite large relative to τ_r , the field-induced changes in n^u and n^l can be countered by rotational and vibrational energy exchange. It is

found that the extractable energy in this limit is determined by the appreciably larger population inversion density $\gamma(M+1)[n^u(0) - n^g(0)]$. The factor $(M + 1)$ arises from rotational energy transfer while the factor γ is contributed by the intramode V-V process (slower types of vibrational relaxation are neglected).²⁻⁴¹ In a typical case, M is about 15 and γ about 3.

The principal results in these limits are summarized in Fig. 2-26. The curve labeled 2LS refers to the two-level-system limit²⁻⁴⁰ and is given by the formula

$$\begin{aligned} (E_{\text{out}} - E_{\text{in}})/(E_{\text{in}}[e^{\alpha_0 L} - 1]) \\ = \left\{ E_{\text{sat}} e^{\alpha_0 L} / (E_{\text{in}}[e^{\alpha_0 L} - 1]) \right\} \\ \times \ln \left\{ 1 + e^{\alpha_0 L} [\exp(E_{\text{in}}/[E_{\text{sat}} e^{\alpha_0 L}]) - 1] \right\}. \quad (2-66) \end{aligned}$$

The curve RR represents the limit, $\tau_p/\tau_i \gg 1$, of full utilization of the rotational energy reservoir, neglecting any vibrational energy transfer. The curve labeled VV

represents the limit in which intramode VV energy transfers contribute fully; i.e., when the duration of the input pulse is long compared to τ_{vv} as well as τ_i . These curves can be constructed simply by translating the 2LS curve to the right by factors of $(M + 1)$ and $\gamma(M + 1)$ respectively; alternatively, they can be obtained from Eq. (2-66) by replacing E_{sat} with $(M + 1) E_{\text{sat}}$ and $\gamma(M + 1) E_{\text{sat}}$, respectively. The energy extraction for values of the pulse width that are intermediate between τ_i and τ_{vv} is obtained by numerical integration.²⁻³⁹

A comparison of the theory with published experimental results of Figueira *et al.*²⁻⁴² is shown in Fig. 2-27. The agreement is satisfactory and leads to an estimate of

$$1/(\tau_{vv} P_{\text{CO}_2}) = (1.0 - 3.5) \cdot 10^6 \text{ s}^{-1} \text{ torr}^{-1}$$

for the rate of intramode VV energy transfer in CO_2 , where P_{CO_2} is the partial pressure of carbon dioxide in a gas mixture.

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3. PULSED POWER AND PLASMA PHYSICS

Introduction

The plasma physics effort in the Division is directed toward developing tools — analytical, numerical and experimental — to provide the Laboratory with a valuable design resource in the areas of pulsed power, energy conversion, and energy transport. Our work includes activities in a broad range of research areas — nonlinear wave propagation, intense microwave generation and interaction, collective ion acceleration, high-intensity relativistic beam dynamics, dense plasma focus phenomena, low-inductance power supply component design, plasma x-ray sources, and plasma beam-field computer code development.

In the past forty years plasma physics has developed from minor branches in statistical mechanics and hydrodynamics into a major discipline. It now exceeds any other field of physics in its richness of nonlinear phenomena and variety of potential applications. At sufficiently high specific energy density, all materials are plasmas. Thus, the technology of energy conversion and transport at high power densities is governed by the laws of plasma physics. Although processes such as

coherent coupling, soliton transport, and caviton formation may presently appear as theoretical curiosities, mastery of such phenomena will provide keys to the efficient release of and control of energy of all forms — nuclear, chemical, mechanical and electromagnetic.

The following description of our activities is divided into two sections. The experimental section describes the continuing collective acceleration work, the plasma focus facility development and experimental design, low-inductance power supply component design and development, and design of intense microwave cavity experiments. Many of these activities are carried out in collaboration with the experimental physics and electronics engineering divisions at the Laboratory. The theoretical section describes current work on the analysis of dense pinch phenomena, the interaction of intense microwave fields with plasmas, the propagation and break-up of solitons in nonplanar geometries, gas imbedded Z-pinches, and the development of efficient simulation codes for studies of intense beam and electromagnetic field interactions with plasmas.

Experiments and Experimental Design

COLLECTIVE ACCELERATION EXPERIMENTS

The first attempt to accelerate positive ions with fields generated by high-energy electrons was made by Alfvén and Wernholm in 1952.³⁻¹ The potential of this exciting new concept was subsequently recognized by many scientists, and by 1956 several schemes had been proposed to accelerate ions by this method. Linear collective field acceleration has up until now been more effective than the Electron Ring Accelerator and other methods being investigated. For the past several

years, we have been developing a linear system that has demonstrated outstanding success — an energy conversion efficiency of better than 15%, accelerated protons with energies of up to 50 MeV, and heavy ion acceleration to energies greater than 7 MeV per nucleon.^{3-2,3-3} The geometry and vacuum conditions of the current system are also particularly favorable to potential fusion and accelerator applications.

The geometry of the experiment is shown in Fig. 3-1. A high-vacuum diode system with an adjustable graphite cathode and an insulated anode has been developed that operates with a relativistic electron beam with v/γ (the ratio of energy in electromagnetic fields to energy in particles) of ~ 1 . Dielectric lenses are used to focus the collectively accelerated electrons and ions which are ejected from a hole in the anode. The dielectric lenses are charged by the electron beam and focus both electrons and ions by convective processes. It has been determined that at least two lenses are needed to optimize ion energy, the lenses having some of the same characteristics as the insulated anode.

When operating with a cylindrically symmetric cathode structure, the current sheet was observed to be strongly, but somewhat irregularly, filamented (Fig. 3-2). The maximum proton energies obtained with this system were on the order of 20 MeV.

To better understand the role of the filamentation process in the system, axial grooves were cut in the cathode to deliberately emphasize the filament structure. It was found that a system with eight grooves resulted in a highly stable eight-fold current structure that persists throughout the entire current path, and that upon proper insulation of the target structure, the proton energy produced in the device is increased to approximately 50 MeV. Since the

operation with insulated targets had little effect in the symmetric cathode system, we conclude that the increased ion acceleration is due to the strong ordering of the electron current into the observed stable structure.

All of the experiments described here were performed on the LLL Pulsed e-beam machine, which delivers 2.5 kJ at 1 MV to the diode in 50 ns.

The current results from these experiments on ion acceleration are in Table 3-1.

Although highly successful, this system does not easily lend itself to detailed theoretical investigation. The overall acceleration process in the device appears to depend on the observed cavity-mode interaction of the e-beam with the dielectric anode structure through inductively-coupled surface currents. There is also a very hot, diffuse, and apparently turbulent region created between the anode and target structures. Only ions emitted from the anode hole region are observed to be accelerated to significant energies. Our present hypothesis is that the major ion acceleration occurs from plasma waves strongly coupled to the anode-beam system in the anode hole region. As they accelerate (in group velocity) down the axial plasma density gradient, they finally deposit their residual energy by Landau damping in the hot, low-density region. Although we have begun to study the nature of the current filament structures in more detail, we do not

Fig. 3-1. Geometry of the collective field acceleration experiment.

Fig. 3-2. Flow of current near the surface of the dielectric anode (image converter photo).

yet have an hypothesis that explains the strong dependence of the ion energy upon the stabilization of the filament structure. It may be significant that whereas with the cylindrically symmetric cathode, the ion energy achieved scaled roughly with ion mass, this no longer seems to be the case with the stabilized system.

Besides the obvious need for more detailed diagnostics to compare with acceleration mechanism hypotheses, the most important factor for applications is determination of the scaling law for ion energy as a function of input energy to the diode of the collective accelerator. The energy range of the LLL Pulsarad 422 is too small to do this measurement.

Table 3-1. Experimental results: collective field acceleration (LLL Pulserad e-beam machine)

Proton energy	45 MeV
Number of protons	10^{14} per burst
Heavy ion energy	80 MeV (C, F, and Cl)
DD neutrons	10^{11} per burst
Fn neutrons	10^{10} per burst

However, it can be done on the Boeing FX 175,² and we plan to do this experiment as soon as possible.

Another important fundamental investigation for some applications is the study of beam propagation

in vacuum for about 10 m. This experiment could also be done conveniently at Boeing, and possibly at LLL with some experimental modifications.

A third important parameter is the degree of focusing achievable in a propagating collectively accelerated beam. Magnetic, electrostatic and other focusing systems are being considered. It is believed that the stabilized filaments will play an important role in focusing when the beam is propagated over large distances. This experiment can not be undertaken meaningfully until scaling laws have been established and propagation of the beam achieved.

PLASMA FOCUS FACILITY AND EXPERIMENTS

The plasma focus was discovered in the USSR in the mid-1950's by Filippov^{3,4,5} and rediscovered several years later by Mather at Los Alamos.^{3,6} Since no one had predicted such a small diameter (about 1 mm), short pinch (about 1 cm), its discovery came as a surprise to experimentalists and theoreticians alike. Considerable interest was generated by declassification of this phenomenon at the 1958 Geneva Conference. Since that time plasma focus devices have proliferated and a number of them are in operation in various countries. In this country the largest device planned is the LLL 1 MJ "Rook" capacitor bank configuration, which eliminates capacitor bank cables. In Europe, 1-MJ devices are under construction in Poland and Italy. Filippov has proposed a 10-MJ device, the status of which is not known.

The plasma focus is a device that effectively accepts energy from a capacitor bank and transforms it into magnetic and kinetic energy of a plasma current sheet. When the current sheet collapses on axis, this stored energy is available at the Alfvén speed for conversion

into internal energy of the dense plasma region (focus) formed by the collapsing sheet. By control of the system parameters and geometry, a wide variety of energy couplings can be achieved in the focus — high intensity x rays ($>1/2$ kJ), neutrons ($>10^{12}$ DD), and energetic electron and ion bursts have all been observed in focus experiments in the 200- to 500-kJ range.

A primary motivation for the development of the LLL facility is the prospect of coupling the stored energy of the focus system, either directly or through the intense particle bursts, into suitable "targets." The goal of these studies will be to increase the fusion energy yield over that achievable from the focus itself. Even without targets, however, a DT fusion yield of about 10^{15} reactions is predicted for conservative scaling at the 1-MJ level, making the facility *the most potent laboratory pulsed neutron source in this country*. When combined with a suitably designed prompt multiplier, fluences on the order of 10^{15} neutrons/cm² delivered in 10^{-6} s have been shown to be achievable over volumes of about 1 liter. This could be interesting for materials studies, in laser pumping experiments, and as a radiation (neutron and gamma) source.

*Reference to a company or product name does not imply approval or recommendation of the product by the University of California or the U.S. Energy Research & Development Administration to the exclusion of others that may be suitable.

Fig. 3-3. The LLL plasma focus.

A further purpose of the focus experiments is that the plasma dynamics represented in the system will allow detailed comparison of theory and experimental data in the run-down and collapse phases and in the strongly turbulent behavior in the focus and disrupted-focus phases. We believe that the modeling of such effects as arc-starvation and radiation collapse (the Pease-Braginskii limit) lies within the range of current plasma physics theory and calculational tools, provided they are amply girded and supported by experimental data.

Preliminary check-out of the focus facility below 100 kJ was started late in 1975 (Fig. 3-3). No difficulties were encountered during these initial tests, except for a flashover in the gun itself, which occurred on the 44th shot. The quarter-section bank and switches are performing with excellent shot-to-shot reproducibility over the pressure range of 6 to 10 Torr D_2 fill, with peak neutron yield ($\sim 5 \times 10^{10}$) occurring at 8 Torr, as anticipated. These shakedown runs will be continued with increasing operating energy up to about 250 kJ. Experiments at this level with targets (CD_2 pellets and DT microbubble) will be

carried out early next year, primarily to gain experience with mounting procedures. The bank will then be assembled to the 0.5-MJ level and extensive design optimization and data gathering will commence. The operation at full 1-MJ capability will be guided by the results of the 0.5-MJ operating results, depending upon which coupling mode appears most favorable for optimizing the yield in target-coupled systems.

Extensive compilation and study of data, from a large number of plasma focus facilities, strongly support a reaction yield which scales as the fifth power of peak current (see Fig. 3-4). This scaling is also predicated on theoretical arguments for one burn model (the "deflagration" burn) of the plasma focus. If this scaling, rather than the second power dependence predicted by more conventional theories, is verified, fusion breakeven might be achieved in a sufficiently low-inductance system at energies $\lesssim 1$ MJ. Such a facility could provide substantial net power and energy gains in a hybrid configuration. A repetitively pulsed system utilizing these design concepts could also provide a valuable fusion reactor materials test facility.

FAST SWITCH DEVELOPMENT

Most high-energy plasma physics is dependent upon energy compression in space and time. Such energy compression is the product of the coherent interaction of matter with energy storage modes such as kinetic energy and electromagnetic energy. Thus, we can envision the energy compression process as a series of compression stages starting at the utility outlet (where a few megawatts of power may be delivered and fields and energy densities are moderate) and progressing to the limit of material properties in unionized matter, and then into the plasma state where still different processes are used to continue the compression processes. Since there is a premium on maximizing space-time compression in the early stages of compression, we have supported the investigation of

fast switches in the electronics engineering department.³⁻⁷

The most important characteristics of such a switch are: power handling capacity, rise time, and lifetime. Another consideration for large systems is the ability of many switches to function simultaneously.

Solid dielectric switches currently handle the highest power and have short rise times. However, they are single shot devices and have simultaneity problems. The best currently available repetitive device is the high-pressure spark gap. It can carry up to 1 MA per channel (0.1 μ s) and hold off 500 kV/cm (100 psi). The inductance is around 0.05 nH/kV (25 nH at 500 kV), and the simultaneity is in the nanosecond regime.³⁻⁸

Fig. 3-4. Neutron yield vs peak current per pulse, and corresponding energy output (see following page for legend).

In the past, silicon switches (thyristors) have been able to obtain current rise times of the order of 1 to 3 kA/ μ s. Westinghouse Research Laboratories have demonstrated that light-activated silicon switches

(LASS) have current rise times of about 20 kA/ μ s (up to 3 kA).

Because we suspected that the rise time for the LASS device would only be limited by the length of

Legend for Fig. 3-4:

- AJ Aerojet Nuclear. 250 kJ, 20 kV, 320 μ F.
- Da Darmstadt. 0.34 - 1.35 kJ; 10 - 20 kV; C = 6.7 μ F; inductance = 24 nH; circuit frequency = 400 kHz; Mather type gun length = 10 cm, diam = 5 and 1.6 cm; hollow center electrode.
- H Hoboken. Electrode structure is identical to that of Darmstadt group. 14 - 18 kV; C = 6 μ F; hollow center electrode. Now in operation at University of Buenos Aires.
- H' Hoboken. About 5 kJ; 45 μ F; 14 kV; time to current peak 1.8 μ s; Mather type gun; length = 14 cm, diam = 10 cm and 3.4 cm. Hollow center electrode.
- A Aerospace Corporation.
- J Jülich. 25 kJ; 40 kV; C = 22.4 μ F; center electrode 3 cm long; 6 cm diam; outer electrode = 11 cm diam.
- Lj Limell. 96 kJ, 40 kV, inductance = 27 nH; 1/4 cycle time = 2.5 μ s.
- Lj' Limell. Plasma focus driven by explosive generator.
- LA¹ Los Alamos. DPF-6; 420 kJ.
- LA² Los Alamos. DPF-5; 120 kJ.
- LA³ Los Alamos. DPF-6; 210 kJ.
- M Moscow. $\gamma \rightarrow 10^{10}$ to 10^{11} DD neutrons; I = 1 MA.

the actuating laser pulse, we have undertaken an experimental investigation which has demonstrated current rise times in excess of 750 kA/ μ s at 10 kA.³⁻⁸ The results are summarized in Table 3-2.

Note that the LASS possesses the high power capability and short rise times needed for energy compression applications. Furthermore, the experiments summarized in Table 3-3 were performed using only a 0.1 cm² photo-actuation area; existing LASS devices have potential photo-actuation areas up to 50 cm² and thus current switching capabilities in the MA range are probable.

The other switch requirements for high power applications are long life and the ability of many switches to function simultaneously. Silicon switches have demonstrated long life in other applications. The nature of the LASS triggering mechanism makes it possible to predict that near perfect simultaneity can be achieved by ensuring that the light pulse reaches all switches at the same time.

Table 3-3 gives a qualitative comparison of currently available switches with the LASS.

The LASS device should lend itself very easily to the design of improved MARX generators. The inductance of the device is low (0.1 nH/kV or less) since practically all the magnetic flux can be external to the device. Triggering arrays of switches is particularly easy since laser triggering provides both high voltage isolation and perfect simultaneity (subnanosecond laser pulses are readily available).

Table 3-2. Summary of results^a

Z Ω	V, volts	I = V/Z, amps	τ , 10^{-9} s	I = 1/ τ , 10^9 (kA/ μ s)	P = VI, MW
50	750	15	4	3.75	0.011
25	750	30	4	7.5	0.022
0.156	1110	7115	11	647	7.9
0.104	1020	9820	13	755	10
↑ On line					

^aDefinition of symbols: Z = line impedance
V = pulse voltage
I = peak current
 τ = rise time
I = rate of current rise
P = power

Thus, the erection and discharge times of MARX generators can be substantially reduced, thereby providing higher fields and higher power densities in liquid dielectric transmission lines or Blumlein applications.

The discharge of megajoule capacitor banks on a repetitive basis is now feasible. The charge transfer capability of the LASS is in excess of 10 C, which is adequate. The primary limitation on a high repetition rate is the cooling of the devices. The flat geometry (providing a large surface area) and the low dissipation rate (between 0.1 and 1% of transferred energy) makes these devices particularly promising. For example a 1 kV to 100 kA switch can deliver 10⁸ W

Table 3-3. Qualitative comparison of switching devices

Switch type	High power	Long life	Simultaneity	Short rise time
Pressurized spark gap	✓✓✓			✓
Vacuum spark gap	✓✓		✓	✓
Thyatron		✓	✓	✓
Ignatron		✓	✓	✓
Transistor		✓✓✓	✓	✓
Solid dielectric	✓✓			✓✓
Liquid dielectric	✓✓✓			✓✓
Thyristor	✓✓✓	✓✓✓✓		
LASS	✓✓✓	✓✓✓✓	✓✓✓	✓✓✓

of instantaneous power. If the dissipation is 1 MW and we can cool the device by convection or heat sinking at a 1-kW rate, then the duty cycle could be 10^{-3} . This result implies a 1-kHz repetition rate for a 100-MW/1- μ s pulse or a 100-kHz rate for a 100-MW/10-ns pulse. Currently available silicon switches typically have junction cooling rates of 100 W/cm².

Another interesting potential development would be to modify the geometry of the device to improve the coupling of the device to the circuit. The self inductance associated with the switch could be significantly reduced. Another possible geometrical modification is to optically integrate either a Ga-As laser or amplifier to the device. The device could then be triggered electrically or by a relatively weak light pulse, thereby maintaining electrical isolation of the trigger.

Turn-on with picosecond laser pulses in silicon has been demonstrated by Johnson and Auston of Bell Laboratories.³⁻⁹ There is no reason to suspect that turn-on in junction devices would be slower than in bulk intrinsic material. A crude estimate of the turn-on time is the light transit time in the depletion layer, which is about 1 to 2 ps.

MICROWAVE STORAGE, SWITCHING, AND HEATING

Plans have been developed during the past year to establish a new LLL facility to study intense microwave generation and interaction with plasmas. Design work and calculations for this system have been carried out over the past several years.³⁻¹⁰⁻³⁻¹² Previous experimental achievements include surface fields of 0.2 Tesla and power levels of about 3×10^8 W into a dummy load. Basic technological requirements of operating at liquid helium temperatures were also met.

The basic concepts and motivation for this work follow from the extremely high field intensities that can be created and stored within superconducting

The turn-off characteristics in single- and dual-junction devices should be similar to the performance of the storage or snapoff diode. These diodes generate gigahertz harmonics when the charge in the depletion layer is swept out and the diode snaps off. In a typical application, such a junction (biased at 1 kV) would be turned on with a picosecond rise time laser pulse. Depending on the waveguide impedance, amperes to kiloamperes could be conducted. When the light turns off the carriers are swept out and the device snaps off. This snap off can be timed accurately since both the number of carriers and the recombination rates are known. Thus, a resonant cavity could be excited with precise phasing. This phasing could be controlled by varying the spacing between the laser pulses. This can be done quite easily with electrooptic techniques. Thus, megawatts per device of microwave power can be generated at extremely broad bandwidth. We could construct phased array radar sources of very high powers. Finally, the use of these devices as programmed nonlinear elements in waveguides would make it possible to achieve high-power compression of microwave energy.

cavities with small losses; the apparently favorable containment/heating interaction possible between such fields and dense plasmas; and the high-power fluxes with which the stored microwave energy can be made available for coupling. Anticipated applications range from production of dense, relatively massive hot plasmas to ultra-high-power microwave beam pulses.

The three methods proposed for generating the intense cavity field are:

- Klystron excitation of a superconducting cavity (Fig. 3-5)
- Excitation of a small normal conducting cavity with a high-power e-beam

Fig. 3-5. Conceptual microwave fusion power generator for producing pulsed x rays and neutrons.

• Generation of high power, microwave frequency pulses using solid state switches.
Present e-beam machines ($P \sim 10^{12}$ W) can provide ≥ 100 -Tesla fields and close to 1 MJ of energy.

The present superconducting-cavity-based proposal is aimed at producing switched power levels in the range of 10^{12} to 10^{14} W, with stored energy ≥ 1 MJ. These are extremely interesting power levels for transmission into an interaction region for hot plasma production and for coupling into a radiating system

for production of intense propagating beams. Previous concepts and theories of "linearized" interaction of EM radiation with plasmas require drastic revision to describe the dynamics of systems in which the radiation pressure is comparable to or greater than the particle pressure. Some of the new theoretical results are presented in the theoretical section of this report. Many of the problems remain to be worked out, but a close coupling between theory and experiment will be required to explore the most interesting cases.

Theory and Analysis

MICROWAVE-PLASMA INTERACTIONS

To investigate the nature of the interaction of intense microwave fields with plasmas and evaluate the potential for applications of microwave-plasma systems, several new computer programs have been completed. One of these, ORBIT, tracks both electrons and ions in an approximate self-consistent field configuration. The details of the self-consistent fields themselves were determined with the aid of another program, as outlined in the paper by Ensley and White.³⁻¹³

A new heating mechanism, which we call field-reversal heating, and which is several orders of magnitude greater than the classical corona-collisional heating (inverse bremsstrahlung) and "PdV" heating for microwave confined systems, has been verified by the ORBIT code calculations. Field-reversal heating is greatest for plane polarized incident waves and is absent if the fields are circularly polarized. Field intensities corresponding to field pressures $\geq$ the plasma pressure are required.

The field reversal mechanism can be understood as follows: The interface between plasma and fields is a layer of thickness about c/ω_{pe} , where ω_{pe} is the electron plasma frequency. This layer, the corona, is sufficiently tenuous and has a small enough linear dimension for collisions to be ignored. We also have ignored radiation reaction forces.

Therefore, the Hamiltonian for the interaction of an electron with the fields is

$$H_e = -e\phi + (p_x + \frac{e}{c} A_x)^2 / 2M_e, \quad (3-1)$$

where e is the electronic charge, M_e is the electronic mass, P_x , P_y , and P_z are the canonical momenta, and $\vec{A} = [A_x(z,t), 0, 0]$ is the plane polarized field that is incident on the plasma from the $-z$ direction. ($A_z = 0$ is a consequence of the self-consistent field approximation.) And ϕ is the scalar "plasma sheath" potential due to charge separation.

In the paper previously cited, we have shown that the self-consistency of the fields requires (for a hydrogen plasma) that

$$e\phi = \frac{1}{4} \frac{e^2 A^2}{M_e c^2}. \quad (3-2)$$

The reflection of a particle "evaporated" from the plasma surface occurs where $p_z = 0$; hence, a thermal electron with $P_x = P_y = 0$ reflects where

$$kT = \frac{1}{4} \frac{e^2 A^2}{M_e c^2}. \quad (3-3)$$

(To see this, set P equal to 0, use Eq. (3-2) for ϕ in Eq. (3-1), and set H_e equal to kT .)

At times near field reversals, A_x is small everywhere and particles can penetrate deeply into the field region where, as the fields begin to rise after reversal, A_x will be much larger than the value given by Eq. (3-3). The electrons (and ions) are, in effect, lifted to higher potential energies by the rapidly increasing fields. When A_x vanishes, the transverse electric field ($E_x = -1/c \partial A_x / \partial t$) is at maximum. The electrons (and ions) which have penetrated deeply into the sheath region are, therefore, subjected to large transverse accelerations. For example, at the field intensities studied, E_x reaches 10^8 V/cm for select electrons according to the ORBIT calculations.

The behavior of electrons caught in the rapidly increasing field just after field reversal depends critically upon the field phase at the time of their injection into the fields and on the angle of injection. Some will be headed into the plasma as the fields rise; these are shot directly back into the plasma with energies reaching as much as 20 kT. Others are headed into the field as the field rises; these penetrate even deeper into the field before being reflected and typically achieve energies in excess of 50 kT. This is an important and rather beautiful example of phase

coherence phenomena: those electrons whose cyclotron orbits have just the right phase relation with the incident field achieve the highest energies.

Figure 3-6 shows a typical electron phase coherence resonance at times near the field reversal. Details of the resonance structure depend upon the energy of the injected particle, E_0 , and upon both the polar angle, θ , and the azimuthal angle, ψ , which define the direction of the injection velocity. ($\theta = 0$ is normal to the plasma surface, $\psi = 0$ is parallel to the incident $\vec{A}$ field.) Generally, the number of resonance peaks increases as $\theta \rightarrow 90^\circ$ and as $\psi \rightarrow 0^\circ$ or 180° . (For $\psi \approx 180^\circ$ the resonance occurs at a phase near π rather than 2π .) Electrons injected at times corresponding to the peak on the far right execute 1/2 of a cyclotron orbit before being driven back into the plasma. The penultimate peak corresponds to 3/2 cyclotron orbits, the next peak to the left to 5/2 orbits, etc.

We have studied individual particle orbits in detail and also have operated ORBIT in a Monte Carlo mode to calculate mean heating rates and energy spectra. Figures 3-7 and 3-8 show results of ORBIT calculations for an incident wavelength of 1 cm and a deuterium plasma.

For incident fields of the order of 1 to 10 MG and electron number densities between 10^{18} and $6 \times 10^{20}/\text{cm}^3$ (typical of those expected in the corona-plasma) the net power density in reflected electrons (i.e., power into pellet minus power in the outward thermal flux) is of the order of 1 to 10 TW/cm². For typical pellets — envisioned to have coronal radii on the order of 1 cm — this corresponds to a field-to-plasma coupling with net power in the 10 to 100 TW range.

The energy spectrum (Fig. 3-1) is such that approximately half the electrons reach energies of 30 kT or greater. Thus, field reversal heating offers the possibility of direct collisional heating of a dense pellet core imbedded within the thinner corona plasma. The time to double the pellet's thermal energy by this heating mechanism is estimated to be several orders

Fig. 3-6. A typical electron resonance at times near field reversal. The ordinate is the field phase at the time when the electron first enters the field; the abscissa is the energy increase upon reflection measured in units of the plasma thermal energy. Plasma parameters for this plot are: electron number density = $10^{21}/\text{cm}^3$, $kT = 6.25$ keV. The incident field has a wavelength of 1 cm.

Fig. 3-7. Net power density in reflected electrons as a function of the incident field. The numbers by the circled points are temperatures in keV.

of magnitude less than the hydrodynamic disassembly time.

Field-reversal heating and related phenomena may also be important in other situations; e.g., the plasma focus or the LLL collective ion acceleration experiment. Generally, the phenomenon may occur in any system in which the plasma densities and

Fig. 3-8. Net power spectrum for reflected electrons. Note that half the energy is supplied in electrons with energies ≥ 30 kT.

temperatures are sufficiently high and the electromagnetic field frequencies low enough that

$$(\omega/\omega_{pe}) (c/v_e) \ll 1,$$

where ω is the field frequency and v_e is the electron thermal velocity. Note that the field intensity is sufficient to reflect the thermal electrons.

In the near future we plan to use ORBIT to calculate corrected number density and current distributions to improve our self-consistent field approximation.

DENSE PINCH PHENOMENA AND TARGET DESIGN

Some effort has been directed toward analysis of the dense focus phase, fusion yield scaling, and target design principles appropriate to the plasma focus system described in the experimental section of this chapter (Refs. 3-14 through 3-18). At least five different neutron production mechanisms have been

identified for the plasma focus. One of the most interesting modes is referred to as the deflagration burn mode. This results from an explosion of the dense plasma pinch wire about 10 ns after maximum pinch. A plasma with a density decreased relative to the maximum pinch density by a factor 100 and with a

temperature of 10 to 20 keV and which is contained for a microinstability or Bohm diffusion time by the residual magnetic field. This mode accounts for at least 70% of the yield in the Filippov geometry and the yield in this case may be of a nearly thermonuclear nature. During this pinch explosion, about one-half of the inductive energy or roughly one-fourth of the bank energy is converted into plasma thermal energy. The explosion of the pinch is due to the onset of anomalous resistivity as a result of intense Langmuir turbulence. This causes an increase in the resistivity of the plasma wire by 2 to 3 orders of magnitude in a time $0.1 \text{ ns} \leq t \leq 1 \text{ ns}$.

If the deflagration burn yield scales as the 5th power of the current then the DT yield — at 1 MJ — should be at least 10^{15} neutrons or 2800 J. If this scaling is correct, break-even would be approached for a system driven by a 25-MJ capacitor bank. One form of the deflagration burn mode scaling is given by

$$Y = 10^{21} \frac{(fE_b)^{2.5} F(T)}{R\ell^3},$$

where Y is the DT neutron yield, F_b is the bank energy in MJ, R , and ℓ are respectively the exploded pinch radius and length in cm, T is the temperature in KeV and f is the fraction of bank energy that goes into plasma heating during the pinch explosion. The Maxwell averaged velocity cross section product $\langle\sigma v\rangle$ has been written in the form $\langle\sigma v\rangle = 10^{-16} F(T)$. Ideally $f \rightarrow 1/4$, while an experimental value of f tends to be more nearly $f = 1/8$. The factor $F(T)/T^3$ has an optimum value at about 8 keV. For the exploded plasma deflagration burn, the $R\ell$ product is about 1.

It can be seen that a substantial increase in the yield resulting from deflagration burn at fixed bank energy can only be obtained by decreasing the $R\ell$ product. A decrease in $R\ell$ by a factor of 100 could result in a DT yield approaching the 1-MJ bank energy.

By operating at lower pressure, the factor, $f \rightarrow 1/4$, of the bank energy that goes into plasma heating for high-density operations can be substantially converted

into a small-diameter, relativistic electron burst and oppositely directed ion burst that is concentrated in an axial cone with a half angle of $\leq 104^\circ$. The accelerated ions have been observed to exceed the bank voltage by a factor of more than 100. The entire pinch current — several MA — can be carried by the accelerated electrons and ions for low density mode operation. By use of a hollow anode, an additional source of gas for the ion acceleration of the pinch is provided. This permits an increase in the ion current substantially greater than the ratio $\sqrt{M_e/M_i}$ times the electron current dictated by simple space charge considerations.

In addition to the low-density mode electron and ion bursts obtained from the focus, substantial energy compression into material degrees of freedom is provided by the snowplowed plasma, particularly in the high-density mode operation. This collapsing plasma shell reaches a final velocity prior to stagnation in axis of $3 \text{ to } 5 \times 10^7 \text{ cm/s}$. The snowplow can have a thickness of 0.2 cm resulting in a stagnation time as short as $4 \times 10^{-9} \text{ s}$. The collapsing plasma shell can contain at least 5% of the bank energy or plasma kinetic energy. This corresponds to enough stagnation power — in excess of 10^{13} W — to drive a small diameter cylindrical or pseudospherical microexplosion placed on axis. Final direct coupling of the inductive stored energy of the disrupted sheet should dramatically increase the final power available to the implosion.

Numerous target ideas have been evolved from the focus. Figure 3-9 shows an example of a target that illustrates many of the principles of interest. The target is a 1-mm-i.d., 1-cm-long glass tube with 100- μm -thick walls, containing D^2 gas at 100 atm. In the ideal case, the DT should be present as a uniform frost layer on the inside surface of the glass wall.

The sequence of events imagined for this target begins with pinch formation between the hollow anode and the target end and results in injection of a large burst of 300-kV to 1-MeV ions into the target end. This is rapidly followed by stagnation of the current

Fig. 3-9. The plasma focus and target.

sheet on the outer wall of the target cylinder, which causes the wall to implode as an exploding pusher. A second pinch forms off the far end of the target and injects a relativistic electron burst along axis into the target. Initially a return current is induced back along the path of the relativistic current. However, conditions favoring development of strong Langmuir turbulence exist — particularly if the ion burst and the shock heating resulting from current sheet stagnation have resulted in an ion temperature of about

1 keV. In this case, large amplitude plasma oscillations develop before substantial ion damping of the Langmuir turbulence can occur. The turbulence results in suddenly increased resistivity and an increased rate of diffusion of the return current relative to the relativistic current. The return current is explosively expelled to the inner wall of the imploding glass tube in the form of filaments.

This so-called Weibel instability results in strong field penetration into the target plasma and a propagating axial-induced electric field accelerates ions that in turn can help to cause ignition. The resulting current field configuration constitutes a toroidal vortex 10-keV plasma structure that is being imploded by the exploding glass wall. Computer calculation for this and other targets are in progress.

A fully correct treatment of this and similar targets will require removing certain inadequacies of existing codes. Specifically, a correct, fully self-consistent formulation of strong turbulence effects is required. In addition, net charge, space charge separation effects, as well as strong excitation of electrostatic and electromagnetic modes of target cavities may be of considerable importance. Also, at present no adequate computational treatment of strong field coupled burn exists. Two codes under development — ORBIT and VOA^{3-19,3-20} — will provide a basis for the required improvements in computational techniques, and — combined with existing codes such as ANIMAL, MOKU and LASNEX — will ultimately permit the important strong turbulence and strong field effects to be properly computed.

SOLITONS

The solitary wave is a well known phenomenon in the area of shallow water waves. It is a surface wave consisting of a single bump with a symmetric profile, which propagates over long distances without changing its shape. It was first observed by Scott-Russell in 1834.³⁻²¹

This phenomenon occurs in the diverse areas of ion acoustic waves in plasmas, the anharmonic lattice, pressure waves in liquid-gas bubble mixtures, rotating flow down a tube, heat flow in low-temperature, nonlinear crystals, and propagation of laser pulses in a nonlinear dielectric fiber.³⁻²² Solutions have been

obtained for a wide class of problems where weak nonlinear and weak dispersive effects determine the propagation of an initial disturbance. The initial disturbance first steepens and then breaks into a sequence of pulses that are called solitons. Each of these pulses then propagates with its own characteristic amplitude, width, and propagation speed while preserving its shape.

All of the above results were carried out for one-dimensional systems (planar solitons). Recently, the first results for two and three dimensions were obtained at LLL. It was predicted³⁻²³ that cylindrically and spherically symmetric ingoing ion acoustic waves would break up into a sequence of cylindrical or spherical solitons. These solitons are localized pulses of density, fluid velocity, and electric field which propagate through the plasma. However, the cylindrical and spherical solitons differ from the planar cases. In addition to a dependence of the amplitude and width of a single soliton on radial position, it was discovered that the cylindrical and spherical solitons leave a wake.

The amplitude of a single cylindrical (spherical) soliton increases faster than $r^{-1/2}$ (r^{-1}) while the width decreases so that the square root of the amplitude multiplied by the width is constant. The propagation speed increases as r gets smaller. Figure 3-10 shows the breakup of an initial disturbance into four spherical solitons. The amplitude is plotted vs spatial coordinate in ξ frame moving toward the origin at sound speed.

Cylindrical solitons were observed in a series of experiments at the University of Iowa.³⁻²⁴ The experimental results showed the breakup of a half-sine wave into cylindrical solitons and verified the theoretical amplitude-width relationship to an accuracy of 10%. Further work with the experimental group at

Fig. 3-10. Breakup into four spherical solitons. Dimensionless amplitude U vs spatial coordinate ξ at (a) initial time showing the initial disturbance and (b), a time somewhat later than the "breaking" time. Note the difference in vertical scale at the two times. The profile (b) evolves in time so that the four solitons separate from each other.

Iowa is planned to investigate the acceleration and containment of plasma ions using cylindrically convergent ion acoustic waves.

PLASMA SIMULATION BY MOMENTS EXPANSION

We have been developing a two-dimensional plasma physics code, VOA,³⁻²⁵ which treats relativistic

charged particle transport by expanding the particle distribution function in terms of moments taken over

momentum space. Appropriate combinations of these moments are dynamic quantities which evolve with time and which are calculated in the code. The evolution of the zero moment (the scalar average of the distribution function) is identical with the hydrodynamic evolution of particle density. The first moments yield the hydrodynamic equations for particle momentum and energy. Higher order moments give information about the nonthermal nature of the distribution function. The moments are truncated by a physically realistic closure procedure at an order selected by the user.

Electromagnetic fields are treated by solving Maxwell's equations, including displacement current. The algorithm for solving Maxwell's equation is, presently, explicit; consequently, the time step is limited by the time for light to traverse the smallest zone.

VOA is based upon the framework of the code BBC, which includes nonrelativistic multifluid hydrodynamics and radiation transport. In the future, BBC will be expanded to include fusion reaction physics, and this option will then be automatically available in VOA. Parts of either or both codes may be utilized together for any specific problem.

An optional version of VOA exists, which allows electrons to come into self-consistent equilibrium with the ions and fields. This, in turn, allows calculations on time scales approaching those for hydrodynamic (ion) motion.

The VOA code is intended to solve the basic plasma physics problems connected with the interaction of relativistic matter or fields with a plasma. These

problems concern phenomena at the time scale of plasma oscillations, including turbulent nonequilibrium plasma evolution and the full electromagnetic field description. In this form the code is intended for use to model Z pinches, relativistic electron beams and targets, and basic plasma target physics. Calculations on these problems are now underway. Analysis of plasma focus phenomena will start soon, with comparisons to appropriate MHD and plasma simulation codes planned in the early stages.

A variation of the code has been developed to allow the ions to move according to the basic plasma algorithms while the electrons are assumed to come into quick self-consistent equilibrium with the ions and EM fields. This bypasses the electron plasma oscillations and the electromagnetic time scale restriction. This version of the code may be considered to be a "plasma hydrodynamics" code. This modified code has been used to calculate soliton behavior in cylindrical geometry for comparison with the analytic theory.

The calculations of soliton behavior yield essentially perfect agreement with analytic results when taken from an ideal initial state corresponding to the analytic solution for a propagating soliton. Calculations were also run on problems with ideal initial density profiles but which had an initially flat temperature profile. It was found that the soliton developed the temperature profile of the analytic solutions after traveling only a few Debye lengths. It then propagated stably, but left a modified wake of particles from which internal energy had been removed to build the correct temperature profile.

RADIATION REACTION IN INTENSE LOW-FREQUENCY FIELDS

A measure of the ability of an electromagnetic wavefield to accelerate particles of a given charge-to-mass ratio (e/m) is provided by the dimensionless parameter

$$\xi = \frac{eE_{\max}}{m\omega_0}, \quad (3-4)$$

where $E_{\max}$ denotes the maximum value of the electric vacuum field strength, and ω_0 is the frequency

of the wave field. In terms of the parameter ξ , the maximum kinetic energy of the oscillatory motion of the charged particle driven by the wave field is

$$\epsilon_{\text{kin}} = mc^2[(1 + \xi^2/n^2)^{1/2} - 1]. \quad (3-5)$$

Here, n designates the refractive index of the medium – in our case quasineutral or nonneutral plasma – in which the charged particle under consideration is embedded. To estimate the effect of radiation damping on the orbit of a charged particle moving in an electromagnetic wavefield, it is instructive to compare the above expression for the kinetic energy to the energy, ΔW , which the charged particle loses by emission of radiation during an oscillation period. For a relativistic particle ($\xi \gg 1$), this energy loss is approximately

$$\Delta W = \frac{e^2 \omega_0}{96\pi c} \left(\frac{\epsilon_{\text{kin}}}{mc^2} \right)^6 \approx \frac{e^2 \omega_0}{96\pi c} \left(\frac{\xi}{\sqrt{n^2}} \right)^6. \quad (3-6)$$

The electromagnetic field created by motion of the charged particle can certainly not be neglected if ΔW is comparable with ϵ_{kin} . The value ξ^0 of the dimensionless field strength parameter ξ , Eq. (3-4), for which

$$\Delta W = \epsilon_{\text{kin}} \quad (3-7)$$

is according to Eqs. (3-5) and (3-6)

$$\xi^0 = \sqrt{n^2} \left[\frac{96\pi mc^3}{\omega_0 e^2} \right]^{1/5}. \quad (3-8)$$

Equation (3-4) yields for the corresponding electric field strength

$$E_{\text{max}}^0 = \sqrt{n^2} \left(96\pi n^6 c^8 \omega_0^4 / e^2 \right)^{1/5}. \quad (3-9)$$

This relation shows that the critical wavefield intensity beyond which reradiation cannot be neglected

decreases with decreasing field frequency. At a given field intensity, reradiation effects are therefore more pronounced for microwave fields than for the fields of laser radiation. For an electron driven by the radiation field of a neodymium glass laser ($\omega_0 = 1.78 \times 10^{15} \text{ s}^{-1}$) we obtain from Eq. (3-9)

$$E_{\text{max}}^0 / \sqrt{n^2} \approx 2 \times 10^{12} \text{ V/cm}.$$

For an electron moving in a microwave field with $\omega_0 = 10^{11} \text{ s}^{-1}$, however, we find

$$E_{\text{max}}^0 / \sqrt{n^2} \approx 8 \times 10^8 \text{ V/cm}.$$

Field intensities on the order of 10^{10} V/cm would be necessary for the microwave confinement of a thermonuclear plasma at a temperature $T = 15 \text{ keV}$ and at a density $n = 5 \times 10^{22} \text{ cm}^{-3}$.

The presence of the single-particle reradiation fields modifies the dynamics of a plasma inside a microwave cavity – not only through the radiative reaction force, term which has to be included in the equations of motion for the electrons and possibly ions, but also by changing the characteristic electromagnetic modes of the cavity resonator. In a careful description of the interference between the reradiation fields and the characteristic cavity fields, the near fields produced by the charged particles must be taken into account since the cavity wall belongs to the near zone. Furthermore, stimulated reradiation by groups of particles moving in unison will enhance the single-particle reradiation effects.

To account for various shapes (cylindrical, spherical, toroidal) of the cavity resonators, in which the plasma is to be confined and heated, we have constructed the relativistic Vlasov equation for radiation damping in covariant form (thus allowing for an arbitrary curvilinear coordinate system). In particular, we apply our formalism to a spherical configuration and calculate the radiative reaction modification of the ponderomotive force exerted by the microwave field on the plasma.

We have assisted in the numerical modeling of the gas embedded Z-pinch, using one- and two-dimensional magnetohydrodynamic codes. The concept involves the creation of a narrow preheated current-carrying channel in a dense gas, as might be formed, for example, by a laser or relativistic electron beam. The central core is then preferentially heated to thermonuclear temperatures by a capacitor discharge. The surrounding dense neutral gas blanket serves to retard the growth of MHD instabilities and to insulate the hot core region from first wall impurities.

One-dimensional calculations were used to find optimum conditions for the pinch without exceeding the electrical breakdown strength of the neutral gas. A typical pinch is described in Ref. 1 where the channel expands and is ohmically heated during the resistive preheat phase. The current is then suddenly increased, compressing the hot plasma to densities and temperatures of interest for thermonuclear fusion. In these calculations it is important to minimize the rate of mass accretion to the hot core from the surrounding gas, since the maximum temperature is limited by the mass of the pinch plasma for a given current.

Reference 3-26 also describes the results of two-dimensional magnetohydrodynamic calculations of the sausage ($m = 0$) instability. The calculations on an initial sheet current distribution show the growth of vortex motion and the subsequent relaxation of the system to a profile marginally stable to $m = 0$ perturbations. The broadening of the pressure profile occurs on the time scale for coalescence and dissipation of the vortices rather than the much shorter time predicted by linear growth theory. Estimates of the effects of end losses were also obtained by

two-dimensional calculations. It was found that the end loss velocity is about 0.1 of the ion sound speed when the pinch terminates in rigid conducting walls.

The one-dimensional code was modified to include the effects of plasma heating by alpha particles³⁻²⁷ from fusion reactions. The alpha particles were assumed to be lost to the system by end losses from magnetic field gradient drifts, and to deposit energy in the plasma at a rate given by classical small angle collisions. Radial expansion of the pinch due to alpha particle heating limited the ratio of the output energy (neutron plus alpha) to the pinch energy (magnetic plus thermal) to values of about 4 or 5.

Two-dimensional calculations are also being carried out on a Z-pinch experiment at Naval Research Laboratory involving a capacitor discharge through a laser preheated channel in hydrogen gas. Here, approximate agreement with experiment is obtained because of sausage instability effects while a one-dimensional calculation predicts too high a temperature and strong skin currents.

We are also studying one-dimensional calculations of exploding tubes to assess the feasibility of preheated channel formation by radially converging shock waves.³⁻²⁸

Analytic calculations³⁻²⁹ show that a possibly important effect in the gas embedded Z-pinch is the electric breakdown of the neutral gas blanket. Ohmic heating by photoelectrons produced by radiation from the central hot core or direct energy deposition by the radiation can heat the gas to sufficient temperatures so that it becomes conducting. Code modifications to include this effect are being completed.

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4. ENERGY AND ENVIRONMENT

Introduction

As a result of our participation in the Department of Transportation's Climatic Impact Assessment Program (CIAP), we are studying physical systems involving coupled chemical kinetic and dynamic transport processes. Some LLL programs that deal with such systems are:

- *In situ* coal gasification
- *In situ* oil shale retorting
- Fundamental combustion research
- Stratospheric and tropospheric pollution modeling

We have developed a broad multidisciplinary research program to solve the systems of coupled nonlinear partial differential equations which form the theoretical models for these systems, taking advantage of their underlying similarities to apply similar numerical methods to their solution.

We are now studying three kinds of physical systems:

- Natural and perturbed distributions of minor trace constituents in the stratosphere
- The analysis of flows in porous media, with particular application to *in situ* coal gasification
- Basic combustion studies

The first modeling effort is a continuation of the earlier CIAP program and is carried out in collaboration with other divisions of the Laboratory. In support of this work we developed a one-dimensional model of the stratosphere and used it to study the stratospheric effects of:

- Exhaust from the supersonic transport^{1,4-2}
- Injection of NO_x from past atmospheric nuclear tests⁴⁻³
- Injection of NO_x from nuclear war⁴⁻⁴

Currently we are applying this one-dimensional model to analyze the stratospheric impact of the chlorofluoromethane industry, and we are developing a two-dimensional model of the stratosphere.

The second modeling effort is aimed at studying chemically reactive flow in porous media. Two complementary models have been developed. The first is a one-dimensional model describing gas flow and chemical kinetics in a coal bed. This model is currently being tested against experimental results in coal gasification. If the tests are successful, the computer program will be expanded to a more useful two-dimensional model. A second approach studies the flow of multiphase, multicomponent fluids in porous media. The current emphasis is on the analysis of air-water-steam systems and two-phase geothermal flows. This model has been very successful in describing some experimental systems. We plan to eventually combine these two models in order to describe the multiphase, multicomponent flow found in *in situ* coal gasification processes. In addition, results from such studies are directly applicable to the simulation of multiphase flow in an internal combustion engine.

The principal goal of the combustion program is to acquire a basic understanding of combustion processes in order to analyze and design practical combustion systems. Our initial work has concentrated on some specific aspects of the internal combustion engine: the behavior of fuel spray in a stratified charge engine configuration; the detailed chemical kinetics of methane (CH_4) and (CO_2H_2) combustion; the development of a one-dimensional model of an internal combustion engine. We hope to extend and unify these models to obtain a realistic description of a practical engineering system.

Stratospheric Models

Introduction

One-dimensional parameterized models can contribute significantly to our understanding of the governing physico-chemical processes occurring in the atmosphere. They can be particularly useful in studying the globally averaged vertical distributions of minor chemical constituents of the atmosphere, both in its natural state and when responding to perturbations.

In a vertical one-dimensional model of the atmosphere, the conservation equation governing the temporal variation of the number density of the i^{th} constituent, $c_i = c_i(z, t)$, is

$$\frac{\partial c_i}{\partial t} = P(c) - L(c) c_i - \frac{\partial}{\partial z} \left[k_z \rho \frac{\partial}{\partial z} \left(\frac{c_i}{\rho} \right) \right] \quad (4-1)$$

where $P(c)$ is the production rate of c_i from photochemical interactions with the other species, $L(c)c_i$ is the loss of c_i due to the chemical interaction of c_i with the other species, k_z is the vertical transport coefficient (often referred to as the "eddy" diffusion coefficient), $\rho = \rho(z)$ is the ambient air density, and t and z are, respectively, the time and the altitude.

The domain of the model extends from the ground to a height of 55 km, comprising most of the troposphere and stratosphere. Primary emphasis has been placed on the calculation of stratospheric distributions of minor chemical species, particularly ozone.

At present, the concentrations of 23 minor atmospheric species are computed. For 20 of these species, $O(^3P)$, O_3 , NO , NO_2 , N_2O , HNO_3 , OH , HO_2 , H_2O_2 , Cl , ClO , Cl_2 , ClO_2 , $OCIO$, $CINO$, $CINO_2$, HCl , CCl_4 , $CFCl_3$, CF_2Cl_2 , we solve an equation of the form of Eq. (4-1) to obtain its vertical profile. The other three species, $O(^1D)$, H , and N are assumed to be in instantaneous equilibrium. The vertical distributions of five constituents, N_2 , O_2 , CH_4 , H_2O , and H_2 are presently assumed to be time independent

and are held constant. The distributions of these species are based on published measurements.

There are presently 87 photochemical reactions included in the model. All relevant data on these reactions are obtained from the published literature or pre-publication communications. Much of the computational and other physical details have been discussed in the literature.^{4-1,4-2}

Applications of the One-Dimensional Stratospheric Model

In the past several years the one-dimensional model has been used to study the stratospheric impact of many man-made events⁴⁻¹⁻⁴⁻⁴ and to analyze results obtained by other investigators. Recently, after a considerable expansion of the model, it has been used to study the impact of anthropogenic chlorofluoromethanes on stratospheric ozone. Because of the wide global use of the chlorofluoromethanes (CF_2Cl_2 , and $CFCl_3$), there is now a sufficient quantity in the atmosphere to be a source of stratospheric chlorine comparable to the known natural sources. Since there is no apparent tropospheric sink for these compounds, any further increase could have a significant effect on the structure of the stratosphere. After these compounds are released into the atmosphere, they eventually reach the stratosphere and undergo photodecomposition. The product free chlorine atom then becomes a catalytic agent for the destruction of natural ozone. With a sufficiently large man made source of free chlorine in the stratosphere, the natural balance of ozone production and destruction can be altered to result in a reduction of the total ozone. This, in turn, is thought to lead to undesirable environmental consequences such as an enhanced level of ultraviolet radiation at the earth's surface. Figure 4-1 illustrates some typical results. Maintaining the 1973 chlorofluoromethane production level through the year 2000 leads to a 6% decrease in total ozone. Under steady state conditions, the

reduction could be as high as 14%. At half the chlorofluoromethane production level the effect on ozone will be approximately halved. The width of the individual curves represents that part of the current uncertainty in the one-dimensional results due to different assumptions for the vertical one-dimensional eddy diffusion coefficients. There are additional uncertainties in the chemical kinetics rate coefficients which could alter the model predictions by a factor of two or more. A systematic analysis of these uncertainties has been carried out⁴⁻⁵ and will be a major part of a forthcoming report by a panel of the National Academy of Sciences.

Another application of the one-dimensional model has been to the possible effects that a very large number of high-yield atmospheric nuclear explosions could have on stratospheric composition, primarily on ozone concentration due to NO_x production. Since the model is only one dimensional and utilizes a highly parameterized transport prescription, it is highly limited. While the SST and past nuclear tests caused relatively small perturbation to the ozone, the effect of a very large number of high-yield atmospheric nuclear explosions is expected to be greater. Since significant perturbation of ozone (the solar energy absorption of which is the primary mechanism governing stratospheric motions) might well cause the assumed transport prescription to be inadequate, our results must be viewed as preliminary. The actual effects will probably be less because of the expected transport response of the real atmosphere. For better accuracy a model is needed in which transport calculations are performed internally based on the perturbed state of the ozone and temperature fields.

In determining a reasonable maximum number of nuclear explosions (and their yield) that might be exploded in the atmosphere, we used estimates from an Institute of Strategic Studies (1972) analysis that looked at the total deliverable payloads of the U.S.S.R. and the U.S.A.⁴⁻⁶ A gross estimate of the maximum total yield is approximately 1.5×10^4 Mt (Case A) for very large-yield, megaton-range weapons

Fig. 4-1. The calculated decrease in the ozone concentration as a function of time under the assumption that the chlorofluoromethane production remains constant at its 1973 rate (top band), and at half that rate (lower band). The width of each band represents the uncertainty arising from different assumptions about the eddy diffusion rates.

and about 1.1×10^4 Mt (Case B) for smaller-yield, megaton-range weapons, depending on various assumptions concerning delivery systems. Table 4-1 shows some of these possibilities in terms of yield, an important consideration in studying the height of injection. We have also used the model to simulate the effect of half of each of these cases to provide an initial

Table 4-1. Yield mixture for various case studies^a

Estimated total yield	Number of detonations	Yield/detonation (Mt)	Total yield (Mt)
Case A:	290	20	5,800
	54	10	540
	250	9	2,250
	2,030	2	4,060
	2,820	1	2,820
Total:			15,470
Case B:	1,134	5	5,670
	5,282	1	5,282
Total:			10,952

^aSee Ref. 4-6.

evaluation of the importance of absolute amount (i.e., Case C is one-half the input of Case A, and Case D is one-half the input of Case B). Results for these cases are shown in Figs. 4-2 through 4-5.

In general, for the lowest total yield with the lower individual yield devices (Case D, Fig. A-4), using one-dimensional models the nuclear explosions are calculated to cause at least a 5% reduction in ozone

after 5 or 6 years and as much as a 8% to 21% effect after 2 years. The changes for other cases with larger total yield and larger individual yield per device are correspondingly larger as shown in Fig. 4-2, 4-3, and 4-4, with as much as a 24% to 43% reduction in ozone after 2 years for the worst case (Case A). In all of these cases, the first-year maximum reduction should not be considered realistic because in the

Fig. 4-2. Model-predicted changes in the globally averaged ozone column due to a very large number of high-yield atmospheric nuclear explosions: Case A.

Fig. 4-4. Model-predicted changes in the globally averaged ozone column due to a very large number of high-yield atmospheric nuclear explosions: Case C.

Fig. 4-3. Model-predicted changes in the globally averaged ozone column due to a very large number of high-yield atmospheric nuclear explosions: Case B.

Fig. 4-5. Model-predicted changes in the globally averaged ozone column due to a very large number of high-yield atmospheric nuclear explosions: Case D.

one-dimensional model one has to inject the NO_x uniformly over the globe over a layer dictated by the injection cloud stabilization height. This assumption is primarily responsible for the large first-year perturbation. In reality, it takes about a year to achieve uniform, horizontal spread and during that year there would be substantial vertical spreading as well. In Case A, this reduction in the first-year effect is probably of less climatic and biological significance than the few percent reduction still present after 10 years.

The upper and lower lines in each graph show the perturbation that is computed to result when using approximately the maximum and minimum estimates of Gilmore (1974) for NO_x production per megaton yield. Thus, the curves (from top to bottom) are for injection rates of 0.5, 0.9, and 1.5×10^{32} molecules/Mt, respectively.

Although this rather limited study must be viewed as preliminary, it does indicate that a very large number of high-yield nuclear explosions in the atmosphere could cause a significant reduction in stratospheric ozone. Considerably more research, including seasonal and latitudinal dependence, is needed to provide more definitive results.

One-dimensional models can, at best, provide globally averaged results and a general characterization of the structure of the stratosphere. Any detailed analysis requires at least a two-dimensional model, and we are now developing such a model with essentially the same structure as the one-dimensional model. We are currently testing the model through a sequence of validation studies, by simulating the known distribution of radioactive tracers injected in past atmospheric nuclear tests. After verifying the accuracy of the model, we will use it for studies that are beyond the capability of the one-dimensional models.

Computational Modeling of Flow in Porous Media

Introduction

The flow of gases and liquids in underground porous media is of importance to a number of LLL programs. Among these are: nuclear containment, where high-pressure superheated steam from a nuclear cavity condenses in the surrounding rocks; geothermal wells, where the flow consists of high-pressure saturated water and steam and the LLL *in situ* coal gasification program, where gases, tars, and condensing and evaporating steam flow through, and react with, a packed bed of rubblized coal.

Despite the diverse nature of their constituents, all these flows take place in "porous" media, i.e., solids containing connecting voids. On a small scale the structure of these media is quite irregular, with void spaces made up of cracks and holes randomly connected. Since detailed flow calculations on this scale would be impossible, the simplifying assumption is made that each porous medium is locally

homogeneous, the flow being determined entirely by the local porosity and permeability and by the viscosities of the gases.

Flows of this type are governed by Darcy's law — an empirically derived relation that replaces the usual momentum equation — which states that the fluid velocity is proportional to the local pressure gradient. This has the effect of converting the advection terms that appear in the mass and energy conservation equations into diffusion-like terms. Under these assumptions, the above described flows are all described by coupled systems of time-dependent nonlinear diffusion equations, complicated by multiphase effects when condensible fluids are present, and by chemical reactions in the case of coal gasification.

These common features suggest that a unified approach be taken in modeling them computationally. For maximum usefulness such models should be

(a) time-dependent, so that transient effects can be studied, and (b) ultimately have two or even three space dimensions. Hence, in developing the one-dimensional models described below, we have used numerical methods capable of being efficiently extended to two or three dimensions.

Coal Gasification Model

The conservation equations describing gas flow and chemical kinetics in a coal bed are:

- Gas chemical species continuity

$$\frac{\partial}{\partial t}(\phi c_i) = -\vec{\nabla} \cdot (c_i \vec{u}) + S_i, \quad (i = 1, 2, \dots, I) \quad (4.2)$$

where

ϕ = porosity

c_i = concentration of the i^{th} chemical species

$\vec{u}$ = gas bulk velocity

S_i = reaction rate for i^{th} species

I = number of gas species

- Gas energy conservation

$$\frac{\partial}{\partial t}(\phi \rho \epsilon) = -\vec{\nabla} \cdot (h \vec{u}) - a(T - T_s) + Q, \quad (4.3)$$

where

ρ = gas density

ϵ = gas specific energy

h = gas specific enthalpy

T = gas temperature

T_s = solid temperature

a = convective heat transfer coefficient

Q = energy source rate from chemical reactions

- Solid energy conservation:

$$\frac{\partial}{\partial t}[(1 - \phi)\rho_s \epsilon_s] = \vec{\nabla} \cdot [(1 - \phi) K_s \vec{\nabla} T_s] + a(T - T_s) + Q_s, \quad (4.4)$$

where

ρ_s = solid density

ϵ_s = solid specific energy

K_s = solid coefficient of heat conduction

Q_s = solid energy source rate

To these we add the material properties:

- Darcy's law:

$$\vec{u} = -\frac{k}{\mu} \vec{\nabla} p, \quad (4.5)$$

where

k = permeability

μ = gas viscosity

P = gas pressure

- Gas equations of state:

$$h = h(T) = \sum_{i=1}^I h_i^0 + \int_{T^0}^T c_{p_i}(T') dT'$$

$$p = \rho RT / \bar{A}$$

$$\epsilon = h - p/\rho \quad (4.6)$$

where

c_{p_i} = specific heat at constant pressure of i^{th} gas species

R = gas constant

$\bar{A}$ = average molecular weight (we are assuming a mixture of ideal gases, so that ϵ and h are functions of temperature only)

- Solid equation of state:

$$\epsilon_s = \int_{T_{0s}}^{T_s} c_s(T') dT'. \quad (4.7)$$

Making use of Darcy's law we can rewrite the conservation equations

$$\phi \frac{\partial c_i}{\partial t} = -\vec{\nabla} \cdot (c_i \vec{u}) + S_i \quad (i = 1, 2, \dots, I) \quad (4-8)$$

$$\phi \frac{\partial \rho}{\partial t} = \vec{\nabla} \cdot (K \rho \vec{\nabla} P) + S$$

$$\phi \rho c_v \frac{\partial T}{\partial t} = \vec{\nabla} \cdot (K h \vec{\nabla} P) - a(T - T_s) + Q$$

$$(1 - \phi) \rho_s c_s \frac{\partial T_s}{\partial t} = \vec{\nabla} \cdot [(1 - \phi) K_s \vec{\nabla} T_s] + a(T - T_s) + Q_s \quad (4-9)$$

We have assumed that ϕ changes sufficiently slowly that its time derivative may be neglected; $K \equiv k/\mu$.

The first part of Eq. 4-9, representing gas continuity, is in fact redundant, since it is obtained simply by adding up the individual species continuity equations. However, it proves to be useful in the numerical solution.

Numerical Solution

The equations given above are split into two systems, labeled (4-8) and (4-9). Each system is solved by a fully implicit iterative method, as follows:

System (4-8). Holding T , T_s , and $\vec{u}$ fixed, we calculate the new c_i 's using a fully implicit upstream method for the advection terms, and functional iteration for the source terms.

System (4-9). Holding fixed the gas mass source terms S and the energy source terms Q and Q_s , we solve three coupled nonlinear diffusion equations for the variables T , T_s , and ρ by a fully implicit iterative scheme, in which we linearize around each iteration. The above method has been carried out so far in one space dimension, and both iterative schemes seem to converge reasonably well.

Numerical Results

Figure 4-6 is a series of graphs of pressure, velocity, density, and temperature vs position for a test problem

in which nonreacting gas flows through a heated solid region. The numerical scheme, although only first order, is able to follow steep gradients in these variables without spurious oscillations. Typical results for a combustion problem (with ignition at the center of the bed) are shown in Fig. 4-7. The absorption of the O_2 , depletion of the dry coal, and buildup of char, CO , and CO_2 are clearly seen.

Multicomponent Two-Phase Flow. We assume that a mixture containing a gas (e.g., air), a vapor (e.g., steam) and a miscible liquid (e.g., water) is diffusing through the porous medium. Besides the usual thermodynamic variables, we now have the saturation of a vapor, S_v , defined as the fraction of the void volume occupied by vapor. Similarly we define the saturation of the liquid, $S_l = 1 - S_v$; both S_v and S_l are unaffected by the presence of the background gas.

If liquid and vapor are both present in a given zone, they are assumed to be in instantaneous thermodynamic equilibrium, since the equilibration time is short compared to the time scales of the problems of interest. If no liquid is present we have superheated steam, which we treat as an ideal gas.

The conservation laws are analogous to those in the coal gasification system:

- Gas continuity

$$\phi \frac{\partial \rho_g}{\partial t} + \frac{\rho_g \phi u_m}{\partial x} = 0 \quad (4-10)$$

- steam-water continuity

$$\phi \frac{\partial}{\partial t} (\rho_l S_w + \rho_v (1 - S_l)) + \frac{\partial}{\partial x} (\rho_l u_l + \rho_v u_m) = 0 \quad (4-11)$$

- energy equation

$$\phi \frac{\partial}{\partial t} \left(\frac{1 - \phi}{\phi} \right) \rho_s c_s + \rho_l c_l S_l$$

Fig. 4-6. Pressure, velocity, density, and temperature vs position.

Fig. 4-7. Results of a combustion problem (see text).

Fig. 4-8. Condensation front location from maximum temperature data.

Fig. 4-8. Condensation front location from maximum temperature data.

$$+ (\rho_v e_v + \rho_g e_g) (1 - S_g)) \\ + \frac{\partial}{\partial x} (\rho_\ell h_\ell u_\ell + (\rho_v h_v + \rho_g h_g) i_m) = 0 \quad (4-12)$$

- Darcy's law

$$u_\ell = -\frac{k_c k}{u_\ell} \frac{\partial P}{\partial x} \\ u_m = -\frac{k_m k}{u_m} \frac{\partial P}{\partial x} \quad (4-13)$$

The equation of state for the gas is $P_g = P_g(\rho_g, T)$. For superheated steam, $P_v = P_v(\rho_v, T)$ and $S_w = 0$. For saturated steam-water, $P_v = P_v(T)$. The internal energy $e_\alpha = e_\alpha(T)$ and enthalpy $h_\alpha = e_\alpha + P_\alpha/\rho_\alpha$, where $\alpha = g, v, \ell$ for gas, vapor, and liquid respectively, and the total pressure $P_\ell = P_v + P_g$. The symbols are: Q porosity, ρ_α density, u_α velocity, S_w water saturation, k_α relative permeability, k permeability, μ_α viscosity, T temperature, and m mixture of vapor and gas.

The finite difference form of Eqs. 4-10 to 4-13 are obtained in a manner similar to that described for coal combustion. We then have a system of algebraic equations, which we solve — by iteration — for the appropriate three variables in each zone, depending on whether or not liquid water is present.

Verification of this program is provided by modeling an experiment in which saturated steam is injected into a pipe filled with sand at atmospheric pressure. Figure 4-8 shows a plot of the steam condensation front as a function of time. The calculated and experimental results are in excellent agreement. A second example is the flow of superheated steam from a nuclear cavity following an underground nuclear test. Figure 4-9 is a plot of the penetration distance of the condensed steam calculated in both spherical and planar geometry. This plot agrees with the planar calculations of Morrison⁴⁻⁷; the spherical results are believed to be more realistic.

One-Component Two-Phase Flow (Geothermal)⁴⁻⁸

Geothermal reservoirs can be described by Eqs. (4-11) to (4-13) without the gas component, leaving a saturated steam-water mixture defined by the equation of state $P_v = P_v(T)$. This simplifies the solution procedure, permitting use of a direct method, which is a considerable improvement over iterative methods because the latter offer convergence difficulties when following steep gradients. Figure 4-10 shows a typical calculation of an evaporation wave when high-pressure saturated water is released from a pipe filled with sand.

Two-Dimensional Modeling.⁴⁻⁹ Two-dimensional finite element and finite difference simulations of porous flow are currently being investigated, in particular isothermal compressible flow:

$$\frac{\partial P}{\partial t} = \vec{\nabla} \cdot \left(\frac{k}{u} P \vec{\nabla} P \right) \quad (4-14)$$

and incompressible flow:

$$\frac{\partial P}{\partial t} = \vec{\nabla} \cdot \left(\frac{k}{u} \vec{\nabla} P \right) + Q, \quad (4-15)$$

where Q is a source term.

Fig. 4-9. Saturation front penetration distance vs. time.

In an oil field or geothermal reservoir, the Q term may contain many logarithmically singular point sources and sinks representing wells. Ordinarily, fine zoning would be required for accuracy near each singularity. However, since the character of the singularity is known, it can be embedded in the finite difference scheme without mesh refinement.⁴⁻¹⁰ An alternating-direction two-dimensional code using this technique is currently being written.⁴⁻¹

Fig. 4-10. Calculation of an evaporation wave when high-pressure saturated water is released from a pipe filled with sand (see text).

Combustion Research

During the past year we have begun a program of theoretical combustion research. This research is directed toward a wide variety of applications, ranging from analysis and understanding of fundamental physical processes to engineering design computer models to be used for specific combustors. Coordinated programs with other Laboratory divisions are being developed, as well as a relationship with the Sandia Combustion Center.

The principal goal of the combustion research program is to develop computer programs which can be used to analyze and to design practical combustion systems. The specific requirements of these programs depend somewhat on the particular systems to which they are applied. Thus, the needs of a computer model for a turbine combustor may be slightly different from those for an internal combustion engine model. In spite of such variations, the same physics is important in nearly all combustors. As a result, our approach has been to take each physics subsystem and develop a simple numerical model for it. Concurrently, we examine a variety of geometrical configurations appropriate to specific combustors. Then the geometry is combined with the necessary physics models to construct a simple computer model of a particular

combustor. Specific components of the resulting model can be refined as the need arises. This refinement process, and the subsystem modeling progress, are described below.

Submodels

In most combustors the important physics systems which must be included are the chemical kinetics of the burning, the hydrodynamics of the fluid motion, energy production and transfer, and energy losses to the combustor walls. Since the great majority of practical combustors produce a strongly turbulent environment, this turbulence must also be included in any complete description. Since turbulence couples together the hydrodynamics, the energy transfer, and the chemical kinetics, a unified treatment of these processes may be necessary. In combustion systems in which liquid fuel is introduced into a chamber where it vaporizes and burns, the physical processes of liquid atomization and spray vaporization and motion must also be included. It must be emphasized that while simplifying assumptions may be appropriate in specific cases, all of the physics subsystems must be included, with a treatment that is sufficiently detailed for that particular case.

The detailed chemical kinetics of methane (CH_4) has been examined and modeled numerically during the past year. The chemical reaction scheme included 16 chemical species and 24 reactions, each with forward and reverse reaction rates. This system was chosen for several reasons. First, the reaction mechanism is relatively well understood. Also, fairly reliable reaction rates have been published for most of the reactions included. Reaction rates and mechanisms for fuels more complicated than methane, such as propane or gasoline, are not well established, so that results with other fuels would be subject to more uncertainty than with methane. Another motivation for the use of methane is its similarity to methanol, which has been widely suggested as a feasible automotive fuel alternative to gasoline. Methane combustion has been studied under a wide variety of conditions. Adiabatic

constant volume and adiabatic constant pressure calculations at high density, and at atmospheric density and pressure, have been performed, and the results compare favorably with both experimental results and calculations carried out elsewhere. Calculations of adiabatic flame temperatures and of equilibrium chemical composition as a function of temperature also agree well with published results. Our current efforts involve coupling the detailed kinetics with hydrodynamic model, in stratified charge reciprocating engines and in flow reactors. Additional plans include extension of the chemical system to include additional chemical species and reactions, progressing towards the methanol system. We are also examining the applicability and limitations of conventional one-step kinetics treatments or the less restrictive assumption that the fuel molecule breaks up into its constituent

Fig. 4-11. Mole fractions for selected chemical constituents in a typical methane combustion calculation.

atoms with some average reaction rate. Results for a typical methane combustion calculation are shown in Fig. 4-11.

Turbulence modeling has been approached from several directions. For inclusion in simplified, preliminary composite models, a conventional mixing length theory has been applied. With this model, mass and energy transport result from the motion of turbulent eddies. These transport properties are averaged over the entire spectrum of eddy sizes and velocities, resulting in average transport coefficients. These eddy diffusivities are included as coefficients of energy and chemical species diffusion terms in the total energy and mass conservation equations. In this simplified form these equations may be integrated numerically to give useful results in many cases. This is currently the approach being taken in the combustor model being developed for simple applications. The second direction from which turbulence modeling is being approached is from a detailed treatment of the

Navier-Stokes equation. Statistical mechanical methods have been used to describe the properties of a turbulent fluid in terms of a distribution of turbulence cells. Physical properties of the fluid which are needed are then calculated from the distribution function by established mathematical operations. Details of the statistical mechanical method and the mathematical and computational techniques remain to be refined, and work in this area is continuing. Another approach being examined is a somewhat more conventional closure model of the Navier-Stokes equation. A two-equation closure model is currently being developed, along with the numerical methods necessary for the efficient and accurate solution of the appropriate equations. One turbulence model or the other, or a combination of the two, will eventually replace the simplified eddy diffusion model.

Fuel spray motion and vaporization in a gaseous medium has been extensively examined during the past year. Prior research had used a method of

Fig. 4-12. Cross section of a combustion chamber for a stratified charge, liquid fuel injected engine, showing results for a computer calculation of liquid fuel vaporization. Contours of constant vaporization rate are shown. The piston and injector configuration at the time the fuel is injected is indicated schematically in the inset.

characteristics to solve the time independent thin spray equation for problems with one space dimension. This method was limited in its applicability to real environments and did not generalize readily to include more complicated geometry or time dependence. In its place we have developed a new solution method for the spray equation, treating the full seven-dimensional (three space dimensions, three velocity dimensions, droplet radius) droplet distribution function, including its time dependence. Calculations have been performed for a fuel spray in a rocket motor and for fuel injection into an actual chamber of an internal combustion engine currently being developed, the Ford PROCO chamber. Other applications to different geometries can and will be made in the next year. These calculations provide, for the first time, an opportunity for the engineer or designer to examine the fuel distribution in such a chamber at ignition time as a function of gas swirl, nozzle characteristics, and relative nozzle position. Results for a typical calculation of liquid fuel vaporization are shown in Fig. 4-12. We are working on the inclusion of a complete two-phase description of the fluid development in a combustion chamber, using the above spray model.

Geometrical Configurations

For most theoretical combustion research in the past, geometrical considerations have been neglected in favor of zero-dimensional or thermodynamic models. These models have been useful but their

applicability is limited. We have undertaken to develop multidimensional computer models for use in actual design studies. Most real combustors are quite sensitive to geometrical factors, including the generation of turbulence, chemical reaction quenching in boundary layers, gas swirl, compressional heating, spark timing, wall heat losses, and many other details with which geometrical factors interact. We already have the means of treating reciprocating or rotary engine geometries and flow reactor. For some applications a degree of symmetry is assumed to simplify calculations, while for other applications such as the spray motion and vaporization the full three-dimensional geometry is retained. Currently being tested is a one-dimensional combustion model, including detailed chemical kinetics, turbulent mass and energy transfer using a mixing length model, energy transport by means of molecular diffusion, and liquid spray motion and vaporization. This model will be applied to study stratified charge internal combustion engines, both reciprocating and rotary type, and flow reactors used in laboratory experiments. In most cases some experimental data are available with which to compare and calibrate calculations. We hope to be able to cooperate with combustion device design engineers in a variety of areas in applying these design models to actual combustors of interest. We also intend to develop a number of two-dimensional composite computer models, which will be even more useful in aiding design efforts of a wide variety of practical combustors.

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5. RELATED RESEARCH

Introduction

In a number of scientific areas the Laboratory's extensive computational facilities and codes provide an unparalleled research capability. In astrophysics, for example, many phases of stellar evolution are similar to those occurring in a nuclear explosion. Molecular dynamics, a technique for numerically simulating classical many-body phenomena in statistical

mechanics, was developed at the Laboratory and has remained an active research topic. The general subject of computational techniques underlies many of our applied programs. Some work has also been carried out in such diverse fields as geophysics and economic modeling. In this section we describe recent work in some of the above areas.

Astrophysics

Our efforts in astrophysics during the last year have covered a variety of topics: star formation,⁵⁻¹ protostellar evolution,⁵⁻² studies of quasar absorption and emission red shifts,^{5-3,5-4} x-ray astronomy,⁵⁻⁵ and the physics of the early universe.⁵⁻⁶ The first two research topics are of special interest because they represent applications of general Laboratory codes to astrophysical problems.

Star Formation

We have carried out detailed calculations⁵⁻¹ that relate to a possible mechanism for star formation in spiral galaxies. We computed the implosion of a standard interstellar cloud, which occurs after such a cloud encounters a shock in the inter-cloud medium. The physical parameters were chosen to represent a cloud flowing into a spiral arm. Although the work

Fig. 5-1. Views of the originally spherical cloud at a time of 1.7×10^6 years.

Fig. 5-2. Close up view of the cloud at a time of 5.35×10^6 years.

was motivated by spiral density-wave theory, the results should also be indicative of the evolution of a cloud struck, for instance, by a supernova shock. The CEL code⁵⁻⁷ has been used for the calculations because of its facility for coupled Lagrange and Eulerian calculations. The very thin, dense shell of shocked cloud gas that moves inward during the implosion can be followed because a Lagrangian grid

is used to describe the cloud. Also, the motion of the shocked intercloud gas past the cloud and the development of vortices in this flow can be computed because an Eulerian grid is used to describe the intercloud gas. The numerical mesh used was also sufficiently fine-grained to follow the development of the larger-wavelength modes of the Kelvin-Helmholtz and Rayleigh-Taylor instabilities of the cloud surface.

Fig. 5-3. Expanded view of the flow around the cloud at the end of the calculation.

In Figs. 5-1 through 5-3 we show the evolution of a typical interstellar cloud as it encounters a strong shock. Initially, the spherical interstellar cloud has a radius of 15 pc, a density of $1.5 \text{ particles/cm}^3$, a temperature of 140°K , and a total mass of 500 solar masses. It is in pressure equilibrium with a surrounding intercloud gas that has a temperature of about $11,000^\circ\text{K}$ and a density of $0.019 \text{ particles per cm}^3$. The cloud's self-gravity is negligible, and it is confined by the pressure of the intercloud gas. A shock in the intercloud gas is fed in at the right-hand end of the computational grid. The shocked intercloud gas has a velocity of 18 km/s and a sound speed of about 20 km/s. After this shock has passed over the cloud, the motion of the cloud through the shocked intercloud gas is subsonic.

In Fig. 5-1 we show the originally spherical cloud at a time $t = 1.7$ (time is in units of 10^6 years). The shock struck the front cloud surface at $t = 0.2$, and has now passed over the cloud. A reflected shock can be seen at the back of the cloud, and along the sides

ripples are growing from the Kelvin-Helmholtz instability. In all of the figures the velocity vectors and isodensity contours (labeled by the value of the particle density) are plotted in the Eulerian region, and the Lagrangian grid representing the cloud is shown. The cloud shock can usually be located by a compression of that grid. The coordinate distances are measured in parsecs and VMAX is the value in km/s of the longest velocity vector shown.

Figure 5-2 shows a close-up of the cloud at $t = 5.35$. The Rayleigh-Taylor instability of the front surface has caused previous Kelvin-Helmholtz modes to grow into long, dense tongues of compressed material. These contain a substantial fraction of the gas swept up by the cloud shock. A view of the cloud at the termination of the computations ($t = 6.16$) is shown in Fig. 5-3. Near the symmetry axis the larger Rayleigh-Taylor mode has overtaken the smaller one, and the dense clump contains 26.5 solar masses of material. The self-gravitational energy of this clump just exceeds its thermal energy, so that it will now

presumably collapse gravitationally to form a star or stars.

Protostellar Evolution

Assuming that some mechanism (such as the one described above) creates a gravitationally bound clump of gas, it is of interest to follow its subsequent evolution and find out whether it becomes a star. We have investigated the evolution of spherically symmetric gravitationally bound clumps (protostars) with initial masses ranging between 0.1 and 50 solar masses.⁵⁻² To perform the calculations, a numerical technique was developed in which rapid dynamical motions in one region of the star and quasi-static evolution in another region could be simultaneously computed. This scheme was implemented in a 1-D code, and the computations were performed with a version of that code which includes gravitational forces.

The general evolutionary features of the protostellar collapse are:

- An initial free-fall collapse followed by the creation of a core in hydrostatic equilibrium
- The core's subsequent accretion of the surrounding envelope
- Quasi-static contraction to the main sequence (i.e., to the configuration of a normal star).

We found significant quantitative differences between the evolution of low and high mass stars. For protostar with less than about one solar mass, the luminosity remained relatively small until late evolutionary times, and the evolution was very sensitive to the treatment of convective energy transport. The properties of such stars at the beginning of the calculation and at the time when they first reach hydrostatic equilibrium are listed in Table 5-1. Note that the radius at the latter time is large compared with the value it will have when the star reaches the main sequence (for the sun, for example, the radius is about ninety times larger than the present value).

For protostars whose initial mass is greater than a few solar masses, convective energy transport is no

Fig. 5-4. The mass fraction, M_{fin}/M_{in} , which forms the final core of the protostar as a function of the initial protostellar mass M_{in} . The remaining mass is ejected by the protostar. For initial mass greater than $10 M_{\odot}$, the significance of the computed points is somewhat uncertain because of the sensitivity of the results to the assumed boundary conditions. The dashed curve is simply an extrapolation of the curve based on the computed points.

Fig. 5-5. H-R diagram of the effective core temperature for massive protostars. The final core masses (in units of $M_{\odot}$) are indicated for each curve, and the last computed points for each model are at times of 1.7×10^6 , 1.3×10^6 , 2.0×10^6 , 4.3×10^6 , and 1.1×10^7 yr for initial masses of 3, 5, 10, 20, and $50 M_{\odot}$, respectively. The open circles labeled 115, 19, 15, and 13 are the points at which Iben's (1965) pre-main-sequence models (with masses 15, 9, 5, and $3 M_{\odot}$) cross the $\log T_{eff} = 4.0$ line on their now nearly horizontal approach to the main sequence.

Table 5-1. Initial and hydrostatic equilibrium properties of low-mass protostars^a

M/M	R ₀ (cm)	ρ ₀	t _{hc} (yr)	R _{hc} /R	ρ _c	T _c	ρ _b	T _b	T _{eff}	L/L
0.1.....	1.71(+16)	1.0(-17)	2.94(+4)	10.2	5.0(-2)	1.5(+5)	7.1(-6)	1.6(+4)	1.6(+3)	0.6
0.2.....	3.42(+16)	2.5(-18)	5.56(+4)	19.0	7.0(-3)	2.0(+5)	2.5(-6)	1.5(+4)	1.7(+3)	2.6
0.5.....	8.56(+16)	4.0(-19)	1.34(+5)	43.7	3.4(-3)	2.5(+5)	5.5(-7)	1.4(+4)	2.1(+3)	32
1.0.....	1.71(+17)	1.0(-19)	2.67(+5)	90.0	3.0(-4)	3.5(+5)	1.4(-7)	1.3(+4)	2.2(+3)	165

^aThe various columns are, respectively, the protostellar mass, the initial radius, the initial density, the time at which complete hydrostatic equilibrium is reached, and the values of the ρ_{c} , central density, central temperature, last zone density, last zone temperature, effective temperature, and luminosity at the time of hydrostatic equilibrium. All densities are in grams cm⁻³, all temperatures in kelvins and the units for the other quantities are shown; the number in parentheses indicates the power of 10 by which the tabular entry is to be multiplied.

longer significant and the luminosity reaches quite large values during early stages of the evolution. Radiation pressure can also become important, and for sufficiently high initial masses it can reverse the infall of the outer layers, ejecting them back into the ambient surrounding medium. In Fig. 5-4 we have plotted the fraction of the initial mass which eventually forms a star. Although the physics is somewhat idealized, it appears evident that radiation pressure limits the mass of a normal star to

approximately 100 solar masses. In Fig. 5-5 we show the evolutionary tracks in a Hertzsprung-Russell diagram in which the luminosity is plotted against temperature for protostars of various masses. As indicated, there is good agreement with conventional calculations⁵⁻⁸ of early stellar evolution. The high luminosities of such massive protostellar objects should have several observational consequences, and we plan to investigate some of these possibilities in the future.

Molecular Dynamics

The computer program, STEP,⁵⁻⁹ which solves the simultaneous classical equations of motion of several hundred particles, has been used to study a number of diverse physical situations involving both equilibrium and nonequilibrium phenomena. Here we discuss three examples for which interesting results have already been obtained, but further work is underway to gain a deeper understanding.

The first problem concerns the calculation of the band shape and intensity of depolarized light when laser light impinges on rare gases.⁵⁻¹⁰ Light scattering is, in general, due to dipoles produced by a fluctuating anisotropic field. The primary cause of such a field is a temporary asymmetric configuration of the spherical atoms. Such an asymmetric density fluctuation can, however, also distort the electron

density distribution of an atom so that it is no longer spherically symmetric. The calculation of the purely asymmetric density fluctuations, ignoring electron distortions, was carried out by computer evaluations of the dipolar density fluctuation autocorrelation function,

$$\rho(t) = \left\langle \left(\sum_{i < j} T_{ij}^{xy} \right)_t \left(\sum_{i < j} T_{ij}^{xy} \right)_0 \right\rangle,$$

where

$$T_{ij}^{xy} = \frac{1}{r_{ij}^3} \left(\delta_{xy} - \frac{x_{ij} y_{ij}}{r_{ij}^2} \right)$$

is the xy component of the dipole tensor; r_{ij} is the distance between particle i and j ; X_{ij} and Y_{ij} are the x and y cartesian components of that distance; δ_{xy} is the Kronecker delta; and the subscripts t and o stand for the evaluation of these sums at two different times, one arbitrarily considered the origin of time. Finally the angular brackets represent the statistical mechanical averaging; that is, the process is repeated for many origins of time and the results are averaged. The calculations were carried out for particles interacting as hard sphere and with some more realistic interatomic potential that included attractive forces

The calculation of the intensity of the depolarized light, which is proportional to $\rho(0)$, were disappointing while the band shapes, given by the Fourier transform of $\rho(t)$, were quite accurate when compared to experiments over a wide range of conditions of temperature and density.⁵⁻¹¹ The only exception to this good comparison for band shapes occurred in the solid phase for hard spheres where the calculations gave no evidence of the phonon structure that is apparent from experiments. However, introduction of the more realistic intermolecular potential led to agreement with experiments so that it might be guessed that the absence of short range attractive restoring forces in hard spheres leads to a rather different phonon structure in the solid phase. We are investigating this interpretation in a much more direct fashion through the calculation of the neutron scattering function where phonons can be readily identified.

The agreement found for the band shape implies that the electronic distortion almost instantaneously follows the atomic density distortions; hence, the decay of the anisotropic fluctuations is dominated by the much slower atomic motion. This picture is also consistent with the observations on the intensity, namely that the discrepancy between calculation and experiment becomes larger at higher density, such that in the normal liquid state the disagreement is an order of magnitude. The expectation is that the higher the density the larger the electronic distortion, because of the larger overlap of the wave functions. This

distortion is in such a direction that it opposes the anisotropic density fluctuation and is of the same angular characteristic. Hence, by introducing electronic distortion through an atomic polarizability that depends only on the radial distance from another atom, one ought to be able to explain the intensity provided the pairwise additivity of the electronic distortion is an adequate approximation. This hypothesis has been tested by introducing a theoretically calculated pair polarizability into the calculations. Preliminary computations of the intensity agree with experiments within the rather large uncertainty of the data.

Equation of State for Dense Mixtures

The second problem arose in connection with the state of matter in the interior of Jupiter. Jupiter is believed to consist primarily of hydrogen with about 10% helium mixed in. At the center of Jupiter, where the pressure is about 40 million atmospheres, hydrogen is almost certainly metallic (although there is still considerable controversy about the lowest pressure needed for the transition from a diatomic hydrogen insulating system to a monatomic metallic state). The question then arises as to whether helium, which is still predicted to be an insulating material at the center of Jupiter, is soluble in the metallic hydrogen. If not, it would gravitate to the center of Jupiter and form an insulating core, with the core temperature estimated to be about 10,000°K.

At these temperatures metallic hydrogen is predicted to be a fluid due to the quantum mechanical zero point energy of the nuclei. This prediction is based on the molecular simulation computer calculation for melting a one-component quantum mechanical plasma.⁵⁻¹² The one-component plasma is a good description of metallic hydrogen at high pressures since it consists of a system of nuclei interacting repulsively with the Coulomb potential in which the electrons form a uniform background. For this system we found that the proton nuclei cannot exist as a solid at any density for temperatures above 3000°K.

To study the solubility question, two extreme models were investigated. The first model treated helium as a one-component metallic (completely unscreened) plasma.⁵⁻¹³ The second assumed that helium retains its electron around it (completely screened) and is treated as a spherical neutral atom (hard sphere). In the former case it was shown that a mixture of two one-component plasmas separates into two fluid phases below a critical temperature; for the special case of hydrogen and 10% helium mixture, that temperature is considerably above 10,000°K. The reason for the phase separation could be traced to the lack of local charge neutralization in the mixture and its much better realization in the separate pure components. On the other hand, the neutral helium atom was found to be completely soluble under the conditions expected at the center of Jupiter, and we believe this model corresponds more accurately to the real situation.

Nevertheless, it is clear that in any real situation the degree of screening of the atoms is crucial in determining the solubility. A crude model to incorporate screening under various physical situations is now being formulated. It should then be possible to determine the state of matter in other stellar objects such as the sun, which also consists of a mixture of hydrogen and helium. Furthermore, we should be able to determine whether the above predicted phase separation played a significant role during the evolution of white dwarfs.

Generalized Hydrodynamics

The last example concerns the microscopic investigation of the region of validity of macroscopic hydrodynamics. A few years ago we discovered, very surprisingly, that in two dimension the Navier-Stokes equations are not applicable because the presumptions of the existence of transport coefficients was unjustified.⁵⁻¹⁴ For example, we found that the

diffusion coefficient diverges in two dimensions because of persistence of velocity. This persistence was traced back to the generation by a moving particle of a vortex, which in turn fed part of its original momentum back into the particle. The persistence of velocity in three dimensions is somewhat weaker, because in higher dimensions less of the momentum is fed back. However, it could be theoretically demonstrated that due to this same effect, the Navier-Stokes equations in three dimensions are valid only asymptotically; that is, only when the external gradients causing the transport phenomena are in the limits of small amplitude, of long wavelength, and of time invariance.

To gain a better understanding of how to generalize hydrodynamics, the wavelength dependence of the diffusion coefficients has been investigated via a computer study of the distribution of displacements of particles as a function of time. The second moment of this displacement divided by the time is the ordinary diffusion coefficient. It was found that the second cumulant (the fourth moment minus the square of second moment) divided by the time diverges in three dimensions, confirming the nonanalytic nature of the wavelength dependence of the Navier-Stokes equations. Moreover, it was found that the distribution of the displacements in the long time limit deviated from the expected Gaussian in the sense that fewer particles reached large distances than would have been expected in a random walk picture. It seems physically reasonable to assume that the vortex motion previously found might explain this result, since on the average the vortex has the effect of causing particles to move back toward the center. Hence a model is now being numerically investigated in which a Fick's diffusion law is modified by a vortex to see whether the resulting displacement distribution agrees with that found from molecular simulation. If it does, a beginning would have been made concerning the manner in which hydrodynamics has to be generalized.

Computational Methods

ARTIFICIAL VISCOSITY

Artificial viscosities have played a major role in our hydrodynamic codes and we have recently been studying the question of which artificial viscosities should be used in our finite-difference schemes for solving hyperbolic equations. Some difference schemes, such as upstr 1 differencing and Lax-Wendroff, already have viscosity built into them. This frees the user from the necessity of choosing an artificial viscosity, but it also makes these difference schemes very inflexible. For example, the upstream difference method is so viscous that it gives reasonably accurate results only for problems in which very strong source terms occur.

Perhaps one should say something about why we need any artificial viscosity at all. It is true that nondissipative difference schemes, such as leapfrog and Crank-Nicolson, conserve energy, while dissipative schemes don't. (It is common in this context to use the terms "viscous" and "dissipative" interchangeably.) The trouble is that if a nondissipative scheme is used on a problem with a discontinuous solution, the energy is shifted to spurious grid-sized oscillations. (See Ref. 5-15 and Fig. 5-6.) These oscillations aren't so bad for linear problems or for nonlinear problems with only contact discontinuities: In those cases the oscillations stay bounded.⁵⁻¹⁶ For nonlinear problems with shocks, however, the energy may grow and the oscillations in a nondissipative scheme may grow rapidly.⁵⁻¹⁷ In fact, Fig. 5-6 shows the solution of the nonlinear equation $u_t + uu_x = 0$ by a difference scheme with just enough artificial viscosity to maintain stability. One way to view this phenomenon is to say that a nondissipative difference scheme introduces a dispersive medium. That is, waves of different frequencies travel at different velocities. In this case energy is carried along at the group velocity, and between a shadow region and an illuminated region there is a transition region called a caustic. This is

discussed in Ref. 5-18, where the group velocities and caustics are determined for the solution of $u_t + u_x = 0$ by a Galerkin method.

We have recently found that the only difference schemes that track a discontinuity with exactly the right speed are those for which the order of dissipation is no larger than the order of accuracy. This means that if we want to track a discontinuity with a fourth-order scheme, we must use either a second-order artificial viscosity, $\epsilon \Delta u_{xx}$, or a fourth-order artificial viscosity, $-\epsilon(\Delta x)^3 u_{xxxx}$. (We may of course use an ϵ which depends on u_x .)

We have also found that the only way to have no overshoot at a discontinuity (that is, no Gibbs phenomenon) is to use a second-order artificial viscosity with a large enough ϵ . This point can be important for waves in an elastic-plastic medium, such as rock. For example, if the computations say that the material has deformed enough to become plastic, we want to be certain that this isn't just the result of a numerical Gibbs phenomenon.

Fig. 5-6. Result of a nondissipative scheme used on a problem with a discontinuous solution.

Fig. 5-7. Solution of the wave equation with artificial viscosity (see text).

The TENSOR and HEMP codes for two-dimensional wave computations are based on second-order difference schemes with three ad hoc artificial viscosities.⁵⁻¹⁵ The reason for using so many viscosities is that none of them alone is truly dissipative. We have found that the discrete Laplace operator is a fine artificial viscosity. Figure 5-7 shows the solution (w) at time $t = 1$ of the problem

$$u_t = w_x + \epsilon \Delta x (u_{xx} + u_{yy}), \quad u(x, y, 0) = 0,$$

$$v_t = w_y + \epsilon \Delta x (v_{xx} + v_{yy}), \quad v(x, y, 0) = 0,$$

$$w_t = u_x + v_y, \quad w(x, y, 0) = 1 \text{ if } x^2 + y^2 < 1, \\ w(x, y, 0) = 0 \text{ if } x^2 + y^2 \geq 1.$$

We have taken $\epsilon = 0.05$. Notice that there still are some small grid-sized oscillations. In this setting the oscillations are sometimes called hour glasses.⁵⁻¹⁵ If $\epsilon = 0$, our system is equivalent to the wave equation, and because of the focusing the true solution at time $t = 1$ behaves like $\ln(x^2 + y^2)$ at the origin. Figure 5-7 does indeed show a hole at the origin, but the singularity is considerably smoothed out. For the sake of comparison we show in Fig. 5-8 the result of the same computation with no artificial viscosity ($\epsilon = 0$). It is clear that the grid-sized oscillations give us nonsense. In this case the artificial viscosity helps a lot, but the singularity at the origin is so strong that there is probably no difference scheme that will resolve it.

Fig. 5-8. Solution of the wave equation with no artificial viscosity.

INTEGRODIFFERENCE METHODS

A systematic procedure has been developed⁵⁻¹⁹ for deriving difference schemes of high accuracy. This procedure applies to two-point boundary-value problems as well as to mixed initial-boundary-value problems for partial differential equations. It is particularly useful on nonuniform grids and for

differential equations which are quasilinear or singular or both. These new difference schemes are a little more complicated to set up than the standard difference schemes, but once they are set up, the computing times and storage requirements are the same. Hence, we obtain increased accuracy at very little cost.

The main idea of the method is as follows. For a two-point boundary-value problem the differential equation may be integrated to form an integrodifference equation which is exactly equivalent to the original equation. That is, we obtain an equation involving integrals and differences. Our new difference schemes are then obtained by interpolating under the integrals by linear functions or by parabolas. For a uniform grid the linear functions give a scheme which is second-order accurate, and the parabolas a

third-order or a fourth-order scheme. In this case the standard central difference scheme is also of second order accuracy. On the other hand, for a nonuniform grid the standard scheme becomes of first order, while our linear-interpolation scheme remains of second order and our parabolic-interpolation scheme becomes of third order.

As an example we show in Figs. 5-9 and 5-10 the local truncation errors for the central difference method and for our integrodifference method with

Fig. 5-9. Local truncation errors for the central difference method.

linear interpolation and with parabolic interpolation. For the function

$$\psi(r) = \exp(-r^2) \quad (0 \leq r \leq 3)$$

each figure shows, first, the Laplacian of ψ in cylindrical coordinates

$$g(r) = \frac{d}{dr} (r \, d\psi/dr) = -4(1 - r^2)\psi$$

and then the difference between this exact value g and the number obtained by replacing

$$\frac{d}{dr} (r \, d\psi/dr)$$

by standard central differences and by our new difference schemes. Figure 5-9 shows the case of a uniform grid, while Fig. 5-10 shows the case of a nonuniform grid with

Fig. 5-10. Local truncation errors for the integrodifference method.

$$(r_{i+1} - r_i)/(r_i - r_{i-1}) = 1.01.$$

These graphs illustrate that:

- The central difference formula is of comparable accuracy with our method of linear interpolation when the grid is uniform, but the central difference method becomes progressively worse as the degree of nonuniformity increases.

- The method of parabolic interpolation provides substantially better results than the other methods, whether the grid is uniform or nonuniform.

It would be useful to compare our difference schemes with other methods which produce difference schemes of high accuracy, such as the Galerkin or finite-element methods.

Based on our new methods, we have developed several user-oriented codes for problems of optical propagation and self-focusing.

Acknowledgments

This report describes the work of many individuals in the Division, not all of whom are specifically mentioned in the Contents. However, all persons responsible for the various subjects discussed here are listed in the references at the end of each major section.

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