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ALEGRA-HEDP Simulations of the Dense Plasma Focus

C.S. Kueny, D.G. Flicker, and D.V. Rose

Prepared by Sandia National Laboratories Albuquerque, New Mexico 87185 and Livermore, California 94550

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C. S. Kueny Hewlett-Packard Company

D. G. Flicker Sandia National Laboratories

> D.V. Rose Voss Scientific, LLC

Sandia National Laboratories P. O. Box 5800 Albuquerque, New Mexico 87185-1135

ABSTRACT

We have carried out 2D simulations of three dense plasma focus (DPF) devices using the ALEGRA-HEDP code and validated the results against experiments. The three devices included two Mather-type machines described by Bernard *et. al.* [1] and the Tallboy device currently in operation at NSTec in North Las Vegas. We present simulation results and compare to detailed plasma measurements for one Bernard device and to current and neutron yields for all three. We also describe a new ALEGRA capability to import data from particle-in-cell calculations of initial gas breakdown, which will allow the first ever simulations of DPF operation from the beginning of the voltage discharge to the pinch phase for arbitrary operating conditions and without assumptions about the early sheath structure. The next step in understanding DPF pinch physics must be three-dimensional modeling of conditions going into the pinch, and we have just launched our first 3D simulation of the best-diagnosed Bernard device.

TABLE OF CONTENTS

1. Introdu	ection	9
2. DPI	F Operation and Simulation	11
3. Ove	rview of Targeted Experiments	13
4. ALEG	RA-HEDP	. 15
5. Problei	n Set-up	17
6. Sim	ulation Results	19
	Bernard Long	
	Bernard Short	21
6.3	Tallboy	23
7. Discuss	sion	25
8. Distrib	ution	27
	LIST OF FIGURES	
_	Schematic of DPF operation, showing sheath creation (I), lift-off (II), run-down (III) and collapse (IV)	11
Figure 2.	Plasma density plots for Bernard Long device, showing the lift-off, run-down and pinch phases.	19
Figure 3.	Computed current traces for open- and closed-cathode models of Bernard Long, and accompanying thermonuclear neutron yields between 1 and 2×10^5 . Experimental values were 0.6 MA and 1.5×10^9 neutrons.	20
Figure 4	Density plot for pinch phase in Bernard Short device	
	Computed current traces and thermonuclear neutron yields for Bernard Short	
C	device	22
Figure 6.	Plasma density during run-down in Tallboy closed-cathode configuration,	
D: 5	showing plasma tendril that disrupted the simulation.	
	Plasma density during pinch for open-cathode Tallboy simulation.	23
	Plot of electron temperatures near Bernard Long insulator, computed by LSP	25
	and imported to ALEGRA-HEDP	
J		
	LIST OF TABLES	
Table 1.	Peak Currents and Neutron Yields from Experiment and from ALEGRA	
	Simulations, for all Three Test Devices	24

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NOMENCLATURE

2D two-dim ensional 3D three-dimensional 3D three-dimensional

ALE Arbitrary Eulerian-Lagrangian

DOE Department of Energy DPF dense plasma focus

DTRA

EOS equation -of-state

HEDP

LANL Los Alamos National Laboratory

LSP MHD

NNSA National Nuclear Security Administration

NSTec

PIC particle -in-cell

QEOS

SNL Sandia National Laboratories

1. INTRODUCTION

The dense plasma focus is a pulsed power device that accelerates and compresses plasma along a coaxial cavity and into a small pinch, which (depending upon the material) may emit intense bursts of neutrons, x-rays and charged particles. DPFs were invented independently by Mather [2] and Filippov [3] in the 1960s and are still studied intensely in laboratories around the world as inexpensive sources of neutrons, ion beams and x-rays, and as platforms for the study of high energy-density physics phenomena. [4,5,6]. Our interest is in their use as a compact neutron source, and to that end we have carried out simulations of three DPF experiments using Sandia National Laboratories' (SNL's) ALEGRA-HEDP code [7]. We validate the code as an accurate modeling tool and describe coming enhancements, we describe the need for a three-dimensional capability and our first launch of a three-dimensional (3D) simulation, and we suggest the next steps needed in order to provide an adequate predictive and design capability for higher neutron yields.

2. DPF OPERATION AND SIMULATION

A schematic of a DPF is shown in Figure 1. A high voltage discharge across the anode-cathode gap in a low-pressure, static gas fill initiates gas breakdown along the insulator and current flow along the path indicated by (I). The current interacts with its self magnetic field, providing lift-off (II) of a plasma sheath some millimeters thick and propelling it down the tube in phase (III), the run-down. As the sheath passes the anode tip, it is forced into a hot, dense pinch (IV), which must be timed via machine geometry, input voltage and fill pressure to coincide with the peak of the current flow. Pinch size is typically one mm wide and a few mm long, with particle densities of $10^{19-}10^{20}/\text{cm}^3$ and temperatures of hundreds of eV or more, lasting tens of nanoseconds [1]. For devices studied in this paper, we consider gas fills of 3–10 Torr, discharge voltages of 20-50 kV and currents of 0.6-1.8 MA, producing neutron yields of up to 5×10^{11} .

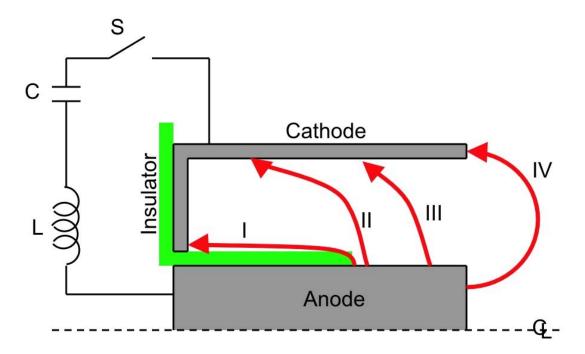


Figure 1. Schematic of DPF operation, showing sheath creation (I), lift-off (II), rundown (III) and collapse (IV).

Several aspects of DPF function are still poorly understood. Optimal neutron production requires the creation of a uniform, relatively thin sheath [8,9]. Choosing the correct gas fill to achieve this for new geometries is a still matter of trial and error. Outside of the ideal range the sheath may appear diffuse and reach across the cavity, or secondary sheaths or filaments may appear [8], both apparently harmful to performance. Voss Scientific has recently carried out 2D, fully electromagnetic particle-in-cell (PIC) simulations of sheath creation [10] using their code LSP, modeling the creation of the plasma sheath for arbitrary operating conditions. This is an important step toward a design tool for choosing DPF operating conditions. The ALEGRA team is completing work on a new capability to directly import data derived from these PIC simulations and use it to initiate our MHD simulations.

Current knowledge of pinch physics is even spottier. Plasma densities and temperatures, both predicted and measured, are insufficient to produce thermonuclear neutrons in the quantities observed, and the anisotropy and energy spectra of neutrons, and the ejection of high-energy charged particles all indicate non-thermonuclear mechanisms [1,11-27,49]. The pinch is subject to a variety of instabilities, producing complex structures, hot spots, strong electric fields and axial particle acceleration, all of which may contribute to neutron production [11,12,14,28-32,44]. In some experiments neutron emission has been observed in two discrete bursts, the first occurring at maximum pinch compression and a much larger, apparently non-thermonuclear burst as the pinch expands [12,49]. Yield saturation at higher energy inputs has been observed in some experiments [33-35] and is still not understood. Explanations for the high yields have focused on beam-target fusion driven by deuteron acceleration from MHD instabilities [11-13,22,24], but other observed features such as small, high-temperature hot spots [4,5,36,37] have not been explained and may be relevant.

MHD simulations can model conditions only up to the early pinch stage, when charge separation and instabilities occur, MHD approximations break down and the simulation must be stopped [42,43,45-48]. 2D simulations also miss many critical details: parallel cathode bars cannot be modeled, nor filamentation or other structuring in the sheath and pinch. An accurate simulation would require a three-dimensional MHD model up to the early pinch stage, where one might gain insight into the 3D structure as a starting point for further, particle-based simulations to follow the non-thermal plasma evolution. Ref. 26 documents a three-dimensional (3D), fully electromagnetic PIC simulation of sausage and kink instabilities in z-pinch-like plasmas for an idealized situation. We believe that PIC calculations guided by 3D MHD modeling of DPF pinch physics could shed new light on the mechanisms of neutron production. ALEGRA-HEDP is fully capable of high-resolution, massively parallel 3D simulations, and with the 2D benchmarks described in this paper completed, we are ready to carry out this 3D modeling.

3. OVERVIEW OF TARGETED EXPERIMENTS

Three experimental devices were chosen for modeling by agreement with DTRA/NumerEx/SNL. Two of these were documented by Bernard *et al.* [1]; the third device currently operated by NSTec in North Las Vegas. All three geometries are of the common "Mather" design. The center electrode is a solid copper anode, the outer electrode a cage of parallel copper bars (which appear as a solid wall in 2D cross-section). The base of the anode is wrapped in a 1/4"-thick pyrex insulator reaching 5 cm into the cavity. All three machines have a coaxial cavity of approximately one inch radial extent, and differ mainly in the anode length and width, and input power. We will refer to them as Bernard Long (25-cm anode, 27 kJ), Bernard Short (15-cm anode, 96 kJ) and Tallboy (nearly 66-cm anode, 270 kJ). The cathode length and insulator width for both Bernard devices had to be estimated from descriptions that were not clear and sometimes contradictory. Cross-sections of the three geometries from our 2D simulations are shown in Figures 2, 4 and 6, and the geometry for an upcoming 3D simulation of the Bernard Long machine is seen in Figure 9.

The documentation of the Bernard experiments included measurements of density and temperature obtained from holographic interferometry and laser scattering for one of the machines, and peak current and neutron yield for both machines. NSTec provided us current vs. time traces and total neutron yield for Tallboy.

As discussed earlier, neutron production in DPFs appear to be largely non-thermonuclear in origin. MHD codes such as ALEGRA can model only the thermonuclear contribution arising from hot, dense plasma, and only through the early part of the pinch phase after which the MHD approximation fails. We therefore expect that computed predictions of neutron yield will fall far below the experimental observations.

4. ALEGRA-HEDP

ALEGRA-HEDP [7] is a 2D/3D ALE (Arbitrary Eulerian-Lagrangian) code featuring coupled, operator-split models for hydrodynamics, magnetics, thermal conduction and radiation physics; multi-material, multiphase equation-of-state (EOS) models; material strength and fracture models; MHD including advanced thermal/electrical conductivity and lumped circuit models; two-temperature physics (separate ion and electron temperatures); emission, multi-group diffusion and implicit monte-carlo for radiation modeling; neutron yield and time-of-flight diagnostics; and a very full complement of output diagnostics. The ALEGRA code family runs both in serial and massively parallel mode on a wide variety of platforms, and has been successfully used to model a wide variety of experiments with high fidelity in both two and three dimensions [refs].

5. PROBLEM SET-UP

Simulations were carried out on meshes fitted to each geometry, with deuterium gas completely filling the computational domain. ALEGRA-HEDP provides extensive control over the computational approximations used, requiring a detailed knowledge of the assumptions involved and how these controls work. Our greatest challenge involved the equation-of-state model. We began with the widely used Los Alamos National Laboratory (LANL) Sesame model containing tabulated EOS data for deuterium down to a lowest meaningful density of .01 kg/m³, below which thermodynamic consistency is guaranteed not to hold. For DPF simulations, the initial gas fill and the low-density region behind the sheath are both in this thermodynamically inconsistent regime. We found that the plasma sheath would not propagate stably using this model, apparently due to this lack of consistency. An ideal gas model allowed modeling of sheath dynamics for a single-temperature approximation but did not handle two-temperature physics well. We finally employed the analytic QEOS model with parameters chosen for gaseous deuterium. Evaluating the equations in this model slow the computation significantly compared to a tabular EOS, so we carried out simulations with a tabularized version of this model, generated by Kyle Cochrane of SNL. Simulations using the table and the full QEOS model were found to differ very little.

Cell size was roughly 0.5 mm, with finer meshing along the rounded end of the anode. This is the minimum for capturing the pinch structure; with the code now validated for a series of geometries, higher-resolution simulations should be carried out. We modeled the insulator both as fully embedded in the anode and more accurately as 0.25 in. thick, with little effect on the results. Estimate of photon mean free paths indicates that radiation diffusion should be of little consequence, so a thermal emission model was used to avoid the heavy computations of full radiation diffusion.

As already mentioned, one limitation of 2D simulations involves the cathode bars. The cathode consists of a cage of parallel bars, and much of the plasma is lost between the bars while the rest accumulates against the bars. When modeling a 2D slice of this geometry in ALEGRA, we must choose between representing the bars as a solid impermeable boundary, or as completely open to mass flow while maintaining the correct boundary conditions for current flow. Running in these two modes produced different details for the current rise and the timing of the pinch. We expect the two results to bracket the correct value, which would only be obtained by a full 3D model of the bars (Figure 9). It is interesting to note that early DPF experiments were done with solid cathode walls, but these were abandoned in favor of porous walls and then parallel bars, because residual gas accumulating against the cathode could sometimes form a second current path behind the sheath that would disrupt power flow. This is indeed what happened in our Tallboy simulation when carried out with a solid wall model.

Each problem was set up with a circuit model comprising appropriate values of capacitance, inductance, resistance and charging voltage. The problem was initialized with a uniform, room-temperature deuterium gas fill, and a thin layer of higher-temperature gas in a thin layer along the insulator. MHD DPF simulations require choosing this seed ionized gas rather arbitrarily; we chose a thin layer of 1 eV temperature. Again, we are in the process of importing a first-principles PIC description of the sheath from LSP (Figure 8).

6. SIMULATION RESULTS

We relate the simulation results in turn for the Bernard Long, Bernard Short and Tallboy devices, and compare to all available experimental data. All three devices were run with both open and closed cathode boundaries, as discussed in the last section, to bound the peak current and the timing.

6.1 Bernard Long

The Bernard Long device featured a 135 microF capacitor bank at 20 kV charging voltage, for total stored energy of 27 kJ. We ran our circuit model with 27 nH stray inductance and 3.3 m Ω resistance, values not given in the paper but estimated from measurements on other machines. We ran with a 3 Torr gas fill for comparison to experiment.

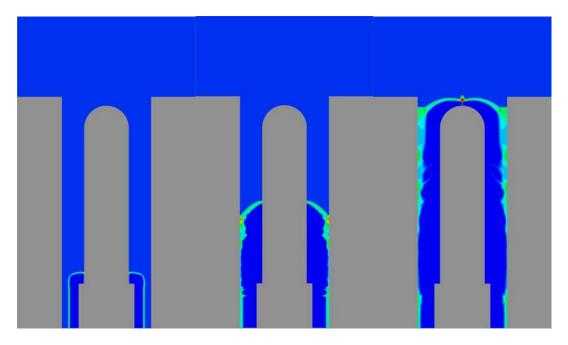


Figure 2. Plasma density plots for Bernard Long device, showing the lift-off, run-down and pinch phases.

Plasma density for this device is plotted for closed-cathode-boundary conditions in Figure 2, showing the lift-off, rundown and pinch phase. (The computational domain was just one side of the region shown; we plot a reflection of the data about the vertical axis to make the geometry more clear.) A substantial amount of residual plasma is seen against the cathode wall. Figure 3 displays current traces for the open- and closed-cathode boundary cases along with neutron yields of between 1 and 2×10^5 and rising at the end of the simulation, compared to 1.5×10^9 reported from the experiment. We see that the presence or absence of residual plasma strongly affects the current peak and timing. Neutron yields differ for the two simulations, but since the yield was rising at the end of the simulation the difference is not meaningful. Again, the discrepancy between computed and experimental neutron yields was expected due to the inability of MHD to model non-thermonuclear production mechanisms.

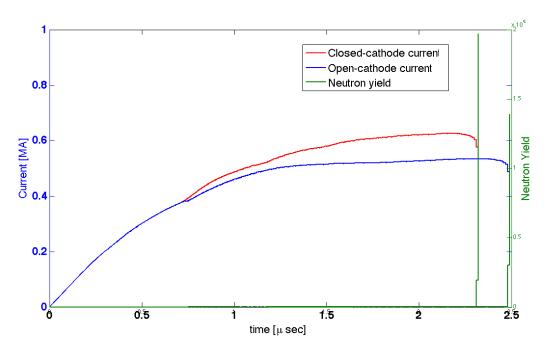


Figure 3. Computed current traces for open- and closed-cathode models of Bernard Long, and accompanying thermonuclear neutron yields between 1 and 2 x 10⁵. Experimental values were 0.6 MA and 1.5 x 10⁹ neutrons.

Bernard *et al.* measured peak current, neutron yield, estimated ion and electron temperature and plasma density during rundown and pinch. Some detailed pinch observations were made at times beyond the reach of our MHD code and are not discussed here. The peak current reported was 0.6 MA, with 0.5 MA quoted for their neutron yield of 1.5×10^9 . Our simulation produced a peak current of 0.60 MA. They report a maximum ion temperature of 300 eV before the plasma pinches, with "much lower" electron temperature, and a collapse velocity of 1.8×10^7 cm/s, although they don't specify exactly where this was measured. Immediately before the pinch in Figure 2, computed peak ion and electron temperatures in the densest part of the sheath were in the ranges 250–650 eV and 200-360 eV respectively (lower temperature farther from the anode), with sheath radial speed of 6×10^7 cm/s. Very shortly before that, when the sheath was approximately $^{3}/_{4}$ of the way around the curved tip of the anode, sheath radial velocity was 1.8×10^7 cm/s, and total speed 2.2×10^7 cm/s, much closer to the experimental figure. The simulation produced higher temperatures in the extremely low-density plasma behind the sheath, but densities there are so low—more or less at the density floors imposed on the simulation—that the temperatures not considered meaningful.

Bernard reports a pinch lifetime of 20–50 ns, experiencing "large variations in size and density" during that time, with number densities ranging from 10^{18} to 5×10^{19} /cm³, and ion temperatures roughly estimated to be 700 eV. The simulation produced peak ion temperatures of 9 keV in the pinch, and peak mass density of .045 kg/m³, corresponding to a number density of 1.4 × 10^{19} /cm³. From the time the sheath hits the axis to the time our circuit solver fails is only a few ns, as long as we can reasonably hope to follow the pinch evolution with an MHD code. The cause of the anomalously high ion temperatures in the pinch simulation has not been determined

yet. Similarly high temperatures were reported by Degnan *et al.* from the MACH2 code in the April 30, 2009 DTRA briefing at SNL [40].

Bernard *et al.* observed neutron yield of 1.5×10^9 for this experiment, and this pulse was not observed until after the pinch had broken up. They point out that the peak measured ion densities and temperatures in the pinch could produce only 5×10^5 neutrons (in the neighborhood of what ALEGRA predicted), which is negligible compared to the observation.

For the closed-cathode case the leveling off of current for the open case was due to an apparently random sheath non-uniformity that developed into a tendril and affected current flow as it exited the boundary. The collapse speeds, densities and temperatures were similar to the closed-cathode-boundary case. The pinch came out somewhat thinner, with density close to the axis reaching .079 kg/m³, and temperature reaching 9 keV. This very high-density region only spanned one cell radially, so these simulations should be done at higher resolution in order to confirm these numbers.

Bernard *et al.* also relate experiments on this device with an 8-Torr gas fill, but the data presented mainly comprises interferometric observations of pinch stages later than what can be accessed with our simulations. They present visible-light photos of very prominent radial filamentation in the plasma sheath during rundown, documentation of high-energy, anisotropic neutron emissions, and speculative discussion of the apparently non-thermonuclear origins of the emitted neutrons. They also point out from estimates of electron drift speeds that the pinch plasma would be subject to cyclotron drift, Buneman and beam-plasma instabilities.

6.2 Bernard Short

This device was powered by a 120 microF capacitor bank charged to 40 kV for a stored power of 96 kJ, and the circuit model was run with same resistance and inductance as Bernard Long. Gas fill was 10 Torr. The experiment produced a peak current of 1.5 MA and total neutron yield of 3×10^{10} . In Figures 4 and 5 respectively we show a snapshot of plasma density in the pinch phase for the closed-cathode configuration, and the current trace and neutron yields for open and closed configuration. The open- and closed-cathode cases both agreed precisely with peak current value, and were much closer to one another than in the Bernard Long case, presumably because the compact size of Bernard Short doesn't allow the discrepancies to accumulate over time. Neutron yields for both were around 3.5×10^6 at the end of the simulation.

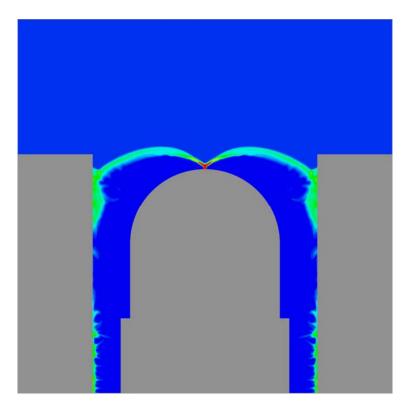


Figure 4. Density plot for pinch phase in Bernard Short device.

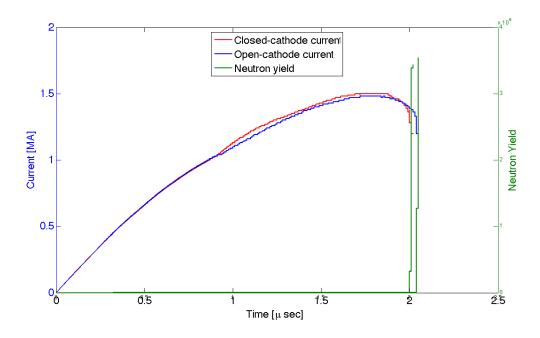


Figure 5. Computed current traces and thermonuclear neutron yields for Bernard Short device. Peak current was 1.5 MA and neutron yields around 1.5×10^6 , compared to experimental values of 1.5 MA and 3×10^{10} neutrons.

6.3 Tallboy

We modeled Tallboy in its then-current configuration with geometry and experimental parameters provided by NSTec: 270 kJ stored energy, with 216 microF capacitor bank, 50 kV charging voltage, 50 nH inductance, and resistance set to the 3.3 m Ω guess for the Bernard machines. We were not able to obtain Tallboy experimental data until September 14, 2009 (one week ago). When our first simulation did not agree with experiment, we made inquiries and learned that the cathode length and gas fill for the experiments were different from that we had originally been advised, necessitating a rapid setup of a new simulation with the correct parameters. We are still verifying the veracity of the data.

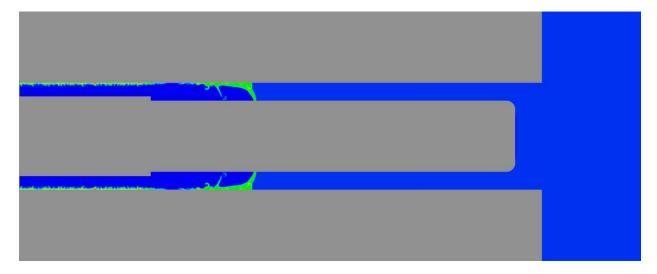


Figure 6. Plasma density during run-down in Tallboy closed-cathode configuration, showing plasma tendril that disrupted the simulation.

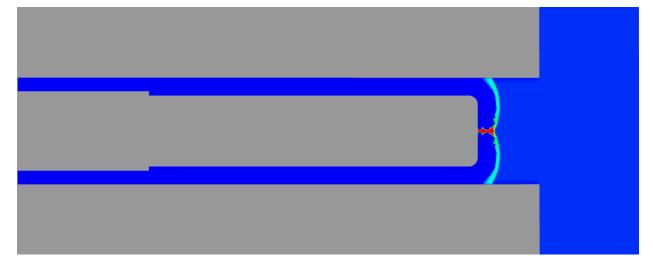


Figure 7. Plasma density during pinch for open-cathode Tallboy simulation.

Simulations were carried out with both open and closed cathode boundaries. The closed-cathode case experienced a disruption to the current flow, after which that simulation was terminated. The culprit is seen in Figure 6. Closed-cathode cases frequently exhibited thin plasma tendrils extending out from the residual plasma on the cathode boundary; shortly after the time shown in Figure 6, the large tendril immediately behind the sheath touched the anode surface, providing a second current path which caused the disruption. As already mentioned, this is why solid-wall cathodes were abandoned. In Figure 7 we see the pinch phase for the open-cathode Tallboy simulation, apparently showing an m=0 instability.

Experimental data for thirteen shots was very recently obtained and compared to our open-cathode simulation. We were surprised at a large discrepancy between ALEGRA's prediction of 1.8 MA peak current and the experimental value of 2.3 MA. MACH2 results presented by Degnan *et al.* at the April 30, 2009 DTRA briefing [40] were also close to ALEGRA's prediction. We are currently tracking down whether there could be an error in what is being compared, as previous experience with both ALEGRA and MACH2 indicate that we should be able to predict the current quite closely. The computed neutron yield at job finish was 3.7×10^7 , compared to an average experimental value of 3.5×10^{11} .

Table 1. Peak Currents and Neutron Yields from Experiment and from ALEGRA Simulations, for all Three Test Devices

	Peak Current (MA)		Neutron Yield	
	Experiment	ALEGRA	Experiment	ALEGRA
Bernard Long	0.6	0.5 – 0.6	1.5 × 10 ⁹	1.2 × 10 ⁵
Bernard Short	1.5	1.5	3 × 10 ¹⁰	1.5 × 10 ⁶
Tallboy	2.3	1.8	3.5 × 10 ¹¹	3.7×10^7

7. DISCUSSION

2D ALEGRA-HEDP simulations accurately reproduced most of the key characteristics of the three devices tested. Computed pinch temperatures for the Bernard experiments were higher than those estimated from experiments; the reason for this is still under investigation. Timing, peak currents, sheath speed and temperatures in the collapse phase were in good agreement for the Bernard devices; the Tallboy comparisons are still under review. The computed and experimental peak currents and neutron yields for all three machines are shown in Table 1. Neutron yields were underestimated, as we expected since MHD can only predict the thermonuclear portion of neutron production. We have confirmed the ability of ALEGRA-HEDP to perform accurate simulations of DPF operation in 2D, an ability that should extend to 3D simulations, and establishes the code as a powerful tool for other applications in the DTRA loads effort.

The ALEGRA capability to import existing 2D LSP data for the early time-sheath is very nearly in place: ALEGRA can now import ion and electron densities and temperatures, and the magnetic field import capability is being completed. Figure 8 shows electron temperatures during sheath initiation for the Mather Long device imported from LSP, which will be used to initiate a 2D simulation. The ability to easily couple electromagnetic PIC calculations and resistive MHD simulations is a new and powerful tool that should have applications in many areas



Figure 8. Plot of electron temperatures near Bernard Long insulator, computed by LSP and imported to ALEGRA-HEDP.

The ultimate goal of this work was to optimize DPF designs for increased neutron yields. The successful simulations presented here confirm our ability to address this task. With validation on the Bernard devices and a first Tallboy simulation completed, we can easily increase the driving voltage and gas fills, and scale up and modify the geometry to predict machine behavior. We have launched a first 3D simulation of the Bernard Long device, with Figure 9 showing the copper and insulator geometry, which should provide a more realistic glimpse of conditions going into the pinch and point the way for future computational efforts.

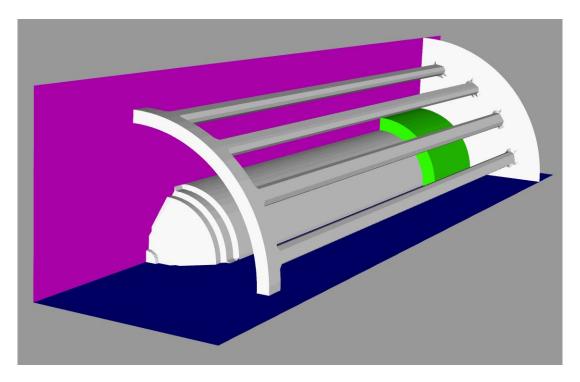


Figure 9. Copper and insulator surfaces for 3D simulation of Bernard Long device.

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