Optimization of critical-density gas jet targets for laser ion acceleration in the collisionless shockwave acceleration regime

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Abstract. Laser ion acceleration induced by high-power laser systems is nowadays an important research subject due to the large potential range of applications it could satisfy. Most of the available high-power laser facilities deliver only a few laser pulses per hour. The new facilities under development will operate at higher repetition rates (up to 10 Hz). Conventional target technologies (solid targets) and acceleration mechanisms (Target Normal Sheath Acceleration – TNSA) used so far in laser-based ion acceleration are difficult to implement at high repetition rate. New ion acceleration mechanisms such as Collisionless Shockwave Acceleration (CSA) using high density gas jets represent therefore a promising alternative. Dense gas jet targets show several advantages such as constant refresh and negligible debris production. However, full comprehension of the fluid dynamics involved in the gas jet target production is fundamental for its optimization, and at present precise data is scarce. An ongoing study of design and optimization of supersonic gas jet nozzles for laser-based ion acceleration is presented.

1. Introduction

Up to now, Target Normal Sheath Acceleration is the main laser-based mechanism used to accelerate ions from the rear side of targets (usually solid foils) [1-8]. However, other acceleration mechanisms exist which require more complex targets and laser configurations [9-13]. Most of these acceleration mechanisms produce continuous ion energy distributions. Recent studies show that an intense laser pulse can induce a collisionless shock-wave in the interaction with a critical density target [14, 15]. This shock is generated during the interaction of the high energy laser pulse with a sharp target density gradient. Ions can be accelerated by this electrostatic shock to high energies with peaked distributions (CSA regime) [16]. A gas jet nozzle at high pressure can provide the critical density needed [8, 17, 18]. It is important to note that in the experiments different mechanisms may compete and only optimization of the laser-matter interaction parameters will bring CSA to lead the acceleration process [19-20].

Recent studies show that the optimum gas jet target for a consistent pure CSA regime has to be close to the critical density or over-dense [21-23]. The critical density is defined as $n_c = \frac{\varepsilon_0 m_e \omega_0^2}{e^2}$, where $\varepsilon_0$ is the vacuum permittivity, $m_e$ the electron mass, $\omega_0$ the angular frequency of the laser, and $e$ is the electron charge. For a near infrared laser (1053 nm) the critical density is approximately $10^{21}$ cm$^{-3}$. This will be used as a reference in the calculations of the gas density produced by the nozzles.
Besides the density requirements, the width of the gas puff should be long enough for a proper shock-wave formation and transport in order to achieve stable acceleration. However, it should not be too long to avoid depletion and slow down of the shock-wave. In addition, the gas jet shape may also play an important role and in some cases could improve the acceleration process [24]. One may conjecture that a steep slope faced to the laser beam will raise a stronger electrostatic shock-wave. On the other side of the gas jet profile, a longer relaxation will lead into a longer propagation of the shock-wave. A systematic numerical study of supersonic gas jet nozzle design is required to reach the optimal conditions for CSA mechanisms.

2. Nozzle geometry and computational fluid dynamics simulations

A convergent-divergent supersonic conical nozzle is one of the simplest geometries one can use. The simulated geometry (figure 1) consists of a reservoir where the backing pressure arrives, a convergent section, a throat, a divergent section and a chamber that mimics the experimental vacuum chamber. Systematic simulations are performed varying the backing pressure $P$ and the nozzle parameters: diameter of the throat $d$, diameter of the nozzle exit $D$, nozzle length $L$ and half-angle of the divergent section $\alpha$, which is calculated from the previous parameters.

Computational fluid dynamics (CFD) simulations are performed using the commercial software ANSYS FLUENT [25]. An implicit density-based coupled solver (DBCS) is used with double precision accuracy green-Gauss node-based gradients of solution variables, to solve the stationary fluid flow. The standard k-omega model is used to model the turbulence. A 2D axisymmetric grid with quadrilateral cells was used, which typically consist of $1.5 \times 10^5$ cells with $2 \times 10^{-2}$ average skewness ratio. The grid was adapted to the surfaces to maximize its quality, and it was checked that further refinement of the grid does not change the results.

![Image: Scheme of the 2D axisymmetric nozzle geometry used in CFD simulations. The nozzle has a convergent section, a throat, an expansion section and exits to a chamber at vacuum. The parameters studied in this article are the inlet pressure $P$ and the half-angle of the divergent section $\alpha$, which depends on the throat diameter $d$, the nozzle exit diameter $D$ and the length $L$. The distance from the nozzle exit is represented by $Z$.](image)

The boundary conditions are: a high pressure inlet in the reservoir and three low pressure outlets in the vacuum chamber outside the nozzle. The inlet conditions are: constant laminar flux and a free expansion of the gas in the vacuum (steady solution). The medium is diatomic hydrogen, assumed to be ideal gas with a constant specific heat. The temperature of the inlet is $300$ K, and the walls are supposed adiabatic. The outlet pressure was set at $10^{-4}$ mbar to reproduce the experimental conditions. The size of the vacuum chamber was chosen such as the gas can propagate, avoiding dilute flows. In order to verify the independence of the solution, the net imbalance of mass and energy was verified to be less than 1% of the smallest flux through the domain boundary for flux conservation.

2.1. Supersonic flow

The convergent-divergent geometry nozzle produces a supersonic gas flow in the diverging section. The gas flow is compressed at the throat where Mach number $= 1$ is reached. This flow expands and accelerates in the diverging section. The temperature and the pressure drop since the flow expansion is
considered adiabatic. Our interest diverges from the classical sonic/supersonic nozzle design, where the increase of the maximum specific momentum is the main goal. In our case the objective is the increase of the density at the exit of the nozzle, while controlling other conditions such as the gas jet divergence, profile and shape. A proper understanding of the geometry of the nozzle is essential because it strongly impacts the conditions mentioned above.

Furthermore, an important feature of the supersonic propagation is the formation of Mach waves inside the nozzle and their recombination all along the flow direction. The interference of these Mach waves can increase the density in some cases and can also modify the typical Gaussian profile of the supersonic gas jet giving rise to special profiles such as a high-density flat-top.

The evolution of the density with the backing pressure is well known to fit a linear progression [26]. Figure 2a shows the linear evolution of the density as a function of the backing pressure for three nozzle half-angles in the pressure range between 50 and 1000 bars at a distance of 500 μm from the nozzle exit. This range of pressures can be achieved with commercial gas boosters. In order to provide enough density at the nozzle exit, the working pressure has to be bigger than 600 bars. A backing pressure of 1000 bars allows to access a density close to the critical density almost independently of the nozzle parameters and over-critical densities can be reached with optimized geometries. We have chosen to work with an inlet pressure of 1000 bars and optimize the nozzles with respect to their density profile and shape.

As mentioned above, Mach waves created inside the diverging section can create different density profiles. In figure 2b one can observe that the density profile changes with the pressure. The difference between profiles at different pressures increased when the nozzle half-angle α was increased (dashed), however it is negligible for small half-angles (solid).

2.2. Nozzle half-angle and throat diameter
In the experiments, the laser gas jet interaction takes place at a certain distance Z from the nozzle exit (figure 1). This distance is adjusted to avoid nozzle damage due to the plasma plume expansion, while keeping the highest possible density at the laser interaction point. Systematic simulations were performed to optimize the throat diameter d and nozzle length L for sub-millimetric nozzle geometries in order to maximize the density starting from 250 μm above the nozzle exit. A density contour map was plotted for different cone half-angles at several distances from the nozzle exit. The half-angle α was varied from 0° (cylindrical case) to 10.4° by 1.3° steps. Distances Z from the nozzle exit (origin) up to 650 μm by 50 μm steps were investigated. The resulting density was expressed in n_r units (for a wavelength of 1053 nm). Figure 3 shows contour maps comparing three throat diameters d, 2/3d and 1/3d. For each figure L is fixed while D is scanned.
Figure 3. Interpolated contour maps of the density at 1000 bars (for a wavelength of 1053 nm) at different distances from the nozzle exit $Z$ as a function of the half-angle $\alpha$ for three throat diameters ($L$ is fixed): a) density-optimized nozzle throat diameter $d$, b) $2/3d$ throat diameter and c) $1/3d$ throat diameter. The position of $n_c$ is indicated as a solid black line.

A given density can be reached using different couples of half-angle $\alpha$ and distance to the nozzle $Z$. The maximum density for one nozzle cone angle is obtained at a finite number of distances from the nozzle exit. In other words, in order to choose an optimized nozzle geometry, one should define first the interaction distance from the nozzle exit. The optimum conditions (cone half-angle and distance) can be modified in some cases by the converging Mach waves and additional density structures appear in the density contour. In figure 3a one can see the effect of these converging Mach waves at 7º and 250 μm. Figure 3b and 3c show the evolution of the density when the throat diameter is decreased. A smaller throat diameter $d$ implies a slightly higher Mach number and flow velocity with a consequent decrease of density. In fact, the fundamental effect when the throat diameter is decreased is an increase of the relative size of the boundary layer thickness in the divergent section of the nozzle compared to the throat size, which leads to an increase of the turbulent kinetic energy of the flow. A relative thicker boundary layer reduces the propagation of the core flow and decreases the Mach waves rebounding off the walls [27]. This results in a drastic decrease of the density, which is a major drawback for CSA.

Figure 4 shows the contour maps for the FWHM (Full Width at Half Maximum) of the gas jet profiles performed with the same parameters as in figure 3. One can observe that a maximum density corresponds to a minimum FWHM, as a result of the converging waves. The FWHM decreases with the decrease of the gas jet throat diameter which can be advantageous to control the depletion of the laser-target interaction in CSA. However, as it was already commented, a decrease of the throat diameter can also decrease the density. A balance between these two behaviours has to be found for further optimization. Figure 4 also represents the divergence of the flow for a chosen $\alpha$ value.

Figure 4. The FWHM interpolated contour maps at 1000 bars at different distances from the nozzle exit $Z$ as a function of the half-angle $\alpha$ for three throat diameters ($L$ is fixed): a) optimized throat diameter $d$, b) $2/3d$ throat diameter and c) $1/3d$ throat diameter.
The gas jet profile is therefore a fundamental parameter of the shock-wave formation and propagation. Some profiles can be more advantageous than others. Small angle (close to 0º) nozzles show Gaussian-like profiles. These evolve to a more pointed distributions at the minimum FWHM, and to flat-top distributions when the angle further increases (figure 5). In the contour map plot, Gaussian-like profiles are on the left border, pointed profiles correspond to minimum FWHM and flat-top profiles are on the right border. The flap-top profile can be inhomogeneous depending on how the Mach waves converge and it can present dips or wavy structures. Figure 5 shows the density profiles for a half-angle close to 0º with a Gaussian profile, pointed profile at 2.6º and flat-top profile for bigger angles.

2.3. Nozzle length

Figure 6 shows the change of the density contour maps for different nozzle lengths. The length does not change drastically the density, but it changes the position of the convergence of the Mach waves. A longer nozzle will dissipate more Mach waves and a shorter nozzle will not confine the flow, with a consequent decrease of density and increase of divergence.

Figure 5. Transversal density profiles at 1000 bars for a half-angle $\alpha$ between 0º and 5.2º at 250 µm from the nozzle exit ($d$ and $L$ are fixed). In this case the maximum density is reached around $\alpha = 2.6º$ with a pointed profile. For angles smaller than this value (0º) the profiles are Gaussian-like. In the case of bigger values (3.9º and 5.2º) the profiles are flat-top.

2.4. Reservoir and electro-valve design

Special care has to be taken in the design of the gas transportation system (connections, tubes, valve, nozzle, etc.). An occasional formation of a supersonic flow section inside the transport system can generate instabilities in the flow that lead to turbulences and flow-blocking zones. The general rule is to avoid relatively big gas reservoir areas before the nozzle throat, use conical profiles between sections of different diameters, avoid sharp discontinuities or surface irregularities and propagate the flow from big diameters to lower diameters.
Figure 7 compares the effect of a conical transition (figure 7a) and a sharp transition (figure 7b). A sharp transition led to a perturbed flow propagation in the subsequent sections of the nozzle. In the simulation with a sharp discontinuity (figure 7b) the flow was blocked and mass conservation could not be reached due to the instabilities of the fluid flow.

3. Conclusion
An evaluation of different conical nozzle design parameters expected to be used for laser ion acceleration in the CSA regime was performed. It was shown that CFD simulations are fundamental for a complete understanding and optimization of supersonic gas jet targets. High pressure gas jet targets offer several advantages to set up critical density targets. Small cone half-angles provided higher densities (also observed by other authors [28]) and smaller profile FWHM. The nozzle throat diameter parameter is still to be fully optimized. PIC (Particle-In-Cell) simulations will be coupled to the present study in order to investigate the relative importance between density and profile FWHM in the acceleration process.

The next step will be to compare the density and profiles obtained during this study with experimental data from interferometry density measurements [26]. Moreover a development of the simple conical nozzle to more complex designs will also require characterization. Several high-resolution tomographic techniques are currently under development that could be implemented [29-32]. It is also interesting to note the advancements in nozzle rapid machining which could ease the access to complex nozzle geometries [33].

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