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**R.R.** Peterson

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UNIVERSITY OF WISCONSIN

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# Initial Computer Simulations of Vaporization of Material in Experiments Meant to Mimic Divertor Plates During Tokamak Disruptions

Robert R. Peterson

Fusion Technology Institute Department of Nuclear Engineering and Engineering Physics University of Wisconsin-Madison Madison, WI 53706

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#### 1. Introduction

The vaporization of material from the surface of a tokamak divertor during a disruption is an important issue in the design of a tokamak reactor such as ITER. During the disruption, plasma ions with a energy of about 5 keV reach the divertor surface with a fluence of several hundred to a few thousand J/cm<sup>2</sup> over a pulse width of 0.1 to 3 ms. This is enough to cause vaporization of any material. If all of the energy were used to vaporize a graphite divertor first surface, 500 J/cm<sup>2</sup> would erode 38  $\mu$ m per shot, or 1.9 mm over the expected 50 disruption lifetime of ITER. Since, in the divertor design, the thinnest possible surface coating is favored because it leads to better steady-state heat conduction, adding a few mm of material to account for erosion will hurt the design. Understanding the phenomena occuring during disruption vaporization may lead to a lower calculated erosion and to designs that control the erosion.

The phenomena important to the material erosion are shown in Fig. 1. The ions early in the pulse deposit in solid material and vaporize a portion of it. Ions later in the pulse are stopped in the already vaporized material. Ion energy is continually deposited in the vapor for the rest of the pulse. The temperature of the vapor is determined by a balance between ion energy deposition and cooling due to conversion of the vapor internal energy into kinetic energy through decompression expansion. As the vapor heats up, it begins to radiate. The opacity profile of the vapor will determine where the radiant energy is deposited. Any radiant energy reaching the unvaporized surface of the divertor can cause additional vaporization. Thermal conduction from the vapor to the divertor surface is usually far less than the radiant heat transfer but it should be considered.

To understand these phenomena, experiments are being performed. Since reactor scale tokamaks have not yet been constructed, other means of achieving relevant energy fluences must be used. This paper will begin with a summary of ongoing experiments to simulate tokamak disruptions. Computer simulations of these experiments is the main topic of this paper. I will discuss the CONRAD computer code, which has been used in these simulations and the results for experimental conditions. Finally, I will discuss the validity of the code's assumptions and compare with another code.

# 2. Experiments

The combined use of laboratory experiments and computer simulation will improve the understanding of these phenomena. Experiments in Russia and in the U.S. [1] are in



Figure 1. Schematic of phenomena occuring in vaporization during tokamak disruptions.

progress. The most common is some form of gas gun, which is shown schematically for a typical experiment in Fig. 2. Here, a fluence of  $0.5-2.0 \text{ kJ/cm}^2$  over 0.1 ms has been achieved on a typically 1 in diameter sample. However, the average ion energy is typically 100 eV instead of 5 keV. This leads to an ion stopping range in the divertor material that is much shorter than what is expected in a tokamak. Also, because the energy per ion is so small in the experiments, a much greater plasma density from the ion source, typically  $10^{17}$  atoms/cm<sup>3</sup>, is required. This will cause some differences between the experiment and the tokamak conditions in the hydrodynamic motion of the vapor. The hydrodynamic motion and the radiation flow is probably not one-dimensional. Another type of experiment injects plasma into a small radius long tube with a plasma gun [2]. In this experimental geometry, the plasma radiates energy to the inside wall of the tube, vaporizing whatever coating is applied to that surface. The hydrodynamic motion of the vapor and the radiation flow is one-dimensional. In this experiment, energy is transferred to the material surface via radiation and not through ion deposition. Even with these concerns, these experiments do exhibit the same set of phenomena that occur in a tokamak. Since these experiments are currently in operation, there is an opportunity to test computer code calculations.

The typical parameters for some experiments are shown in Table 1. Typical ITER parameters are shown for comparison. The parameters vary significantly and each machine is unique.

#### 3. The CONRAD Computer Code

CONRAD is a one-dimensional radiation-hydrodynamics computer code [3] that can be used in slab, cylindrical or spherical geometry. CONRAD was originally written to analyze the response of inertial confinement fusion target chambers to the target explosions. Hydrodynamics is calculated with a Lagrangian differencing scheme. The hydromotion is driven by pressure that includes gas pressure and a Von Neumann artificial viscosity. The gas pressure is calculated as  $\frac{3}{2}(1+Z)nkT$ , where Z is the local average charge state, n is the total local number density of ions and neutrals, and T is the local gas temperature. In CONRAD, the electron and ion temperatures are assumed to be equal. Z and T are calculated from equation-of-state table lookups. The tables either come from the SESAME library [4] or are calculated with the IONMIX code [5]. The artificial viscosity provides a mechanism for shock heating. The radiation transport is calculated with flux-limited multigroup diffusion. The flux-limitting method smoothly imposes a

PLADIS Gas Gun Experiment at the University of New Mexico



Figure 2. Schematic picture of a gas gun experiment to simulate material vaporization during a tokamak disruption.

					Source	
	Ŧ	Ion	Pulse	Energy	Plasma	Sample
Facility/Location	Type	Energy	Duration	Fluence	Density	Size
		(eV)	(ms)	$(J/cm^2)$	$(\mathrm{cm}^{-3})$	(cm)
ITER Divertor	Thermal Quench	5000	0.1-3.0	500-2000	$10^{14}$	
VIKA/Efremov	Gas Gun	100	0.1	500-5000	?	2
SPRUT/Efremov	Gas Gun	100	0.15-1.0	1000	?	10
MK-200/Troitsk	Cusp Trap	5000	20	250-1000	$1-5 \times 10^{17}$	$1 \times 3$
MKT/Troitsk	Gas Gun	100-5000	20	60-100	$3 \times 10^{15}$	10
PLADIS/UNM	Gas Gun	100	0.1	2000	$1 \times 10^{17}$	5
SIRENS/NCSU	Gas Gun into tube	1-6 photons	0.1-0.2	20-2400	$1 \times 10^{20}$	large

# Table 1. Experimental Parameters for Disruption Simulators

decrease in the radiation diffusion coefficient so that in the limit of a very optically thin plasma, the radiation flux is equal to the radiation energy density times the speed of light. 20 radiation energy groups are normally used in CONRAD, though as many as 200 have been used. Thermal conduction is calculated with the Spitzer model [6].

There are several energy, momentum and mass sources in CONRAD. A timedependent, energy-dependent source of ions can be defined in CONRAD. The time-offlight of the ions is included in the analysis. The ion energy is deposited as calculated with a model that includes collisions with free electrons, bound electrons, and nuclei [7]. Once the ion speed drops below the local electron thermal speed, the remaining ion energy is deposited instantaneously. The momenum and energy of the ions are deposited in the stopping medium, but the ion mass is not. A time-dependent, energy-dependent photon source is also available, though it is not relevant to the tokamak divertor problem. Mass is added to and removed from the gas phase by vaporization and condensation at a surface. Vaporization is calculated with any one of several models, the most applicable to the tokamak divertor vaporization being a kinetic model with the rate at which mass is ablated from a surface being equal to

$$\dot{m} = \left(\frac{m_a}{2\pi T_s}\right)^{1/2} \left(P_{sat}(T_s) - P_g\right) \,.$$

 $T_s$  is the surface temperature,  $P_{sat}$  is the saturation pressure, and  $m_a$  is atomic mass. The surface temperature is calculated with a thermal conduction away from the surface competing with radiation, conduction, and condensation energy from the gas/vapor phase.

#### 4. Computational Results

Three computer simulations are presented here. They attempt to mimic the vaporization that would occur in a graphite lined divertor in ITER and in experiments. There are two experimental situations that are considered; one of high density and low density gas in the experimental chamber. The parameters for these three simulations are given in Table 2. The ITER simulation is meant to provide a basis for comparison to test if the experiments are indeed mimicking the physics of tokamak disruption vaporization. The two simulations of experiments are to test the fidelity in mimicking ITER conditions and to test the sensitivity of the results to the initial gas density in the experimental chamber. This is important because CONRAD does not currently add the ion mass to the stopping medium as energy is deposited. The density for run disr.expt.c.5  $(10^{14} \text{ cm}^{-3})$ 

	disr.iter.c.3	disr.expt.c.10	disr.expt.c.5
Beam Proton Energy (eV)	5000	100	100
Ion Power $(MW/cm^2)$	12	5	5
Pulse Length $(\mu s)$	100	100	100
Ion Fluence $(J/cm^2)$	1200	500	500
Vaporizing Material	Graphite	Graphite	Graphite
Init. Material Temp. (C)	500	30	30
Init. Material Thickness	$21~\mu{ m m}$	$6 \mathrm{mm}$	$6 \mathrm{mm}$
Init. Gas Density $(cm^{-3})$	$10^{14}$	$10^{17}$	$10^{14}$
Simulation Geometry	Cylindrical	Slab	Slab
Problem Size (cm)	339	40	40

 Table 2. Parameters for CONRAD Simulations

is typical of experimental chambers before a shot. The density for run disr.expt.c.10 ( $10^{17}$  cm<sup>-3</sup>) is what the gun gas must apply to the samples to achieve 500 J/cm<sup>2</sup>. The ITER simulation, disr.iter.c.3, is done in cylindrical symmetry because it was thought that this was the best one-dimensional approximation to the tokamak divertor situation. A cylinder 339 cm in radius has the same cross sectional area as the ITER vacuum chamber in the CDA design [8]. The gas gun experiments are closest to a slab; though there are quite possibly two-dimensional effects. I assume that the end of the gas gun is 40 cm from the target. The initial thickness of the ITER graphite liner is taken to be 21  $\mu$ m, where the temperature at the back of the liner is assumed fixed at 500 C by a good conducting substrate.

The results of these simulations are sumarized in Table 3. There are a number of ways in which the simulations can be compared. The energy radiated to the surface is one important basis for comparison because the self-shielding effect is closely tied to it. The energy radiated to the surface is also able to be experimentally measured through calorimetry. The amount of wall erosion is a good comparison because it is easily measured in experiments, though erosion can occur for reasons other than vaporization.

It is clear from Table 3 that the two simulations for the gas gun experiments are significantly different. There is much more radiation transported to the surface in the high gas density case, and therefore more vaporization. This is, to a large degree, due to

	disr.iter.c.3	disr.expt.c.10	disr.expt.c.5
Run Time $(\mu s)$	100	400	103
Deposited Ion Energy $(J/cm^2)$	1200	500	500
Energy Radiated			
to Surface $(J/cm^2)$	305	230	99
Erosion $(\mu m)$	4.5	7.6	2.7
~ /			

 Table 3. CONRAD Simulation Results

the difference in run time. disr.expt.c.5 only runs to  $103 \,\mu$ s because the time step becomes greatly reduced when the leading edge of the vapor collides with the opposite side of the experimental chamber. To understand the differences in these runs, one needs to study the details of the simulations. The results for the high gas density run (disr.expt.c.10) are shown in Fig. 3. The hydrodynamic motion is shown in frame a, where the Lagrangian zone boundary positions are plotted against time. The Lagrangian zone boundaries act like markers fixed in the moving fluid. The position 0 is the end of the gas gun and 40 is the surface of the sample being tested. In frames b, c, and d, the ion temperature, mass density and radiation temperature are plotted over the same space as in frame a. Similiar plots are made in Fig. 4 for the low gas density run (disr.expt.c.5). More detail of the plasma and radiation temperature profiles near the vaporizing surface is shown in Figs. 5, 6, 7 and 8. The width of material lost from the surface is plotted against time in Figs. 9 and 10. The accumulated energy fluence radiated to the material surface is shown in Figs. 11 and 12.

The most obvious difference between these two calculations is that there is much more hydrodynamic expansion of the vapor in the low gas density simulation (disr.expt.c.5). The gas pressure in the high density vapor is much higher and prevents the rapid expansion seen in the low density case. In 400  $\mu$ s, the vapor in the high gas density case expands slightly more than 10 cm. In the low gas density case, the leading edge of the vapor traverses the 40 cm wide chamber in about 80  $\mu$ s, though the density plot shows that the bulk of the vapor begins to reach the other side of the chamber after 100  $\mu$ s. The density of the vapor in disr.expt.c.10 remains much higher than in the other case.



Figure 3. Results of the CONRAD simulation disr.expt.c.10: (a) Positions of Lagrangian zone boundaries versus time (red represents vapor, black hydrogen gas), (b) gas temperature, (c) mass density, (d) radiation temperature.







Figure 5. Plasma temperature versus position for CONRAD run disr.expt.c.10. Profiles are plotted at various times.



Figure 6. Plasma temperature versus position for CONRAD run disr.expt.c.5. Profiles are plotted at various times.



Figure 7. Radiation temperature versus position for CONRAD run disr.expt.c.10. Profiles are plotted at various times.



Figure 8. Radiation temperature versus position for CONRAD run disr.expt.c.5. Profiles are plotted at various times.



Figure 9. Ablated thickness versus time for CONRAD run disr.expt.c.10.



Figure 10. Ablated thickness versus time for CONRAD run disr.expt.c.5.



Figure 11. Cumulative energy fluence radiated to unvaporized surface versus time for CONRAD run disr.expt.c.10.



Figure 12. Cumulative energy fluence radiated to unvaporized surface versus time for CONRAD run disr.expt.c.5.

The gas temperature profiles are considerably different in the two simulations. In the high gas density case, the ion mean free path is short compared to the size of the gas and energy remains in the hydrogen gas for a long time, which is shown by the high temperature in the gas. In the low gas density case, the ion range is long in the gas, so the ions are deposited in the vapor, which is shown by the ridge of high temperature moving away from the sample surface. Figs. 5 and 6 show that, in the high gas density simulation, the vapor temperature is initially about 3 eV and drops to below 2 eV, while in the low gas density case the vapor temperature is fairly constant at 3 eV. Both simulations have very thin layers of cold gas near the material surface. The opacity of the vapor is quite sensitive to the vapor temperature so the radiation transport in the vapor, as shown by the radiation temperature plots in Figs. 7 and 8, is different in the two cases. The radiation temperature, which is defined as  $(E_r c/4\sigma)^{1/4}$  (with  $E_r$  being the radiation energy density,  $\sigma$  being the Stefan-Boltzmann constant, and c being the speed of light), has somewhat steeper profiles in the high gas density case. This is due to a higher opacity in the vapor in the high gas density case, which is due, in part, to the higher vapor density. From the plots of material ablation and accumulated radiation energy fluence, one sees that the increased opacity leads to somewhat lower radiation fluence to the surface by 100  $\mu$ s. At 100  $\mu$ s, more energy is actually radiated to the surface in the low gas density case. The eroded thickness at 100  $\mu$ s is higher for the low gas density than the high gas density (2.7  $\mu$ m versus 1  $\mu$ m).

The same material is plotted for the ITER simulation (disr.iter.c.3) in Figs. 13 through 17. The hydrodynamic motion for the ITER simulation is similar to the low gas density experimental simulation in that both simulations show that much of the vapor moves several tens of cm in 100  $\mu$ s. The magnitude of the density in the vapor is roughly the same in ITER and low gas density experimental simulations, though there are structures present in the ITER density profiles due to the in-depth deposition of ions that are not present in the low gas density experimental density profiles. The plasma temperature is somewhat higher in the ITER case than in either experimental simulation because of the higher ion energy fluence. The shapes of the plasma temperature profiles differ from either gas gun simulation because of the great disparity in the energy per ion and, therefore, the ion deposition length. The radiation temperature is also higher in the ITER simulation. By 100  $\mu$ s, the energy re-radiated to the surface is much higher than either experimental case. The surface thinning stops in the ITER simulation at about 70  $\mu$ s because the re-radiated power density at that point drops to the level that





Figure 14. Plasma temperature versus position for CONRAD run disr.iter.c.3. Profiles are plotted at various times.



Figure 15. Radiation temperature versus position for CONRAD run disr.iter.c.3. Profiles are plotted at various times.



Figure 16. Ablated thickness versus time for CONRAD run disr.iter.c.3.



Figure 17. Cumulative energy fluence radiated to unvaporized surface versus time for CONRAD run disr.iter.c.3.

can be carried away by heat transfer through the solid graphite. This feature is not seen in either experimental case because the graphite is much thicker in those simulations and heat transfer through the graphite is much slower. In this ITER simulation, it has been assumed that a perfect conductor sits in back of the graphite layer that maintains a constant temperature of 500 C.

#### 5. Discussion

The relevance of these simulations to experiments is now discussed. Also, some similar simulations, performed with another computer code, LASNEX, are discussed. Finally, some suggestions for additional work are made.

#### 5.1. Comparison with Experiment

Even though the methodology for performing computer simulations is still under consideration, some comparisons with experiments are valuable. Gas gun experiments have been performed on graphite on several devices, one being PLADIS at the University of New Mexico [9]. On PLADIS, the ablation of POCO graphite was measured to be between 0.6 and 1.4  $\mu$ m for 800 J/cm<sup>2</sup> of 100 eV protons in a 100  $\mu$ s pulse. The low gas density simulation, disr.expt.c.5, was not run to the point where vaporization stopped but it predicted 2.7  $\mu$ m vaporized by 500 J/cm<sup>2</sup> after 100  $\mu$ s. This is well above what one would expect from the same energy fluence of PLADIS. The SIRENS experiment [2] measured about 7  $\mu$ m of Pyrographite ablated by 500 J/cm<sup>2</sup> of energy fluence over 100  $\mu$ s, which is very close to the 7.6  $\mu$ m predicted in the high gas density CONRAD simulation, disr.expt.c.10.

The SIRENS experiment is essentially in one-dimensional cylindrical geometry, while the gas guns may have significant radiation transport and hydrodynamic motion of vapor transverse to the ion beam direction. Transverse radiation transport can significantly reduce the amount of vaporization and could explain why the PLADIS measurements are below the CONRAD predictions and why the SIRENS experiments do agree with CONRAD.

#### 5.2. Other Computer Codes

Calculations have been performed with the LASNEX computer code at Sandia National Laboratories in Albuquerque, similar to the CONRAD simulations presented in this paper. Because LASNEX is a two-dimensional radiation transport code with physics similar to CONRAD, it might be useful in tokamak disruption simulations where twodimensional effects are important. LASNEX is designed for much higher energy densities than are present either in gas gun experiments or in tokamak disruption plasmas. It is an open question whether the physics assumptions in LASNEX are appropriate for this class of problems.

Three sample one-dimensional calulations have been performed with LASNEX to test the low energy density behavior of this code. The first problem, labeled DR02, is meant to test the ion energy deposition in LASNEX. 500 J/cm<sup>2</sup> of 100 eV protons in a 100  $\mu$ s square pulse are deposited in a 40 cm thick hydrogen gas at a density of 10<sup>18</sup> cm<sup>-3</sup>. The second and third problems, DR03 and DR04, test the vaporization physics by depositing 500 J/cm<sup>2</sup> of 100 eV protons in a 100  $\mu$ s pulse in a 6 mm thick piece of solid graphite at a density of 3.5 g/cm<sup>3</sup>. DR03 and DR04 use different ways of modeling vaporization.

The results of simulation DR02 are shown in Fig. 18. Comparing with CONRAD run disr.expt.c.10, one sees that the temperatures reached in the gas are much lower than that calculated in the hydrogen gas by CONRAD. The ion deposition model used in LASNEX is designed for ion energies in the neighborhood of 1 MeV/amu, while CONRAD uses a model that includes corrections needed at low ion energies. LASNEX would need an improved ion stopping model to be useful for tokamak disruption problems.

The results for simulation DR03 are shown in Figs. 19 and 20. In this simulation, a vaporization method is used in which material cannot perform hydrodynamic motion until it reaches the vaporization temperature (4100 K for graphite). In this model, latent heat of vaporization is ignored. The temperature profiles are noisy in the solid material due to rapid density oscillations. These oscillations are not physical. The material that is vaporized (on the right side of the plots) cools due to decompression and recondenses. This may in fact occur, but the latent heat of vaporization must play an important role. For these reasons this vaporization is not useful for these types of problems.

The results of LASNEX run DR04 are shown in Figs. 21 and 22. In this simulation, vaporization is calculated in an ablation model where the vaporization temperature and latent heat of vaporization are both included. One can see that the temperatures in the vapor are of the same order as calculated in CONRAD run disr.expt.c.3. The density and temperature profiles are smooth. This is a much better way to do these simulations



Figure 18. Electron, ion and radiation temperatures (in keV) as calculated by LASNEX in run DR02 versus position at time 100  $\mu$ s. The ion beam is incident from left. Position is measured in cm.



Figure 19. Electron, ion and radiation temperatures (in keV) as calculated by LASNEX in run DR03 versus position at time 400  $\mu$ s. The ion beam is incident from right. Position is measured in cm.



Figure 20. Mass density (in g/cm<sup>3</sup>) as calculated by LASNEX in run DR03 versus position at time 400  $\mu$ s. The ion beam is incident from right. Position is measured in cm.



Figure 21. Electron, ion and radiation temperatures (in keV) as calculated by LASNEX in run DR04 versus position at time 2.5  $\mu$ s. The ion beam is incident from left. Position is measured in cm.



Figure 22. Mass density (in g/cm<sup>3</sup>) as calculated by LASNEX in run DR02 versus position at time 2.5  $\mu$ s. The ion beam is incident from left. Position is measured in cm.

than in the previous run. LASNEX would have an advantage over CONRAD in problems where two-dimensional hydro and radiation transfer are important.

LASNEX will be useful for these problems only if a new ion deposition model is developed. There is also considerable question as to the utility of the equations of state used. At low temperature and solid densities the pressure can be negative, which raises some questions in this author's mind.

#### 5.3. Future Work

This study has been preliminary in nature and has posed more questions than it has answered. Therefore, several items could be suggested for future work:

- 1. Parametric study of the ablation of graphite versus energy fluence. This is how experimental studies are performed and would provide a better basis for comparison with experiment.
- 2. Investigate other materials. Tungsten and molybdenum have been experimentally studied, have well-known properties, and have high melting temperatures so splashing might not be a problem in experiments. Beryllium is a possible divertor material, but experiments have shown that splashing is a significant source of mass loss.
- 3. Two-dimensional simulations. LASNEX could perform 2-D simulations for the gas gun geometry to compare with 1-D simulations. Comparison with experiments might not be useful until an improved ion deposition package is installed in LASNEX. The ion deposition package may work better for Doublet-III or ITER ion energies, so 2-D LASNEX simulations may be useful in these cases.
- 4. Improvements to the CONRAD computer code. The first two items may lead to discrepancies between code predictions and experiments. There are several areas in which CONRAD uses models which are out of date. These include radiation transport, equations of state, the addition of ion mass to zones absorbing ions, and electron and ion temperature coupling. A 1-D code like CONRAD is a good test bed for physical models when 1-D experiments can be found for comparison.

### 6. Conclusions

Three CONRAD and three LASNEX runs are presented in this paper. The CONRAD runs have been compared with each other, with LASNEX, and with experiment. The following results have been noted:

- 1. The mass of the energy depositing ions has been found to limit the hydrodynamic expansion of the vapor and, therefore, change the properties of the vapor.
- 2. The mass of the gun gas causes the hydrodynamic expansion of the vapor in the gas gun to differ from what will occur in ITER. The reduced expansion in the gas gun experiments may affect the fidelity of these devices in mimicking tokamak disruptions because of changes in the temperature and density of the vapor.
- 3. LASNEX has been found to have an ion deposition package that needs to be improved to simulate gas gun experiments. The ablation package in LASNEX seems adequate for disruption problems.

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