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for Simulating High Energy Density ICF
Plasmas**

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THE BUCKY AND ZEUS-2D COMPUTER CODES FOR SIMULATING HIGH ENERGY DENSITY ICF PLASMAS

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ABSTRACT

BUCKY and ZEUS-2D are two radiation hydrodynamics codes under development at the University of Wisconsin for the simulation of the behavior of high energy density plasmas found in ICF targets and target chambers. The ZEUS-2D code was originally developed at the National Center for Supercomputer Applications. BUCKY is a 1-D Lagrangian code which models many physical phenomena. Verification of these models in BUCKY with experiments is in progress. ZEUS-2D is a 2-D Eulerian radiation magnetohydrodynamics code written for astrophysical applications. It contains relatively simple radiation physics models which are being enhanced by implementing models from the BUCKY code.

I. INTRODUCTION

This paper describes the present state of ICF radiation hydrodynamics code development at the University of Wisconsin. Computer codes for the study of ICF plasma physics and radiation transport have been under development at the University of Wisconsin for about twenty years. Presently, two radiation hydrodynamic computer codes and an atomic physics code are being used, maintained and improved upon. BUCKY¹ is a 1-D radiation-hydrodynamics computer code. ZEUS-2D, written at NCSA, is a 2-D radiation MHD code.^{2,3,4} EOSOPA⁵ is an atomic physics computer code for calculation of equations-of-state and opacities for BUCKY and ZEUS-2D.

BUCKY¹ is a 1-D Lagrangian radiation-hydrodynamics computer code in slab, spherical, and cylindrical geometry. BUCKY uses table lookups for detailed equations-of-state and opacities from

EOSOPA⁵ or SESAME.⁶ Radiation transport is calculated several possible ways, including multigroup diffusion and CRE line transport. Thermonuclear burn, neutron and fusion product transport, laser, thermal radiation, and ion source deposition are modeled. BUCKY calculates the response of a solid surface to x-rays and ions including vaporization and melting.

ZEUS-2D is a two-dimensional, Eulerian-mesh radiation-magnetohydrodynamics code.² The fundamental hydrodynamic equations can be solved separately or augmented with magnetohydrodynamics, radiation, or both. In its published condition, ZEUS-2D had single group radiation transport, ideal gas equations-of-state and minimal energy source physics. ZEUS-2D is being modified to include the physics capabilities of BUCKY.

BUCKY has been used in the simulation of high and moderate energy density plasma phenomena. BUCKY has been used to model ICF target implosions and explosions. It has been useful in the study of ion beam driven physics experiments on PBFA-II at Sandia National Laboratories⁷ and on KALIF at Forschungszentrum Karlsruhe.⁸ Laser driven physics experiments on Nova at Lawrence Livermore National Laboratory have also been studied with BUCKY. Moderate energy density applications of BUCKY include fireballs in gases, and vaporization and melting of solids by x rays and ions. These applications are often related to an ICF target chamber, such as in power plant concepts and in the National Ignition Facility.⁹

Recently, there has been significant development of the BUCKY 1-D radiation-hydrodynamics code. The ZEUS 2-D radiation-magnetohydrodynamics

code is still in development and has not yet been used for problems of interest to ICF. BUCKY results have been compared with experiments at high and moderate energy densities, that are relevant to ICF targets and target chambers. These are discussed in this paper.

II. BUCKY 1-D CODE

A. Radiation Transport and Hydrodynamics

The BUCKY code has been compared with radiation burnthrough experiments performed on the Nova laser at LLNL.¹⁰ In these experiments, x rays produced in a gold Hohlraum with the Nova laser beams are allowed to burn through a thin gold foil. The Hohlraums are cylinders 0.16 cm in diameter and 0.275 cm long with walls 25 μm thick. Gold foils and observation holes are placed in the Hohlraum walls near the center. Ten laser beams enter the Hohlraums through holes at each end of the cylinder and shine on the inside of the walls. The laser pulse shape is assumed to be trapezoidal, with a 0.8 ns flat top. The x rays create a Marshak wave in the gold, whose speed is a function of the opacity and equation of state of the gold. The transit time of the Marshak wave is measured for foil thicknesses from 1 to 3 μm by observing the history of the x-ray emissions from the back of the foils with a Streaked X-ray Imager (SXI). Simultaneously, the drive radiation inside the Hohlraum is measured with the DANTE x-ray diode array. DANTE observes the x-ray power emitted by a given area on the inside of the Hohlraum wall in several energy channels. This can be converted into an effective wall temperature that is reported as a function of time.¹⁰

These experiments have been modeled with the BUCKY code in 1-D. The Nova Hohlraum is modeled as two slabs of solid gold separated by 0.15 cm of low density gold vapor. BUCKY models the deposition of the laser in the vapor and on the inside edge of one of the walls, assuming that the beams are incident at 45°. By simulating the laser deposition, the radiation burning into the gold is in a spectrum calculated by the code and is not assumed to be Planckian. Radiation transport is modeled with 100 energy group flux-limited diffusion. Equations-of-state come from SESAME tables, and opacities from tables generated with the EOSOPA code, where the Unresolved Transitions Array method is used to calculate high atomic number opacities.

The proper intensity of the laser is uncertain, because in a Hohlraum the lasers are focused in distinct spots which is a 3-D problem. The intensity has been varied until the code predicts the wall temperature measured by DANTE. The wall temperature is calculated as the blackbody temperature that would create the emitted flux predicted by the BUCKY simulations. The simulations used flux limited diffusion for the radiation transport, which only provides the net flux across the wall surface, so the emitted flux is calculated as the difference between the net flux and the flux from the center of the Hohlraum, σT_r^4 (center). The radiation temperature in the center of the Hohlraum or drive temperature, the calculated wall temperature, and the DANTE measured wall temperature are plotted in Fig. 1 for a laser intensity of 150 TW/cm². One can see that this intensity is close to agreeing with the DANTE measurements. The effect of losses on the holes is accounted for through the adjustment of the laser power. A 1-D model like this is only useful when it is tied to a measurement of the wall temperature. The advantage of modeling the laser, as it has been in these calculations, over modeling the drive radiation as a blackbody spectrum is the inclusion of non-Planckian features. Because the calculated wall temperatures are forced to agree with the measure values, the drive fluxes on the sample foil are correct, and the spectrum is closer to correct than a Planckian would be.

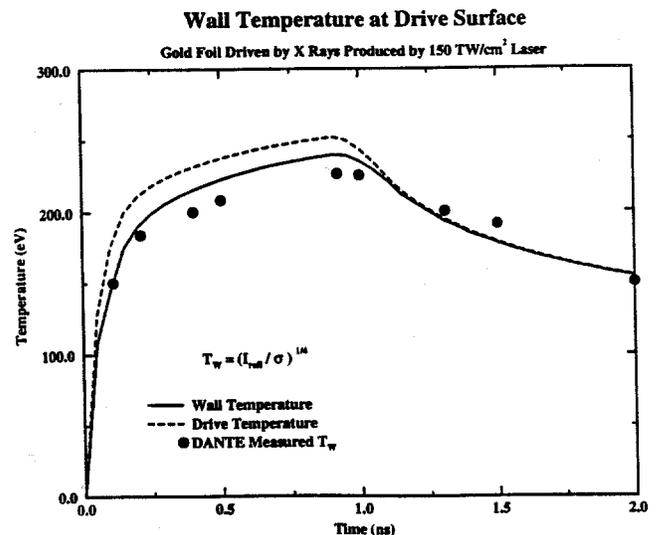


Fig. 1. Wall and drive temperatures in Nova Hohlraums. Drive and wall temperatures calculated by BUCKY for 150 TW/cm² laser. Wall temperatures are measured with DANTE.

Using 150 TW/cm^2 as a laser intensity, the burn-through of various thicknesses of the gold foils has been simulated with BUCKY. The burnthrough time is defined as the time between when the drive flux reaches 10% of its maximum and when the flux at the back of the foil reaches 50% of its peak. The SXI measures the flux in channels between 210 and 240 eV and 430 and 570 eV. BUCKY group structure allows channels between 208 and 236 eV and 451 and 547 eV. The comparisons of the burnthrough times for radiation in these channels are shown in Fig. 2, plotted against foil thickness. One can see that the BUCKY simulations show excellent agreement with the experimental results. This is a confirmation of the radiation diffusion method in BUCKY and the opacities calculated by EOSOPA for use in the simulation of radiation transport in dense high atomic number plasmas.

B. Ion Stopping, Vaporization and Melting

The calculation of the deposition of ions in solids by the BUCKY code has been improved. The code divides material into two parts: hydrodynamic regions where the material is allowed to move and solid or liquid regions, where hydrodynamic motion does not occur. Heat transfer is calculated in both parts, though radiation transport is not calculated in solids. Photons reaching the interface between vapor and solid are deposited in the first solid zone. The ion deposition is calculated in the solid material as a function of distance using the Bethe model at high particle velocity and the Lindhard model at low velocities, with a transition region that smoothly transfers between the two models. BUCKY uses a model which is an improvement over Mehlhorn's¹¹ model by improving the smoothness of the transition region. Also, BUCKY calculates the charge state of the ions during their transit. The ion stopping in BUCKY has been compared favorably with experiments in hot stopping media.

The ion stopping in BUCKY has been compared with the TRIM code¹² for cold stopping media, relevant in target chamber walls. The TRIM code uses fits to measured cold stopping results to obtain range as a function of energy, while BUCKY is an ab initio calculation. TRIM does a 3-D Monte Carlo calculation of ion trajectories, including direction change scattering, while BUCKY assumes 1-D normal incidence ion trajectories and does a deterministic calculation. Therefore, TRIM can include the straggling effect while BUCKY cannot.

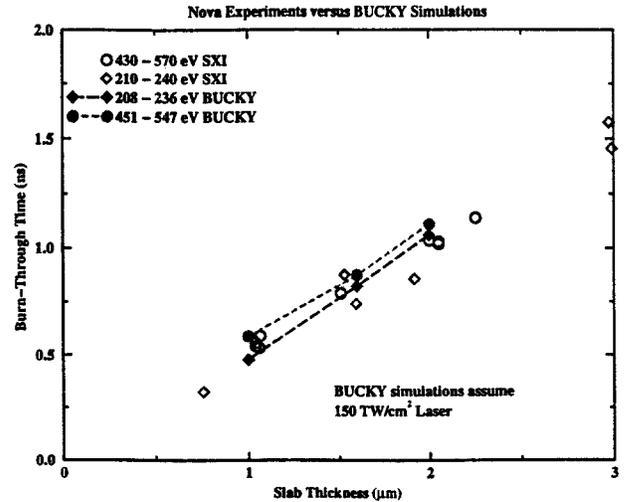


Fig. 2. X-Ray burnthrough times in gold versus thickness. Radiation flux is measured with the SXI and calculated with BUCKY at the back of a gold foil in two photon energy bands.

Vaporization is calculated in BUCKY by determining the rate that atoms leave the surface, as a function of surface temperature and lattice separation energy. This is offset by the rate that vapor atoms near the surface are condensed, as determined by the properties of the vapor when enough mass has been converted to vapor, additional vapor Lagrangian zones are created. The ability of BUCKY to model the vaporization of materials by ions has been tested by comparing a simulation with an experiment performed at Sandia National Laboratories. Tim Renk of SNL has irradiated a pure aluminum sample with 4 J/cm^2 of mixed carbon ions and protons and has measured the melt depth. The experiment was performed with a light ion diode focusing a beam onto a sample across a distance of 25 cm. This produces a beam of mixed protons and carbon ions, each with a maximum energy of 500 keV. The carbon ions carry most of the energy (3.40 J/cm^2). The carbon ions arrive after the protons because they are moving more slowly. The experiment yields a $5 \mu\text{m}$ thick melt layer.

The results of a BUCKY simulation of this experiment show that the peak surface temperature is about 2800 K and is reached at 160 ns after the start of the protons reaching the sample. The temperature profile at 60 ns is due to the protons, which have a range of a few μm in aluminum. The profile has a temperature peak of 770 K about $2.1 \mu\text{m}$ into the material. The melting temperature of aluminum is 933 K, so the

protons do no melting. The profile at 100 ns is dominated by carbon ions. The peak in temperature is at the surface because the range of carbon is so much shorter. The melt depth is estimated by just considering all material above the melting temperature to be melted. This ignores the effect of latent heat in melting. Latent heat is included in vaporization. The results are summarized in Fig. 3, where the temperature profiles in the material are plotted against position at various times. The melt depth at 100 ns is about $3 \mu\text{m}$. The maximum temperature is reached at 160 ns and the melt depth at this time is about $5 \mu\text{m}$. At 400 ns, the maximum melt depth of about $7 \mu\text{m}$ is released. The density of beam ions in the aluminum builds throughout the shot due to deposition. The carbons are much closer to the surface. This is compared with the TRIM code densities where 500 keV protons and carbons (monoenergetic) are deposited in aluminum. TRIM calculations include the effects of straggling, which are seen to be important for 500 keV carbon. The maximum ranges predicted by BUCKY and TRIM are quite close.

The BUCKY calculations agree reasonably well with the TRIM calculations and with the SNL experiments. BUCKY predicts $0.05 \mu\text{m}$ of vaporization. This has not been detected in the SNL experiments.

C. X-ray Vaporization

X-ray vaporization is predicted by the BUCKY code. The time-dependent deposition of a multigroup spectrum of x rays is calculated in the solid and vapor materials, using cross sections from fits to experimental values.¹³ Heat transfer in the materials is simultaneously performed. Vaporization is modeled by converting zones of solid into zones of vapor. The zones of vapor are Lagrangian and exhibit hydrodynamic motion; the solid zones do not move. A zone makes this conversion either when the zones have sufficient internal energy to overcome the sensible heat and latent heat of vaporization, or when the surface vapor pressure has been high enough for a long enough time that the zone has evaporated. This model assumes that mass is lost as individual atoms or molecules, not as large chunks.

The x-ray vaporization in BUCKY has been compared with experiments done on the Helen laser. In these experiments, a laser strikes a foil, creating x rays with approximately a 160 eV blackbody spectrum. At this photon energy, most of the x-ray attenuation of Al_2O_3 is due to the Al,¹³ so BUCKY uses the x-ray stopping power of Al at 3.9 g/cm^3 . The x rays are assumed to be emitted in a Gaussian pulse 1 ns wide.

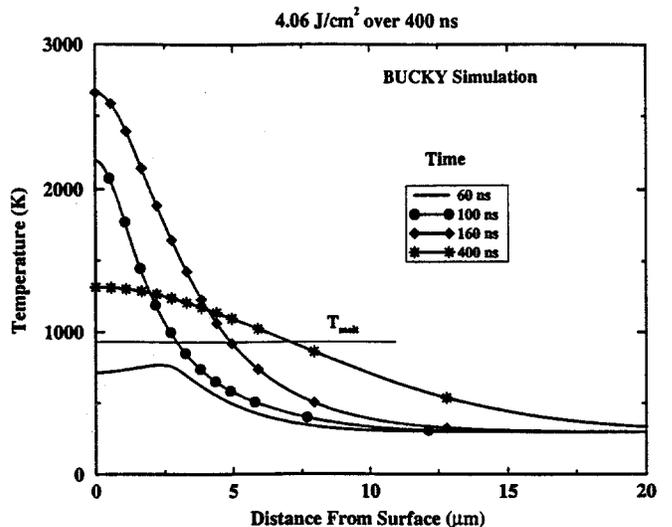


Fig. 3. Temperature profiles in aluminum plotted against depth at various times. SNL experimental conditions are assumed.

The fluence on a sample material is adjusted by varying the position of the sample relative to the x ray producing foil. The material loss is then measured. For Al_2O_3 , BUCKY calculations were performed and compared with the Helen experimental results. The actual uncertainty in the results is not known, but near the vaporization threshold the uncertainty must be at least $0.05 \mu\text{m}$. The Helen data points at about 0.6 and 0.8 J/cm^2 are shown to have zero depth removed, but to have some surface damage. This may mean a small depth removed that could not be measured. The Helen results show a threshold for vaporization of between 0.25 and 0.6 J/cm^2 . The BUCKY simulations predict a vaporization threshold of 0.25 J/cm^2 . At about 1.1 J/cm^2 , Helen had a removal of $0.1 \mu\text{m}$ and BUCKY predicted $0.12 \mu\text{m}$. So the agreement between BUCKY and Helen experiments was within experimental uncertainty.

III. ZEUS 2-D CODE

The ZEUS-2D radiation-magnetohydrodynamics code^{2,3,4} is being augmented to add the key capabilities of the University of Wisconsin's 1-D BUCKY code, including multiple materials, multigroup radiation diffusion, and table lookup of detailed opacities and equations of state. ZEUS-2D is a two-dimensional, Eulerian-mesh code, written in covariant orthogonal coordinates and solved by finite differences with operator splitting into implicit source and

explicit transport steps. The finite-difference mesh can be modified dynamically, although ZEUS-2D is not an adaptive-mesh code, and the mesh spacing can be varied independently in both dimensions.

The unmodified ZEUS-2D code has been tested on simple radiation diffusion, microexplosion, and Hohlraum test problems, and it appears to be a suitable code upon which to base the desired modifications. Multiple materials have been implemented by including the solution of a separate equation of continuity for each species. The modifications to the difference equations required to add multigroup frequency dependence have been developed and tested in a small auxiliary code, using the same variable names and covariant differencing scheme presently in ZEUS-2D. These modifications are in the process of being introduced into ZEUS-2D. The table lookup subroutines from the BUCKY code for equations of state and opacities have been merged with the ZEUS-2D code, and debugging of this merger is in its final stages.

IV. CONCLUSIONS

Verification of ion stopping, radiation transport, atomic physics, vaporization, and melting are in progress for the BUCKY code. The physics models in BUCKY agree with experiments in several regimes. The ZEUS-2D code is being modified to include multigroup radiation diffusion, multiple material tracking and realistic equations-of-state and opacities. Models developed in BUCKY will be inserted into ZEUS-2D, allowing the accurate simulation of 2-D target and target chamber phenomena.

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