The Acceleration of Thermal Ions at a Strong, Quasi-Parallel Interplanetary Shock: A Hybrid Simulation

Joe Giacalone
Lunar & Planetary Laboratory, University of Arizona, Tucson, AZ 85721

giacalon@lpl.arizona.edu

Abstract. Using a self-consistent hybrid simulation, with kinetic protons and fluid electrons, we investigate the acceleration of thermal protons and minor ions (alphas, 3H\(^{++}\), and C\(^{++}\)) by a quasi-parallel collisionless shock. The results are compared to spacecraft observations of a strong interplanetary shock seen by the Advanced Composition Explorer on DOY 94, 2001, which was associated with significant increases in the flux of > 50 keV/nuc ions. Our simulation uses similar plasma and shock parameters to those observed. The densities of minor ions for two of the species (alphas and C\(^{++}\)) were based on observations at thermal energies for this shock, and we used a nominal value for the density of 3H\(^{++}\), since no observations at thermal energies was available to us. Acceleration of the ions by the shock leads to a high-energy tail in the distribution in the post-shock plasma for all ion species. We find that by extrapolating the simulated tails to the higher energies measured by ACE/EPAM and ACE/ULEIS, the intensity matches well the observations for protons, alphas, and carbon. This suggests that thermal solar wind, accelerated directly at the shock, is a significant source of the observed high-energy protons and these minor ions.

1. Background
The origin and acceleration mechanism involved in creating non-thermal charged-particle distributions in astrophysical, solar, and heliospheric plasmas is an important unsolved problem. Spacecraft observations of particle distributions have noted the existence of a non-thermal tail, even in the absence of an obvious source, like a collisionless shock [4,5,17,9]. It has been reported that non-thermal tails in the distribution often form just behind strong interplanetary shocks [18] suggesting that the formation of the tail is related to plasma heating, particle acceleration, and energy dissipation across the shock. Self-consistent plasma simulations of shocks in which the ions are treated kinetically have also shown this [27,28,14,12]. However, it has also been noted that in the solar wind, particles with energies well above the peak in the thermal distribution have intensities that vary by a few orders of magnitude, which is far more than the variation in the density in the solar wind [25,7]. Moreover, the isotopic composition of “suprathermal” particles can differ considerably from that of the solar wind at 1AU [24,26,6,22]. In some cases of strong interplanetary shocks driven by coronal mass ejections and associated with large intensities of energetic particles the ratio of 3H\(^{++}\)/4H\(^{++}\) is far greater than the same ratio at thermal energies, based on typical solar wind conditions [24]. This suggests that the source is a pre-existing suprathermal population of particles rather than solar wind.

Collisionless shocks provide an excellent “laboratory” to the formation of non-thermal particle distributions. For one, shocks heat the plasma, and broaden the particle distribution. Moreover, strong interplanetary shocks are known to be associated with large intensities of high-energy particles [12].
Moreover, there is a widely accepted theory for particle acceleration at shocks – diffusive shock acceleration [23,1,2,3]. In this mechanism, particles are accelerated by diffusively moving in the irregular magnetic fields embedded in the plasma flows on both sides of the shock and cross the shock many times gaining energy at the large plasma compression. The theory only addresses acceleration from some initial energy, but does not specifically address what this energy is, or what the value of the distribution is at this energy. Thus, the theory does not address the injection mechanism. Hybrid simulations have shown that shocks naturally accelerate low-energy particles, even those from the thermal distribution [27,28,14,12].

It is the purpose of this paper to address the source of accelerated minor ions at an interplanetary shock. We do this by simulating an interplanetary shock in which multiple ion species are treated kinetically and whose un-shocked, initial distributions are Maxwellian. We then compare the distribution resulting from their interaction with the shock with spacecraft observations of a particular event.

2. Numerical Model

We use the hybrid model described in [15,10] to simulate a quasi-parallel interplanetary shock. The ions are treated kinetically and the electrons as a massless fluid. The bulk flow velocity, number density, electric and magnetic fields are all functions of one spatial coordinate, x. The average magnetic field upstream of the shock, $B_x$, is in the x direction. The magnetic field consists of this mean plus a fluctuating component derived from a discrete sum of many plane Alfvén waves that propagate along the mean field. The amplitudes of each is determined from an assumed Kolmogorov-like power spectrum with variance of $0.3|B|^2$, and an outer scale of 0.01AU, similar to that observed in the interplanetary magnetic field [21].

The shock is created by forcing plasma to reflect off a boundary at one end of the simulation domain. The shock then propagates back into the flow. The calculation is performed in a frame at rest with respect to the reflecting boundary, but results are transformed to the spacecraft frame to compare results with observations. Table 1 lists the input parameters, which are consistent with ACE MAG and SWEPAM observations for the interplanetary shock that crossed ACE at 14:22:27 UT on DOY 94, 2001. Averaged over the hour before the shock crossing, ACE observed the number density, field strength, and flow speed to be 4.6 cm$^{-3}$, 7 nT, and 490 km/s, respectively. The shock speed was estimated to be 690 km/s. Using these parameters, the proton inertial length, $c/\omega_p$, and cyclotron period, $\Omega_p^{-1}$, the characteristic length and time scales of the hybrid simulation, corresponds to 1.1x10$^{-7}$ cm and 1.6 s, respectively.

We also identify a boundary that co-moves with the shock, a distance $\Delta_{\text{beh}}$ upstream, which acts as a “free-escape” boundary for any particles that move from the shock back upstream and allowing them to escape. The reason for this boundary is to ensure that the “escape distance” upstream remains constant with time. Note that the shock moves in the simulation frame. For the parameters used, this corresponds to $\Delta_{\text{beh}} = 0.025$ AU, and the entire simulation domain, $x_{\text{max}}$, is 0.035 AU. Such a boundary has been used in diffusive shock calculations previously [8], and can even be made to be a function of energy by setting it to be some number of diffusive skin depths ahead of the shock [31]. The latter requires prior knowledge of the diffusion coefficient’s dependence on energy, which we do not have.

The maximum simulation time, $t_{\text{max}}$ in Table 1 corresponds to 5.3 hrs of real time. The time step is 0.005 $\Omega_p^{-1}$. The grid spacing is 0.5 $c/\omega_p$. There are 100,000 grid cells in the entire domain.

The initial distributions, and also injected at the inflow boundary, of all ions are drifting Maxwellians. All ions are assumed to have (initially) the same thermal speed. The proton thermal speed is related to the plasma beta, $\beta_p$, given in the table. The inflow speed is related to $M_A$, the Mach

| Table 1. Simulation Parameters |
|--------------------------------|
| $M_A$                      | 3 |
| $M_A$                      | 4 |
| $\beta_e$                  | 0.6 |
| $\beta_p$                  | 0.3 |
| $\omega_p / \Omega_p$      | 4500 |
| $t_{\text{max}}$           | $12,000\Omega_p^{-1}$ |
| $x_{\text{max}}$           | $50,000c/\omega_p$ |
| $\Delta_{\text{beh}}$      | $35,600c/\omega_p$ |
| $n(4H_e^+)/n_p$            | 0.022 |
| $n(3H_i^+)/n_p$            | $9.4x10^6$ |
| $n(C^{++})/n_p$            | $4.3x10^5$ |
number in the simulation frame of reference. A total of 190 particles per grid cell are initially loaded into the simulation domain. Of these, 100 are protons, and 30 each of $4H^{++}$, $3H^{++}$, and $C^{5+}$. We also performed a few other simulations with more minor ions per grid cell, doing each species and protons together without including the other species, and found essentially the same results as those presented below. The proton density is $4.6cm^{-3}$, and Table 1 lists the abundance ratios for the other ions that were used in our calculation. The alpha to proton abundance ratio, $n(4H^{++})/n_p$, is chosen to match ACE/SWEPAM observations, and the carbon to proton ratio, $n(C^{5+})/n_p$, is also consistent with observations from ACE/SWICS (not shown, but determined from phase-distributions functions provided by S. Lepri). Observations of the $3H^{++}$ to proton ratio were not available, so a nominal value was used [16].

As the simulation evolves, the upstream plasma, fields, and ion distributions evolve self-consistently according the fundamental physical equations that govern the hybrid simulation [30].

3. Results

Figure 1 shows some simulated results transformed to the spacecraft frame of reference in real units. The two panels on the left show the differential intensity (upper left) and plasma flow speed (lower left) as functions of the time relative to the shock crossing. This was accomplished by relating the position within the simulation domain, $x$, at the end of the simulation to “spacecraft time”, $\tau$, by $\tau = (x-x_{\text{shock}})/V_{\text{sh}}$, where $x_{\text{shock}} = 38,844 c/\omega_p$ is the position of the shock in the simulation domain at $t_{\text{max}}$. The alternate axis at the top of the upper left panel indicates position relative to the simulation domain. $V_{\text{sh}} = 690 km/s$ is the observed interplanetary shock speed. The right panel shows the simulated proton differential energy spectrum as a function of kinetic energy as a solid histogram, determined by averaging over the region indicated with the yellow shaded region in the left panels. This is downstream of the shock. The symbols are ACE/EPAM observations averaged over a 15-minute time interval immediately after the shock crossed ACE at 14:22.27UT DOY 94, 2001.

Figure 1. Upper left: Simulated flux of 20-30 keV protons as a function of time relative to the shock crossing. The symbols are averages over $50c/\omega_p$, and the solid curve is a 20-pt running average of this. The upper axis shows the corresponding position within the simulation domain. Lower left: simulated plasma flow speed as a function of time. Right: (Solid histogram) Differential intensity as a function of energy for protons over the region indicated by the yellow shaded region in the left figures. (Symbols) 15-minute-avarged ACE/EPAM LEMS30 and LEMS120 data at the time of the crossing of the interplanetary shock on DOY 94, 2001.
The downstream proton spectrum reveals a high-energy tail. These are shock-accelerated thermal protons [15,10]. The spectrum is approximately a power law from about 8 keV to 30 keV. Above this, the spectrum falls off approximately exponentially, which is the result of particles escaping the free escape boundary (as discussed in the references above). Had we used a larger simulation domain, and run the simulation longer, we expect that the spectrum would have been a power law to larger energies. In fact, it seems by comparing with the ACE/EPAM observations that the simulated high-energy tail would match the observations if it extended to higher energies. The energy where this tail emerges in the distribution is related to the efficiency of the acceleration of thermal protons [15]. In this case, it seems the acceleration efficiency is such that it matches well the observations, suggesting that the source of the high-energy protons observe by ACE/EPAM is accelerated solar wind protons. It is also noteworthy, however, that the acceleration is, in fact, quite slow. The characteristic energy, where the spectrum rolls over from a power law to exponential, is only ~30 keV for a maximum simulation time corresponding to 5.5 hours of real time. This slow acceleration time is because the simulated shock is quasi-parallel, and such shocks are quite slow at accelerating particles. Quasi-perpendicular shocks, in contrast, are much faster [19,20,11,12].

Figure 2 shows downstream energy spectra, averaged over the same region indicated by the yellow-shaded region of the left panels of Figure 1, for the minor ions in our simulation. We only show the spectra up to 30 keV/nuc., and do not show the exponential part of the spectrum, which, as indicated above, is the result of particle escaping our small computational domain. Also shown are ACE/ULEIS observations of the differential flux of the same minor ions. This data was obtained from the ACE science center which provides 1-hour averages. We took the time that most-closely coincided with the passage of the shock, but still downstream of it.

As in the case of the protons, the simulated spectra have a high-energy tail that, when extended to high energies, matches reasonable well with the spacecraft observations for at least two of the minor ions.

![Figure 2](image-url)
ion species (4He\textsuperscript{++} and C\textsuperscript{5+}). The tail does not match very well the 3He\textsuperscript{++} data at high energies. It should be noted, however, that this is the only species for which we had no observations of the initial distribution, and, instead had to use a ‘nominal value’. For the other two species, which we did have observations at thermal energies upstream of the shock, the simulated energy spectra, if extrapolated to high energies, match quite well with the ACE/ULEIS observations. This suggests that the source of these high-energy ions, as well as the protons, mentioned above, is the solar wind.

Assuming the upstream distribution of solar-wind 3He\textsuperscript{++} is similar to that which we assumed, then our results would indicate that the source of the high-energy 3He\textsuperscript{+} would have to be a pre-existing suprathermal population. However, although we do not show it here, inspection of ACE/ULEIS observations of the 160-310 keV/nuc. 3He\textsuperscript{++} flux over ~36 hour interval of this interplanetary shock (using data obtained from the ACE science center) reveals that the flux increased by almost 2 order of magnitude from far upstream to the peak at the shock. Thus, the high-energy tail would have to be enhanced by this factor across the shock, which is a challenge to understand theoretically. We suggest, alternatively, that it is perhaps more likely that the 3He\textsuperscript{++} thermal distribution upstream of the shock is larger than we assumed. If this is the case, then our results would also suggest that the source of accelerated 3He\textsuperscript{++} is solar wind as well. This requires further analysis for verification.

If the source of accelerated 3He\textsuperscript{++} is indeed thermal solar wind, it would be quite surprising given that previous studies have noted that the abundance ratio of 3He\textsuperscript{++}/4He\textsuperscript{++} at high energies is far greater than the same value at thermal solar wind energies, especially at large solar-energetic particle events [24]. We have found that the acceleration efficiency, which is related to where in the spectrum the high-energy tail emerges, depends on the species, and that 3He\textsuperscript{++} is the most efficiently accelerated of the ions. This is shown in Figure 3. This figure shows energy spectra, normalized in such a way to give the same total abundance, or number density – the proton density, in this case. Note that at high energies, the 3He\textsuperscript{++} is the largest, indicating it is the most efficiently accelerated. Interestingly, the protons are the least efficiently accelerated. A possible interpretation is that the efficiency of the proton acceleration is constrained by the total ‘energy budget’ since the protons are the dominant species. Total energy must be conserved, and the available energy is that which is swept up by the shock. The shock converts most of this energy into enthalpy flux by heating the protons (and electrons), but a fraction of this is in high-energy protons as shown by [15]. These authors noted that this fraction, related to the acceleration efficiency, does not exceed about 20% in hybrid simulations of strong quasi-parallel shocks. Moreover, a significant fraction of the accelerated particles escape the upstream boundary, representing an energy sink. These authors also noted that a significant energy loss leads to a very large change in the nature of the shock, with a density compression ratio, for example, that is considerably larger than that expected from the standard Rankine Hugoniot jump conditions. The minor ions, however, contribute a negligible amount of energy to the system and, as such, do not have the same restriction as the protons. The minor ions are all accelerated very efficiently, but 3He\textsuperscript{++}, by far is the most efficient. We note that 3He\textsuperscript{++} is lighter than 4He\textsuperscript{++}, yet 3He\textsuperscript{++} is accelerated far more efficiently than 4He\textsuperscript{++}, which is not consistent with previous findings showing the acceleration efficiency increasing with mass per charge [8]. The cause of this is not yet determined, but we have found that all the minor ions, especially 3He\textsuperscript{++}, are significantly heated upstream, before they encounter the shock (not shown). We also find

![Figure 3. Downstream energy spectra of protons and minor ions, as indicated, normalized so that the density is the same for all species.](image)
that the protons are slightly cooled relative to their injected temperature. Recall that only the distribution at the start of the simulation, and that injected at one boundary of the simulation, have equal thermal speeds for the ions. As the ions move with the flow, before encountering the shock, their distributions evolve in time. The cause of this heating/cooling is not presently understood. It is possibly caused by fluctuations in both the magnetic and electric fields upstream of the shock. These fluctuations are caused, partly, by back-streaming protons accelerated at the shock and evolve non-linearly in time, often forming large magnetic fluctuations such as SLAMS [29]. There also fluctuations in the electrostatic field caused by variations in the electron (equal to the ion) number density. For ions of equal charge, electrostatic fluctuations would preferentially heat lighter particles, which may explain why $3\text{He}^{++}$ is heated more than $4\text{He}^{++}$ in our simulations. We are not aware of observations of minor ions heated prior to the passage of interplanetary shocks.

4. Conclusions

We used a one-dimensional hybrid simulation of a shock using input parameters consistent with those observed for an interplanetary shock which crossed the ACE spacecraft at 14:22:27UT on DOY 94, 2001 to investigate the acceleration of thermal protons and minor ions. The simulation treats the ions kinetically, and requires that the ion cyclotron period and thermal ion gyroradius are well resolved. These are very small compared to the typical temporal and spatial scales involved with the acceleration to ions to high energies at a quasi-parallel collisionless shock. We find that acceleration by the shock leads to a high-energy tail in the ion distribution that is approximately a power law up to a characteristic energy where the spectrum becomes exponential. This is consistent with diffusive shock acceleration theory. This change in spectrum is caused by the finite spatial domain of the simulation. Because the shock we studied was only marginally supercritical ($M_s$ $\sim$ 4), and because the simulation domain was finite (although still many thousands of ion inertial lengths) the characteristic energy in our calculations was only about 30 keV/nuc for all ion species, although maximum energies were over 100 keV/nuc. We compared our simulation results to observations. The lowest energy of ACE/EPAM and ACE/ULEIS is higher than the power-law part of our simulated distributions given our computational constraints. Thus, our results could only be compared by extrapolating to higher energy, assuming that a larger simulation domain and longer run time would lead to a power-law part that extended to higher energies and overlap with the observations.

We find that the high-energy tail, caused by acceleration of particles at the shock, emerges from the thermal distribution with an intensity that when extrapolated to higher energies matches well the observed intensities for all ions, except $3\text{He}^{++}$. The initial distributions in our simulations were assumed to be Maxwellian in the upstream plasma frame. Moreover, we used initial densities and thermal speeds consistent with observed values at thermal energies of all particles (except $3\text{He}^{++}$). Thus, the results of our simulations suggest strongly that the source of accelerated minor ions at the interplanetary shock seen by ACE on DOY 94, 2001 is thermal solar wind. The source of $3\text{He}^{++}$ remains a question since we did not have observations of the density and temperature of this ion species. But assuming nominal values, there are fewer high-energy $3\text{He}^{++}$ in our simulation than that observed by ACE/ULEIS. This suggests the source is pre-existing suprathermal particles.

We also find that the acceleration efficiency depends on the ion species. The protons are the least efficiently accelerated. Their efficiency is constrained by the amount of energy contained in high-energy particles compared to the energy incident on the shock. The minor ions, however, do not have the same constraint because, due to their low density, contribute very little to the total energy. We find that $3\text{He}^{++}$ is the most efficiently accelerated ion species. We suggest that this may be related to the electrostatic field in the hybrid simulation, which is caused by gradients in the electron density. An electrostatic field effects more significantly particles with a larger charge to mass ratio, and $3\text{He}^{++}$ has the largest ratio ($(Z/A)_{\text{thle}} = 2/3$) of the three minor ions we simulated ($(Z/A)_{\text{thle}} = 2/4; (Z/A)_{\text{thle}} = 5/12$). In our simulations, the electrostatic field has both a fluctuating part, as well as a steady part, in the shock front, known as the cross-shock electric field.
Our simulations suggest that solar wind is likely a significant source of acceleration particles at strong interplanetary shocks. We also emphasize the importance of measuring the entire distribution function, from thermal energies, to the suprathermal tail, and high energies in order to understand the source of accelerated particles. Future instrumentation with such capabilities will significantly advance our understanding of the origin and physical mechanisms involved in the acceleration of high-energy particles.

Acknowledgements
I thank J. R. Jokipii, J. Kota, and F. Fraschetti, for useful conversations relevant to this study. This study was supported, in part, by NASA under grants NNX15AJ71G and NNX15AJ72G. Numerical simulations were performed with the support of NASA SMD High-End Computing on the Pleiades cluster, under the award SMD-16-7631

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