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Journal of Nuclear Materials 313–316 (2003) 579–583

journal of nuclear materials

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Fluid simulation on pellet ablation with atomic process

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Abstract

A new type of a hydrodynamic code applicable to solid, liquid and gas states, 'CAP' has been developed in order to investigate an ablation process of pellets in hot plasmas under various atomic process (dissociation and ionization) and heat fluxes. One of the most important features of the code is to be able to treat recession of the pellet surface by ablation without any artificial boundary condition between the pellet and ablation cloud. It is clearly known that a stationary shock wave is induced by ionization, and that the Maxwellian heat flux more enhances ablation than a conventional mono-energetic heat flux. Nonuniform of the ablation pressure induced by nonuniform heating along *B*-field leads to a deformation of the pellet, so that the pellet lifetime is found to be shorter than one predicted by an ablation model.

Keywords: Ablation; Pellet; Shock; Ionization; Dissociation; CiP

1. Introduction

Refueling is one of essential methods in order to control plasma density and sustain steady state plasmas. A gas puffing has been successful for building and sustaining a plasma density in an experimental system of past generation. However, in a large scale experimental system, e.g., LHD, the plasma sources induced by the gas puffing are strongly localized near the plasma surface. Then, a pellet injection is placed as a fundamental tool and has been mainly used to obtain a high density plasma and control a density profile [1].

A theoretical analysis of the pellet injection was started by Rose [2], and several ablation models for the pellet based on different physics were developed, e.g., a neutral gas shielding (NGS) model set up by Parks and Turnbull [3]. The NGS model is derived by applying one dimensional, spherically symmetric and quasi-steady gas dynamics to the fluid ablating from a pellet in a thermonuclear plasma. And the model supposes the ablation cloud to consist of only one species, such as ground-state deuterium molecules. Though the model is very simplified, it has been providing many useful predictions and contributing to experiments of the pellet injection. However, more detailed analysis is required in these days when the pellet injection plays an important role in high-β plasmas in a large scale experimental system. Our final goal is to investigate the bulk plasma motion induced by the pellet injection including pellet dynamics itself, by developing a three-dimensional fluid code dealing with both a neutral fluid and MHD plasma. As a first step, a new type of hydrodynamic code CAP has been developed where a various states of pellet are treated without assumptions, although electromagnetic forces are ignored for simplicity.

The model of CAP is constructed as follows. When a pellet consisting of solid hydrogen is heated by an energy flux, it changes to liquid and gas during phase transition and subsequently to plasma during atomic process. In the present work, it is assumed that the ablation cloud consists of four species particles, namely, molecules, atoms, ions and electrons, and it behaves as one fluid due to charge neutrality and strong charge exchange except for incident plasma electrons encountering the cloud. The incident electron heat flux is considered by a kinetic treatment with a half-space Maxwellian distribution

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PII: S0022-3115(02)01414-9

[4]. In addition, the equation of state (EOS) [5] is used to treat solid, liquid and gas. Dissociation and ionization are also included to cause deuterium to change to plasma. Since domain of the numerical simulation includes solid and gas regions, the cubic-interpolated psudoparticle method [6] is used in the code. The most essential point of the method is that it can calculate simultaneously incompressible and compressible regions without any artificial boundary conditions between them. It is shown numerically that a stationary shock wave is driven by ionization and the pellet deforms by nonuniform heating along B-field. And the numerical results are compared with the NGS model predictions on the ablation rate and pellet lifetime for several parameters.

2. Basic equations

All species in the cloud are assumed to be treated as fluids, though there is some doubt as to the validity of this assumption in the bulk plasma. Since the ablation cloud has a very high density and low temperature, it has a high collisional rate required for the validity of a fluid treatment. The hot bulk plasma, which is not accurately treated as a fluid, has a minimal effect on the ablation process, except for an effect as the source of the heat flux which drives the ablation. The ablation cloud consists of molecules, atoms, ions and electrons. Effects of atomic physics on the ablation process, in particular dissociation and ionization in the ablation cloud, are considered. It is assumed that the species have same velocity (u) and temperature (T) due to high collision and charge exchange rate, so that they are regarded as one fluid with different densities. An electromagnetic force is ignored for simplicity. The dynamics in not only gas (ablation cloud) region but also solid (pellet) region are given by the following equations of mass, momentum and energy conservations:

$$\frac{d\rho}{dt} = -\rho\nabla u, \tag{1a}$$

$$\rho\frac{du}{dt} = -\nabla p, \tag{1b}$$

$$\rho\frac{de}{dt} = -p\nabla u + H, \tag{1c}$$

where ρ is the total density; u, the velocity; p, the total pressure; e, the total specific internal energy, and H the heat source. When a solid is heated, it is transformed to gas (molecules) by absorbing the sublimation energy ($\varepsilon_s = 0.01$ eV). Subsequently, when the molecules are transformed to atoms by absorbing the dissociation energy ($\varepsilon_d = 4.48$ eV), the number density of the molecules decreases but one of the atoms increases. When the ablation cloud is more heated, the atoms are transformed to ions and electrons by absorbing the ionization energy ($\varepsilon_i = 13.6$ eV) and the number density of the atoms decreases but ones of the ions and electrons increase. Since the ablation cloud can be regarded as one fluid, p and e are respectively given by the following equations:

$$p = p_s + \left(\frac{1}{2}f_s + \frac{1}{2}f_d + f_i\right)\frac{\rho kT}{m}, \tag{2a}$$

$$e = (1-f_s)e_s + \left[\frac{f_s - f_d}{2(\gamma_m - 1)} + \frac{f_d + f_i}{\gamma - 1}\right]\frac{kT}{m} + \frac{1}{2}f_s\frac{k\varepsilon_s}{m} + \frac{1}{2}f_d\frac{k\varepsilon_d}{m} + f_i\frac{k\varepsilon_i}{m}, \tag{2b}$$

where p_s and e_s is the pressure and specific internal energy in the solid, respectively, that should be determined by the EOS of the solid. γ_m and γ are ratios of the specific heats for molecules and atoms, respectively. k and m are the Boltzmann constant and nuclei mass, respectively. Fractions f_s, f_d and f_i are defined by $f_s = (2n_g + n_a + n_i)/n_t$, $f_d = (n_a + n_i)/n_t$ and $f_i = n_i/n_t$, respectively, where $n_t = 2n_s + 2n_g + n_a + n_i$. n_s, n_g, n_a and n_i are nuclei number densities of solid, gas, atoms and ions, respectively. These fractions are given by assuming the local thermodynamic equiriblium [7]. The atomic process induced by the incident electrons encountering the cloud is not considered.

In the present model, only Ohmic (no runaway) discharges are considered so that the distribution of energies of electrons and ions of the bulk plasma may be taken as Maxwellian. Owing to the lower thermal velocity and shorter mean free path of ions, the thermal ion heat flux is too small to penetrate the ablation cloud and drive ablation. Since the electron gyroradius is much smaller than the size of the ablation cloud surrounding the pellet, orbits of the electrons are strongly tied to a single magnetic field line, when the electrons penetrate the ablation cloud. Then, the heating of the cloud can be calculated field line by field line. The heat flux, q, is solved by using a kinetic treatment for the deposition energy by plasma electrons incident to the cloud with a half-space Maxwellian distribution as shown in Ref. [4]. When z is supposed to be the spatial co-ordinate along the field line directed into the ablation cloud, the heat source H in Eq. (1c) is given by $\partial q/\partial z$.

3. Ablation in one-dimensional spherical symmetric system

In order to investigate features in the case with atomic process and compare them with the NGS model, Eq. (1) is solved by assuming one-dimensional (1D) spherical symmetry. Initial conditions are the pellet radius $r_p = 2$ mm, electron temperature $T_{e\infty} = 2$ keV and number density $n_{e\infty} = 10^{20}$ m^{-3} in the bulk plasma. The pellet is placed at the center of 1D spherical symmetry and is isotropically irradiated by the heat flux from the bulk plasma. $T_{e\infty}$ and $n_{e\infty}$ are assumed to be constant through temporal evolution. A quasi-steady state is obtained because the ablation is self-regulating. Fig. 1(a) and (b) show spatial profiles at 8 μs without and with atomic process, respectively. In other words, the former expresses ablation including only one species, namely, ground-state D_2 molecules ($f_d = 0$ and $f_i = 0$), and the latter expresses one including molecules, atoms, ions and electrons. Fig. 1(a) shows normalized pressure p/p_s, temperature T/T_s and Mach number M as functions of normalized radius r/r_s, where p_s, T_s and r_s are the pressure, temperature and radius at the sonic point. The pressure decreases, and the temperature and Mach number increase in the radius direction out of the pellet because the ablation cloud expands by the heat flux. On the other hand, the pressure is constant within the pellet because the pellet is not moved and incompressible. Fig. 1(b) shows p/p_s, T/T_s, M, fractional dissociation f_d and ionization f_i as functions of r/r_s. It is clear that the ablation phenomena is changed by including the atomic process in ablation phase. The fact that the spatial profiles have jump structures is a most different point from the profiles in Fig. 1(a). There are two features in this fact. The first feature is that the flow is supersonic ahead of the jump structure and subsonic behind one. This means that the jump structure obviously expresses a shock wave. The shock is found to be driven in the region where the ablation particles ionize. In this region, since the neutral particles loose their energy by ionization, their kinetic and internal energies are hard to increase compared with ones in the other region. Then, ionization reduces the expansion of the ablation cloud and the shock is driven. The second feature is difference between dissociation and ionization. The ablation cloud

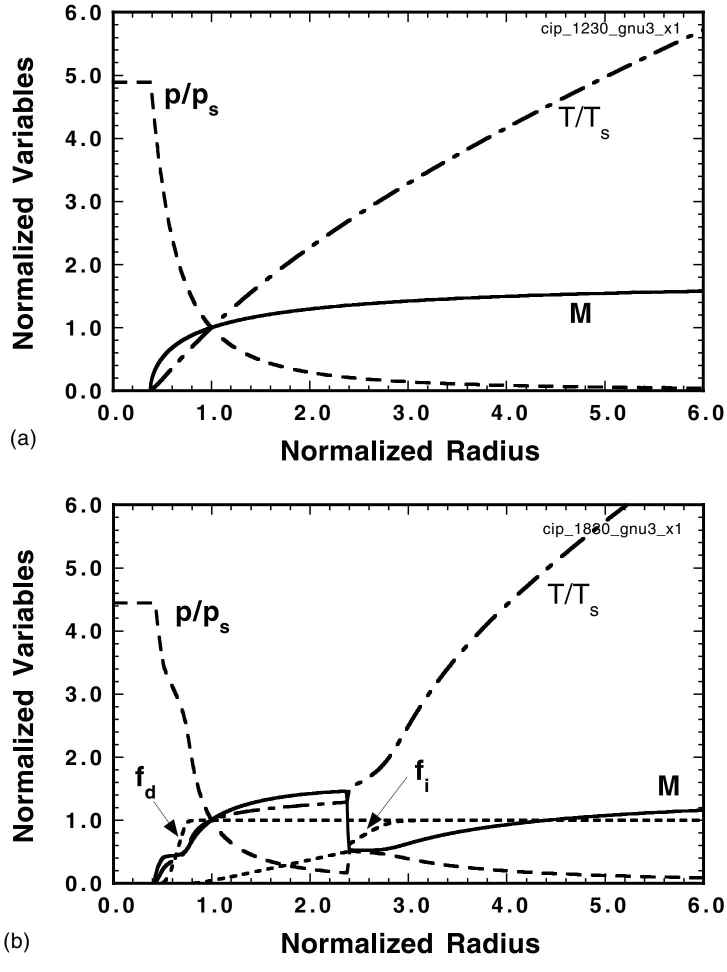

Fig. 1. Normalized fluid profiles at 8 μs in 1D simulation of (a) ablation without atomic process and (b) one with it. A solid, dashed and dot-dashed lines are M, p/p_s and T/T_s as functions of r/r_s, respectively. Dot lines in (b) show f_d and f_i.

Table 1
Parameters used in the simulation (cases are corresponding to numbers in Figs. 2 and 4)

Case	r_p (mm)	T_e (keV)	n_e (m^{-3})
1	0.5	0.5	1.0×10^{19}
2	0.5	0.5	5.0×10^{19}
3	1	0.5	5.0×10^{19}
4	1	2.0	5.0×10^{19}
5	2	2.0	1.0×10^{20}
6	2	5.0	1.0×10^{20}

loose its energy for dissociation similarly to ionization, but the shock dose not appear in the region where dissociation is dominant. Comparing Fig. 1(b) with Fig. 1(a), it is found that the region dominated by dissociation is subsonic and the region dominated by ionization is supersonic. Then, though the shocks are driven in both regions at first, it is flattened by the sound wave in the dissociation region. On the other hand, the shock is kept due to supersonic flow in the ionization region because it is no longer affected by the sound.

In order to investigate difference between the simulation results and the NGS model predictions on the ablation rate, the simulations are carried out for several parameters shown in Table 1. Fig. 2 shows comparison of the simulation results, G_{code}, and the NGS model predictions, G_{NGS}. Circles and squares show the simulation results without and with the atomic process, respectively. Since the NGS model uses a mono-energetic heat flux that overestimates the deposition energy compared with the Maxwellian heat flux used in the code, expansion of the ablation cloud is enhanced and the density decreases. As a result, the ablation rate proportional to the density is underestimated. Therefore, the simulation results are about three times greater than ones of the NGS model [8]. The atomic process is found to be not so essential on evaluating the ablation rate, but essential on determining the spatial structure as mentioned above [9].

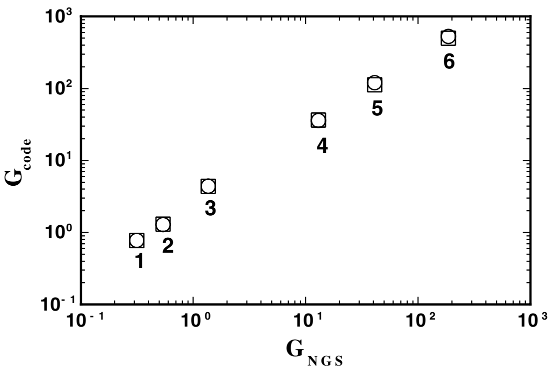

Fig. 2. Comparison between the ablation rate G_{NGS} by the NGS model and G_{code} by the simulation. Circles and squares show the simulation results without and with the atomic process, respectively. Numbers correspond to cases in Table 1.

4. 2D simulation

In this section, the results of 2D simulation are shown to investigate geometrical effects, where the cylindrical geometry (r, θ, z) is used. A spherical pellet is placed at the center of it and the plasma heat flux propagates along the magnetic field (z) to the pellet. Physical quantities are assumed to be uniform in the θ-direction. No effect of the magnetic field (except for setting the direction of the electron heat flux) is included. The contrast in Fig. 3 shows the isodensity contour at 8 μs. The parameters used are $r_p = 2$ mm, $T_{e\infty} = 2$ keV and $n_{e\infty} = 10^{20}$ m^{-3} corresponding to the case 5 in Table 1. The white region at the center represents the pellet. It is clear that the pellet changes to the shape as a disk in temporal evolution. This fact comes from nonuniform ablation pressure on the pellet surface. The heat flux around the pole of the pellet ($r = 0$) is almost completely absorbed before it reaches the pellet surface. On the contrary, the heat flux around the equator of the pellet could penetrate the cloud before its significant absorption. Then, the ablation pressure at the pole becomes much higher than one at the equator due to the difference of deposition energy from the heat flux. The

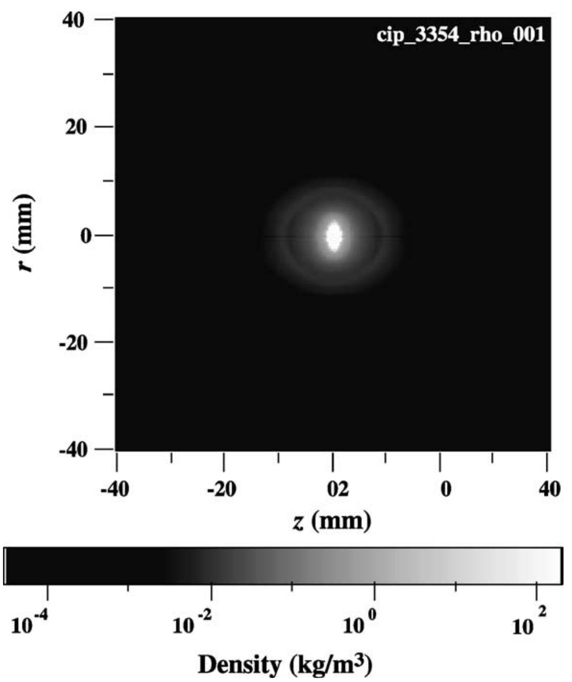

Fig. 3. Isodensity contour on the r–z plane in the cylindrical symmetry at 8 μs.

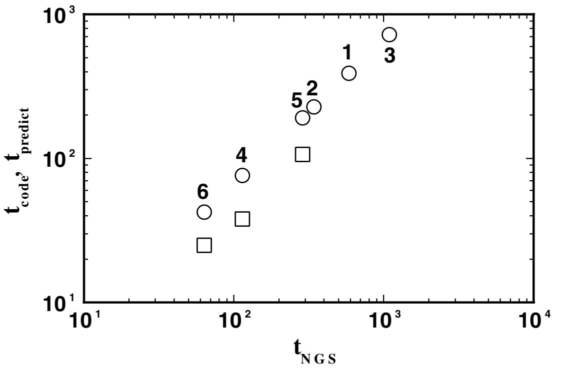

Fig. 4. Pellet lifetime. Squares show comparison between t_{NGS} by the NGS model and t_{code} by the simulation. Circles show comparison between t_{NGS} by the NGS model and $t_{predict}$ by the prediction. Numbers correspond to cases in Table 1.

difference of these pressure reaches more than 10 MPa in the simulation. The pellet is possible to deform by such an ablation pressure because it is known that solid deuterium behaves like incompressible fluid in the pressure more than 0.5 MPa [10], However, since this calculation dose not include thermal conduction, viscosity and elastic–plastic effect in the pellet, calculation by an advanced code including those effects is required in order to predict more detail about the deformation. The pellet size is reduced as the ablation proceeds, and finally ablation is almost completely reduced up to 110 μs. A spherical shape contrast produced around the pellet shows the shock wave driven by ionization mentioned in the previous section.

In order to investigate the pellet lifetime, the several runs are carried out for parameters shown in Table 1. Circles in Fig. 4 shows comparison between the pellet lifetime t_{code} by the simulation and t_{NGS} by the NGS model. t_{code} is found to be about one third of t_{NGS}. The NGS model is derived by assuming 1D spherical symmetry and using the mono-energetic heat flux. As shown in Fig. 2, the mono-energetic heat flux underestimates the ablation rate by one third of that with the Maxwellian heat flux. On the other hand, the assumption of 1D spherical symmetry could overestimate the ablation rate by twice of that in 2D cylindrical symmetry due to difference of an effective pellet surface area irradiated by the heat flux and difference of a spatial distribution of the heat flux [11]. In result, the NGS model could estimate the ablation rate by two third of that in the case using the Maxwellian heat flux and 2D cylindrical symmetry. The pellet lifetime $t_{predict}$ evaluated by this prediction is shown by circles in Fig. 4. It is clear that the simulation results are less than those by the prediction. Though the prediction supposes the pellet to be reduced as its spherical shape is kept, the pellet changes to a disk shape as shown in Fig. 3. This fact means that an effective pellet surface area irradiated by the heat flux in 2D simulation is larger than that in the prediction. Therefore, the heating in the former is enhanced compared with the latter, and the lifetime t_{code} becomes shorter than $t_{predict}$.

5. Conclusions

Two dimensional fluid code CAP, treating with a neutral in various states of matter and plasma simultaneously, has been developed to investigate the pellet ablation with atomic processes and nonuniform heating from bulk plasmas. It is shown that a stationary shock wave is induced by ionization. The ablation rate dose not change so much (up to several percentage) even if those atomic processes are included. A Maxwellian heat flux enhances the ablation rate by a factor of about three compared with a mono-energetic source. The pellet is deformed by nonuniform ablation pressure on its surface coming from the nonuniform heat flux along *B*-field, so that the pellet lifetime becomes shorter than the prediction by the ablation model.

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