Time-dependent and radiation field effects on collisional-radiative simulations of radiative properties of blast waves launched in clusters of xenon

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Abstract

Radiative shock waves are ubiquitous throughout the universe and play a crucial role in the transport of energy into the interstellar medium. This fact has led to many efforts to scale the astrophysical phenomena to accessible conditions. In some laboratory experiments radiative blast waves are launched in clusters of gases by means of the direct deposition of the laser energy. In this work, by using a collisional-radiative model, we perform an analysis of the plasma level populations and radiative properties of a blast wave launched in a xenon cluster. In particular, for both the shocked and unshocked material, we study the influence of different effects such as LTE, steady-state or time-dependent NLTE simulations, plasma self-absorption or external radiation field in the determination of those properties and also in the diagnosis of the electron temperature of the blast wave.

Keywords: laboratory astrophysics, radiative blast waves, xenon plasmas, collisional-radiative simulations

1. Introduction

The growth of laboratory astrophysics is directly related to the progress achieved with high-energy density facilities. These ones permit either to reproduce conditions identical to the ones of the astrophysical phenomena or to recreate in laboratory versions of those phenomena on condition that the hydrodynamics is scaled correctly between laboratory and astrophysical scenarios [1, 2, 3, 4, 6]. Laboratory experiments permit to explain and to predict what occurs in astrophysical phenomena and they also provide useful data for the verification and validation of many aspects of numerical codes such as the atomic physics, equation of state and hydrodynamics.

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An area of particular interest is that of the radiative shocks, which are very common in astrophysics. Thus, they are observed in accretion shocks, pulsating stars, supernovae in their radiative cooling stage or bow shocks of stellar jets in galactic medium. The dynamics of the radiative shock can be significantly modified due to the radiative cooling of the postshock region. If the upstream material ahead of the shock is optically thick to some parts of the emission spectrum, then the radiation is absorbed and heats and ionizes the unshocked medium leading to the creation of a radiative precursor [7], which is an example of photoionized plasma. A method used in laboratory to create radiative shocks is based on a sudden release of energy in a zero-extension and instantaneous explosion. In this case, a shock moves into the surrounding medium creating a blast wave, usually defined as an expanding shock that sweeps up the material that is ahead of the shock. One manner to launch the shock in this context is to irradiate a gas formed by atomic clusters by intense lasers directly [8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19]. Clustered gases exhibit extremely efficient absorption of intense laser light creating a hot, high energy density plasma in a low average density target. This plasma subsequently explodes into the ambient gas creating a cylindrical blast wave [8]. This way, high Mach numbers shocks can be launched with high intensity lasers ($10^{17}$ W cm$^{-2}$) but with low energies ($< 1$ J). For given shock velocity and initial gas pressure, materials with medium or high atomic numbers are the best candidate for the shock to achieve the radiative regime, and for this reason xenon is commonly used as the medium in which the radiative shock propagates.

In a previous work [20] we carried out an analysis of the thermodynamic regime, the average ionization and charge state distribution (CSD) of plasmas of Xe in the range of plasma conditions typically found in the laboratory experiments commented above. Furthermore, in other previous works [21, 22, 23] we made an analysis of microscopic properties such as the monochromatic opacities and emissivities, mean opacities, optical depths, radiative power losses, cooling times, specific intensities and also a collisional-radiative diagnosis of the electron temperature for a particular experiment in which a blast wave was launched in a clustered gas of Xe irradiated by an intense laser [16]. All those simulations were performed solving a collisional-radiative model assuming steady state situation and without including the effect of the radiation coming from the shocked material in the radiative precursor. In this work we analyze the influence of both effects on the collisional-radiative simulation of the microscopic properties and the diagnosis of the electron temperatures of the blast wave of that experiment. The remainder of the paper is structured as follows: in the next section a brief description of the experiment under analysis is presented. In section 3, the theoretical model employed for the simulations is described. In Section 4 the results and the analysis of the collisional-radiative simulations including time and radiation effects are presented. Finally, last section is devoted to the conclusions and main remarks.

2. Brief description of the experimental set up

The blast waves under study in this work were launched in a gas of xenon cluster using the THOR laser system at the University of Texas [16]. The gas was irradiated with a laser energy of $\approx 400 \text{mJ}$ at average gas density of $1.6 \times 10^{-3} \text{ g cm}^{-3}$ creating a hot plasma filament approximately $65\mu\text{m}$ in diameter and $4 \text{ mm}$ long. This plasma developed into a strong cylindrical radiative blast wave and a radiative precursor ahead of the shock front was observed. The evolution and morphology of the blast wave were monitored using imaging interferometric and Schlieren techniques. Therefore, electron density profiles for the cylindrical blast waves were obtained. The average ionization values of pre-shock region are direct measurements from the
interferograms since the ambient density of gas is known. Behind the shock the electron density is measured and the average ionization is calculated from the compression of the shocked material, defined as the ratio of the maximum mass density within the shell to the ambient gas density, which was measured from the blast wave electron density profiles given a value of 2 [16, 17]. The weak compression is because of the preheating of the gas ahead of the shock front that reduces the Mach number. Finally, the plasma temperature of the blast wave was not measured in this experiment, although in this kind of experiments this could be measured using X-ray Thomson scattering. A more detailed description of the experiment is found in [16].

3. Theoretical model

The collisional-radiative simulations performed in this work were carried out under the relativistic detailed configuration accounting (RDCA) approach. The atomic data such as the energy levels, transition energies, wave functions and oscillator strengths were calculated using FAC code [24]. The transition energies include the shift associated to the Unresolved Transition Array (UTA) formalism and the line strengths are corrected for configuration interaction within the same non-relativistic configurations. In the range of plasma conditions considered in this work which is matter densities between \(10^{-3} \times 10^{-3}\) g cm\(^{-3}\) and electron temperatures between 1-20 eV, the ions found in the plasma are the ones ranged between Xe\(^{+0}\) to Xe\(^{+12}\) and the electron densities are ranged between \(10^{16} - 10^{19}\) cm\(^{-3}\).

The plasma atomic level populations were obtained by means of a collisional-radiative model (CRM) solving a set of rate equations given by the following expression

\[
\frac{dN_{\xi i}(r, t)}{dt} = \sum_{\xi j} N_{\xi j}(r, t) R_{\xi j \rightarrow \xi i}^+ - \sum_{\xi j} N_{\xi i}(r, t) R_{\xi i \rightarrow \xi j}^- \tag{1}
\]

where \(N_{\xi i}\) is the population density of the atomic configuration \(i\) of the ion with charge state \(\xi\). The terms \(R_{\xi j \rightarrow \xi i}^+\) and \(R_{\xi i \rightarrow \xi j}^-\) take into account all the atomic processes which contribute to populate and depopulate the state \(\xi i\), respectively. The atomic processes included are the collisional ionization, three-body recombination, spontaneous decay, collisional excitation and deexcitation, radiative recombination, electron capture and autoionization. The calculation of the rate coefficients of these atomic processes was made using ABAKO code [25], except the one for the spontaneous decay which was obtained from FAC code. In ABAKO they are evaluated by means of analytical expressions widely used (see [25] for a more detailed description). To analyze the effect of the radiation from the shocked material in the radiative precursor, photoexcitation, photo-deexcitation and photo-ionization processes were also included in the CRM. For the last one the Kramers photo-ionization cross section [26] was used. The rates of these processes were obtained assuming that the radiation field can be modeled with a diluted Planck function.

The set of rate equations given by Eq.(1) are coupled to the radiative transfer equation

\[
\frac{1}{c} \frac{\partial I(r, t, v, e)}{\partial t} + e \cdot \nabla I(r, t, v, e) = -\kappa(r, t, v) I(r, t, v, e) + j(r, t, v), \tag{2}
\]

where \(I\) is the specific intensity, \(v\) the photon frequency and \(e\) a unitary vector in the direction of the radiation propagation. The emissivity and the absorption coefficients \((j(r, t, v)\) and \(\kappa(r, t, v)\), respectively) couple the radiative equation with the rate equations. However, in this work they are uncoupled since as we obtained in [23] the plasma self-absorption can be neglected in the
calculation of plasma level populations both in the shocked material and in the radiative precursor regions and, besides, since in the analysis of the effect of the radiation in the kinetics calculations of the radiative precursor the Planck function is used to model the intensity of the radiation field.

Once the plasma atomic level populations are obtained, the radiative properties such as the monochromatic opacities and emissivities, mean opacities, radiative power losses and the specific intensities are calculated using RAPCAL code [27, 28]. For the bound-bound contributions we employed the atomic data generated using FAC code. For the the line shape a Voigt profile was used including natural, Doppler, UTA and collisional broadenings [29]. Bound-free contributions were calculated using the photoionization cross sections provided by FAC code under the distorted wave approach. Finally, for the free-free contribution, the Kramers semi-classical expression for the inverse bremsstrahlung cross section was used [30]. A more detailed description of the calculation of the radiative properties can be found in [27].

4. Results

4.1. Time effects in the collisional-radiative simulations of the front shock

In a previous work an estimation of the temperature of the shock front was made in local thermodynamic equilibrium (LTE), using Saha-Boltzmann (SB) equations, and in NLTE [23] but in steady-state (CRSS) situation. The procedure employed for that purpose was to generate a database of the average ionizations, both using the SB equations and the CRSS model, as a function of the electron densities and temperatures. Then, they were fitted using polynomial functions using PARPRA code [31]. Therefore, for a given experimental electron density and average ionization the temperature was obtained using the polynomial fittings with the criterion that the difference between the theoretical and experimental average ionizations was lower than 0.1%. In this work we have made an estimation of those temperatures but using the time-dependent collisional-radiative model (CRTD) previously commented. To solve the system of first order differential equations of the CRM we have employed an implicit Euler method. First of all, as from the experiment the electron density and the average ionization are only known at 5 times in the range 3-83 ns, we have made a fitting of both quantities using a polynomial function of third degree. The quality of the fitting is shown in Fig. 1 for the average ionization, where the greatest error obtained is about 3%. Similar fitting and errors were obtained for the electron density.

Then, making use of the fitted time profiles of average ionization and electron density the electron temperature at each time was determined solving the system of rate equations given by Eq. (1) by means of an iterative procedure that ended when the relative difference between the theoretical and experimental average ionizations was lower than 0.1%. In Fig. 2 we show the electron temperatures for the shock front estimated by means of LTE, CRSS and CRTD simulations. The first thing that we observe is that the three simulations provide almost similar temperatures for times later than 15 ns. Furthermore, even for earlier times, the differences between the three temperatures are small, overall between the CRTD and LTE simulations. Thus, for instance, at 5 ns the temperatures given by CRSS, CRTD and LTE simulations are 16.50, 15.50 and 15.40 eV, respectively.

Using the temperatures estimated with the three theoretical models we have analyzed the CSDs provided by them. In Fig. 3 we show the fractional abundance at two times. As the average ionization is the same for the three simulations the main ions that contribute are also the same. At 23 ns the CSDs obtained are very similar to each other. At 6 ns we observe that the CSDs
obtained with LTE and CRTD simulation are close although the most abundant ion predicted by both models disagrees (Xe$^{+9}$ and Xe$^{+8}$, respectively). Thus, although the temperatures provided by the LTE and CRTD simulations are quite similar, according to Fig. 2, there are differences in the CSDs given by the two models. On the other hand, the CRSS simulation agrees with the CRTD one with respect to the most abundant ion but there are discrepancies in the fractional abundance of the ions. Therefore, although the temperatures predicted by the three models at 6 ns are close, we detect differences in the fractional abundance of the ions that contribute to the CSD, which are essentially Xe$^{+8}$, Xe$^{+9}$ and Xe$^{+10}$, provided by the theoretical models.

The analysis of the monochromatic radiative properties is useful to study the effect of the different models in the plasma atomic level populations. In Fig. 4 we have plotted the monochromatic emissivities and opacities calculated with the three models at these two times. Both for the emissivities and the opacities the differences detected are larger at 6 ns than at 23 ns as it is expected according to the discrepancies obtained in the analysis of the CSDs. As the ions that contribute are the same in the three models, the structures in the spectra are also the same, and, therefore, the differences are related to the height of the peaks and to the depth of the valleys in the opacities and emissivities. However, we observe from the figure that the disagreement is greater for the LTE simulation at both times, overall for the case of the emissivity. Thus, at 6 ns the discrepancies are detected both for the monochromatic opacity and emissivity, whereas at 23 ns, the differences are only observed for the emissivity, which means that the ground and low lying excited configurations could be considered in LTE but not the other excited configurations. This result remains true even for later times. In Fig. 5 we present the radiative power loss as a function of time, calculated assuming the plasma as optically thin, where we can observe that the differences in the LTE simulations only vanish for times later than 50 ns. On the other hand, with respect to CRSS and CRTD models we observe that both simulations provide quite similar results even at early times both for the monochromatic and mean opacities and the emissivity and the radiative power loss.

Finally, we have also analyzed the effect of the kinetic model employed in the calculation of the specific intensity emitted by the shock front since this one will affect the radiative precursor.
The solution of Eq. (2) along the beam in the propagation direction is given by

$$I_\nu(\tau_\nu) = I_\nu(0)e^{-\tau_\nu} + \int_0^{\tau_\nu} S_\nu(t_\nu)e^{-(\tau_\nu-t_\nu)}dt_\nu,$$

(3)

where $S_\nu$ is the source function and $\tau_\nu$ is the monochromatic optical thickness measured along the beam

$$\tau_\nu(r) = \int_0^r \kappa_\nu(s)ds.$$

(4)

We have assumed that the shock shell is an homogeneous medium in which the source function does not vary with the location, with planar geometry of thickness $D$ calculated as the full width at half maximum of the shocked shell, which is experimentally measured and is ranged between 86 $\mu$m (at 3 ns) and 167 $\mu$m (at 83 ns) [23]. Assuming $I_\nu(0) = 0$ in Eq.(3) the outgoing specific intensity will be given by

$$I_\nu(D) = S_\nu(1 - e^{-\tau_\nu(D)}).$$

(5)

In Fig. 6 we have represented the outgoing intensity of the shock front at two times (6 and 26 ns) calculated with the three models. Since the specific intensity depends on the emissivity and the absorption coefficient the results obtained when we analyzed these properties will rule the behavior of the specific intensity. Thus, again, bigger differences are observed for the early times and also for the LTE approach. However, the intensities provided by the CRTD and the CRSS models are quite similar. Therefore, from the whole analysis we could conclude that the electron temperature, plasma level populations, and radiative properties of the shocked shell can be obtained using the CRSS model since the differences with respect to the CRTD are not very relevant. This is an interesting result since this fact reduces considerably the complexity of the collisional-radiative simulations and also it would allow use the polynomial parametrization of the average ionizations and the mean radiative properties, that we had already obtained using the CRSS model, for further radiative-hydrodynamics simulations. On the other hand, LTE approach would be only accurate for times later than 50 ns.
4.2. Radiation effects in the collisional-radiative simulations of the radiative precursor

We have made an analysis of the effect of the radiation field on the collisional-radiative simulations of the radiative precursor. First of all, we have studied the opacity of the radiative precursor for its density of matter and for the range of temperatures 1-10 eV which is the one that we estimated for the radiative precursor using the CRSS model in [23]. Thus, in Fig. 7 we show the monochromatic opacities for the density of matter of the radiative precursor and several temperatures of that range. From the figure we observe that for the range of temperature of interest the absorption is much stronger in two ranges of photon energies: around 50-100 eV and 10-20 eV. For the regions of lower temperatures in the radiative precursor the latter range is the most important.

The specific intensity at each point of the radiative precursor has been calculated using Eq.(3) where $I_{\nu}(0)$ is the outgoing intensity of the shocked shell given by Eq. (5) and we have not taken into account the radiation that comes from regions of the radiative precursor that are located ahead of the point considered. Furthermore, the monochromatic opacities and emissivities required in Eq.(3) were calculated at the temperatures estimated using the CRSS model without including the radiation field [23]. A more rigorous study would imply a self-consistent calculation of the rates equations coupled to Eq.(3) in order to introduce the radiation effects in the calculation of the monochromatic emissivities and opacities. However, the scope of this work is just to make a qualitative analysis of the effect of radiation driven processes in the kinetics calculations of the radiative precursor of this experiment, since this study has not been carried out previously. In Fig. 8 we present an example of the specific intensity at 11 ns at several points of the radiative precursor. In particular we compare the specific intensity calculated at each point of the radiative precursor and the one emitted by the shocked shell calculated using Eq.(5). Greater values of the coordinate $r$ imply points of the radiative precursor further away from the shock front. From the figure we observe that there is a contribution of the self-emission of the radiative precursor in the range of photon energies 1-5 eV that produces an increase in the intensity in that
range. On the other hand, we observe that the absorption of the radiation is mainly located in the photon ranges 5-20 eV and 50-100 eV, which is expected according with what we presented in Fig. 7 and that radiative precursor can be considered as optically thin for photons with energies not belonging to those ranges. Furthermore, we observe that the range of photon energies in which the absorption is stronger is shifted toward 5-20 eV as the coordinate increases. This result is also expected since, at a given time, the further we get away from the shock front, the lower the temperature is, and, therefore, according to Fig. 7 the plasma absorbs at lower photon energy ranges.

As we said in the second section we have included in this work radiative driven processes in the CRSS model. As in their calculation the radiation field is assumed as a Planck function, first we have approached the specific intensity calculated by a Planck function. Since the radiative precursor absorbs mainly in two photon energies range we approached the specific intensity by two Planck functions that try to reproduce the values of the specific intensity in that ranges. In Fig. 9 an example of this at 11 ns is shown, where the radiation temperatures of the two Planck functions are 12.20 eV and 6 eV and the dilution factors 0.3 and 0.1.

With this model of the radiation field we estimated the electron temperature of the radiative
precursor and we compared the new results with the ones obtained without including radiative driven processes [23]. In Fig. 10 we have presented the comparison at two times. For a given experimental value of the average ionization, the electron temperature predicted by the model including the radiative field is lower, what it is expected since the radiative driven processes help to ionize the plasma. In Fig. 11 we have presented a comparison between the CSDs for these times calculated with and without including the external radiation field for several points of the radiative precursor. From Figs. 10 and 11 we conclude that the effect of the radiation is more relevant at 3 ns than at 44 ns and this could be related to the fact that the blast wave radiates more strongly at 3 ns, as Fig. 5 shows. Thus, at 3 ns differences both in the temperature estimated and in the CDSs are observed whereas at 44 ns although some differences are detected in the estimated temperatures at points away from the shock, these discrepancies are not great enough to produce variations in the CSD. Therefore, the influence of the radiative driven processes on the ion charge balance will be important mainly at the early times when the blast wave emits
more strongly and it will decay as time goes on.

5. Conclusions

In this work we have made an analysis of the influence of the kinetic model employed to obtain the level populations and radiative properties of the shocked shell of a radiative shock launched in a cluster of xenon. Three different approaches have been considered: LTE, steady-state NLTE and time-dependent NLTE. We have obtained that, although there are some differences between CRSS and CRTD simulations, these ones are not too relevant and, therefore, the CRSS model can be employed to calculate the plasma properties of interest. On the other hand, we have detected that LTE approach would be only accurate for times later than 50 ns. We have also analyzed the effect of the radiation emitted by the shocked shell in the kinetics calculations of the radiative precursor. For this purpose, we calculated the specific intensity emitted by the shock front and it was modeled by two Planck functions. In this work we have only made an approached estimation of the effects of the radiation field since a more rigorous study would imply a self-consistent calculation with coupling of the rate equations and the radiative transfer equation. We have observed that the radiative driven processes included in the kinetics simulations of the radiative precursor modify both the estimation of the temperature and the CSDs mainly at early times, when the blast wave emits more strongly, and therefore they should be included in the collisional-radiative simulations.

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Figure 8: Comparison between the specific intensity emitted by the shock shell and the one propagated through the radiative precursor at 11 ns.

References

Figure 9: Intensity approached by the Planck function.

Figure 10: Estimation of the temperature of the radiative precursor including an external radiation field.


Figure 11: Comparison between the CSDs distribution calculated including radiative driven processes (rad) or not at two times and several positions in the radiative precursor.