Z-Pinch $(LiF)_2$-BeF_2(flibe) Preliminary Vaporization Estimation Using the BUCKY 1-D Radiation Hydrodynamics Code

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The post-explosion material vaporization characteristics of the proposed Z-Pinch reactor design were simulated using the BUCKY 1-D radiation hydrodynamics code. To model the 3-D variations in the reactor chamber design, three separate BUCKY simulations were performed — one in each of the cylindrical coordinate geometries: +z, –z, and r. The simulations were run to a time of 80 μs and the chamber material characteristics were analyzed. These results were compared to a simple analytical model to verify the vaporization radii in each of the three modeled directions. The +z material vaporization has been estimated to be at a radius 53.71 cm, compared to an analytic result of 79.00 cm. The –z material vaporization has been estimated to be at a radius of 101.92 cm, compared to an analytic result of 102.78 cm. The r material vaporization has been estimated to be at a radius of 73.86 cm, compared to an analytic result of 77.63 cm.

These simulation results confirm the idea that we can model the exploding Z-Pinch target and its resulting thermal effects on the reactor chamber using the BUCKY 1-D radiation hydrodynamics code. This model is appropriate for analysis of the Z-Pinch reactor because it is a massive structure and because most of the energy coupling to the surrounding structure is via x-rays (30%) rather than expanding ionic debris (4%). Furthermore, we have confirmed the viability of performing three different 1-D simulations in each of the +z, –z, and r directions and merging the three results. Such an approximation to a 3-D phenomenon is valid for times where the outward blast and energy transfer remain nearly spherical.

***Keywords:** Z-Pinch Reactor; radiation hydrodynamics; material vaporization; Z-Pinch; reactor physics*

I. Introduction

The vaporization characteristics of the proposed Z-Pinch reactor design were simulated using the BUCKY 1-D radiation hydrodynamics code [1]. In order to model the 3-D variations in the reactor chamber design, three separate BUCKY simulations were performed using a radial build in each of the cylindrical coordinate geometry axes: +z, –z, and r, where the center of the exploding target is at the origin for each simulation. The simulations were run to a time of 80 μs and the material characteristics were analyzed. These results were compared to a simple analytical model to verify the vaporization radii in each of the three modeled directions. The results of these calculations demonstrate the viability of using BUCKY to perform integrated target-structure simulations.

II. Overview of the Z-Pinch Reactor Geometry

The proposed Z-Pinch reactor design (Fig. 1) consists of a recyclable transmission line (RTL) assembly to which the fusion capsule is attached. The RTL is inserted into a reaction chamber which is protected by jets of liquid flibe on the sides of the chamber and a pool of liquid flibe on the bottom of the chamber. The RTL contains a solid open-celled flibe foam (~8% solid density) which acts as a thermal barrier and mechanical shock absorber [2].

III. Analytical Estimation of Material Vaporization

In order to assess the first-order accuracy of the BUCKY results, an analytical model of material vaporization was developed. This analytical model solves a thermodynamic conservation of energy equation to estimate the mass of material that would be vaporized in each of three directions: +z, –z and r. Two equations were developed in this model — the first for flibe starting in the solid phase (1) and the second for flibe starting in the liquid phase (2), where E_{in} is given as 3.0275 gigajoules for both equations. For these equations the values of T_{melt} and T_{boil} were 459 ºC and 1435 ºC, respectively [3]. The heat capacities at constant pressure used in the solid and liquid phases are given by (3) and (4). The values used for l_f and l_v were 448 J/g and 5540 J/g, respectively [3].

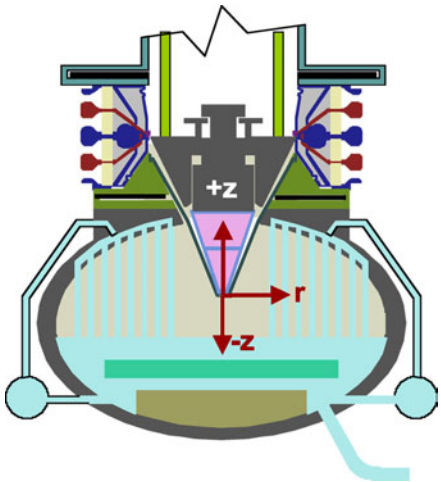

Figure 1. Z-Pinch Reactor Diagram

$$m_{vap} = \frac{E_{in}}{l_f + l_v + \int_{T_{melt}}^{T_{boil}} C_{p,l}(T')dT' + \int_{T_0}^{T_{melt}} C_{p,s}(T')dT'} \quad (1)$$

$$m_{vap} = \frac{E_{in}}{l_v + \int_{T_0}^{T_{boil}} C_{p,l}(T')dT'} \quad (2)$$

$$C_{p,s}(T) = (1.326 + 0.0015T)\frac{J}{g \cdot °C} \quad (3)$$

$$C_{p,l}(T) = 2.384\frac{J}{g \cdot °C} \quad (4)$$

Once the vaporized mass of material in each direction was calculated, the volume of material vaporized based on the initial flibe density (where ε is the flibe solid fraction) for each direction was calculated (5). Given an initial flibe region radius, the flibe vaporization radius in each direction was calculated (6).

$$V_{vap} = \frac{m_{vap}}{\varepsilon\left(2.28 - T_0 \cdot 4.884 \times 10^{-4}\frac{1}{°C}\right)\frac{g}{cm^3}} \quad (5)$$

$$r_{vap} = \left(\frac{3}{4\pi}V_{vap} + r_0^3\right)^{1/3} \quad (6)$$

Given the initial conditions from Table I, r_{vap} was calculated to be 79.00 cm from the center of the target for the +z direction, r_{vap} was calculated to be 102.78 cm from the center of the target for the –z direction and r_{vap} was calculated to be 77.63 cm from the center of the target. Using these values and the initial radii given in Table I, the vaporization depth into the flibe layer, Δr_{vap}, for each of the three directions was calculated and is shown in Table I.

IV. BUCKY Simulation of Material Vaporization

The BUCKY target input deck provided by R.R. Peterson was modified to include the materials and initial conditions proposed for the Z-Pinch reactor target. Table II shows the bare target materials and initial conditions. The BUCKY target radial build is shown in Fig. 2.

A. +z Input Parameters

For the BUCKY simulation representing the material vaporization in the +z direction, two materials were added to the input deck, shown in Table III. The RTL steel layer is a 10 μm layer that represents the structure to which the target capsule is physically attached. The flibe foam layer is the thermal insulator and shock absorber used to protect the rest of the RTL from damage.

B. –z Input Parameters

For the BUCKY simulation representing the material vaporization in the –z direction, two materials were added to the input deck, shown in Table IV. The 10 torr argon gas is used as a buffer and the flibe layer represents the pool of liquid flibe that resides in the bottom of the chamber.

C. r Input Parameters

For the BUCKY simulation representing the material vaporization in the r direction, two materials were added to the input deck, shown in Table V. The 10 torr argon gas is used as a buffer gas and the flibe layer represents the 50% void fraction liquid flibe jets that are used to protect the chamber wall.

TABLE I. Analytical Equation Parameters and Resulting Vaporization Depth

Parameter	Value		
	+z	–z	r
T_0 (eV)	0.05	0.09417	0.09417
T_0 (°C)	307.25	819.84	819.84
r_0 (cm)	1.02	101.01	71.01
ε	0.08	1.00	0.50
Δr_{vap} (cm)	77.98	1.76	6.62

TABLE II. BUCKY Simulation Parameters

Target Layer	Simulation Parameter Value			
	T_0 (eV)	ρ_0 (g/cm^3)	r_f (cm)	Δr (cm)
DT Vapor	0.01	5.00×10^{-04}	0.408	0.408
DT Ice	0.01	0.25	0.466	0.058
Be Shell	0.05	1.85	0.499	0.033
CH Foam	0.05	2.45×10^{-03}	1.000	0.501
Au Electrode	0.05	19.3	1.010	0.010

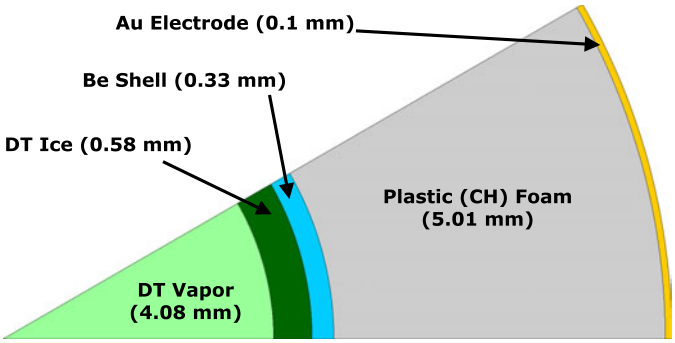

Figure 2. Z-Pinch Target Diagram

D. *BUCKY Simulation Results*

Simulation output was plotted at times of 20, 40 and 80 μs so that the time-dependent evolution of the plotted quantities could be observed. Figures 3, 4 and 5 show material temperature in electron-volts for the +z, –z and radial simulations, respectively.

V. Revised Estimation of Material Vaporization using 80 Microsecond BUCKY Results

The computed ion temperatures and vaporization radii at 80 μs were analyzed to create a revised estimate of the vaporization radius in each of the three simulated directions. A mass-averaged temperature was computed (7) for the simulation zones greater than the vaporization temperature of the flibe (0.147 eV). For (7), the variable m_{gas} is the total mass of all of the gaseous zones in grams. The values Δm_i and T_i are the mass of each zone in grams and temperature of each gas zone in electron-volts, respectively. The revised vaporization mass was computed using an ideal gas mass-energy balance (8). The revised vaporization radii were then recalculated using Equations (5) and (6).

$$\overline{T}_{gas}(eV) = \frac{1}{m_{gas}} \sum_{i=1}^{N} T_i(eV) \cdot \Delta m_i \tag{7}$$

$$m_{vap} = \left(\frac{\overline{T}_{gas}(eV) - 0.147eV}{0.147eV - T_0(eV)} - 1 \right) m_{gas} \tag{8}$$

Given the initial conditions and the simulation results in Table VI, r_{vap} was calculated to be 53.71 cm from the center of the target in the +z direction, r_{vap} was calculated to be 101.92 cm from the center of the target in the –z direction and r_{vap} was calculated to be 73.86 cm from the center of the target in the r direction.

Table VI shows the revised vaporization depth in each direction resulting from the extrapolation of vaporization radius based on the ion temperatures at 80 μs into the simulation.

TABLE III. +z BUCKY Simulation Chamber Parameters

Material Layer	Chamber Parameters			
	T_0 (eV)	ρ_0 (g/cm^3)	r_f (cm)	Δr (cm)
RTL Steel (Fe)	0.05	7.80	1.02	0.01
Flibe Foam (ε=0.08)	0.05	0.17	100.00	98.98

TABLE IV. –z BUCKY Simulation Chamber Parameters

Material Layer	Chamber Parameters			
	T_0 (eV)	ρ_0 (g/cm^3)	r_f (cm)	Δr (cm)
10 torr Ar Gas	0.09417	2.35x10^{-5}	101.010	100.000
Liquid Flibe (ε=1.00)	0.09417	1.94	140.010	39.000

TABLE V. r BUCKY Simulation Chamber Parameters

Material Layer	Chamber Parameters			
	T_0 (eV)	ρ_0 (g/cm^3)	r_f (cm)	Δr (cm)
10 torr Ar Gas	0.09417	2.35x10^{-5}	71.010	70.000
Liquid Flibe (ε=0.50)	0.09417	0.97	171.010	100.000

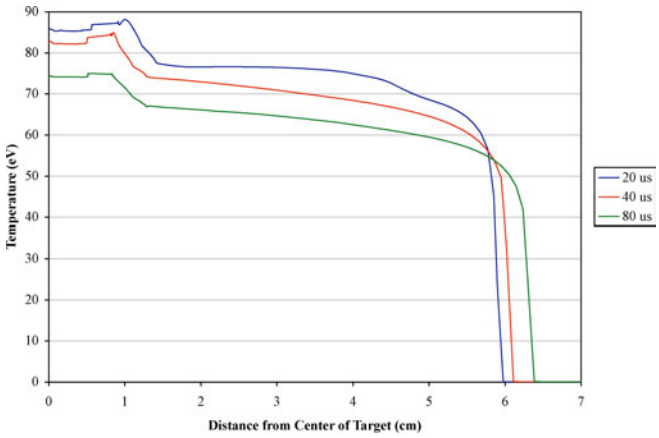

Figure 3. BUCKY Simulation +z Temperature Profile at 20, 40 and 80 μs

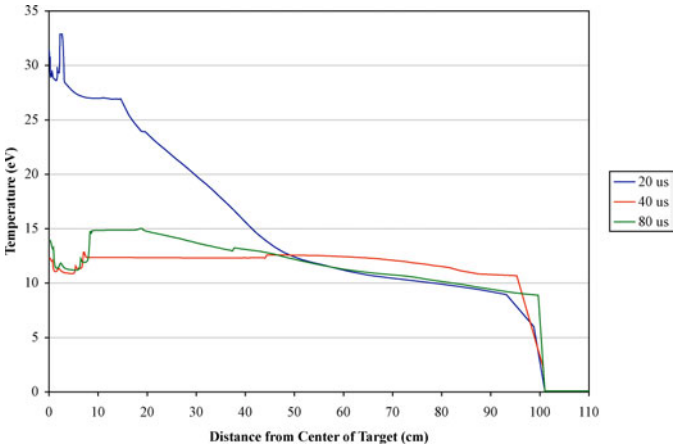

Figure 4. BUCKY Simulation –z Temperature Profile at 20, 40 and 80 μs

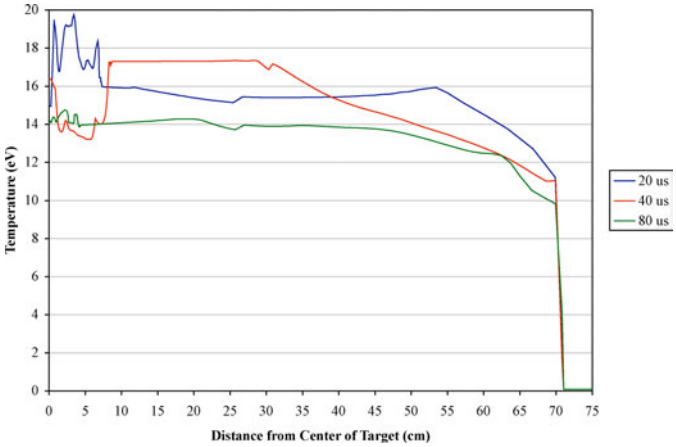

Figure 5. BUCKY Simulation r Temperature Profile at 20, 40 and 80 μs

Table VII shows a comparison between the analytical vaporization depth and the vaporization depth calculated from the BUCKY simulation results at 80 μs.

VI. Conclusion

As expected, the vaporization depths calculated from the result of the BUCKY simulations are less than those given by the analytical model, as is shown by Table VII. This is due to the fact that the analytical equation used the total yield of the target to calculate the vaporization depth. In the BUCKY simulations, only x-ray and ion energies are used to calculate the heating in the simulated materials; neutron heating effects are ignored.

These results indicate the idea that we can model the exploding Z-Pinch target using the BUCKY 1-D radiation hydrodynamics code to perform an integrated target-structure simulation has been confirmed. This model is appropriate for analysis of the Z-Pinch target because it has such a large mass and because most of the energy coupling to surrounding structure is via x-rays (30%) rather than expanding ionic debris (4%). Furthermore, we have confirmed the viability of using three different 1-D simulations in each of the +z, –z, and r directions and merging the three results. Such an approximation to a 3-D phenomenon is valid for times where the outward blast and energy transfer remain nearly spherical.

Further refinement of the BUCKY simulations will allow us to run the simulation for a longer time, providing higher confidence estimates of vaporized mass of the Z-Pinch target explosion.

TABLE VI. Revised Vaporization Parameters and Resulting Vaporization Depth

Parameter	**Value**		
	+z	*–z*	*r*
T_0 *(eV)*	0.05	0.09417	0.09417
$\overline{T}_{gas}$ *(eV)*	55.49	10.62	10.66
r_{gas} *(cm)*	6.3149	101.0123	71.01238
m_{gas} *(g)*	181.74	1,044.56	823.74
Δr_{vap} *(cm)*	52.69	0.91	2.85

TABLE VII. Vaporization Depth Comparison

Direction	Δr_{vap} ***(cm)***	
	Analytical	***Simulated***
+z	77.98	52.69
–z	1.76	0.91
r	6.62	2.85

References

[1] R.R. Peterson, J.J. MacFarlane and G.A. Moses, "BUCKY — A 1-D radiation hydrodynamics code for simulating inertial confinement fusion high energy density plasmas," UWFDM-984 (University of Wisconsin, August 1995).

[2] W.R. Meier, R.P. Abbott, J.F. Latkowski, R.W. Moir, S. Reyes and R.C. Schmitt, "Analyses in support of Z-IFE," LLNL Progress Report for FY-04, UCRL-TR-207101, September 2004.

[3] S.J. Zinkle, "Summary of physical properties for Lithium, Pb-17Li, and $(LiF)_nBeF_2$ coolants," APEX Study Meeting, Sandia National Lab, July 27-28, 1998.